



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:44 PM UTC

PDB ID : 3KR5 / pdb_00003kr5
Title : Structure of a protease 4
Authors : McGowan, S.; Whisstock, J.C.
Deposited on : 2009-11-17
Resolution : 2.56 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

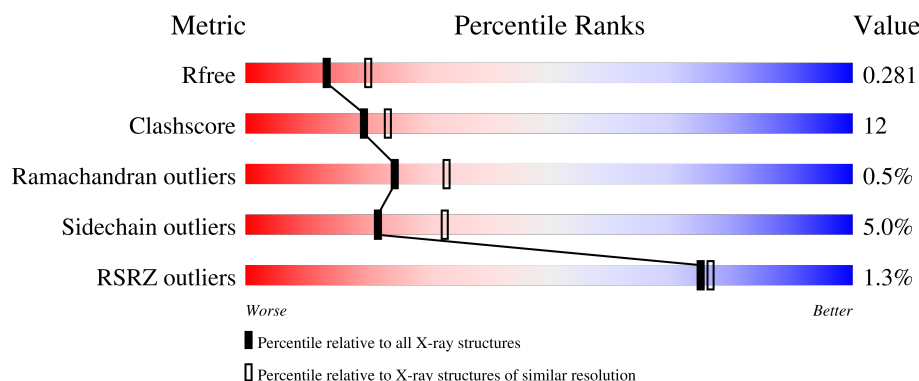
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	528	
1	B	528	
1	C	528	
1	D	528	
1	E	528	

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Mol	Chain	Length	Quality of chain
1	F	528	
1	G	528	
1	H	528	
1	I	528	
1	J	528	
1	K	528	
1	L	528	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CO3	D	1002	-	-	X	-
2	CO3	K	1002	-	-	X	-
5	SO4	E	7	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 50444 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called M17 leucyl aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	518	Total	C	N	O	S	0	0	0
			3980	2556	639	765	20			
1	B	518	Total	C	N	O	S	0	0	0
			3929	2527	635	747	20			
1	C	518	Total	C	N	O	S	0	0	0
			3953	2544	637	752	20			
1	D	513	Total	C	N	O	S	0	0	0
			3928	2531	633	744	20			
1	E	510	Total	C	N	O	S	0	0	0
			3897	2509	626	743	19			
1	F	510	Total	C	N	O	S	0	0	0
			3873	2492	624	738	19			
1	G	516	Total	C	N	O	S	0	0	0
			3989	2560	650	760	19			
1	H	509	Total	C	N	O	S	0	0	0
			3938	2531	640	748	19			
1	I	518	Total	C	N	O	S	0	0	0
			4006	2569	651	766	20			
1	J	513	Total	C	N	O	S	0	0	0
			3954	2539	639	756	20			
1	K	509	Total	C	N	O	S	0	0	0
			3930	2525	637	749	19			
1	L	513	Total	C	N	O	S	0	0	0
			3932	2526	634	753	19			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	GLN	ASN	engineered mutation	UNP Q8IL11
A	515	GLN	ASN	engineered mutation	UNP Q8IL11
A	546	GLN	ASN	engineered mutation	UNP Q8IL11
A	606	HIS	-	expression tag	UNP Q8IL11
A	607	HIS	-	expression tag	UNP Q8IL11

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Chain	Residue	Modelled	Actual	Comment	Reference
A	608	HIS	-	expression tag	UNP Q8IL11
A	609	HIS	-	expression tag	UNP Q8IL11
A	610	HIS	-	expression tag	UNP Q8IL11
A	611	HIS	-	expression tag	UNP Q8IL11
B	152	GLN	ASN	engineered mutation	UNP Q8IL11
B	515	GLN	ASN	engineered mutation	UNP Q8IL11
B	546	GLN	ASN	engineered mutation	UNP Q8IL11
B	606	HIS	-	expression tag	UNP Q8IL11
B	607	HIS	-	expression tag	UNP Q8IL11
B	608	HIS	-	expression tag	UNP Q8IL11
B	609	HIS	-	expression tag	UNP Q8IL11
B	610	HIS	-	expression tag	UNP Q8IL11
B	611	HIS	-	expression tag	UNP Q8IL11
C	152	GLN	ASN	engineered mutation	UNP Q8IL11
C	515	GLN	ASN	engineered mutation	UNP Q8IL11
C	546	GLN	ASN	engineered mutation	UNP Q8IL11
C	606	HIS	-	expression tag	UNP Q8IL11
C	607	HIS	-	expression tag	UNP Q8IL11
C	608	HIS	-	expression tag	UNP Q8IL11
C	609	HIS	-	expression tag	UNP Q8IL11
C	610	HIS	-	expression tag	UNP Q8IL11
C	611	HIS	-	expression tag	UNP Q8IL11
D	152	GLN	ASN	engineered mutation	UNP Q8IL11
D	515	GLN	ASN	engineered mutation	UNP Q8IL11
D	546	GLN	ASN	engineered mutation	UNP Q8IL11
D	606	HIS	-	expression tag	UNP Q8IL11
D	607	HIS	-	expression tag	UNP Q8IL11
D	608	HIS	-	expression tag	UNP Q8IL11
D	609	HIS	-	expression tag	UNP Q8IL11
D	610	HIS	-	expression tag	UNP Q8IL11
D	611	HIS	-	expression tag	UNP Q8IL11
E	152	GLN	ASN	engineered mutation	UNP Q8IL11
E	515	GLN	ASN	engineered mutation	UNP Q8IL11
E	546	GLN	ASN	engineered mutation	UNP Q8IL11
E	606	HIS	-	expression tag	UNP Q8IL11
E	607	HIS	-	expression tag	UNP Q8IL11
E	608	HIS	-	expression tag	UNP Q8IL11
E	609	HIS	-	expression tag	UNP Q8IL11
E	610	HIS	-	expression tag	UNP Q8IL11
E	611	HIS	-	expression tag	UNP Q8IL11
F	152	GLN	ASN	engineered mutation	UNP Q8IL11
F	515	GLN	ASN	engineered mutation	UNP Q8IL11

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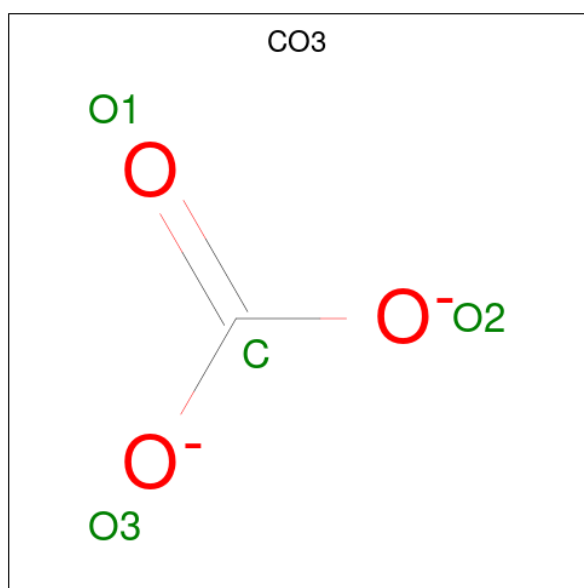
Chain	Residue	Modelled	Actual	Comment	Reference
F	546	GLN	ASN	engineered mutation	UNP Q8IL11
F	606	HIS	-	expression tag	UNP Q8IL11
F	607	HIS	-	expression tag	UNP Q8IL11
F	608	HIS	-	expression tag	UNP Q8IL11
F	609	HIS	-	expression tag	UNP Q8IL11
F	610	HIS	-	expression tag	UNP Q8IL11
F	611	HIS	-	expression tag	UNP Q8IL11
G	152	GLN	ASN	engineered mutation	UNP Q8IL11
G	515	GLN	ASN	engineered mutation	UNP Q8IL11
G	546	GLN	ASN	engineered mutation	UNP Q8IL11
G	606	HIS	-	expression tag	UNP Q8IL11
G	607	HIS	-	expression tag	UNP Q8IL11
G	608	HIS	-	expression tag	UNP Q8IL11
G	609	HIS	-	expression tag	UNP Q8IL11
G	610	HIS	-	expression tag	UNP Q8IL11
G	611	HIS	-	expression tag	UNP Q8IL11
H	152	GLN	ASN	engineered mutation	UNP Q8IL11
H	515	GLN	ASN	engineered mutation	UNP Q8IL11
H	546	GLN	ASN	engineered mutation	UNP Q8IL11
H	606	HIS	-	expression tag	UNP Q8IL11
H	607	HIS	-	expression tag	UNP Q8IL11
H	608	HIS	-	expression tag	UNP Q8IL11
H	609	HIS	-	expression tag	UNP Q8IL11
H	610	HIS	-	expression tag	UNP Q8IL11
H	611	HIS	-	expression tag	UNP Q8IL11
I	152	GLN	ASN	engineered mutation	UNP Q8IL11
I	515	GLN	ASN	engineered mutation	UNP Q8IL11
I	546	GLN	ASN	engineered mutation	UNP Q8IL11
I	606	HIS	-	expression tag	UNP Q8IL11
I	607	HIS	-	expression tag	UNP Q8IL11
I	608	HIS	-	expression tag	UNP Q8IL11
I	609	HIS	-	expression tag	UNP Q8IL11
I	610	HIS	-	expression tag	UNP Q8IL11
I	611	HIS	-	expression tag	UNP Q8IL11
J	152	GLN	ASN	engineered mutation	UNP Q8IL11
J	515	GLN	ASN	engineered mutation	UNP Q8IL11
J	546	GLN	ASN	engineered mutation	UNP Q8IL11
J	606	HIS	-	expression tag	UNP Q8IL11
J	607	HIS	-	expression tag	UNP Q8IL11
J	608	HIS	-	expression tag	UNP Q8IL11
J	609	HIS	-	expression tag	UNP Q8IL11
J	610	HIS	-	expression tag	UNP Q8IL11

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Chain	Residue	Modelled	Actual	Comment	Reference
J	611	HIS	-	expression tag	UNP Q8IL11
K	152	GLN	ASN	engineered mutation	UNP Q8IL11
K	515	GLN	ASN	engineered mutation	UNP Q8IL11
K	546	GLN	ASN	engineered mutation	UNP Q8IL11
K	606	HIS	-	expression tag	UNP Q8IL11
K	607	HIS	-	expression tag	UNP Q8IL11
K	608	HIS	-	expression tag	UNP Q8IL11
K	609	HIS	-	expression tag	UNP Q8IL11
K	610	HIS	-	expression tag	UNP Q8IL11
K	611	HIS	-	expression tag	UNP Q8IL11
L	152	GLN	ASN	engineered mutation	UNP Q8IL11
L	515	GLN	ASN	engineered mutation	UNP Q8IL11
L	546	GLN	ASN	engineered mutation	UNP Q8IL11
L	606	HIS	-	expression tag	UNP Q8IL11
L	607	HIS	-	expression tag	UNP Q8IL11
L	608	HIS	-	expression tag	UNP Q8IL11
L	609	HIS	-	expression tag	UNP Q8IL11
L	610	HIS	-	expression tag	UNP Q8IL11
L	611	HIS	-	expression tag	UNP Q8IL11

- Molecule 2 is CARBONATE ION (CCD ID: CO3) (formula: CO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	1	3		
2	B	1	Total	C	O	0	0
			4	1	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 4 1 3	0	0
2	D	1	Total C O 4 1 3	0	0
2	E	1	Total C O 4 1 3	0	0
2	F	1	Total C O 4 1 3	0	0
2	G	1	Total C O 4 1 3	0	0
2	H	1	Total C O 4 1 3	0	0
2	I	1	Total C O 4 1 3	0	0
2	J	1	Total C O 4 1 3	0	0
2	K	1	Total C O 4 1 3	0	0
2	L	1	Total C O 4 1 3	0	0

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

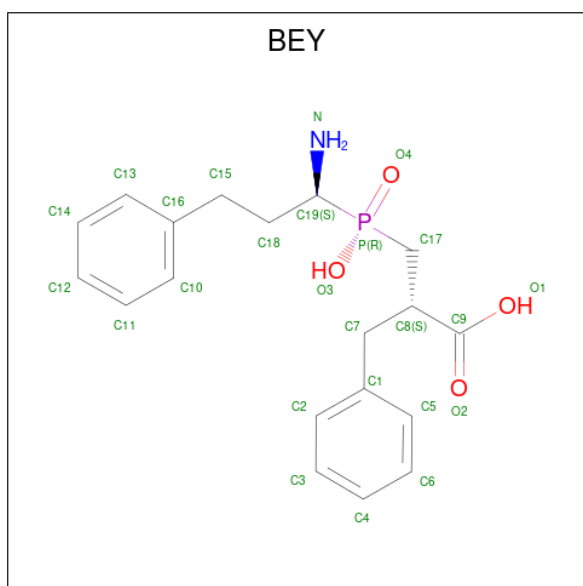
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Zn 2 2	0	0
3	B	2	Total Zn 2 2	0	0
3	C	2	Total Zn 2 2	0	0
3	D	2	Total Zn 2 2	0	0
3	E	2	Total Zn 2 2	0	0
3	F	2	Total Zn 2 2	0	0
3	G	2	Total Zn 2 2	0	0
3	H	2	Total Zn 2 2	0	0
3	I	2	Total Zn 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	2	Total	Zn	0	0
			2	2		
3	K	2	Total	Zn	0	0
			2	2		
3	L	2	Total	Zn	0	0
			2	2		

- Molecule 4 is (2S)-3-[(R)-[(1S)-1-amino-3-phenylpropyl](hydroxy)phosphoryl]-2-benzylpropionic acid (CCD ID: BEY) (formula: C₁₉H₂₄NO₄P).



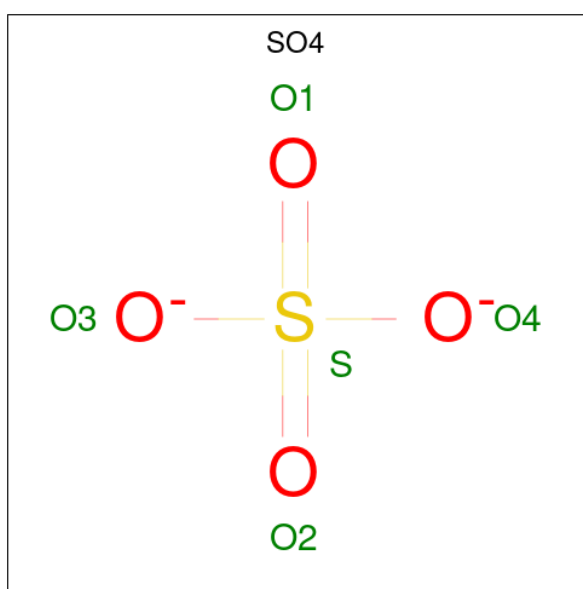
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			25	19	1	4	1		
4	B	1	Total	C	N	O	P	0	0
			25	19	1	4	1		
4	C	1	Total	C	N	O	P	0	0
			25	19	1	4	1		
4	D	1	Total	C	N	O	P	0	0
			25	19	1	4	1		
4	E	1	Total	C	N	O	P	0	0
			25	19	1	4	1		
4	F	1	Total	C	N	O	P	0	0
			25	19	1	4	1		
4	G	1	Total	C	N	O	P	0	0
			25	19	1	4	1		
4	H	1	Total	C	N	O	P	0	0
			25	19	1	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	I	1	Total	C	N	O	P	0	0
			25	19	1	4	1		
4	J	1	Total	C	N	O	P	0	0
			25	19	1	4	1		
4	K	1	Total	C	N	O	P	0	0
			25	19	1	4	1		
4	L	1	Total	C	N	O	P	0	0
			25	19	1	4	1		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



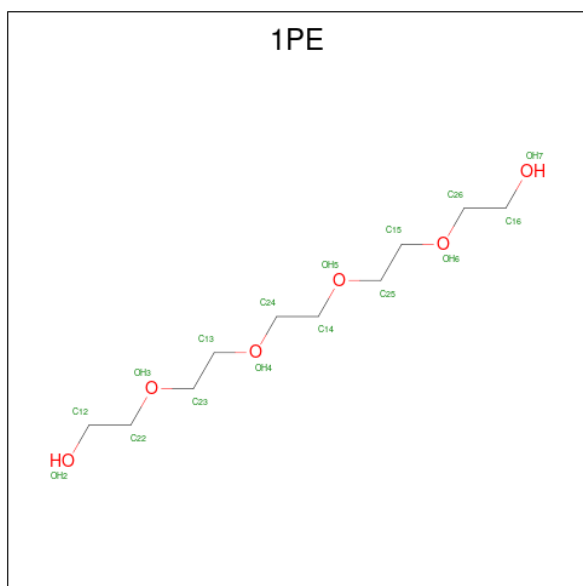
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	1	Total O S 5 4 1	0	0
5	G	1	Total O S 5 4 1	0	0
5	G	1	Total O S 5 4 1	0	0
5	I	1	Total O S 5 4 1	0	0
5	J	1	Total O S 5 4 1	0	0
5	J	1	Total O S 5 4 1	0	0
5	K	1	Total O S 5 4 1	0	0
5	L	1	Total O S 5 4 1	0	0

- Molecule 6 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 9 6 3	0	0
6	A	1	Total C O 12 8 4	0	0
6	B	1	Total C O 10 7 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			10	7	3		
6	B	1	Total	C	O	0	0
			10	7	3		
6	C	1	Total	C	O	0	0
			13	9	4		
6	C	1	Total	C	O	0	0
			9	6	3		
6	D	1	Total	C	O	0	0
			10	7	3		
6	D	1	Total	C	O	0	0
			11	8	3		
6	D	1	Total	C	O	0	0
			10	7	3		
6	D	1	Total	C	O	0	0
			7	5	2		
6	E	1	Total	C	O	0	0
			12	8	4		
6	E	1	Total	C	O	0	0
			12	8	4		
6	E	1	Total	C	O	0	0
			8	5	3		
6	F	1	Total	C	O	0	0
			10	6	4		
6	F	1	Total	C	O	0	0
			10	6	4		
6	F	1	Total	C	O	0	0
			10	6	4		
6	G	1	Total	C	O	0	0
			9	6	3		
6	G	1	Total	C	O	0	0
			7	4	3		
6	G	1	Total	C	O	0	0
			6	4	2		
6	G	1	Total	C	O	0	0
			6	4	2		
6	G	1	Total	C	O	0	0
			15	10	5		
6	H	1	Total	C	O	0	0
			10	7	3		
6	H	1	Total	C	O	0	0
			10	7	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	I	1	Total	C	O	0	0
			15	10	5		
6	I	1	Total	C	O	0	0
			11	8	3		
6	I	1	Total	C	O	0	0
			7	5	2		
6	J	1	Total	C	O	0	0
			11	7	4		
6	J	1	Total	C	O	0	0
			10	6	4		
6	J	1	Total	C	O	0	0
			10	7	3		
6	K	1	Total	C	O	0	0
			12	8	4		
6	K	1	Total	C	O	0	0
			12	8	4		
6	K	1	Total	C	O	0	0
			11	7	4		
6	K	1	Total	C	O	0	0
			6	4	2		
6	L	1	Total	C	O	0	0
			10	6	4		
6	L	1	Total	C	O	0	0
			12	8	4		
6	L	1	Total	C	O	0	0
			11	7	4		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	217	Total	O	0	0
			217	217		
7	B	158	Total	O	0	0
			158	158		
7	C	188	Total	O	0	0
			188	188		
7	D	182	Total	O	0	0
			182	182		
7	E	203	Total	O	0	0
			203	203		
7	F	165	Total	O	0	0
			165	165		

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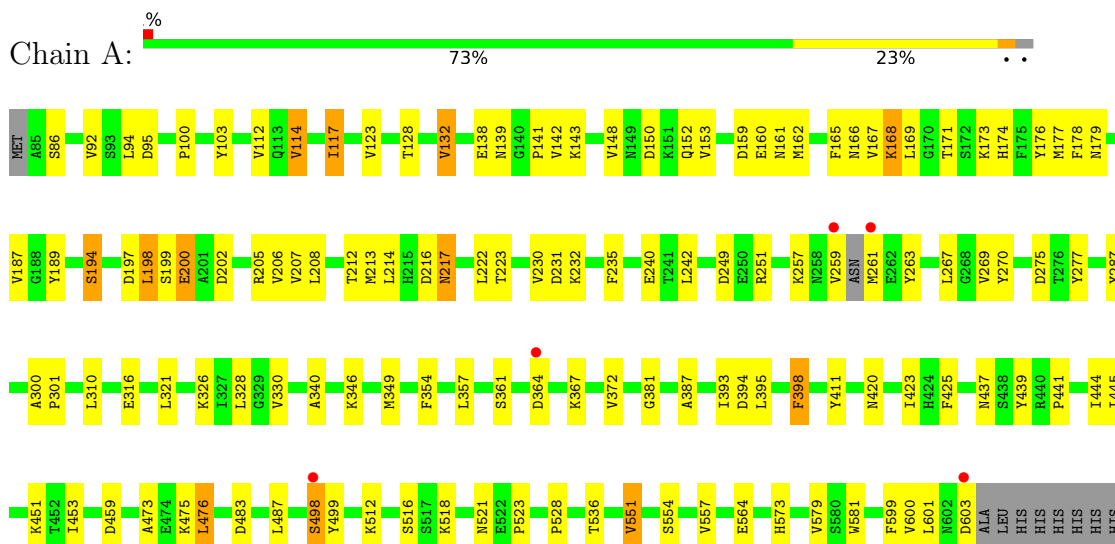
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	204	Total 204	O 204	0	0
7	H	203	Total 203	O 203	0	0
7	I	207	Total 207	O 207	0	0
7	J	207	Total 207	O 207	0	0
7	K	222	Total 222	O 222	0	0
7	L	158	Total 158	O 158	0	0

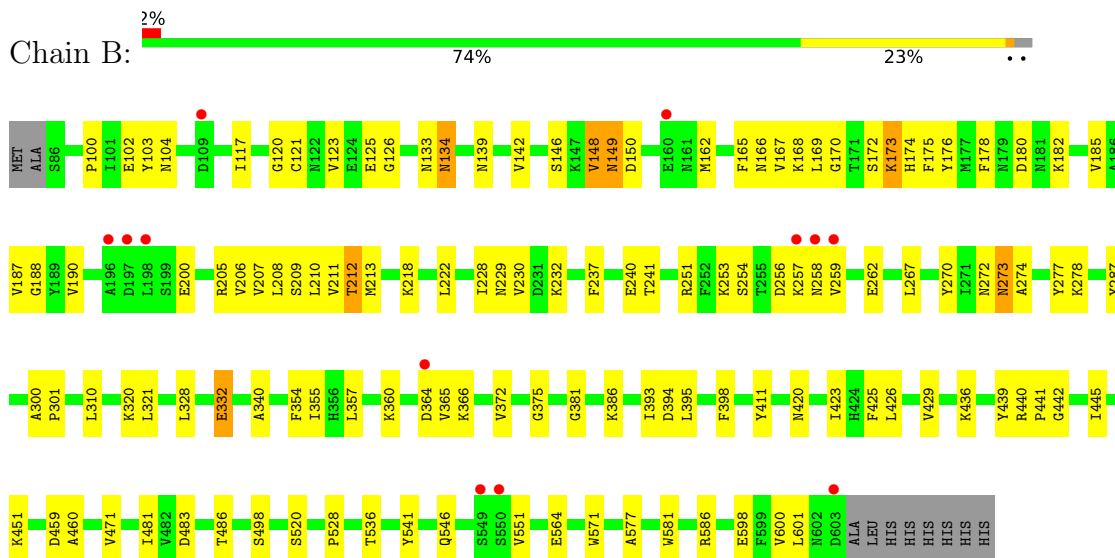
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: M17 leucyl aminopeptidase

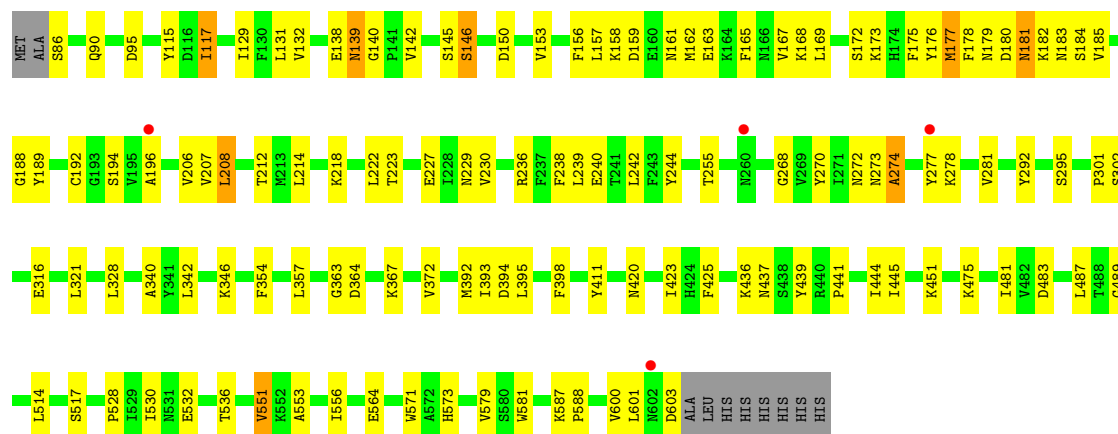


- Molecule 1: M17 leucyl aminopeptidase

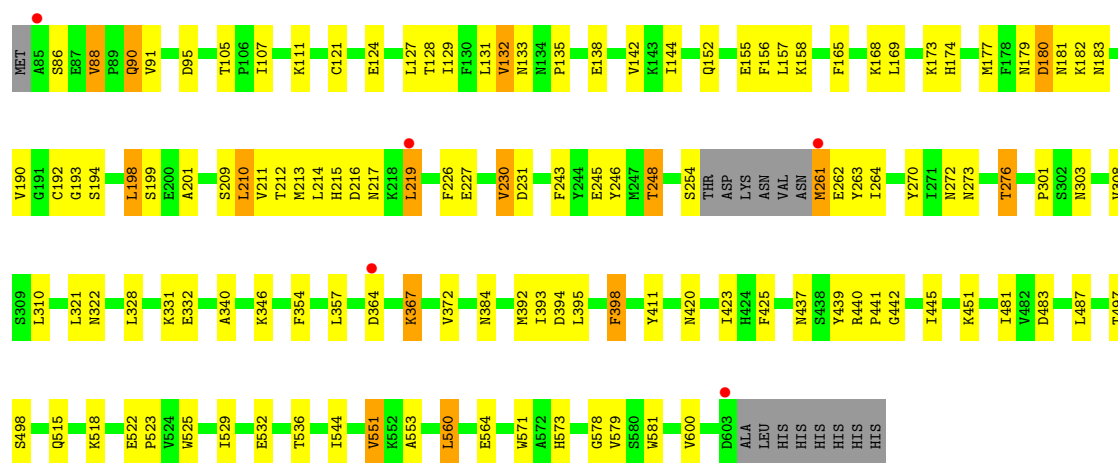
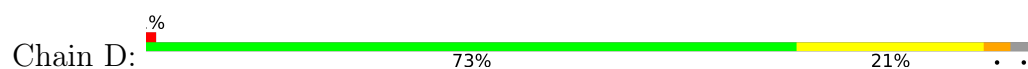


- Molecule 1: M17 leucyl aminopeptidase

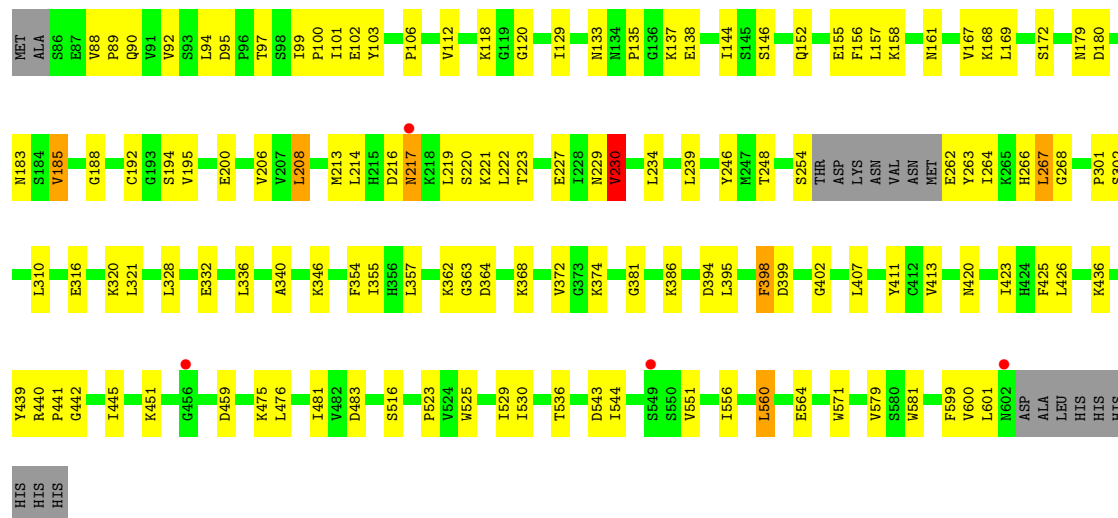




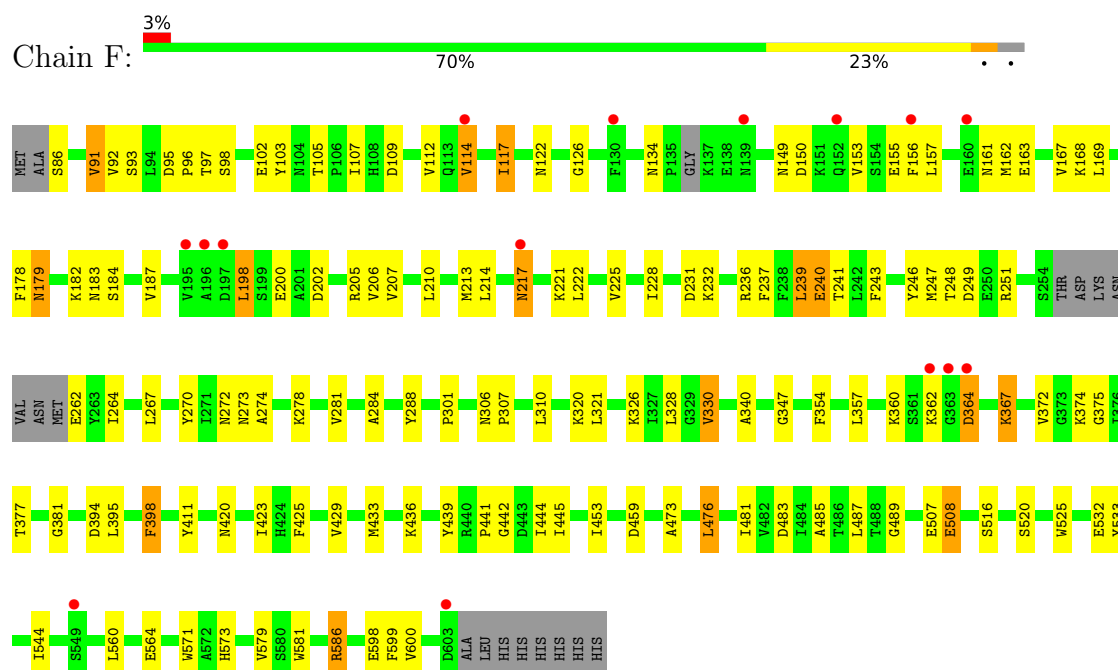
• Molecule 1: M17 leucyl aminopeptidase



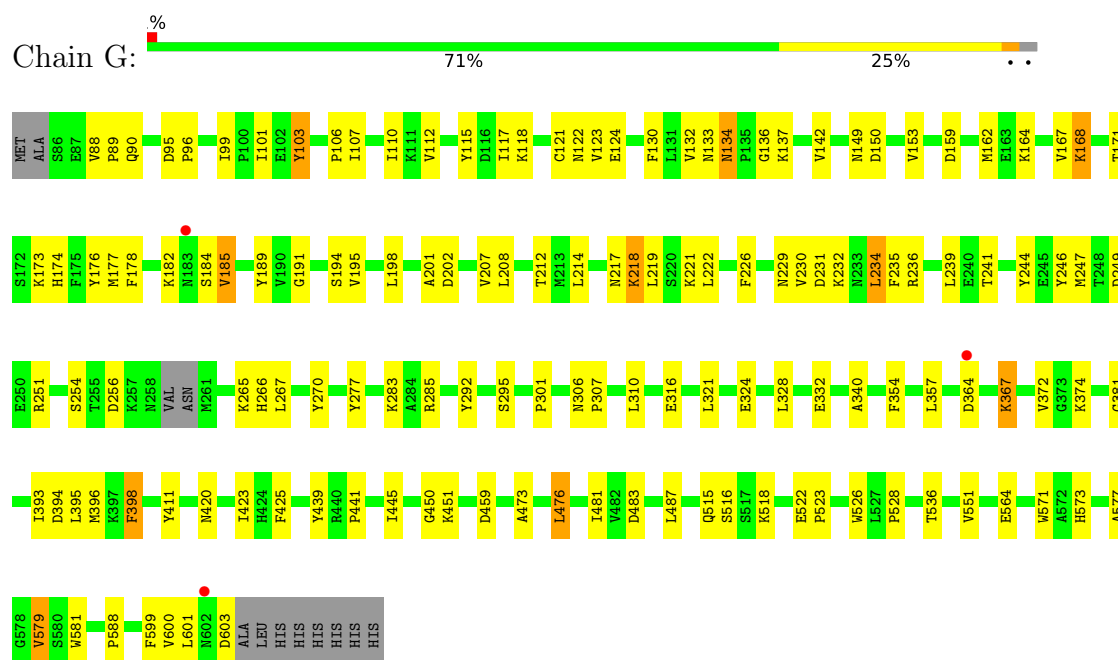
• Molecule 1: M17 leucyl aminopeptidase



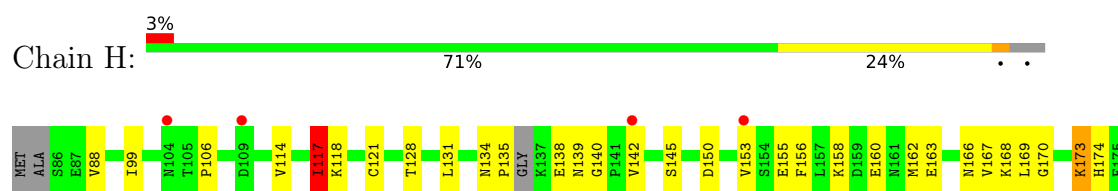
• Molecule 1: M17 leucyl aminopeptidase

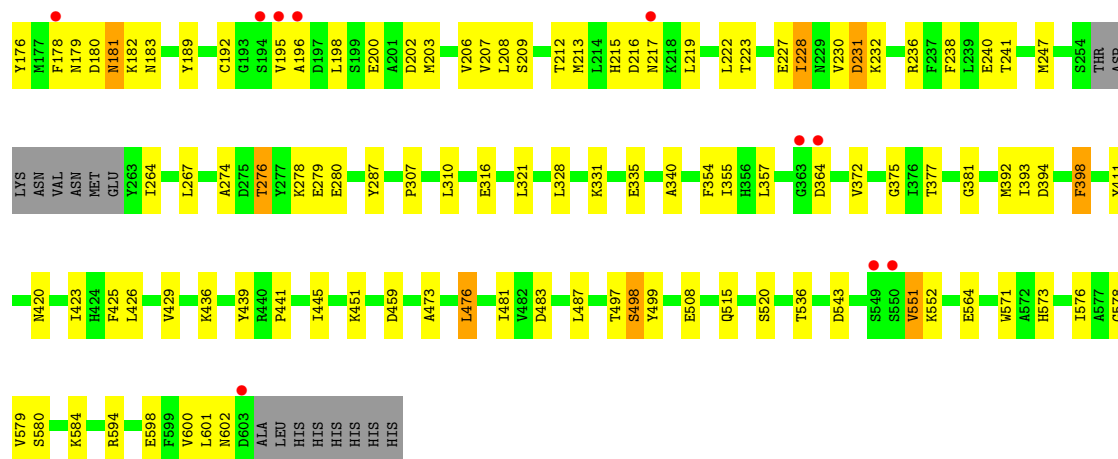


• Molecule 1: M17 leucyl aminopeptidase



• Molecule 1: M17 leucyl aminopeptidase

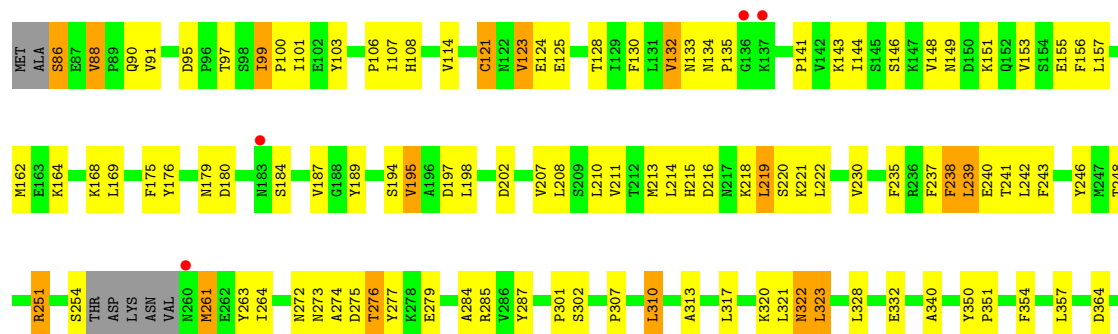


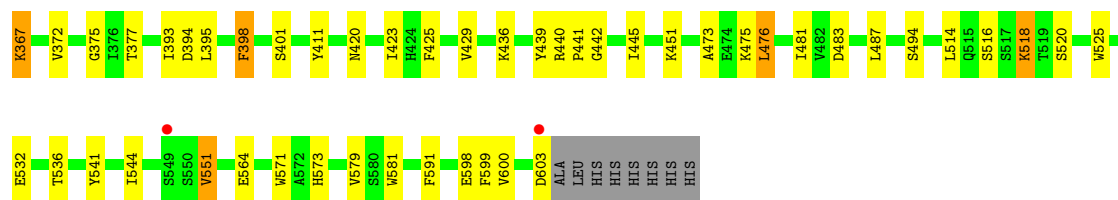


• Molecule 1: M17 leucyl aminopeptidase

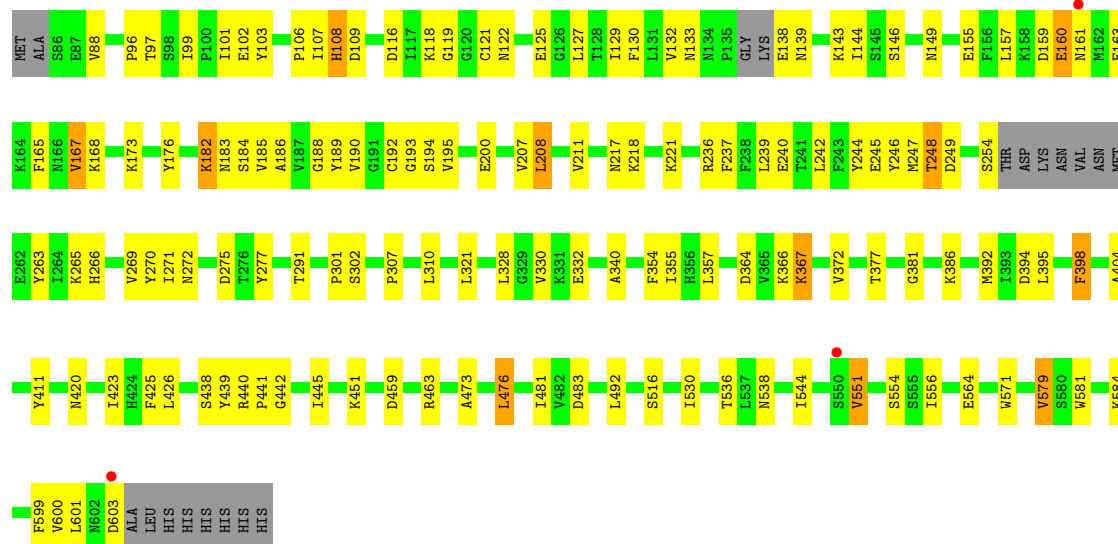


• Molecule 1: M17 leucyl aminopeptidase

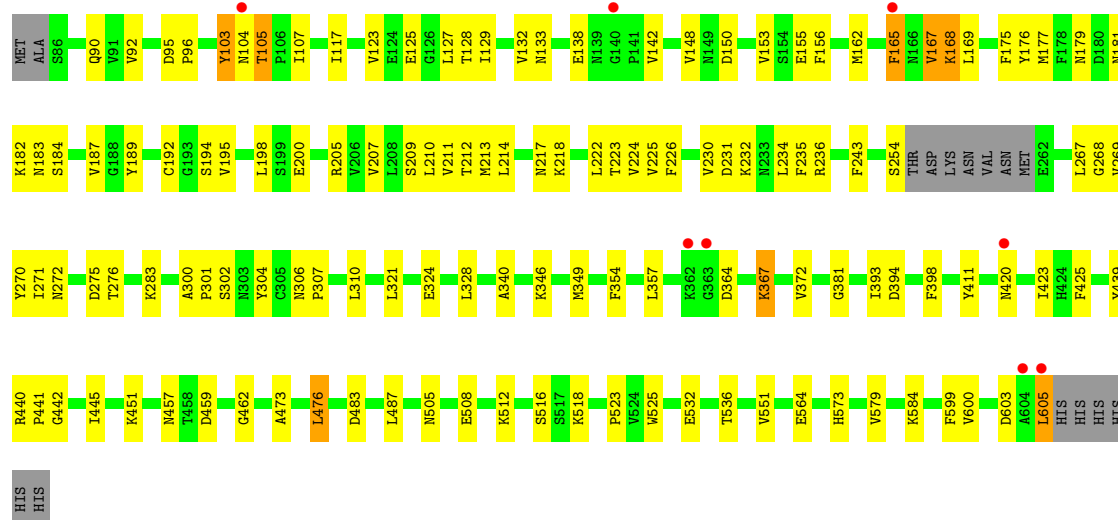




• Molecule 1: M17 leucyl aminopeptidase



• Molecule 1: M17 leucyl aminopeptidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	172.08Å 174.16Å 227.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	77.70 – 2.56 77.70 – 2.56	Depositor EDS
% Data completeness (in resolution range)	98.8 (77.70-2.56) 99.2 (77.70-2.56)	Depositor EDS
R_{merge}	0.55	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.55Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.220 , 0.278 0.224 , 0.281	Depositor DCC
R_{free} test set	10910 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	50444	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.88 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.3151e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BEY, ZN, CO3, 1PE, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.82	0/4057	0.98	1/5500 (0.0%)
1	B	0.82	0/4007	0.95	1/5442 (0.0%)
1	C	0.84	1/4031 (0.0%)	0.96	5/5469 (0.1%)
1	D	0.84	1/4005 (0.0%)	0.98	5/5429 (0.1%)
1	E	0.87	1/3974 (0.0%)	0.98	4/5393 (0.1%)
1	F	0.80	0/3949	0.99	4/5364 (0.1%)
1	G	0.85	1/4066 (0.0%)	0.98	7/5505 (0.1%)
1	H	0.81	0/4014	0.94	7/5434 (0.1%)
1	I	0.83	1/4084 (0.0%)	0.98	5/5531 (0.1%)
1	J	0.86	2/4031 (0.0%)	0.97	7/5461 (0.1%)
1	K	0.90	6/4006 (0.1%)	1.02	11/5427 (0.2%)
1	L	0.84	3/4009 (0.1%)	0.95	2/5440 (0.0%)
All	All	0.84	16/48233 (0.0%)	0.97	59/65395 (0.1%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	183	ASN	C-O	-6.73	1.15	1.24
1	L	105	THR	C-O	-6.37	1.17	1.24
1	K	184	SER	C-O	-6.35	1.16	1.23
1	K	183	ASN	C-O	-6.15	1.16	1.23
1	L	218	LYS	C-O	-6.04	1.16	1.24
1	K	404	ALA	CA-CB	-5.80	1.44	1.53
1	C	218	LYS	C-O	-5.80	1.16	1.23
1	L	103	TYR	CA-C	-5.62	1.48	1.52
1	K	160	GLU	C-O	-5.62	1.17	1.24
1	J	323	LEU	C-O	-5.60	1.17	1.23
1	J	323	LEU	CA-C	-5.54	1.45	1.52
1	D	217	ASN	C-O	-5.49	1.17	1.24
1	I	218	LYS	C-O	-5.48	1.17	1.24
1	K	182	LYS	C-O	-5.45	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	218	LYS	C-O	-5.45	1.17	1.24
1	K	161	ASN	C-O	-5.03	1.18	1.24

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	586	ARG	NE-CZ-NH2	11.10	129.19	119.20
1	F	586	ARG	NE-CZ-NH2	10.52	128.66	119.20
1	I	586	ARG	NE-CZ-NH1	-9.74	111.76	121.50
1	K	161	ASN	N-CA-C	9.69	121.44	111.07
1	F	586	ARG	NE-CZ-NH1	-9.25	112.25	121.50
1	H	99	ILE	CA-C-N	-8.21	111.56	119.76
1	H	99	ILE	C-N-CA	-8.21	111.56	119.76
1	K	99	ILE	CA-C-N	-7.87	111.89	119.76
1	K	99	ILE	C-N-CA	-7.87	111.89	119.76
1	F	586	ARG	CD-NE-CZ	7.46	134.84	124.40
1	G	134	ASN	CA-C-N	-7.41	111.38	119.98
1	G	134	ASN	C-N-CA	-7.41	111.38	119.98
1	K	200	GLU	N-CA-C	-7.33	103.36	111.36
1	I	586	ARG	CD-NE-CZ	7.32	134.65	124.40
1	J	238	PHE	N-CA-C	-7.15	103.09	111.03
1	K	119	GLY	N-CA-C	-6.96	105.59	114.37
1	D	105	THR	N-CA-C	-6.81	101.48	110.40
1	E	99	ILE	CA-C-N	-6.50	112.97	119.92
1	E	99	ILE	C-N-CA	-6.50	112.97	119.92
1	C	551	VAL	N-CA-C	6.19	117.29	108.93
1	I	271	ILE	N-CA-C	6.17	116.39	107.88
1	J	551	VAL	N-CA-C	5.98	117.00	108.93
1	D	551	VAL	N-CA-C	5.96	116.98	108.93
1	L	230	VAL	CA-C-N	5.94	129.72	120.75
1	L	230	VAL	C-N-CA	5.94	129.72	120.75
1	H	228	ILE	N-CA-C	-5.85	100.17	109.17
1	H	88	VAL	CA-C-N	-5.76	114.03	119.85
1	H	88	VAL	C-N-CA	-5.76	114.03	119.85
1	H	551	VAL	N-CA-C	5.65	116.30	108.84
1	C	177	MET	N-CA-C	5.64	116.00	108.38
1	C	140	GLY	CA-C-N	5.58	125.89	119.92
1	C	140	GLY	C-N-CA	5.58	125.89	119.92
1	K	269	VAL	CA-C-N	-5.57	115.31	123.00
1	K	269	VAL	C-N-CA	-5.57	115.31	123.00
1	E	579	VAL	CB-CA-C	-5.44	102.89	110.95
1	J	218	LYS	N-CA-C	-5.44	106.31	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	579	VAL	N-CA-CB	-5.33	105.00	112.35
1	J	121	CYS	N-CA-C	5.32	117.19	108.52
1	K	551	VAL	N-CA-C	5.27	115.80	108.84
1	J	146	SER	N-CA-C	5.25	117.85	110.23
1	G	246	TYR	N-CA-C	-5.25	106.02	112.90
1	D	515	GLN	N-CA-C	-5.22	105.67	111.36
1	A	551	VAL	N-CA-C	5.22	115.73	108.84
1	I	402	GLY	N-CA-C	-5.21	106.47	112.73
1	K	190	VAL	N-CA-C	-5.20	100.99	108.48
1	D	88	VAL	N-CA-CB	5.19	115.33	109.99
1	F	330	VAL	N-CA-CB	5.19	117.59	110.54
1	E	402	GLY	N-CA-C	-5.18	106.51	112.73
1	K	146	SER	N-CA-C	5.16	117.96	110.42
1	G	99	ILE	CA-C-N	-5.12	114.64	119.76
1	G	99	ILE	C-N-CA	-5.12	114.64	119.76
1	G	103	TYR	N-CA-C	-5.08	105.92	112.68
1	J	219	LEU	N-CA-C	5.08	116.52	109.31
1	B	134	ASN	N-CA-C	-5.07	99.47	108.55
1	G	579	VAL	N-CA-CB	-5.04	105.39	112.35
1	D	209	SER	N-CA-C	-5.03	105.50	111.69
1	C	579	VAL	CB-CA-C	-5.03	103.51	110.95
1	H	121	CYS	N-CA-C	5.02	116.35	107.61
1	J	275	ASP	N-CA-C	5.01	116.74	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3980	0	3912	101	0
1	B	3929	0	3828	93	1
1	C	3953	0	3882	94	0
1	D	3928	0	3876	107	0
1	E	3897	0	3822	98	0
1	F	3873	0	3772	100	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	3989	0	3976	100	0
1	H	3938	0	3931	87	0
1	I	4006	0	3986	98	0
1	J	3954	0	3923	126	0
1	K	3930	0	3901	89	0
1	L	3932	0	3862	95	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	2	0
2	E	4	0	0	0	0
2	F	4	0	0	0	0
2	G	4	0	0	0	0
2	H	4	0	0	1	0
2	I	4	0	0	1	0
2	J	4	0	0	1	0
2	K	4	0	0	2	0
2	L	4	0	0	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
4	A	25	0	21	4	0
4	B	25	0	22	3	0
4	C	25	0	21	5	0
4	D	25	0	22	6	0
4	E	25	0	22	2	0
4	F	25	0	21	2	0
4	G	25	0	21	3	0
4	H	25	0	22	7	0
4	I	25	0	22	2	0
4	J	25	0	22	3	0
4	K	25	0	22	3	0
4	L	25	0	22	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	15	0	0	0	0
5	C	5	0	0	1	0
5	D	5	0	0	0	0
5	E	10	0	0	3	0
5	F	5	0	0	1	0
5	G	10	0	0	0	0
5	I	5	0	0	1	0
5	J	10	0	0	2	0
5	K	5	0	0	0	0
5	L	5	0	0	0	0
6	A	21	0	22	2	0
6	B	30	0	30	3	0
6	C	22	0	24	1	0
6	D	38	0	38	5	0
6	E	32	0	36	4	0
6	F	30	0	39	1	0
6	G	43	0	47	4	0
6	H	20	0	20	1	0
6	I	33	0	37	6	0
6	J	31	0	36	9	0
6	K	41	0	44	8	0
6	L	33	0	40	5	0
7	A	217	0	0	13	0
7	B	158	0	0	7	0
7	C	188	0	0	6	0
7	D	182	0	0	5	1
7	E	203	0	0	15	0
7	F	165	0	0	14	0
7	G	204	0	0	11	0
7	H	203	0	0	6	0
7	I	207	0	0	6	0
7	J	207	0	0	18	0
7	K	222	0	0	7	0
7	L	158	0	0	11	0
All	All	50444	0	47344	1107	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (1107) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:436:LYS:HE2	7:I:3958:HOH:O	1.43	1.15
1:B:257:LYS:HA	1:B:258:ASN:HB3	1.34	1.09
1:J:518:LYS:HE2	7:J:2650:HOH:O	1.52	1.08
1:I:214:LEU:HD21	1:I:222:LEU:HD22	1.39	1.03
1:G:136:GLY:HA3	1:G:137:LYS:CB	1.86	1.02
1:J:320:LYS:NZ	6:J:3:1PE:H142	1.74	1.02
1:B:436:LYS:HE2	7:C:3093:HOH:O	1.59	0.99
1:J:254:SER:HB2	7:L:2793:HOH:O	1.61	0.99
1:B:586:ARG:HA	7:B:1076:HOH:O	1.62	0.98
1:A:361:SER:HB3	7:A:755:HOH:O	1.63	0.98
1:E:230:VAL:HG22	1:E:234:LEU:HB3	1.47	0.96
1:A:259:VAL:O	1:A:261:MET:N	2.00	0.94
1:K:133:ASN:HA	1:K:167:VAL:HG11	1.48	0.94
1:C:230:VAL:O	1:C:277:TYR:OH	1.86	0.93
1:A:173:LYS:NZ	1:D:216:ASP:OD2	2.01	0.92
1:I:230:VAL:O	1:I:277:TYR:OH	1.89	0.89
1:B:274:ALA:O	1:B:278:LYS:HG3	1.76	0.86
1:K:96:PRO:HA	6:K:50:1PE:H142	1.58	0.86
1:D:254:SER:HB2	7:F:1110:HOH:O	1.75	0.86
1:J:320:LYS:HZ3	6:J:3:1PE:H142	1.40	0.86
1:B:178:PHE:HZ	1:F:155:GLU:HG2	1.42	0.83
1:J:411:TYR:HE1	6:J:2:1PE:H151	1.44	0.82
1:I:328:LEU:HB2	1:I:354:PHE:HB3	1.61	0.82
1:I:121:CYS:SG	1:I:225:VAL:HG21	2.19	0.82
1:F:231:ASP:HB2	7:F:3092:HOH:O	1.79	0.82
1:D:127:LEU:HD11	1:D:129:ILE:HD11	1.60	0.82
1:E:229:ASN:O	1:E:230:VAL:HB	1.79	0.81
1:F:117:ILE:HG13	1:F:270:TYR:HB3	1.60	0.81
1:L:90:GLN:NE2	1:L:95:ASP:O	2.13	0.81
1:G:178:PHE:HZ	1:J:155:GLU:HG2	1.45	0.81
1:J:401:SER:HB3	7:J:748:HOH:O	1.81	0.80
1:B:175:PHE:CD2	1:B:188:GLY:HA2	2.17	0.80
1:L:328:LEU:HB2	1:L:354:PHE:HB3	1.62	0.79
1:G:328:LEU:HB2	1:G:354:PHE:HB3	1.64	0.79
1:G:367:LYS:HG2	1:G:603:ASP:OD1	1.83	0.79
1:F:114:VAL:HG21	1:F:278:LYS:HG2	1.63	0.79
1:C:532:GLU:OE1	1:D:498:SER:OG	1.99	0.79
1:H:392:MET:HE3	4:H:1003:BEY:H12	1.65	0.79
1:C:328:LEU:HB2	1:C:354:PHE:HB3	1.66	0.77
1:A:216:ASP:O	1:D:173:LYS:HE3	1.85	0.77
1:K:328:LEU:HB2	1:K:354:PHE:HB3	1.65	0.77
1:K:538:ASN:HB2	7:K:5283:HOH:O	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:173:LYS:HA	7:K:1921:HOH:O	1.84	0.77
1:L:349:MET:HB2	7:L:2456:HOH:O	1.84	0.77
1:J:328:LEU:HB2	1:J:354:PHE:HB3	1.65	0.76
1:B:175:PHE:HD2	1:B:188:GLY:HA2	1.50	0.76
1:I:340:ALA:HA	1:I:445:ILE:HD12	1.68	0.76
1:B:328:LEU:HB2	1:B:354:PHE:HB3	1.66	0.75
1:J:394:ASP:HA	1:L:441:PRO:HB2	1.68	0.75
1:H:328:LEU:HB2	1:H:354:PHE:HB3	1.66	0.75
1:E:144:ILE:HG13	1:E:157:LEU:HD22	1.68	0.75
1:D:90:GLN:HB3	1:D:95:ASP:HB2	1.66	0.74
1:E:230:VAL:HG23	1:E:234:LEU:HD23	1.67	0.74
1:J:164:LYS:HE2	7:J:944:HOH:O	1.86	0.74
1:E:103:TYR:HB2	5:E:22:SO4:O3	1.88	0.74
1:K:441:PRO:HB2	1:L:394:ASP:HA	1.68	0.74
1:E:441:PRO:HB2	1:F:394:ASP:HA	1.69	0.74
1:G:441:PRO:HB2	1:H:394:ASP:HA	1.70	0.74
6:J:45:1PE:H242	7:J:3061:HOH:O	1.88	0.74
1:G:168:LYS:O	1:G:171:THR:HG22	1.87	0.74
1:A:340:ALA:HA	1:A:445:ILE:HD12	1.71	0.73
1:H:192:CYS:HB3	1:H:198:LEU:HD11	1.71	0.72
1:J:207:VAL:HG11	1:J:241:THR:HG22	1.71	0.72
1:A:178:PHE:CZ	1:D:155:GLU:HG2	2.23	0.72
1:D:328:LEU:HB2	1:D:354:PHE:HB3	1.71	0.72
1:A:178:PHE:HZ	1:D:155:GLU:CG	2.02	0.72
1:C:363:GLY:HA3	7:C:4562:HOH:O	1.90	0.72
1:D:219:LEU:HD13	1:D:219:LEU:H	1.54	0.72
1:E:328:LEU:HB2	1:E:354:PHE:HB3	1.71	0.72
1:F:328:LEU:HB2	1:F:354:PHE:HB3	1.69	0.72
1:G:321:LEU:HD11	1:G:411:TYR:HA	1.71	0.72
1:L:340:ALA:HA	1:L:445:ILE:HD12	1.72	0.72
1:C:172:SER:O	1:C:173:LYS:HD2	1.90	0.72
1:C:274:ALA:O	1:C:278:LYS:HG3	1.89	0.71
1:D:394:ASP:HA	1:F:441:PRO:HB2	1.72	0.71
1:E:321:LEU:HD11	1:E:411:TYR:HA	1.72	0.71
1:E:475:LYS:HD3	7:E:4546:HOH:O	1.89	0.71
1:I:215:HIS:O	1:I:216:ASP:HB2	1.88	0.71
1:J:237:PHE:HA	1:J:240:GLU:OE1	1.91	0.71
1:L:132:VAL:HG21	1:L:142:VAL:HG13	1.72	0.71
1:L:176:TYR:OH	1:L:217:ASN:OD1	2.04	0.71
1:F:117:ILE:HD11	1:F:225:VAL:HG13	1.72	0.71
1:I:178:PHE:HZ	1:K:155:GLU:HG2	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:LYS:HD2	1:B:256:ASP:HB3	1.73	0.71
1:K:144:ILE:HG13	1:K:157:LEU:HD22	1.73	0.71
1:K:451:LYS:HD3	6:K:42:1PE:H231	1.73	0.71
1:A:321:LEU:HD11	1:A:411:TYR:HA	1.71	0.70
1:C:132:VAL:HG21	1:C:142:VAL:HG13	1.73	0.70
1:J:321:LEU:O	1:J:322:ASN:HB2	1.90	0.70
1:D:179:ASN:OD1	1:D:183:ASN:HB2	1.92	0.70
1:I:128:THR:HB	1:I:187:VAL:HG13	1.73	0.70
1:K:340:ALA:HA	1:K:445:ILE:HD12	1.71	0.70
1:C:321:LEU:HD11	1:C:411:TYR:HA	1.74	0.70
1:H:392:MET:CE	4:H:1003:BEY:H12	2.22	0.70
1:A:173:LYS:CE	1:D:216:ASP:OD2	2.40	0.70
1:F:340:ALA:HA	1:F:445:ILE:HD12	1.72	0.70
1:K:321:LEU:HD11	1:K:411:TYR:HA	1.74	0.70
1:D:340:ALA:HA	1:D:445:ILE:HD12	1.74	0.70
1:K:386:LYS:NZ	4:K:1003:BEY:O3	2.23	0.69
1:D:321:LEU:HD11	1:D:411:TYR:HA	1.73	0.69
1:G:396:MET:HE3	7:G:2070:HOH:O	1.92	0.69
1:C:173:LYS:NZ	1:E:217:ASN:OD1	2.25	0.69
1:J:151:LYS:N	1:J:180:ASP:OD2	2.24	0.69
1:L:104:ASN:OD1	6:L:1:1PE:H141	1.92	0.69
1:A:441:PRO:HB2	1:B:394:ASP:HA	1.74	0.69
1:B:218:LYS:HG2	1:B:262:GLU:CD	2.18	0.69
1:H:321:LEU:HD11	1:H:411:TYR:HA	1.73	0.69
1:G:340:ALA:HA	1:G:445:ILE:HD12	1.75	0.69
1:D:441:PRO:HB2	1:E:394:ASP:HA	1.74	0.69
1:B:257:LYS:HA	1:B:258:ASN:CB	2.18	0.69
1:E:100:PRO:O	1:E:101:ILE:HD13	1.92	0.69
1:H:240:GLU:OE2	1:H:287:TYR:HD2	1.75	0.69
1:J:320:LYS:HZ1	6:J:3:1PE:H142	1.58	0.69
1:F:321:LEU:HD11	1:F:411:TYR:HA	1.76	0.68
1:G:207:VAL:HG11	1:G:241:THR:HG22	1.75	0.68
1:I:244:TYR:OH	1:I:588:PRO:O	2.12	0.68
1:H:232:LYS:HE3	1:H:276:THR:HB	1.74	0.68
1:D:174:HIS:CE1	1:D:213:MET:HG2	2.29	0.68
1:H:441:PRO:HB2	1:I:394:ASP:HA	1.75	0.68
1:I:321:LEU:HD11	1:I:411:TYR:HA	1.76	0.68
1:K:133:ASN:HB2	1:K:193:GLY:O	1.94	0.68
1:K:133:ASN:CA	1:K:167:VAL:HG11	2.23	0.68
1:L:321:LEU:HD11	1:L:411:TYR:HA	1.76	0.68
1:H:340:ALA:HA	1:H:445:ILE:HD12	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:63:1PE:C25	7:D:3204:HOH:O	2.42	0.67
1:A:178:PHE:HZ	1:D:155:GLU:HG2	1.58	0.67
1:G:117:ILE:HD11	1:G:226:PHE:O	1.95	0.67
1:J:219:LEU:HD11	7:J:3193:HOH:O	1.94	0.67
1:F:107:ILE:HG21	1:F:243:PHE:HB3	1.77	0.67
1:H:167:VAL:O	1:H:168:LYS:C	2.36	0.67
1:B:332:GLU:HB3	7:B:675:HOH:O	1.93	0.67
1:A:208:LEU:O	1:A:212:THR:HG23	1.94	0.67
1:J:441:PRO:HB2	1:K:394:ASP:HA	1.75	0.67
1:B:441:PRO:HB2	1:C:394:ASP:HA	1.76	0.67
1:E:340:ALA:HA	1:E:445:ILE:HD12	1.75	0.67
1:A:328:LEU:HB2	1:A:354:PHE:HB3	1.76	0.66
1:C:340:ALA:HA	1:C:445:ILE:HD12	1.76	0.66
1:I:169:LEU:HA	1:I:191:GLY:O	1.94	0.66
1:I:274:ALA:O	1:I:278:LYS:HG3	1.95	0.66
1:G:173:LYS:HD2	1:J:176:TYR:HE1	1.61	0.66
1:C:274:ALA:HB1	1:C:278:LYS:HE3	1.78	0.65
1:L:462:GLY:N	2:L:1002:CO3:O2	2.27	0.65
1:J:215:HIS:O	1:J:261:MET:HB3	1.96	0.65
1:B:230:VAL:O	1:B:277:TYR:OH	2.09	0.65
1:L:107:ILE:HG21	1:L:243:PHE:HB3	1.78	0.65
1:F:156:PHE:O	1:F:162:MET:HE3	1.96	0.65
1:B:102:GLU:CG	7:B:4121:HOH:O	2.45	0.65
1:C:173:LYS:HE3	1:E:217:ASN:OD1	1.97	0.65
1:B:139:ASN:O	1:B:166:ASN:HB2	1.97	0.65
1:B:321:LEU:HD11	1:B:411:TYR:HA	1.77	0.65
2:D:1002:CO3:O2	4:D:1003:BEY:H7A	1.97	0.64
1:G:394:ASP:HA	1:I:441:PRO:HB2	1.78	0.64
1:C:153:VAL:HG12	1:C:157:LEU:CD1	2.27	0.64
1:I:129:ILE:HA	1:I:188:GLY:O	1.97	0.64
1:B:232:LYS:HB2	7:B:4536:HOH:O	1.96	0.64
1:I:230:VAL:HG22	1:I:234:LEU:HB3	1.79	0.64
1:A:132:VAL:HG21	1:A:142:VAL:HG13	1.80	0.64
1:H:274:ALA:O	1:H:278:LYS:HG3	1.97	0.64
1:H:240:GLU:OE2	1:H:287:TYR:CD2	2.51	0.64
1:B:142:VAL:HG23	1:B:162:MET:HB3	1.80	0.63
1:D:451:LYS:HE2	6:D:44:1PE:H151	1.79	0.63
1:G:136:GLY:CA	1:G:137:LYS:CB	2.72	0.63
1:H:150:ASP:OD2	1:H:153:VAL:HG23	1.98	0.63
1:D:423:ILE:HD11	1:D:600:VAL:HG13	1.80	0.63
1:J:123:VAL:HG23	1:J:123:VAL:O	1.96	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:176:TYR:OH	1:K:217:ASN:OD1	2.14	0.63
1:J:321:LEU:O	1:J:322:ASN:CB	2.43	0.63
1:D:331:LYS:CD	1:D:331:LYS:H	2.09	0.63
1:J:88:VAL:HG11	1:J:97:THR:O	1.98	0.63
1:A:372:VAL:O	1:A:483:ASP:HA	1.99	0.63
1:I:118:LYS:HE3	7:I:4080:HOH:O	1.98	0.63
1:J:340:ALA:HA	1:J:445:ILE:HD12	1.81	0.63
1:C:178:PHE:HZ	1:E:155:GLU:HG2	1.64	0.63
1:D:192:CYS:HB3	1:D:198:LEU:HD21	1.79	0.63
1:H:173:LYS:HB2	1:H:189:TYR:CE1	2.33	0.63
1:L:231:ASP:HB3	1:L:234:LEU:H	1.64	0.62
1:A:498:SER:OG	1:F:532:GLU:OE1	2.17	0.62
1:D:124:GLU:HA	1:D:179:ASN:ND2	2.14	0.62
1:D:273:ASN:O	1:D:276:THR:HG23	2.00	0.62
1:I:238:PHE:HD2	1:I:239:LEU:HD13	1.63	0.62
1:K:236:ARG:NE	1:K:240:GLU:OE2	2.27	0.62
1:C:146:SER:OG	1:C:227:GLU:OE2	2.16	0.62
1:J:144:ILE:HG13	1:J:157:LEU:HD22	1.81	0.62
1:A:523:PRO:HA	7:A:1372:HOH:O	1.98	0.62
1:J:198:LEU:HD22	1:J:202:ASP:HB3	1.82	0.62
1:L:367:LYS:HG2	1:L:603:ASP:OD2	1.99	0.62
1:L:451:LYS:HE2	6:L:612:1PE:H241	1.82	0.62
1:A:499:TYR:CZ	1:A:523:PRO:HB3	2.35	0.62
1:L:138:GLU:HA	1:L:194:SER:OG	1.99	0.62
1:B:148:VAL:O	1:B:150:ASP:N	2.28	0.62
1:A:499:TYR:CD2	1:A:523:PRO:HB2	2.34	0.62
1:C:153:VAL:HG12	1:C:157:LEU:HD11	1.80	0.62
1:L:523:PRO:HD3	7:L:644:HOH:O	1.99	0.62
1:H:192:CYS:O	1:H:198:LEU:HD21	1.99	0.61
1:K:554:SER:HB3	7:K:3921:HOH:O	1.99	0.61
1:A:518:LYS:HB2	7:A:3052:HOH:O	2.00	0.61
1:C:173:LYS:CE	1:E:217:ASN:OD1	2.49	0.61
1:F:213:MET:O	1:F:217:ASN:HB2	1.99	0.61
1:H:174:HIS:HB3	1:L:175:PHE:CD1	2.35	0.61
1:D:124:GLU:HA	1:D:179:ASN:HD22	1.66	0.61
1:D:215:HIS:C	1:D:261:MET:HB3	2.26	0.61
1:J:423:ILE:HD11	1:J:600:VAL:HG13	1.81	0.61
1:K:451:LYS:HE3	1:K:564:GLU:O	2.00	0.61
1:J:123:VAL:HG21	1:J:153:VAL:HG21	1.83	0.61
1:G:372:VAL:O	1:G:483:ASP:HA	2.01	0.61
1:B:320:LYS:NZ	6:B:61:1PE:H241	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:ASP:HA	1:C:441:PRO:HB2	1.82	0.60
1:C:223:THR:HA	1:C:268:GLY:O	2.01	0.60
1:E:436:LYS:HG2	5:E:7:SO4:O4	2.00	0.60
1:G:132:VAL:HG21	1:G:142:VAL:HG13	1.83	0.60
1:C:214:LEU:HD21	1:C:222:LEU:HD22	1.82	0.60
1:D:529:ILE:CG2	1:D:560:LEU:HD13	2.31	0.60
1:G:201:ALA:HB1	1:L:532:GLU:OE1	2.01	0.60
1:H:106:PRO:HD2	1:H:247:MET:SD	2.42	0.60
1:H:174:HIS:HB3	1:L:175:PHE:CE1	2.36	0.60
1:I:230:VAL:HG23	1:I:234:LEU:HD23	1.83	0.60
1:D:301:PRO:HB3	1:F:442:GLY:O	2.01	0.60
1:B:176:TYR:OH	1:F:155:GLU:HG3	2.02	0.60
1:D:132:VAL:HG21	1:D:142:VAL:HG13	1.83	0.60
1:F:179:ASN:CG	1:F:183:ASN:HB2	2.26	0.60
2:K:1002:CO3:O2	4:K:1003:BEY:H17A	2.02	0.60
1:D:156:PHE:CD2	1:D:177:MET:HE1	2.37	0.60
1:A:387:ALA:HB1	7:A:5072:HOH:O	2.01	0.60
1:F:237:PHE:HA	1:F:240:GLU:OE1	2.01	0.60
1:L:209:SER:O	1:L:212:THR:HB	2.01	0.60
1:D:155:GLU:O	1:D:158:LYS:HG2	2.02	0.60
1:J:321:LEU:HD11	1:J:411:TYR:HA	1.82	0.60
1:B:272:ASN:O	1:B:273:ASN:C	2.45	0.59
1:E:451:LYS:HE3	1:E:564:GLU:O	2.02	0.59
1:J:215:HIS:C	1:J:261:MET:HB3	2.26	0.59
1:L:451:LYS:HG3	6:L:612:1PE:H131	1.85	0.59
1:A:398:PHE:HZ	4:A:1003:BEY:H13	1.67	0.59
1:G:473:ALA:O	1:G:476:LEU:HB2	2.03	0.59
1:J:123:VAL:CG2	1:J:153:VAL:HG21	2.32	0.59
1:D:219:LEU:HD23	1:D:264:ILE:HG22	1.83	0.59
1:E:152:GLN:HG2	1:E:180:ASP:OD1	2.03	0.59
1:K:122:ASN:OD1	1:K:149:ASN:HB2	2.02	0.59
1:L:605:LEU:HD21	7:L:5436:HOH:O	2.01	0.59
1:C:138:GLU:O	1:C:139:ASN:HB2	2.03	0.59
1:L:162:MET:HE2	1:L:165:PHE:HE1	1.68	0.59
1:B:451:LYS:HE3	1:B:564:GLU:O	2.03	0.58
1:L:169:LEU:HD23	1:L:205:ARG:HH21	1.69	0.58
1:B:340:ALA:HA	1:B:445:ILE:HD12	1.85	0.58
1:C:167:VAL:O	1:C:168:LYS:C	2.46	0.58
1:E:230:VAL:CG2	1:E:234:LEU:HB3	2.27	0.58
1:H:117:ILE:HG23	1:H:118:LYS:N	2.18	0.58
1:J:240:GLU:OE2	1:J:287:TYR:HD2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:423:ILE:HD11	1:D:600:VAL:CG1	2.34	0.58
1:F:372:VAL:O	1:F:483:ASP:HA	2.03	0.58
7:J:3061:HOH:O	1:K:254:SER:C	2.46	0.58
1:H:170:GLY:O	1:H:209:SER:OG	2.21	0.58
1:E:372:VAL:O	1:E:483:ASP:HA	2.03	0.58
1:G:208:LEU:O	1:G:212:THR:HG23	2.03	0.58
1:L:423:ILE:HD11	1:L:600:VAL:HG13	1.85	0.58
1:A:441:PRO:HG2	1:B:393:ILE:HG12	1.84	0.58
1:B:486:THR:O	4:B:1003:BEY:N	2.37	0.58
1:D:107:ILE:HG21	1:D:243:PHE:HB3	1.85	0.58
1:E:386:LYS:NZ	4:E:1003:BEY:O3	2.34	0.57
1:I:138:GLU:O	1:I:139:ASN:HB2	2.04	0.57
1:K:473:ALA:O	1:K:476:LEU:HB2	2.04	0.57
1:G:162:MET:HE2	1:G:162:MET:HA	1.86	0.57
1:A:554:SER:HB3	7:A:2697:HOH:O	2.04	0.57
1:A:117:ILE:HG13	1:A:270:TYR:HB3	1.85	0.57
1:F:179:ASN:OD1	1:F:183:ASN:HB2	2.04	0.57
1:K:125:GLU:HG3	1:K:221:LYS:HD2	1.85	0.57
1:B:123:VAL:HG12	1:B:185:VAL:HG21	1.86	0.57
1:B:207:VAL:HG11	1:B:241:THR:HG22	1.85	0.57
1:B:218:LYS:HG2	1:B:262:GLU:OE2	2.04	0.57
1:F:249:ASP:OD2	1:F:251:ARG:NH2	2.29	0.57
1:F:489:GLY:N	4:F:1003:BEY:O1	2.33	0.57
1:G:324:GLU:HG3	7:G:3727:HOH:O	2.05	0.57
1:J:440:ARG:NH2	7:J:635:HOH:O	2.37	0.57
1:A:321:LEU:CD1	1:A:411:TYR:HA	2.35	0.57
1:C:475:LYS:HD3	7:C:3447:HOH:O	2.04	0.57
1:D:138:GLU:HA	1:D:194:SER:OG	2.05	0.57
1:G:136:GLY:N	7:G:3954:HOH:O	2.38	0.57
1:I:320:LYS:NZ	6:I:21:1PE:OH7	2.37	0.57
1:J:411:TYR:CE1	6:J:2:1PE:H151	2.33	0.57
1:A:487:LEU:O	4:A:1003:BEY:H17A	2.05	0.57
1:J:301:PRO:HB3	1:L:442:GLY:O	2.04	0.57
1:C:244:TYR:OH	1:C:588:PRO:O	2.23	0.56
1:D:215:HIS:O	1:D:261:MET:HB3	2.05	0.56
1:E:213:MET:HG3	7:E:1714:HOH:O	2.04	0.56
1:A:381:GLY:HA2	1:A:459:ASP:OD1	2.05	0.56
1:D:248:THR:HG23	1:D:263:TYR:OH	2.06	0.56
1:F:347:GLY:N	7:F:618:HOH:O	2.38	0.56
1:L:381:GLY:HA2	1:L:459:ASP:OD1	2.05	0.56
1:L:473:ALA:O	1:L:476:LEU:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:TYR:CD1	6:A:20:1PE:H251	2.41	0.56
1:F:381:GLY:HA2	1:F:459:ASP:OD1	2.05	0.56
1:E:332:GLU:HG3	7:E:4802:HOH:O	2.04	0.56
1:F:423:ILE:HD11	1:F:600:VAL:HG13	1.87	0.56
1:J:254:SER:CB	7:L:2793:HOH:O	2.35	0.56
1:K:133:ASN:HA	1:K:167:VAL:CG1	2.29	0.56
1:J:322:ASN:HA	7:J:3618:HOH:O	2.06	0.56
1:B:240:GLU:OE2	1:B:287:TYR:HD2	1.88	0.56
1:E:423:ILE:HD11	1:E:600:VAL:HG13	1.88	0.56
1:D:372:VAL:O	1:D:483:ASP:HA	2.05	0.56
1:I:436:LYS:HG2	5:I:17:SO4:O3	2.06	0.56
1:L:222:LEU:O	1:L:267:LEU:HA	2.06	0.56
1:F:320:LYS:HD3	6:F:31:1PE:H141	1.88	0.56
1:J:211:VAL:HG12	7:J:5351:HOH:O	2.04	0.56
1:L:372:VAL:O	1:L:483:ASP:HA	2.06	0.56
1:J:123:VAL:O	1:J:123:VAL:CG2	2.53	0.55
1:D:451:LYS:HE3	1:D:564:GLU:O	2.06	0.55
1:G:451:LYS:HE3	1:G:564:GLU:O	2.05	0.55
1:K:372:VAL:O	1:K:483:ASP:HA	2.06	0.55
1:K:463:ARG:NE	2:K:1002:CO3:O1	2.27	0.55
1:C:117:ILE:HG22	1:C:272:ASN:HA	1.89	0.55
1:H:145:SER:N	1:H:227:GLU:OE1	2.38	0.55
1:I:127:LEU:HB2	1:I:219:LEU:HD22	1.87	0.55
1:G:236:ARG:HD3	1:G:283:LYS:HD3	1.88	0.55
1:G:357:LEU:HB2	1:G:425:PHE:HB2	1.88	0.55
1:G:487:LEU:O	4:G:1003:BEY:H17A	2.06	0.55
1:H:179:ASN:OD1	1:H:183:ASN:HB2	2.06	0.55
2:J:1002:CO3:O1	4:J:1003:BEY:H7A	2.06	0.55
1:L:133:ASN:HB3	1:L:192:CYS:HB2	1.87	0.55
1:B:121:CYS:HA	1:B:270:TYR:CE2	2.41	0.55
1:F:473:ALA:O	1:F:476:LEU:HB2	2.07	0.55
1:A:216:ASP:O	1:A:217:ASN:HB2	2.06	0.55
1:C:146:SER:N	1:C:227:GLU:OE2	2.21	0.55
1:F:117:ILE:HD11	1:F:225:VAL:CG1	2.37	0.55
1:F:214:LEU:HB3	1:F:246:TYR:CE1	2.41	0.55
1:I:178:PHE:CZ	1:K:155:GLU:HG2	2.41	0.55
1:K:330:VAL:HG21	7:K:5424:HOH:O	2.07	0.55
1:E:146:SER:OG	1:E:227:GLU:OE2	2.11	0.55
1:E:336:LEU:HD21	7:E:4649:HOH:O	2.05	0.55
1:F:114:VAL:HG23	1:F:278:LYS:HE2	1.89	0.55
1:E:321:LEU:CD1	1:E:411:TYR:HA	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:423:ILE:HD11	1:G:600:VAL:HG13	1.88	0.55
1:F:433:MET:HG3	7:F:615:HOH:O	2.07	0.55
1:G:168:LYS:O	1:G:171:THR:CG2	2.55	0.55
1:H:117:ILE:HG23	1:H:118:LYS:H	1.70	0.55
1:E:386:LYS:HA	7:E:623:HOH:O	2.06	0.54
1:J:132:VAL:HG11	1:J:144:ILE:HD13	1.89	0.54
1:B:207:VAL:HG21	1:B:241:THR:HB	1.88	0.54
1:H:372:VAL:O	1:H:483:ASP:HA	2.08	0.54
1:B:222:LEU:HD23	1:B:267:LEU:CD1	2.38	0.54
1:D:254:SER:CB	7:F:1110:HOH:O	2.44	0.54
1:G:90:GLN:NE2	1:G:95:ASP:O	2.40	0.54
1:K:423:ILE:HD11	1:K:600:VAL:HG13	1.90	0.54
1:D:152:GLN:HG2	1:D:180:ASP:OD1	2.07	0.54
1:G:171:THR:HG22	1:G:191:GLY:HA3	1.89	0.54
1:G:176:TYR:CE2	1:J:156:PHE:HB2	2.42	0.54
1:B:180:ASP:C	1:B:182:LYS:H	2.15	0.54
1:D:131:LEU:O	1:D:227:GLU:HB2	2.08	0.54
1:J:357:LEU:HB2	1:J:425:PHE:HB2	1.90	0.54
1:A:100:PRO:HA	7:A:4912:HOH:O	2.07	0.54
1:H:316:GLU:HG3	6:H:65:1PE:H142	1.89	0.54
1:J:442:GLY:O	1:K:301:PRO:HB3	2.08	0.54
1:A:199:SER:O	1:A:200:GLU:C	2.51	0.53
1:A:451:LYS:HE3	1:A:564:GLU:O	2.07	0.53
1:C:156:PHE:O	1:C:161:ASN:HB2	2.08	0.53
1:G:178:PHE:CZ	1:J:155:GLU:HG2	2.36	0.53
1:I:127:LEU:HB2	1:I:219:LEU:CD2	2.38	0.53
1:B:117:ILE:HD11	1:B:146:SER:OG	2.08	0.53
1:I:201:ALA:HB1	1:J:532:GLU:OE2	2.07	0.53
1:J:451:LYS:HG2	6:J:45:1PE:H241	1.89	0.53
1:K:116:ASP:HA	1:K:271:ILE:O	2.08	0.53
1:C:169:LEU:HD11	1:C:206:VAL:HG23	1.91	0.53
1:L:487:LEU:O	4:L:1003:BEY:H17A	2.08	0.53
1:C:372:VAL:O	1:C:483:ASP:HA	2.09	0.53
1:C:530:ILE:HD12	1:C:556:ILE:HD13	1.89	0.53
1:E:221:LYS:HG3	1:E:266:HIS:HB2	1.90	0.53
1:E:451:LYS:HG2	6:E:43:1PE:H141	1.89	0.53
1:F:236:ARG:O	1:F:240:GLU:HG3	2.08	0.53
1:G:173:LYS:HE2	1:J:216:ASP:OD2	2.09	0.53
1:G:381:GLY:HA2	1:G:459:ASP:OD1	2.09	0.53
1:H:222:LEU:HD23	1:H:267:LEU:CD1	2.39	0.53
1:I:150:ASP:OD2	1:I:153:VAL:HG23	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:230:VAL:HG23	1:I:234:LEU:CG	2.38	0.53
1:A:168:LYS:O	1:A:171:THR:HG22	2.09	0.53
1:A:173:LYS:HE2	1:D:216:ASP:OD2	2.08	0.53
1:I:372:VAL:O	1:I:483:ASP:HA	2.09	0.53
1:K:108:HIS:CD2	6:K:5:1PE:H131	2.43	0.53
1:A:240:GLU:OE2	1:A:287:TYR:HD2	1.92	0.53
1:C:451:LYS:HE3	1:C:564:GLU:O	2.09	0.53
1:E:102:GLU:HB3	7:E:2665:HOH:O	2.08	0.53
1:F:360:LYS:CD	7:F:2922:HOH:O	2.56	0.53
1:L:457:ASN:ND2	4:L:1003:BEY:H3	2.24	0.53
1:A:473:ALA:O	1:A:476:LEU:HB2	2.09	0.53
1:A:512:LYS:NZ	7:A:3363:HOH:O	2.41	0.53
1:I:238:PHE:CD2	1:I:239:LEU:HD13	2.43	0.53
1:D:179:ASN:O	1:D:181:ASN:N	2.42	0.53
1:F:362:LYS:CB	1:K:163:GLU:OE1	2.57	0.53
1:L:125:GLU:N	7:L:2009:HOH:O	2.35	0.53
1:A:257:LYS:HG3	7:A:3234:HOH:O	2.08	0.53
1:D:321:LEU:CD1	1:D:411:TYR:HA	2.37	0.53
1:E:90:GLN:NE2	1:E:95:ASP:O	2.41	0.53
1:C:272:ASN:O	1:C:273:ASN:HB2	2.09	0.53
1:B:103:TYR:HB3	6:B:60:1PE:H242	1.91	0.52
1:F:508:GLU:OE2	1:F:508:GLU:HA	2.08	0.52
1:L:225:VAL:HG22	1:L:270:TYR:HB2	1.91	0.52
1:B:372:VAL:O	1:B:483:ASP:HA	2.10	0.52
1:B:423:ILE:HD11	1:B:600:VAL:HG13	1.91	0.52
1:C:165:PHE:CD2	1:C:173:LYS:HG2	2.45	0.52
1:C:184:SER:CB	7:C:2540:HOH:O	2.57	0.52
1:E:262:GLU:N	7:E:5300:HOH:O	2.42	0.52
1:J:130:PHE:O	1:J:189:TYR:HA	2.10	0.52
1:L:451:LYS:HE3	1:L:564:GLU:O	2.10	0.52
1:E:167:VAL:O	1:E:168:LYS:C	2.52	0.52
1:J:215:HIS:ND1	7:J:5351:HOH:O	2.33	0.52
1:K:321:LEU:CD1	1:K:411:TYR:HA	2.40	0.52
1:L:357:LEU:HB2	1:L:425:PHE:HB2	1.90	0.52
1:G:244:TYR:OH	1:G:588:PRO:O	2.28	0.52
1:I:230:VAL:CG2	1:I:234:LEU:HB3	2.38	0.52
1:J:121:CYS:HB2	1:J:148:VAL:HG12	1.91	0.52
1:F:357:LEU:HB2	1:F:425:PHE:HB2	1.91	0.52
1:G:441:PRO:HG2	1:H:393:ILE:HG12	1.91	0.52
1:H:169:LEU:HD23	7:H:3248:HOH:O	2.08	0.52
1:J:451:LYS:HE3	1:J:564:GLU:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:LEU:HB2	1:B:425:PHE:HB2	1.92	0.52
1:E:529:ILE:CG2	1:E:560:LEU:HD13	2.39	0.52
1:H:576:ILE:HD12	1:H:580:SER:HB2	1.91	0.52
1:J:207:VAL:O	1:J:211:VAL:HG23	2.09	0.52
1:A:178:PHE:HZ	1:D:155:GLU:HG3	1.73	0.52
1:I:320:LYS:CE	6:I:21:1PE:H131	2.39	0.52
2:H:1002:CO3:O3	4:H:1003:BEY:H17A	2.10	0.52
1:I:451:LYS:HE3	1:I:564:GLU:O	2.10	0.52
1:J:423:ILE:HD11	1:J:600:VAL:CG1	2.40	0.52
1:D:214:LEU:HB3	1:D:246:TYR:CE1	2.45	0.52
1:B:120:GLY:HA3	1:B:149:ASN:OD1	2.11	0.51
1:D:357:LEU:HB2	1:D:425:PHE:HB2	1.91	0.51
1:D:384:ASN:HB3	7:D:1189:HOH:O	2.10	0.51
1:H:176:TYR:OH	1:L:155:GLU:HG3	2.10	0.51
1:J:106:PRO:HG2	1:J:263:TYR:CE2	2.45	0.51
1:J:210:LEU:HD12	1:J:213:MET:HE3	1.92	0.51
1:F:169:LEU:HD21	1:F:202:ASP:HA	1.90	0.51
1:G:231:ASP:OD1	1:G:234:LEU:N	2.26	0.51
1:K:442:GLY:O	1:L:301:PRO:HB3	2.10	0.51
1:A:139:ASN:HD21	1:A:168:LYS:HG3	1.75	0.51
1:F:169:LEU:HD23	1:F:205:ARG:HE	1.75	0.51
1:L:321:LEU:CD1	1:L:411:TYR:HA	2.39	0.51
1:C:423:ILE:HD11	1:C:600:VAL:HG13	1.92	0.51
1:D:216:ASP:CG	1:D:216:ASP:O	2.53	0.51
1:E:112:VAL:HG13	1:E:267:LEU:HG	1.91	0.51
1:G:256:ASP:O	1:G:256:ASP:CG	2.53	0.51
1:H:357:LEU:HB2	1:H:425:PHE:HB2	1.92	0.51
1:H:473:ALA:O	1:H:476:LEU:HB2	2.10	0.51
1:H:487:LEU:O	4:H:1003:BEY:C17	2.58	0.51
1:B:172:SER:O	1:B:173:LYS:HD2	2.11	0.51
1:B:321:LEU:CD1	1:B:411:TYR:HA	2.40	0.51
1:G:221:LYS:HG3	1:G:266:HIS:HB2	1.92	0.51
1:D:442:GLY:O	1:E:301:PRO:HB3	2.10	0.51
1:E:423:ILE:HD11	1:E:600:VAL:CG1	2.40	0.51
1:G:364:ASP:O	1:G:420:ASN:HA	2.10	0.51
1:I:230:VAL:HG23	1:I:234:LEU:CD2	2.41	0.51
1:L:487:LEU:HD22	1:L:573:HIS:CE1	2.46	0.51
1:A:150:ASP:OD1	1:A:179:ASN:HB2	2.10	0.51
1:C:273:ASN:O	1:C:274:ALA:C	2.54	0.51
1:C:357:LEU:HB2	1:C:425:PHE:HB2	1.92	0.51
1:D:392:MET:CE	4:D:1003:BEY:H12	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:157:LEU:HD21	1:F:187:VAL:HG11	1.93	0.51
1:F:179:ASN:ND2	1:F:183:ASN:HB2	2.25	0.51
1:I:153:VAL:O	1:I:157:LEU:HG	2.10	0.51
1:F:114:VAL:CG2	1:F:278:LYS:HG2	2.37	0.51
1:I:423:ILE:HD11	1:I:600:VAL:HG13	1.93	0.51
1:J:473:ALA:O	1:J:476:LEU:HB2	2.11	0.51
1:C:489:GLY:N	4:C:1003:BEY:O1	2.37	0.51
1:H:423:ILE:HD11	1:H:600:VAL:HG13	1.93	0.51
1:K:357:LEU:HB2	1:K:425:PHE:HB2	1.91	0.51
1:C:238:PHE:HD2	1:C:239:LEU:HD12	1.76	0.50
1:C:392:MET:CE	4:C:1003:BEY:H12	2.40	0.50
1:D:392:MET:HE3	4:D:1003:BEY:H12	1.92	0.50
1:F:112:VAL:HG22	1:F:267:LEU:HB3	1.93	0.50
1:F:364:ASP:O	1:F:420:ASN:HA	2.11	0.50
1:G:235:PHE:CE2	1:G:277:TYR:HB3	2.46	0.50
1:K:129:ILE:HA	1:K:188:GLY:O	2.11	0.50
1:A:240:GLU:OE2	1:A:287:TYR:CD2	2.65	0.50
1:B:176:TYR:CE2	1:F:156:PHE:HB2	2.46	0.50
1:C:176:TYR:CE2	1:E:156:PHE:HB2	2.45	0.50
1:D:219:LEU:HD22	7:D:2082:HOH:O	2.12	0.50
1:H:230:VAL:HG23	1:H:230:VAL:O	2.11	0.50
1:I:167:VAL:O	1:I:168:LYS:C	2.53	0.50
1:A:357:LEU:HB2	1:A:425:PHE:HB2	1.92	0.50
1:H:135:PRO:HA	1:H:196:ALA:HB2	1.93	0.50
1:K:411:TYR:CE1	6:K:5:1PE:H142	2.46	0.50
1:A:150:ASP:OD2	1:A:152:GLN:HB2	2.11	0.50
1:A:476:LEU:CD1	7:A:645:HOH:O	2.59	0.50
1:E:92:VAL:HG23	1:E:94:LEU:H	1.77	0.50
1:F:247:MET:HG2	1:F:288:TYR:OH	2.11	0.50
1:E:179:ASN:HB3	1:E:185:VAL:HG21	1.94	0.50
1:F:262:GLU:HA	7:F:645:HOH:O	2.11	0.50
1:I:121:CYS:SG	1:I:225:VAL:CG2	2.96	0.50
1:A:528:PRO:HB3	1:F:525:TRP:CZ3	2.47	0.50
1:B:240:GLU:OE2	1:B:287:TYR:CD2	2.65	0.50
1:C:321:LEU:CD1	1:C:411:TYR:HA	2.41	0.50
1:E:138:GLU:HA	1:E:194:SER:OG	2.11	0.50
1:E:442:GLY:O	1:F:301:PRO:HB3	2.12	0.50
1:J:372:VAL:O	1:J:483:ASP:HA	2.11	0.50
1:L:423:ILE:HD11	1:L:600:VAL:CG1	2.42	0.50
1:D:398:PHE:CD2	1:D:398:PHE:C	2.89	0.50
1:E:357:LEU:HB2	1:E:425:PHE:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:230:VAL:O	1:H:231:ASP:O	2.30	0.50
1:I:192:CYS:HB3	1:I:198:LEU:HD21	1.93	0.50
1:L:167:VAL:O	1:L:168:LYS:C	2.53	0.50
1:A:249:ASP:CG	1:A:251:ARG:HE	2.20	0.49
1:C:90:GLN:NE2	1:C:95:ASP:O	2.33	0.49
1:D:190:VAL:HG23	1:D:213:MET:HE1	1.93	0.49
1:D:211:VAL:HG21	1:D:245:GLU:HB2	1.93	0.49
1:H:150:ASP:HB3	1:H:153:VAL:HB	1.94	0.49
1:I:320:LYS:HE2	6:I:21:1PE:H131	1.93	0.49
1:J:214:LEU:HD21	1:J:222:LEU:HD22	1.94	0.49
1:K:423:ILE:HD11	1:K:600:VAL:CG1	2.42	0.49
1:D:536:THR:HG21	1:D:551:VAL:HG23	1.94	0.49
1:F:321:LEU:CD1	1:F:411:TYR:HA	2.41	0.49
1:A:94:LEU:HD12	1:C:342:LEU:HD12	1.94	0.49
1:B:320:LYS:HZ1	6:B:61:1PE:H241	1.77	0.49
1:C:156:PHE:O	1:C:161:ASN:CB	2.60	0.49
1:G:130:PHE:O	1:G:189:TYR:HA	2.12	0.49
1:H:321:LEU:CD1	1:H:411:TYR:HA	2.38	0.49
1:J:487:LEU:HD23	7:J:783:HOH:O	2.12	0.49
1:L:129:ILE:HG21	1:L:210:LEU:CD1	2.43	0.49
1:D:133:ASN:HB2	1:D:193:GLY:O	2.13	0.49
1:D:226:PHE:CD2	1:D:230:VAL:HG11	2.47	0.49
1:E:214:LEU:HB3	1:E:246:TYR:CE1	2.47	0.49
1:H:481:ILE:O	1:H:571:TRP:HA	2.13	0.49
1:I:146:SER:OG	1:I:227:GLU:OE2	2.25	0.49
1:A:153:VAL:HG22	1:A:177:MET:SD	2.53	0.49
1:D:529:ILE:HG22	1:D:560:LEU:HD13	1.94	0.49
1:E:346:LYS:HE3	1:F:91:VAL:HG21	1.94	0.49
1:G:321:LEU:CD1	1:G:411:TYR:HA	2.39	0.49
1:H:142:VAL:HG23	1:H:162:MET:HB3	1.94	0.49
1:H:180:ASP:C	1:H:182:LYS:H	2.21	0.49
1:G:526:TRP:CZ3	6:G:30:1PE:H151	2.47	0.49
1:B:100:PRO:O	1:B:251:ARG:HD2	2.12	0.49
1:I:364:ASP:O	1:I:420:ASN:HA	2.13	0.49
1:L:95:ASP:HB3	7:L:4971:HOH:O	2.13	0.49
1:L:117:ILE:HG22	1:L:272:ASN:OD1	2.13	0.49
1:A:487:LEU:HD22	1:A:573:HIS:CE1	2.48	0.49
1:E:346:LYS:HE3	1:F:91:VAL:CG2	2.43	0.49
1:I:236:ARG:HD3	1:I:283:LYS:HD3	1.94	0.49
1:K:88:VAL:HG21	1:K:97:THR:O	2.13	0.49
1:B:237:PHE:HA	1:B:240:GLU:OE1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:117:ILE:CD1	1:G:226:PHE:O	2.61	0.49
1:H:584:LYS:HB2	7:H:4904:HOH:O	2.12	0.49
1:L:226:PHE:HE1	1:L:269:VAL:HG13	1.77	0.49
1:C:236:ARG:NE	1:C:240:GLU:OE2	2.38	0.48
1:D:395:LEU:HD11	1:D:581:TRP:CG	2.48	0.48
1:E:88:VAL:HG21	1:E:97:THR:O	2.13	0.48
1:F:487:LEU:HD22	1:F:573:HIS:CE1	2.48	0.48
1:C:196:ALA:HB1	7:C:2678:HOH:O	2.12	0.48
1:L:226:PHE:CE1	1:L:269:VAL:HG13	2.48	0.48
1:A:207:VAL:HG11	1:A:242:LEU:HA	1.94	0.48
1:H:536:THR:HG21	1:H:551:VAL:HG23	1.95	0.48
1:I:118:LYS:C	1:I:120:GLY:H	2.21	0.48
1:C:367:LYS:HG2	1:C:603:ASP:OD1	2.14	0.48
1:D:273:ASN:HB3	1:D:276:THR:HG23	1.94	0.48
1:B:142:VAL:HG13	1:B:165:PHE:O	2.13	0.48
1:D:364:ASP:O	1:D:420:ASN:HA	2.13	0.48
1:J:124:GLU:HA	1:J:179:ASN:HD22	1.79	0.48
1:J:133:ASN:OD1	1:J:135:PRO:HD3	2.13	0.48
1:J:134:ASN:ND2	1:J:141:PRO:HD2	2.28	0.48
1:L:440:ARG:NH2	7:L:4845:HOH:O	2.46	0.48
1:G:107:ILE:HA	1:G:110:ILE:HD12	1.96	0.48
1:H:487:LEU:HD22	1:H:573:HIS:CE1	2.48	0.48
1:H:451:LYS:HE3	1:H:564:GLU:O	2.13	0.48
1:I:272:ASN:O	1:I:273:ASN:HB2	2.14	0.48
1:B:180:ASP:C	1:B:182:LYS:N	2.72	0.48
1:D:121:CYS:HA	1:D:270:TYR:CE2	2.48	0.48
1:D:144:ILE:HG13	1:D:157:LEU:HD22	1.96	0.48
1:E:216:ASP:C	1:E:217:ASN:ND2	2.71	0.48
1:F:508:GLU:HB3	7:F:1215:HOH:O	2.13	0.48
1:G:177:MET:HG2	1:G:185:VAL:HG23	1.96	0.48
1:H:392:MET:HE3	4:H:1003:BEY:C12	2.41	0.48
1:A:528:PRO:HD3	1:F:525:TRP:CE2	2.49	0.48
1:C:364:ASP:O	1:C:420:ASN:HA	2.14	0.48
1:E:364:ASP:O	1:E:420:ASN:HA	2.14	0.48
1:H:160:GLU:O	1:H:163:GLU:HG2	2.14	0.48
1:I:321:LEU:CD1	1:I:411:TYR:HA	2.42	0.48
1:I:516:SER:OG	1:I:599:PHE:HA	2.14	0.48
1:J:214:LEU:HB3	1:J:246:TYR:CE1	2.49	0.48
1:J:487:LEU:O	4:J:1003:BEY:H17A	2.13	0.48
1:A:423:ILE:HD11	1:A:600:VAL:HG13	1.96	0.48
1:B:207:VAL:O	1:B:211:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:316:GLU:HG3	6:E:612:1PE:H252	1.95	0.48
1:F:423:ILE:HD11	1:F:600:VAL:CG1	2.44	0.48
1:A:207:VAL:CG1	1:A:242:LEU:HA	2.43	0.47
1:A:316:GLU:HG3	6:A:20:1PE:H231	1.96	0.47
1:B:174:HIS:NE2	1:B:213:MET:HE2	2.29	0.47
1:B:222:LEU:HD23	1:B:267:LEU:HD13	1.94	0.47
1:D:199:SER:HB2	7:D:2343:HOH:O	2.13	0.47
1:D:423:ILE:HD13	1:D:600:VAL:HG11	1.94	0.47
1:E:133:ASN:OD1	1:E:135:PRO:HD3	2.14	0.47
1:G:122:ASN:HD22	6:G:47:1PE:H142	1.78	0.47
1:I:357:LEU:HB2	1:I:425:PHE:HB2	1.96	0.47
1:J:99:ILE:HD11	1:J:310:LEU:HA	1.96	0.47
1:J:272:ASN:O	1:J:273:ASN:HB2	2.14	0.47
1:A:275:ASP:HB2	7:A:3251:HOH:O	2.14	0.47
1:D:165:PHE:CD2	1:D:173:LYS:HG3	2.50	0.47
1:E:516:SER:OG	1:E:599:PHE:HA	2.14	0.47
1:E:543:ASP:CG	6:E:43:1PE:H142	2.39	0.47
1:F:364:ASP:HB3	7:I:2655:HOH:O	2.14	0.47
1:B:386:LYS:NZ	4:B:1003:BEY:O3	2.46	0.47
1:G:395:LEU:HD11	1:G:581:TRP:CG	2.49	0.47
1:G:577:ALA:HB1	4:G:1003:BEY:H13	1.96	0.47
1:J:156:PHE:O	1:J:162:MET:HE3	2.14	0.47
1:J:395:LEU:HD11	1:J:581:TRP:CG	2.50	0.47
1:J:487:LEU:O	4:J:1003:BEY:C17	2.63	0.47
1:L:306:ASN:HB2	1:L:307:PRO:HD2	1.97	0.47
1:G:285:ARG:NH2	7:G:633:HOH:O	2.45	0.47
1:G:450:GLY:HA2	7:G:3308:HOH:O	2.13	0.47
1:I:551:VAL:HG12	1:I:553:ALA:H	1.79	0.47
1:A:139:ASN:ND2	1:A:168:LYS:HG3	2.29	0.47
1:A:161:ASN:O	1:A:162:MET:HE2	2.14	0.47
1:A:499:TYR:CE2	1:A:523:PRO:CB	2.97	0.47
1:A:557:VAL:HG11	7:A:37:HOH:O	2.14	0.47
1:B:257:LYS:CB	1:B:259:VAL:N	2.77	0.47
1:C:423:ILE:HD11	1:C:600:VAL:CG1	2.45	0.47
1:D:423:ILE:CD1	1:D:600:VAL:HG11	2.44	0.47
1:I:230:VAL:HG23	1:I:234:LEU:HG	1.95	0.47
1:I:395:LEU:HD11	1:I:581:TRP:CG	2.50	0.47
1:L:236:ARG:HD3	1:L:283:LYS:HD3	1.96	0.47
1:C:131:LEU:HB3	1:C:192:CYS:SG	2.54	0.47
1:D:86:SER:HB2	1:D:308:VAL:HG13	1.95	0.47
6:I:22:1PE:H231	7:I:624:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:440:ARG:CD	1:E:302:SER:HB2	2.44	0.47
6:D:44:1PE:H141	1:E:254:SER:C	2.39	0.47
1:E:381:GLY:HA2	1:E:459:ASP:OD1	2.15	0.47
1:G:423:ILE:HD11	1:G:600:VAL:CG1	2.44	0.47
1:G:536:THR:HG21	1:G:551:VAL:HG23	1.97	0.47
1:H:142:VAL:CG2	1:H:162:MET:HB3	2.44	0.47
1:K:108:HIS:NE2	6:K:5:1PE:H131	2.29	0.47
1:K:367:LYS:HD3	1:K:367:LYS:HA	1.75	0.47
1:B:209:SER:O	1:B:212:THR:HB	2.15	0.47
1:C:150:ASP:OD1	1:C:179:ASN:HB2	2.14	0.47
1:D:133:ASN:OD1	1:D:135:PRO:HD3	2.15	0.47
1:F:95:ASP:O	1:F:96:PRO:C	2.56	0.47
1:G:150:ASP:OD2	1:G:153:VAL:N	2.43	0.47
1:H:203:MET:SD	1:H:238:PHE:HD1	2.38	0.47
1:H:497:THR:HA	1:H:578:GLY:O	2.14	0.47
1:I:473:ALA:O	1:I:476:LEU:HB2	2.15	0.47
1:A:499:TYR:CG	1:A:523:PRO:HB2	2.50	0.47
1:B:257:LYS:CA	1:B:258:ASN:HB3	2.25	0.47
1:C:436:LYS:HG2	5:C:3:SO4:O3	2.14	0.47
1:F:374:LYS:HB3	7:F:622:HOH:O	2.14	0.47
1:J:235:PHE:O	1:J:238:PHE:HB3	2.14	0.47
1:J:364:ASP:O	1:J:420:ASN:HA	2.15	0.47
1:L:169:LEU:HD23	1:L:205:ARG:NH2	2.29	0.47
1:B:355:ILE:O	1:B:426:LEU:HA	2.14	0.47
1:C:168:LYS:O	1:C:169:LEU:C	2.57	0.47
1:D:133:ASN:OD1	1:D:133:ASN:C	2.57	0.47
1:E:529:ILE:HG22	1:E:560:LEU:HD13	1.97	0.47
1:G:398:PHE:CD2	1:G:398:PHE:C	2.93	0.47
1:K:364:ASP:O	1:K:420:ASN:HA	2.15	0.47
1:A:148:VAL:HG11	1:A:153:VAL:HG12	1.97	0.46
1:D:423:ILE:CD1	1:D:600:VAL:CG1	2.92	0.46
1:E:200:GLU:OE1	1:E:523:PRO:HG3	2.14	0.46
1:G:396:MET:HE1	4:G:1003:BEY:C10	2.45	0.46
1:H:215:HIS:O	1:H:216:ASP:HB2	2.15	0.46
1:H:236:ARG:HB2	1:H:280:GLU:HB3	1.97	0.46
1:J:100:PRO:O	1:J:251:ARG:HD2	2.14	0.46
1:L:210:LEU:HA	1:L:213:MET:HE3	1.96	0.46
1:B:170:GLY:O	1:B:209:SER:OG	2.20	0.46
1:F:272:ASN:O	1:F:273:ASN:HB2	2.14	0.46
1:F:347:GLY:CA	7:F:618:HOH:O	2.63	0.46
1:G:124:GLU:O	1:G:185:VAL:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:246:TYR:CE2	1:J:264:ILE:HG12	2.50	0.46
1:J:261:MET:HG2	7:J:2991:HOH:O	2.14	0.46
1:J:451:LYS:HD3	7:J:3214:HOH:O	2.15	0.46
1:E:118:LYS:C	1:E:120:GLY:H	2.23	0.46
4:I:1003:BEY:H10	4:I:1003:BEY:H18A	1.74	0.46
1:K:159:ASP:O	1:K:160:GLU:C	2.53	0.46
1:K:221:LYS:HD3	7:K:1354:HOH:O	2.16	0.46
1:D:487:LEU:O	4:D:1003:BEY:C17	2.64	0.46
1:E:169:LEU:HB3	7:E:5009:HOH:O	2.15	0.46
1:H:134:ASN:HA	1:H:135:PRO:HD2	1.62	0.46
1:I:536:THR:HG21	1:I:551:VAL:HG23	1.98	0.46
1:A:128:THR:HG23	1:A:223:THR:HB	1.96	0.46
1:B:395:LEU:HD11	1:B:581:TRP:CG	2.50	0.46
1:E:476:LEU:HD23	7:E:1550:HOH:O	2.16	0.46
1:F:239:LEU:HB3	1:F:284:ALA:HB1	1.97	0.46
1:G:103:TYR:CD1	6:G:58:1PE:H151	2.51	0.46
1:I:128:THR:O	1:I:188:GLY:N	2.47	0.46
1:I:222:LEU:O	1:I:267:LEU:HA	2.14	0.46
1:K:138:GLU:HA	1:K:194:SER:OG	2.16	0.46
1:B:257:LYS:CB	1:B:259:VAL:H	2.28	0.46
1:D:168:LYS:O	1:D:169:LEU:C	2.57	0.46
1:D:487:LEU:O	4:D:1003:BEY:H17A	2.15	0.46
1:G:254:SER:HB3	1:I:543:ASP:OD2	2.16	0.46
1:G:232:LYS:HB2	7:G:903:HOH:O	2.16	0.46
1:A:364:ASP:O	1:A:420:ASN:HA	2.16	0.46
1:C:162:MET:HA	1:C:162:MET:HE2	1.98	0.46
1:D:179:ASN:C	1:D:181:ASN:H	2.22	0.46
1:G:307:PRO:HG2	7:G:622:HOH:O	2.15	0.46
1:A:169:LEU:HG	1:A:205:ARG:HD2	1.97	0.46
2:D:1002:CO3:O2	4:D:1003:BEY:H17A	2.16	0.46
1:F:516:SER:OG	1:F:599:PHE:HA	2.16	0.46
1:H:138:GLU:HA	7:H:1925:HOH:O	2.15	0.46
1:H:140:GLY:O	1:H:166:ASN:HA	2.16	0.46
1:J:246:TYR:HE2	1:J:264:ILE:HG12	1.80	0.46
1:J:273:ASN:HB3	1:J:276:THR:HG23	1.98	0.46
1:K:101:ILE:HG21	1:K:103:TYR:CE2	2.51	0.46
1:L:516:SER:OG	1:L:599:PHE:HA	2.16	0.46
1:B:167:VAL:O	1:B:168:LYS:C	2.59	0.46
1:C:177:MET:O	1:C:184:SER:HA	2.16	0.46
1:C:392:MET:HE1	4:C:1003:BEY:H12	1.98	0.46
1:G:121:CYS:HA	1:G:270:TYR:CZ	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:602:ASN:HB2	7:H:2166:HOH:O	2.16	0.46
1:K:167:VAL:HG12	1:K:192:CYS:H	1.81	0.46
1:L:224:VAL:N	1:L:268:GLY:O	2.42	0.46
1:F:207:VAL:O	1:F:207:VAL:HG12	2.17	0.45
1:G:106:PRO:HD2	1:G:247:MET:SD	2.56	0.45
1:H:156:PHE:C	1:H:156:PHE:CD2	2.94	0.45
1:I:230:VAL:O	1:I:277:TYR:CZ	2.68	0.45
1:J:125:GLU:CG	1:J:221:LYS:HD2	2.46	0.45
1:J:128:THR:O	1:J:187:VAL:HA	2.16	0.45
1:J:436:LYS:HG2	5:J:18:SO4:O2	2.17	0.45
1:B:577:ALA:HB1	4:B:1003:BEY:H13	1.98	0.45
1:G:217:ASN:OD1	1:G:219:LEU:HG	2.16	0.45
1:H:217:ASN:ND2	1:L:165:PHE:HE2	2.14	0.45
1:I:130:PHE:CD2	1:I:225:VAL:HB	2.50	0.45
1:C:115:TYR:HB2	1:C:270:TYR:CD2	2.52	0.45
1:D:367:LYS:HA	1:D:367:LYS:HD3	1.66	0.45
1:D:451:LYS:HG3	6:D:44:1PE:H151	1.98	0.45
1:F:306:ASN:HB2	1:F:307:PRO:HD2	1.98	0.45
1:K:530:ILE:HD12	1:K:556:ILE:HD13	1.99	0.45
1:E:530:ILE:HD12	1:E:556:ILE:HD13	1.98	0.45
1:E:536:THR:HG21	1:E:551:VAL:HG23	1.98	0.45
1:F:487:LEU:HD23	7:F:617:HOH:O	2.17	0.45
1:G:230:VAL:O	1:G:277:TYR:OH	2.28	0.45
1:J:320:LYS:HZ3	6:J:3:1PE:C14	2.22	0.45
1:L:177:MET:HE3	1:L:187:VAL:HB	1.98	0.45
1:A:143:LYS:HG2	1:A:159:ASP:OD2	2.17	0.45
1:B:375:GLY:O	1:B:429:VAL:HA	2.17	0.45
1:B:451:LYS:HG2	1:C:255:THR:OG1	2.16	0.45
1:K:481:ILE:O	1:K:571:TRP:HA	2.17	0.45
1:B:536:THR:HG21	1:B:551:VAL:HG23	1.99	0.45
1:F:105:THR:C	1:F:107:ILE:N	2.74	0.45
1:H:207:VAL:HG11	1:H:241:THR:HG22	1.99	0.45
1:K:244:TYR:CE1	1:K:291:THR:HG22	2.52	0.45
1:A:141:PRO:HA	1:A:165:PHE:O	2.17	0.45
1:A:216:ASP:O	1:D:173:LYS:CE	2.60	0.45
1:B:142:VAL:CG2	1:B:162:MET:HB3	2.44	0.45
1:C:129:ILE:HA	1:C:188:GLY:O	2.16	0.45
1:D:551:VAL:HG12	1:D:553:ALA:H	1.81	0.45
1:K:165:PHE:CD2	1:K:173:LYS:HG3	2.52	0.45
1:C:153:VAL:HG12	1:C:157:LEU:HD12	1.96	0.45
1:C:536:THR:HG21	1:C:551:VAL:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:497:THR:HA	1:D:578:GLY:O	2.17	0.45
4:E:1003:BEY:H10	4:E:1003:BEY:H18A	1.76	0.45
1:F:487:LEU:O	4:F:1003:BEY:H17A	2.16	0.45
1:H:128:THR:HG23	1:H:223:THR:HB	1.99	0.45
1:I:260:ASN:O	1:I:262:GLU:N	2.50	0.45
1:J:164:LYS:HE3	1:J:164:LYS:HB2	1.65	0.45
1:J:367:LYS:HA	1:J:367:LYS:HD3	1.68	0.45
1:K:130:PHE:O	1:K:189:TYR:HA	2.17	0.45
5:E:7:SO4:O2	1:F:436:LYS:HG2	2.17	0.45
1:F:107:ILE:O	1:F:107:ILE:HG22	2.17	0.45
1:J:107:ILE:HG21	1:J:243:PHE:HB3	1.97	0.45
1:J:536:THR:HG21	1:J:551:VAL:HG23	1.99	0.45
1:K:332:GLU:H	1:K:332:GLU:HG3	1.45	0.45
1:K:355:ILE:O	1:K:426:LEU:HA	2.17	0.45
1:L:156:PHE:CG	1:L:177:MET:HE1	2.52	0.45
1:C:528:PRO:HB3	1:D:525:TRP:CZ3	2.52	0.45
1:H:487:LEU:O	4:H:1003:BEY:H17	2.17	0.45
1:L:181:ASN:O	1:L:182:LYS:C	2.61	0.45
1:L:324:GLU:HA	7:L:970:HOH:O	2.16	0.45
1:E:229:ASN:O	1:E:230:VAL:CB	2.57	0.44
1:G:332:GLU:HB2	7:G:5439:HOH:O	2.16	0.44
1:K:133:ASN:OD1	1:K:133:ASN:C	2.60	0.44
1:K:381:GLY:HA2	1:K:459:ASP:OD1	2.16	0.44
1:A:444:ILE:HA	1:A:453:ILE:O	2.17	0.44
1:B:586:ARG:HB3	7:B:2591:HOH:O	2.17	0.44
1:D:481:ILE:O	1:D:571:TRP:HA	2.16	0.44
1:J:100:PRO:O	1:J:101:ILE:HD13	2.18	0.44
1:J:487:LEU:HD22	1:J:573:HIS:CE1	2.53	0.44
1:B:187:VAL:HG12	1:B:188:GLY:N	2.31	0.44
1:F:202:ASP:O	1:F:206:VAL:HG23	2.17	0.44
1:K:167:VAL:O	1:K:168:LYS:C	2.60	0.44
1:K:516:SER:OG	1:K:599:PHE:HA	2.17	0.44
1:L:232:LYS:HB2	7:L:5173:HOH:O	2.17	0.44
1:B:481:ILE:O	1:B:571:TRP:HA	2.16	0.44
1:C:514:LEU:O	1:C:517:SER:HB3	2.17	0.44
1:E:200:GLU:CD	1:E:523:PRO:HG3	2.41	0.44
1:H:307:PRO:HD3	1:H:377:THR:OG1	2.16	0.44
1:I:210:LEU:HD23	1:I:242:LEU:HD13	1.98	0.44
1:D:152:GLN:O	1:D:155:GLU:HB3	2.18	0.44
1:F:134:ASN:HB2	1:F:167:VAL:HG11	1.99	0.44
1:I:100:PRO:O	1:I:251:ARG:HD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:307:PRO:HD3	1:I:377:THR:OG1	2.18	0.44
1:K:103:TYR:CD1	6:K:4:1PE:H132	2.53	0.44
7:B:2359:HOH:O	1:E:551:VAL:HG13	2.16	0.44
1:E:320:LYS:NZ	6:E:612:1PE:OH4	2.50	0.44
1:E:395:LEU:HD11	1:E:581:TRP:CG	2.53	0.44
1:F:97:THR:O	1:F:98:SER:HB3	2.17	0.44
1:I:528:PRO:HB3	1:J:525:TRP:CZ3	2.52	0.44
1:K:441:PRO:HG2	1:L:393:ILE:HG12	1.99	0.44
1:L:128:THR:HG23	1:L:223:THR:HB	2.00	0.44
1:L:189:TYR:CD2	1:L:189:TYR:C	2.95	0.44
1:L:198:LEU:HD23	1:L:198:LEU:HA	1.60	0.44
1:A:138:GLU:HA	1:A:194:SER:CB	2.47	0.44
1:D:156:PHE:CG	1:D:177:MET:HE1	2.52	0.44
1:D:451:LYS:HE2	6:D:44:1PE:H261	1.99	0.44
1:E:368:LYS:CE	7:E:2241:HOH:O	2.65	0.44
1:F:586:ARG:NH2	7:F:2842:HOH:O	2.36	0.44
1:G:133:ASN:C	1:G:167:VAL:HG11	2.43	0.44
1:H:375:GLY:O	1:H:429:VAL:HA	2.18	0.44
1:I:243:PHE:HB3	1:I:288:TYR:CD1	2.53	0.44
1:I:497:THR:HA	1:I:578:GLY:O	2.18	0.44
1:B:300:ALA:HA	1:B:301:PRO:HD3	1.88	0.44
1:H:335:GLU:CB	7:H:2588:HOH:O	2.65	0.44
1:I:128:THR:HG23	1:I:223:THR:HB	2.00	0.44
1:J:302:SER:HB3	7:J:1429:HOH:O	2.18	0.44
1:J:544:ILE:CD1	1:J:564:GLU:HG3	2.47	0.44
1:K:438:SER:HA	7:K:17:HOH:O	2.18	0.44
1:K:451:LYS:CD	6:K:42:1PE:H231	2.43	0.44
1:B:218:LYS:HG2	1:B:262:GLU:CG	2.48	0.44
1:C:189:TYR:CD2	1:C:189:TYR:C	2.95	0.44
1:C:532:GLU:HG3	1:D:201:ALA:HB1	1.99	0.44
1:D:198:LEU:HD12	1:D:198:LEU:HA	1.86	0.44
1:L:451:LYS:CG	6:L:612:1PE:H131	2.47	0.44
1:A:123:VAL:HG21	1:A:153:VAL:HG11	1.99	0.43
1:D:179:ASN:C	1:D:181:ASN:N	2.76	0.43
1:D:219:LEU:HD22	1:D:219:LEU:N	2.33	0.43
1:E:135:PRO:HA	1:E:194:SER:O	2.18	0.43
1:E:223:THR:HA	1:E:268:GLY:O	2.18	0.43
1:E:368:LYS:HE3	7:E:2241:HOH:O	2.17	0.43
1:F:395:LEU:HD11	1:F:581:TRP:CG	2.53	0.43
1:G:214:LEU:HD21	1:G:222:LEU:HD22	1.99	0.43
1:J:86:SER:HB2	7:J:1689:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:208:LEU:HD13	1:K:245:GLU:HG3	2.00	0.43
1:A:326:LYS:HG2	1:A:328:LEU:HD12	2.00	0.43
4:A:1003:BEY:H10	4:A:1003:BEY:H18A	1.63	0.43
1:C:156:PHE:CE2	1:C:175:PHE:HB3	2.54	0.43
1:C:207:VAL:CG1	1:C:242:LEU:HA	2.48	0.43
1:G:198:LEU:HD22	1:G:202:ASP:HB2	1.99	0.43
1:H:355:ILE:O	1:H:426:LEU:HA	2.18	0.43
1:I:462:GLY:N	2:I:1002:CO3:O1	2.52	0.43
1:J:541:TYR:HE1	1:K:249:ASP:HB3	1.83	0.43
1:K:275:ASP:C	1:K:277:TYR:H	2.26	0.43
1:L:300:ALA:HA	1:L:301:PRO:HD3	1.84	0.43
1:A:174:HIS:CE1	1:A:213:MET:HE2	2.53	0.43
1:B:423:ILE:HD11	1:B:600:VAL:CG1	2.48	0.43
1:F:398:PHE:CD2	1:F:398:PHE:C	2.95	0.43
1:F:520:SER:HB3	1:F:598:GLU:HG3	1.99	0.43
1:G:528:PRO:HD3	1:L:525:TRP:CE2	2.53	0.43
1:H:594:ARG:HG3	7:H:781:HOH:O	2.17	0.43
1:J:99:ILE:HD12	1:J:313:ALA:HB2	1.99	0.43
1:B:440:ARG:HD2	1:C:302:SER:HB2	2.00	0.43
1:D:393:ILE:HG12	1:F:441:PRO:HG2	2.01	0.43
1:E:355:ILE:O	1:E:426:LEU:HA	2.18	0.43
1:F:150:ASP:HB3	1:F:153:VAL:HB	2.00	0.43
1:J:273:ASN:O	1:J:274:ALA:C	2.60	0.43
1:J:516:SER:OG	1:J:599:PHE:HA	2.18	0.43
1:K:395:LEU:HD11	1:K:581:TRP:CG	2.54	0.43
1:K:398:PHE:CD2	1:K:398:PHE:C	2.96	0.43
1:A:214:LEU:HD11	1:A:222:LEU:HD22	1.99	0.43
1:A:230:VAL:O	1:A:277:TYR:OH	2.31	0.43
1:B:364:ASP:O	1:B:420:ASN:HA	2.17	0.43
1:G:232:LYS:N	7:G:903:HOH:O	2.51	0.43
1:I:381:GLY:HA2	1:I:459:ASP:OD1	2.18	0.43
1:J:221:LYS:HE2	7:J:633:HOH:O	2.17	0.43
1:J:520:SER:HB3	1:J:598:GLU:HG3	2.01	0.43
1:E:157:LEU:HD23	1:E:157:LEU:HA	1.87	0.43
1:G:222:LEU:O	1:G:267:LEU:HD12	2.17	0.43
1:I:182:LYS:N	1:I:182:LYS:HD3	2.29	0.43
1:I:320:LYS:NZ	6:I:21:1PE:H131	2.34	0.43
1:A:536:THR:HG21	1:A:551:VAL:HG23	2.01	0.43
1:F:481:ILE:O	1:F:571:TRP:HA	2.19	0.43
1:H:138:GLU:C	1:H:140:GLY:N	2.77	0.43
1:K:536:THR:HG21	1:K:551:VAL:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:VAL:C	1:B:150:ASP:H	2.22	0.43
1:C:238:PHE:CD2	1:C:238:PHE:C	2.97	0.43
1:E:106:PRO:HG2	1:E:263:TYR:CE2	2.54	0.43
1:G:516:SER:OG	1:G:599:PHE:HA	2.18	0.43
1:I:189:TYR:CD2	1:I:189:TYR:C	2.97	0.43
1:J:108:HIS:HA	1:J:285:ARG:HD2	2.00	0.43
1:L:150:ASP:HB3	1:L:153:VAL:HB	2.00	0.43
1:B:133:ASN:C	1:B:167:VAL:HG11	2.43	0.43
1:C:208:LEU:O	1:C:212:THR:HG23	2.19	0.43
1:D:394:ASP:HB3	7:F:3100:HOH:O	2.19	0.43
1:F:423:ILE:HD13	1:F:600:VAL:HG11	2.01	0.43
1:I:138:GLU:C	1:I:139:ASN:HD22	2.26	0.43
1:I:168:LYS:O	1:I:171:THR:HB	2.19	0.43
1:I:530:ILE:HD12	1:I:556:ILE:HD13	2.01	0.43
1:K:246:TYR:CE2	1:K:263:TYR:HD1	2.37	0.43
1:A:167:VAL:O	1:A:168:LYS:C	2.61	0.43
1:B:174:HIS:CD2	1:B:213:MET:HE2	2.54	0.43
1:C:180:ASP:C	1:C:182:LYS:H	2.27	0.43
1:F:103:TYR:HB2	5:F:21:SO4:O4	2.19	0.43
1:G:95:ASP:HA	1:G:96:PRO:HD2	1.90	0.43
1:G:112:VAL:HG22	1:G:267:LEU:HB3	2.00	0.43
1:G:292:TYR:O	1:G:295:SER:HB3	2.18	0.43
1:G:423:ILE:HD13	1:G:600:VAL:HG11	2.01	0.43
1:H:131:LEU:O	1:H:228:ILE:HG23	2.19	0.43
1:H:202:ASP:O	1:H:206:VAL:HG23	2.19	0.43
1:H:364:ASP:O	1:H:420:ASN:HA	2.18	0.43
1:I:324:GLU:H	1:I:324:GLU:HG2	1.68	0.43
1:A:475:LYS:HD3	7:A:2808:HOH:O	2.19	0.42
1:G:306:ASN:HB2	1:G:307:PRO:HD2	2.01	0.42
1:H:498:SER:HB3	1:H:499:TYR:HD2	1.84	0.42
1:J:168:LYS:O	1:J:169:LEU:C	2.62	0.42
1:J:423:ILE:HD13	1:J:600:VAL:HG11	2.01	0.42
1:K:451:LYS:NZ	6:K:42:1PE:H231	2.34	0.42
1:L:512:LYS:HD3	1:L:603:ASP:OD1	2.19	0.42
1:B:134:ASN:HB3	1:B:167:VAL:HG21	2.00	0.42
1:B:229:ASN:ND2	7:B:2947:HOH:O	2.52	0.42
4:C:1003:BEY:H2	4:C:1003:BEY:H8	1.66	0.42
1:G:249:ASP:CG	1:G:251:ARG:HE	2.27	0.42
1:I:273:ASN:O	1:I:274:ALA:C	2.62	0.42
1:J:103:TYR:HB2	5:J:20:SO4:O1	2.19	0.42
1:E:88:VAL:HA	1:E:89:PRO:HD2	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:109:ASP:HB2	7:F:1094:HOH:O	2.19	0.42
1:F:210:LEU:HA	1:F:213:MET:HE3	2.01	0.42
1:F:222:LEU:HB3	1:F:264:ILE:HD13	2.01	0.42
1:G:123:VAL:HG12	1:G:185:VAL:HG11	2.01	0.42
1:G:316:GLU:HG3	6:G:58:1PE:H131	2.01	0.42
1:K:106:PRO:HD2	1:K:247:MET:SD	2.59	0.42
1:B:169:LEU:HD21	1:B:205:ARG:HD3	2.02	0.42
1:C:139:ASN:ND2	1:C:168:LYS:HB2	2.34	0.42
1:E:544:ILE:CD1	1:E:564:GLU:HG3	2.49	0.42
1:F:306:ASN:HB2	1:F:307:PRO:CD	2.48	0.42
1:G:173:LYS:NZ	1:J:176:TYR:OH	2.42	0.42
1:I:316:GLU:CD	6:I:21:1PE:H132	2.43	0.42
1:K:392:MET:CE	4:K:1003:BEY:H12	2.49	0.42
1:L:96:PRO:HB3	1:L:304:TYR:CE1	2.54	0.42
1:A:114:VAL:HA	1:A:269:VAL:O	2.20	0.42
1:A:231:ASP:O	1:A:232:LYS:C	2.62	0.42
1:E:363:GLY:HA3	7:E:1962:HOH:O	2.19	0.42
1:F:374:LYS:HB2	1:F:485:ALA:CB	2.49	0.42
1:G:528:PRO:HD3	1:L:525:TRP:NE1	2.35	0.42
1:H:181:ASN:ND2	1:H:183:ASN:ND2	2.67	0.42
1:H:543:ASP:HA	1:I:256:ASP:HB3	2.00	0.42
1:I:137:LYS:CB	7:I:5069:HOH:O	2.66	0.42
1:J:239:LEU:HB3	1:J:284:ALA:HB1	2.01	0.42
1:K:107:ILE:O	1:K:109:ASP:N	2.52	0.42
1:K:248:THR:HG23	7:K:2935:HOH:O	2.19	0.42
1:D:219:LEU:HD13	1:D:219:LEU:N	2.26	0.42
1:E:362:LYS:N	7:E:1815:HOH:O	2.52	0.42
1:F:544:ILE:CD1	1:F:564:GLU:HG3	2.49	0.42
1:H:423:ILE:HD11	1:H:600:VAL:CG1	2.49	0.42
1:J:317:LEU:HG	1:J:321:LEU:HD12	2.02	0.42
1:J:440:ARG:CD	1:K:302:SER:HB2	2.49	0.42
1:A:112:VAL:HA	1:A:267:LEU:O	2.19	0.42
1:C:395:LEU:HD11	1:C:581:TRP:CG	2.55	0.42
1:E:440:ARG:NH2	7:E:663:HOH:O	2.52	0.42
1:F:444:ILE:HA	1:F:453:ILE:O	2.18	0.42
1:I:423:ILE:HD11	1:I:600:VAL:CG1	2.50	0.42
1:J:273:ASN:HB2	1:J:277:TYR:HE2	1.83	0.42
1:J:321:LEU:CD1	1:J:411:TYR:HA	2.47	0.42
1:K:121:CYS:HA	1:K:270:TYR:CE2	2.54	0.42
1:A:92:VAL:O	1:A:95:ASP:HB2	2.19	0.42
1:C:316:GLU:HG3	6:C:17:1PE:H221	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:169:LEU:HD12	1:E:192:CYS:HA	2.01	0.42
1:F:134:ASN:CB	1:F:167:VAL:HG11	2.50	0.42
1:G:445:ILE:HA	7:G:866:HOH:O	2.19	0.42
1:H:398:PHE:CD2	1:H:398:PHE:C	2.96	0.42
1:J:207:VAL:HG13	1:J:242:LEU:HA	2.00	0.42
1:J:320:LYS:CE	6:J:3:1PE:H142	2.49	0.42
1:J:393:ILE:HG12	1:L:441:PRO:HG2	2.02	0.42
1:J:423:ILE:CD1	1:J:600:VAL:CG1	2.98	0.42
1:D:179:ASN:O	1:D:182:LYS:N	2.51	0.42
1:D:272:ASN:O	1:D:273:ASN:HB2	2.20	0.42
1:E:129:ILE:HA	1:E:188:GLY:O	2.20	0.42
1:F:240:GLU:HG3	1:F:240:GLU:H	1.60	0.42
1:F:533:TYR:HB2	1:F:560:LEU:CD1	2.49	0.42
1:L:150:ASP:OD1	1:L:179:ASN:HB2	2.19	0.42
1:E:222:LEU:O	1:E:267:LEU:HA	2.19	0.42
1:G:134:ASN:O	1:G:194:SER:HB2	2.20	0.42
1:H:381:GLY:HA2	1:H:459:ASP:OD1	2.19	0.42
1:K:207:VAL:CG1	1:K:242:LEU:HA	2.50	0.42
1:L:181:ASN:O	1:L:183:ASN:CG	2.63	0.42
1:A:395:LEU:HD11	1:A:581:TRP:CG	2.54	0.41
1:A:528:PRO:HD3	1:F:525:TRP:NE1	2.35	0.41
1:E:179:ASN:C	1:E:179:ASN:OD1	2.63	0.41
1:I:444:ILE:HA	1:I:453:ILE:O	2.20	0.41
1:A:189:TYR:CD2	1:A:189:TYR:C	2.97	0.41
1:A:346:LYS:HB3	1:A:437:ASN:O	2.19	0.41
1:A:516:SER:OG	1:A:599:PHE:HA	2.20	0.41
1:B:381:GLY:HA2	1:B:459:ASP:OD1	2.19	0.41
1:D:210:LEU:HA	1:D:213:MET:HE3	2.01	0.41
1:D:544:ILE:CD1	1:D:564:GLU:HG3	2.50	0.41
1:F:178:PHE:HD1	1:F:182:LYS:O	2.03	0.41
1:F:198:LEU:HD12	1:F:198:LEU:HA	1.84	0.41
1:F:239:LEU:HD23	1:F:281:VAL:HA	2.01	0.41
1:G:234:LEU:O	1:G:234:LEU:HD12	2.20	0.41
1:H:230:VAL:O	1:H:231:ASP:C	2.60	0.41
1:J:307:PRO:HD3	1:J:377:THR:OG1	2.20	0.41
1:J:350:TYR:HE1	1:L:440:ARG:HH21	1.68	0.41
1:L:214:LEU:HD21	1:L:222:LEU:HD22	2.02	0.41
1:A:300:ALA:HA	1:A:301:PRO:HD3	1.87	0.41
1:B:520:SER:HB3	1:B:598:GLU:HG3	2.01	0.41
1:B:528:PRO:HB3	1:E:525:TRP:CZ3	2.54	0.41
1:C:532:GLU:HB2	7:D:4750:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:346:LYS:HB3	1:D:437:ASN:O	2.19	0.41
1:E:158:LYS:O	1:E:161:ASN:HB3	2.20	0.41
1:E:161:ASN:ND2	7:E:1724:HOH:O	2.53	0.41
1:E:208:LEU:HD12	1:E:208:LEU:HA	1.90	0.41
1:F:375:GLY:O	1:F:429:VAL:HA	2.19	0.41
1:J:90:GLN:NE2	1:J:95:ASP:O	2.53	0.41
1:J:91:VAL:HB	1:L:346:LYS:HE3	2.02	0.41
1:K:118:LYS:NZ	1:K:272:ASN:OD1	2.50	0.41
1:L:142:VAL:HG23	1:L:165:PHE:O	2.20	0.41
1:L:235:PHE:HE1	1:L:269:VAL:HG11	1.86	0.41
1:A:142:VAL:HG21	1:A:189:TYR:CZ	2.56	0.41
1:A:162:MET:HE2	1:A:162:MET:HA	2.03	0.41
1:C:181:ASN:ND2	1:C:183:ASN:ND2	2.67	0.41
1:F:307:PRO:HD3	1:F:377:THR:OG1	2.19	0.41
1:G:174:HIS:HB3	1:J:175:PHE:CD2	2.56	0.41
1:G:487:LEU:HD22	1:G:573:HIS:CE1	2.56	0.41
1:I:225:VAL:HG22	1:I:270:TYR:HB2	2.01	0.41
1:J:494:SER:HB3	7:J:1288:HOH:O	2.19	0.41
1:K:307:PRO:HD3	1:K:377:THR:OG1	2.20	0.41
1:B:541:TYR:OH	1:C:587:LYS:HB2	2.21	0.41
1:F:207:VAL:HG11	1:F:241:THR:HG22	2.03	0.41
1:J:323:LEU:HD23	1:J:323:LEU:HA	1.78	0.41
1:J:514:LEU:O	1:J:518:LYS:HG2	2.21	0.41
1:K:221:LYS:HG3	1:K:266:HIS:HB2	2.03	0.41
1:K:237:PHE:O	1:K:240:GLU:HB2	2.20	0.41
1:C:481:ILE:O	1:C:571:TRP:HA	2.20	0.41
1:E:219:LEU:O	1:E:264:ILE:HG22	2.20	0.41
1:H:487:LEU:O	4:H:1003:BEY:H17A	2.19	0.41
1:I:207:VAL:HG11	1:I:242:LEU:N	2.36	0.41
1:I:497:THR:HB	7:I:4920:HOH:O	2.20	0.41
1:L:232:LYS:HE2	1:L:276:THR:O	2.20	0.41
1:B:133:ASN:CG	1:B:228:ILE:HG22	2.46	0.41
1:B:441:PRO:HG2	1:C:393:ILE:HG12	2.03	0.41
1:C:346:LYS:HB3	1:C:437:ASN:O	2.20	0.41
1:G:88:VAL:HA	1:G:89:PRO:HD2	1.88	0.41
1:H:178:PHE:HZ	1:L:155:GLU:HG2	1.84	0.41
1:I:111:LYS:HE2	1:I:266:HIS:NE2	2.36	0.41
1:I:230:VAL:CG2	1:I:234:LEU:HG	2.51	0.41
1:K:107:ILE:O	1:K:108:HIS:C	2.63	0.41
1:A:176:TYR:CE2	1:D:156:PHE:HB2	2.55	0.41
1:A:301:PRO:CG	1:C:444:ILE:HD12	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:487:LEU:HD22	1:C:573:HIS:CE1	2.56	0.41
1:D:440:ARG:HD3	1:E:302:SER:HB2	2.01	0.41
1:E:374:LYS:HE2	1:E:399:ASP:CG	2.46	0.41
1:E:481:ILE:O	1:E:571:TRP:HA	2.20	0.41
1:G:522:GLU:HA	1:G:523:PRO:HD3	1.92	0.41
1:G:528:PRO:HD3	1:L:525:TRP:CD1	2.56	0.41
1:H:520:SER:HB3	1:H:598:GLU:HG3	2.02	0.41
1:J:481:ILE:O	1:J:571:TRP:HA	2.20	0.41
1:L:364:ASP:O	1:L:420:ASN:HA	2.21	0.41
1:L:536:THR:HG21	1:L:551:VAL:HG23	2.02	0.41
1:A:263:TYR:N	7:A:2776:HOH:O	2.43	0.41
1:A:393:ILE:HG12	1:C:441:PRO:HG2	2.03	0.41
4:A:1003:BEY:H17	4:A:1003:BEY:H18	1.78	0.41
1:B:360:LYS:HE3	1:B:365:VAL:HG21	2.03	0.41
1:C:551:VAL:HG12	1:C:553:ALA:H	1.86	0.41
1:D:487:LEU:HD22	1:D:573:HIS:CE1	2.56	0.41
1:E:133:ASN:OD1	1:E:133:ASN:C	2.64	0.41
1:F:126:GLY:HA3	1:F:221:LYS:O	2.20	0.41
1:F:367:LYS:HD3	1:F:367:LYS:HA	1.83	0.41
1:H:219:LEU:O	1:H:264:ILE:HG22	2.21	0.41
1:H:552:LYS:HE3	1:K:492:LEU:HD13	2.03	0.41
1:I:203:MET:O	1:I:207:VAL:HG23	2.21	0.41
1:I:487:LEU:HD12	1:I:487:LEU:HA	1.95	0.41
1:J:219:LEU:HB3	1:J:220:SER:H	1.62	0.41
1:K:544:ILE:CD1	1:K:564:GLU:HG3	2.51	0.41
1:L:103:TYR:HB3	6:L:1:1PE:H252	2.03	0.41
1:L:162:MET:CE	1:L:165:PHE:HE1	2.32	0.41
1:C:158:LYS:O	1:C:159:ASP:C	2.64	0.41
1:G:177:MET:O	1:G:184:SER:HA	2.21	0.41
1:G:374:LYS:HB3	7:G:636:HOH:O	2.20	0.41
1:I:139:ASN:O	1:I:166:ASN:HB2	2.21	0.41
1:L:207:VAL:O	1:L:211:VAL:HG23	2.20	0.41
1:L:254:SER:O	1:L:254:SER:OG	2.36	0.41
1:A:198:LEU:HB3	1:A:202:ASP:HB2	2.03	0.40
1:A:235:PHE:HE1	1:A:269:VAL:HG11	1.84	0.40
1:E:129:ILE:HA	1:E:129:ILE:HD13	1.84	0.40
1:G:481:ILE:O	1:G:571:TRP:HA	2.21	0.40
1:I:145:SER:OG	1:I:227:GLU:OE1	2.38	0.40
1:I:265:LYS:HA	1:I:265:LYS:HE2	2.03	0.40
1:J:375:GLY:O	1:J:429:VAL:HA	2.21	0.40
1:K:440:ARG:CD	1:L:302:SER:HB2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:MET:HG2	7:C:1438:HOH:O	2.21	0.40
1:B:442:GLY:O	1:C:301:PRO:HB3	2.21	0.40
1:C:239:LEU:HD21	1:C:281:VAL:HG22	2.03	0.40
1:C:292:TYR:O	1:C:295:SER:HB3	2.22	0.40
1:C:392:MET:HE3	4:C:1003:BEY:H12	2.03	0.40
1:D:128:THR:O	1:D:129:ILE:HD13	2.21	0.40
1:D:301:PRO:HB2	1:D:303:ASN:OD1	2.21	0.40
1:G:301:PRO:HB3	1:I:442:GLY:O	2.20	0.40
1:H:138:GLU:O	1:H:140:GLY:N	2.50	0.40
1:H:441:PRO:HG2	1:I:393:ILE:HG12	2.03	0.40
1:J:475:LYS:HB3	7:J:4358:HOH:O	2.21	0.40
1:K:366:LYS:HG3	1:K:420:ASN:HB3	2.03	0.40
1:B:190:VAL:HG11	1:B:206:VAL:HG13	2.02	0.40
1:C:176:TYR:CE1	1:C:184:SER:HB2	2.56	0.40
1:D:522:GLU:HA	1:D:523:PRO:HD3	1.94	0.40
1:I:88:VAL:HG21	1:I:97:THR:O	2.21	0.40
1:I:487:LEU:HD22	1:I:573:HIS:CE1	2.56	0.40
1:J:350:TYR:HA	1:J:351:PRO:HD3	1.97	0.40
1:J:398:PHE:CD2	1:J:398:PHE:C	2.99	0.40
1:L:505:ASN:HA	7:L:2672:HOH:O	2.21	0.40
1:A:200:GLU:HB2	1:A:521:ASN:OD1	2.21	0.40
1:A:326:LYS:HG2	1:A:328:LEU:CD1	2.51	0.40
1:B:125:GLU:HG2	1:B:126:GLY:N	2.36	0.40
1:B:460:ALA:O	1:B:546:GLN:NE2	2.54	0.40
1:C:178:PHE:CZ	1:E:155:GLU:HG2	2.52	0.40
1:G:393:ILE:HG12	1:I:441:PRO:HG2	2.03	0.40
1:I:223:THR:HA	1:I:268:GLY:O	2.22	0.40
1:K:127:LEU:HA	1:K:186:ALA:O	2.20	0.40
1:L:105:THR:C	1:L:107:ILE:N	2.78	0.40
1:L:156:PHE:O	1:L:162:MET:HE3	2.22	0.40
1:C:156:PHE:CZ	1:C:175:PHE:HB3	2.56	0.40
1:E:398:PHE:CD2	1:E:398:PHE:C	3.00	0.40
1:G:115:TYR:O	1:G:270:TYR:HA	2.21	0.40
1:G:159:ASP:OD1	1:G:159:ASP:N	2.55	0.40
1:G:239:LEU:HD23	1:G:239:LEU:HA	1.86	0.40
1:I:399:ASP:OD1	4:I:1003:BEY:N	2.55	0.40
1:J:195:VAL:O	1:J:195:VAL:HG12	2.20	0.40
1:J:591:PHE:CD2	1:J:591:PHE:C	2.99	0.40
1:K:157:LEU:HD23	1:K:157:LEU:HA	1.88	0.40
1:L:123:VAL:HG11	1:L:153:VAL:HG21	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:LYS:NZ	7:D:3762:HOH:O[4_555]	1.84	0.36

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	514/528 (97%)	493 (96%)	19 (4%)	2 (0%)	30	39
1	B	516/528 (98%)	488 (95%)	25 (5%)	3 (1%)	21	28
1	C	516/528 (98%)	495 (96%)	18 (4%)	3 (1%)	21	28
1	D	509/528 (96%)	492 (97%)	16 (3%)	1 (0%)	43	54
1	E	506/528 (96%)	487 (96%)	17 (3%)	2 (0%)	30	39
1	F	504/528 (96%)	484 (96%)	14 (3%)	6 (1%)	10	14
1	G	512/528 (97%)	483 (94%)	27 (5%)	2 (0%)	30	39
1	H	503/528 (95%)	477 (95%)	21 (4%)	5 (1%)	12	17
1	I	516/528 (98%)	493 (96%)	22 (4%)	1 (0%)	43	54
1	J	509/528 (96%)	483 (95%)	24 (5%)	2 (0%)	30	39
1	K	503/528 (95%)	479 (95%)	22 (4%)	2 (0%)	30	39
1	L	509/528 (96%)	484 (95%)	24 (5%)	1 (0%)	43	54
All	All	6117/6336 (96%)	5838 (95%)	249 (4%)	30 (0%)	24	33

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	217	ASN
1	B	149	ASN
1	E	230	VAL
1	H	139	ASN
1	B	273	ASN

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Mol	Chain	Res	Type
1	C	274	ALA
1	E	137	LYS
1	H	231	ASP
1	I	261	MET
1	K	108	HIS
1	D	180	ASP
1	F	163	GLU
1	F	184	SER
1	F	274	ALA
1	J	149	ASN
1	C	139	ASN
1	F	149	ASN
1	F	179	ASN
1	G	149	ASN
1	J	251	ARG
1	K	139	ASN
1	L	168	LYS
1	A	200	GLU
1	B	254	SER
1	F	168	LYS
1	G	218	LYS
1	H	117	ILE
1	H	181	ASN
1	C	117	ILE
1	H	195	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/455 (94%)	404 (95%)	22 (5%)	21	31
1	B	412/455 (90%)	398 (97%)	14 (3%)	32	47
1	C	419/455 (92%)	407 (97%)	12 (3%)	37	53
1	D	417/455 (92%)	392 (94%)	25 (6%)	17	25
1	E	414/455 (91%)	396 (96%)	18 (4%)	26	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	409/455 (90%)	381 (93%)	28 (7%)	14	20
1	G	435/455 (96%)	416 (96%)	19 (4%)	25	37
1	H	430/455 (94%)	409 (95%)	21 (5%)	22	33
1	I	437/455 (96%)	410 (94%)	27 (6%)	16	24
1	J	430/455 (94%)	402 (94%)	28 (6%)	15	22
1	K	427/455 (94%)	405 (95%)	22 (5%)	21	31
1	L	421/455 (92%)	401 (95%)	20 (5%)	23	34
All	All	5077/5460 (93%)	4821 (95%)	256 (5%)	22	33

All (256) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	SER
1	A	114	VAL
1	A	117	ILE
1	A	132	VAL
1	A	160	GLU
1	A	166	ASN
1	A	168	LYS
1	A	187	VAL
1	A	194	SER
1	A	197	ASP
1	A	198	LEU
1	A	206	VAL
1	A	310	LEU
1	A	330	VAL
1	A	367	LYS
1	A	398	PHE
1	A	439	TYR
1	A	476	LEU
1	A	498	SER
1	A	579	VAL
1	A	601	LEU
1	A	603	ASP
1	B	104	ASN
1	B	148	VAL
1	B	173	LYS
1	B	200	GLU
1	B	208	LEU
1	B	210	LEU

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Mol	Chain	Res	Type
1	B	212	THR
1	B	310	LEU
1	B	332	GLU
1	B	398	PHE
1	B	439	TYR
1	B	471	VAL
1	B	498	SER
1	B	601	LEU
1	C	86	SER
1	C	145	SER
1	C	146	SER
1	C	163	GLU
1	C	181	ASN
1	C	185	VAL
1	C	194	SER
1	C	208	LEU
1	C	229	ASN
1	C	398	PHE
1	C	439	TYR
1	C	601	LEU
1	D	88	VAL
1	D	90	GLN
1	D	91	VAL
1	D	111	LYS
1	D	132	VAL
1	D	198	LEU
1	D	210	LEU
1	D	212	THR
1	D	219	LEU
1	D	230	VAL
1	D	231	ASP
1	D	248	THR
1	D	261	MET
1	D	262	GLU
1	D	276	THR
1	D	310	LEU
1	D	322	ASN
1	D	332	GLU
1	D	367	LYS
1	D	398	PHE
1	D	439	TYR
1	D	518	LYS

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Mol	Chain	Res	Type
1	D	532	GLU
1	D	560	LEU
1	D	579	VAL
1	E	172	SER
1	E	185	VAL
1	E	195	VAL
1	E	206	VAL
1	E	208	LEU
1	E	217	ASN
1	E	220	SER
1	E	230	VAL
1	E	239	LEU
1	E	248	THR
1	E	267	LEU
1	E	310	LEU
1	E	398	PHE
1	E	407	LEU
1	E	413	VAL
1	E	439	TYR
1	E	560	LEU
1	E	601	LEU
1	F	86	SER
1	F	91	VAL
1	F	92	VAL
1	F	93	SER
1	F	102	GLU
1	F	114	VAL
1	F	117	ILE
1	F	122	ASN
1	F	161	ASN
1	F	198	LEU
1	F	200	GLU
1	F	217	ASN
1	F	228	ILE
1	F	232	LYS
1	F	239	LEU
1	F	240	GLU
1	F	248	THR
1	F	310	LEU
1	F	326	LYS
1	F	330	VAL
1	F	364	ASP

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Mol	Chain	Res	Type
1	F	367	LYS
1	F	398	PHE
1	F	439	TYR
1	F	476	LEU
1	F	507	GLU
1	F	508	GLU
1	F	579	VAL
1	G	101	ILE
1	G	118	LYS
1	G	164	LYS
1	G	168	LYS
1	G	182	LYS
1	G	185	VAL
1	G	195	VAL
1	G	229	ASN
1	G	234	LEU
1	G	265	LYS
1	G	310	LEU
1	G	367	LYS
1	G	398	PHE
1	G	439	TYR
1	G	476	LEU
1	G	515	GLN
1	G	518	LYS
1	G	579	VAL
1	G	601	LEU
1	H	114	VAL
1	H	117	ILE
1	H	155	GLU
1	H	158	LYS
1	H	173	LYS
1	H	200	GLU
1	H	208	LEU
1	H	212	THR
1	H	213	MET
1	H	276	THR
1	H	279	GLU
1	H	310	LEU
1	H	331	LYS
1	H	398	PHE
1	H	439	TYR
1	H	476	LEU

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Mol	Chain	Res	Type
1	H	498	SER
1	H	508	GLU
1	H	515	GLN
1	H	579	VAL
1	H	601	LEU
1	I	121	CYS
1	I	132	VAL
1	I	145	SER
1	I	154	SER
1	I	163	GLU
1	I	171	THR
1	I	182	LYS
1	I	187	VAL
1	I	195	VAL
1	I	198	LEU
1	I	199	SER
1	I	200	GLU
1	I	208	LEU
1	I	228	ILE
1	I	229	ASN
1	I	239	LEU
1	I	265	LYS
1	I	310	LEU
1	I	324	GLU
1	I	367	LYS
1	I	398	PHE
1	I	439	TYR
1	I	476	LEU
1	I	508	GLU
1	I	579	VAL
1	I	601	LEU
1	I	603	ASP
1	J	86	SER
1	J	88	VAL
1	J	99	ILE
1	J	114	VAL
1	J	123	VAL
1	J	132	VAL
1	J	143	LYS
1	J	184	SER
1	J	194	SER
1	J	195	VAL

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Mol	Chain	Res	Type
1	J	197	ASP
1	J	208	LEU
1	J	230	VAL
1	J	239	LEU
1	J	248	THR
1	J	261	MET
1	J	276	THR
1	J	279	GLU
1	J	310	LEU
1	J	322	ASN
1	J	332	GLU
1	J	367	LYS
1	J	398	PHE
1	J	439	TYR
1	J	476	LEU
1	J	518	LYS
1	J	579	VAL
1	J	603	ASP
1	K	102	GLU
1	K	132	VAL
1	K	143	LYS
1	K	167	VAL
1	K	182	LYS
1	K	185	VAL
1	K	195	VAL
1	K	208	LEU
1	K	211	VAL
1	K	218	LYS
1	K	239	LEU
1	K	248	THR
1	K	265	LYS
1	K	310	LEU
1	K	367	LYS
1	K	398	PHE
1	K	439	TYR
1	K	476	LEU
1	K	579	VAL
1	K	584	LYS
1	K	601	LEU
1	K	603	ASP
1	L	92	VAL
1	L	127	LEU

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Mol	Chain	Res	Type
1	L	148	VAL
1	L	165	PHE
1	L	167	VAL
1	L	184	SER
1	L	195	VAL
1	L	200	GLU
1	L	271	ILE
1	L	275	ASP
1	L	310	LEU
1	L	367	LYS
1	L	398	PHE
1	L	439	TYR
1	L	476	LEU
1	L	508	GLU
1	L	518	LYS
1	L	579	VAL
1	L	584	LYS
1	L	605	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	ASN
1	A	152	GLN
1	A	181	ASN
1	A	215	HIS
1	A	272	ASN
1	B	113	GLN
1	B	122	ASN
1	B	229	ASN
1	B	260	ASN
1	C	134	ASN
1	C	181	ASN
1	C	183	ASN
1	D	139	ASN
1	D	521	ASN
1	E	104	ASN
1	E	602	ASN
1	F	183	ASN
1	F	217	ASN
1	F	266	HIS
1	F	322	ASN

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Mol	Chain	Res	Type
1	F	521	ASN
1	G	122	ASN
1	G	183	ASN
1	H	134	ASN
1	H	181	ASN
1	H	183	ASN
1	I	104	ASN
1	I	113	GLN
1	I	139	ASN
1	I	166	ASN
1	I	531	ASN
1	I	602	ASN
1	J	104	ASN
1	J	113	GLN
1	J	152	GLN
1	J	166	ASN
1	J	174	HIS
1	J	183	ASN
1	J	420	ASN
1	K	149	ASN
1	K	181	ASN
1	K	602	ASN
1	L	122	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 100 ligands modelled in this entry, 24 are monoatomic - leaving 76 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	BEY	D	1003	3	22,26,26	1.00	1 (4%)	24,35,35	1.17	2 (8%)
6	1PE	G	47	-	5,5,15	0.40	0	4,4,14	0.25	0
5	SO4	A	2	-	4,4,4	0.29	0	6,6,6	0.58	0
5	SO4	J	18	-	4,4,4	0.24	0	6,6,6	0.30	0
6	1PE	E	8	-	11,11,15	0.53	0	10,10,14	0.43	0
2	CO3	K	1002	-	3,3,3	0.54	0	2,3,3	0.62	0
6	1PE	E	43	-	7,7,15	0.47	0	6,6,14	0.49	0
6	1PE	K	50	-	5,5,15	0.70	0	4,4,14	0.55	0
5	SO4	A	1	-	4,4,4	0.27	0	6,6,6	0.32	0
6	1PE	G	30	-	6,6,15	0.55	0	5,5,14	0.43	0
2	CO3	H	1002	-	3,3,3	0.85	0	2,3,3	1.16	0
4	BEY	A	1003	3	22,26,26	0.78	0	24,35,35	1.29	3 (12%)
4	BEY	F	1003	3	22,26,26	1.14	1 (4%)	24,35,35	1.01	0
4	BEY	L	1003	3	22,26,26	0.93	1 (4%)	24,35,35	1.02	0
5	SO4	G	26	-	4,4,4	0.23	0	6,6,6	0.07	0
5	SO4	K	19	-	4,4,4	0.25	0	6,6,6	0.20	0
2	CO3	I	1002	-	3,3,3	0.59	0	2,3,3	0.91	0
6	1PE	G	12	-	8,8,15	0.49	0	7,7,14	0.21	0
6	1PE	I	21	-	14,14,15	0.73	0	13,13,14	0.51	0
6	1PE	B	62	-	9,9,15	0.68	0	8,8,14	0.44	0
4	BEY	J	1003	3	22,26,26	0.92	0	24,35,35	0.90	1 (4%)
4	BEY	I	1003	3	22,26,26	0.88	1 (4%)	24,35,35	1.42	3 (12%)
6	1PE	B	61	-	9,9,15	0.72	0	8,8,14	0.93	0
5	SO4	I	17	-	4,4,4	0.18	0	6,6,6	0.13	0
6	1PE	H	65	-	9,9,15	0.59	0	8,8,14	0.23	0
6	1PE	H	64	-	9,9,15	0.62	0	8,8,14	0.27	0
6	1PE	F	31	-	9,9,15	0.50	0	8,8,14	0.50	0
2	CO3	F	1002	-	3,3,3	0.83	0	2,3,3	0.59	0
2	CO3	J	1002	-	3,3,3	0.59	0	2,3,3	0.18	0
4	BEY	C	1003	3	22,26,26	1.15	1 (4%)	24,35,35	1.31	3 (12%)
6	1PE	I	66	-	6,6,15	0.62	0	5,5,14	0.54	0
5	SO4	L	25	-	4,4,4	0.26	0	6,6,6	0.37	0
6	1PE	F	32	-	9,9,15	0.66	0	8,8,14	0.44	0
4	BEY	E	1003	3	22,26,26	0.72	0	24,35,35	1.07	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	1PE	D	9	-	9,9,15	0.60	0	8,8,14	0.57	0
5	SO4	D	5	-	4,4,4	0.24	0	6,6,6	0.13	0
6	1PE	C	18	-	8,8,15	0.59	0	7,7,14	0.37	0
5	SO4	J	20	-	4,4,4	0.21	0	6,6,6	0.32	0
6	1PE	D	44	-	10,10,15	0.71	0	9,9,14	0.44	0
6	1PE	I	22	-	10,10,15	0.57	0	9,9,14	0.52	0
5	SO4	G	23	-	4,4,4	0.21	0	6,6,6	0.21	0
6	1PE	J	2	-	10,10,15	0.61	0	9,9,14	0.36	0
5	SO4	E	7	-	4,4,4	0.17	0	6,6,6	0.39	0
6	1PE	A	19	-	8,8,15	0.61	0	7,7,14	0.20	0
2	CO3	C	1002	-	3,3,3	0.92	0	2,3,3	1.02	0
6	1PE	J	45	-	9,9,15	0.68	0	8,8,14	0.53	0
2	CO3	B	1002	-	3,3,3	0.68	0	2,3,3	1.56	0
2	CO3	G	1002	-	3,3,3	0.62	0	2,3,3	0.77	0
2	CO3	E	1002	-	3,3,3	0.78	0	2,3,3	0.21	0
5	SO4	A	24	-	4,4,4	0.28	0	6,6,6	0.32	0
6	1PE	E	612	-	11,11,15	0.60	0	10,10,14	0.41	0
6	1PE	F	33	-	9,9,15	0.62	0	8,8,14	0.28	0
6	1PE	L	56	-	10,10,15	0.78	0	9,9,14	0.49	0
4	BEY	B	1003	3	22,26,26	0.94	0	24,35,35	1.24	3 (12%)
4	BEY	G	1003	3	22,26,26	1.01	0	24,35,35	1.12	1 (4%)
6	1PE	A	20	-	11,11,15	0.63	0	10,10,14	0.35	0
6	1PE	K	42	-	10,10,15	0.59	0	9,9,14	0.34	0
6	1PE	D	67	-	6,6,15	0.74	0	5,5,14	0.36	0
6	1PE	G	58	-	14,14,15	0.73	0	13,13,14	0.54	0
2	CO3	D	1002	-	3,3,3	1.00	0	2,3,3	0.62	0
5	SO4	C	3	-	4,4,4	0.20	0	6,6,6	0.38	0
2	CO3	L	1002	-	3,3,3	0.61	0	2,3,3	1.30	0
6	1PE	B	60	-	9,9,15	0.54	0	8,8,14	0.29	0
4	BEY	K	1003	3	22,26,26	0.72	0	24,35,35	1.74	6 (25%)
6	1PE	G	48	-	5,5,15	0.64	0	4,4,14	0.79	0
6	1PE	J	3	-	9,9,15	0.59	0	8,8,14	0.54	0
5	SO4	E	22	-	4,4,4	0.31	0	6,6,6	0.31	0
6	1PE	K	4	-	11,11,15	0.74	0	10,10,14	0.64	0
6	1PE	L	612	-	11,11,15	0.65	0	10,10,14	0.34	0
2	CO3	A	1002	-	3,3,3	0.78	0	2,3,3	0.40	0
6	1PE	D	63	-	9,9,15	0.70	0	8,8,14	0.42	0
4	BEY	H	1003	3	22,26,26	0.87	0	24,35,35	1.04	1 (4%)
6	1PE	K	5	-	11,11,15	0.51	0	10,10,14	0.41	0
6	1PE	L	1	-	9,9,15	0.52	0	8,8,14	0.37	0
5	SO4	F	21	-	4,4,4	0.29	0	6,6,6	0.22	0
6	1PE	C	17	-	12,12,15	0.92	0	11,11,14	1.05	1 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BEY	D	1003	3	-	8/18/24/24	0/2/2/2
6	1PE	G	47	-	-	1/3/3/13	-
6	1PE	E	8	-	-	4/9/9/13	-
6	1PE	K	50	-	-	3/3/3/13	-
6	1PE	E	43	-	-	3/5/5/13	-
6	1PE	G	30	-	-	2/4/4/13	-
4	BEY	A	1003	3	-	12/18/24/24	0/2/2/2
4	BEY	F	1003	3	-	10/18/24/24	0/2/2/2
4	BEY	L	1003	3	-	10/18/24/24	0/2/2/2
6	1PE	G	12	-	-	4/6/6/13	-
6	1PE	I	21	-	-	8/12/12/13	-
6	1PE	B	62	-	-	4/7/7/13	-
4	BEY	J	1003	3	-	8/18/24/24	0/2/2/2
4	BEY	I	1003	3	-	8/18/24/24	0/2/2/2
6	1PE	B	61	-	-	5/7/7/13	-
6	1PE	H	65	-	-	2/7/7/13	-
6	1PE	H	64	-	-	5/7/7/13	-
6	1PE	F	31	-	-	3/7/7/13	-
4	BEY	C	1003	3	-	11/18/24/24	0/2/2/2
6	1PE	I	66	-	-	2/4/4/13	-
6	1PE	F	32	-	-	3/7/7/13	-
4	BEY	E	1003	3	-	7/18/24/24	0/2/2/2
6	1PE	D	9	-	-	3/7/7/13	-
6	1PE	C	18	-	-	3/6/6/13	-
6	1PE	D	44	-	-	4/8/8/13	-
6	1PE	I	22	-	-	4/8/8/13	-
6	1PE	J	2	-	-	4/8/8/13	-
6	1PE	A	19	-	-	2/6/6/13	-
6	1PE	J	45	-	-	4/7/7/13	-
6	1PE	E	612	-	-	2/9/9/13	-
6	1PE	F	33	-	-	3/7/7/13	-
6	1PE	L	56	-	-	6/8/8/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BEY	B	1003	3	-	9/18/24/24	0/2/2/2
4	BEY	G	1003	3	-	7/18/24/24	0/2/2/2
6	1PE	A	20	-	-	3/9/9/13	-
6	1PE	K	42	-	-	5/8/8/13	-
6	1PE	D	67	-	-	3/4/4/13	-
6	1PE	G	58	-	-	5/12/12/13	-
6	1PE	G	48	-	-	2/3/3/13	-
6	1PE	B	60	-	-	4/7/7/13	-
4	BEY	K	1003	3	-	10/18/24/24	0/2/2/2
6	1PE	J	3	-	-	3/7/7/13	-
6	1PE	K	4	-	-	1/9/9/13	-
6	1PE	L	612	-	-	7/9/9/13	-
6	1PE	D	63	-	-	1/7/7/13	-
4	BEY	H	1003	3	-	9/18/24/24	0/2/2/2
6	1PE	K	5	-	-	3/9/9/13	-
6	1PE	L	1	-	-	5/7/7/13	-
6	1PE	C	17	-	-	3/10/10/13	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1003	BEY	P-C17	3.87	1.83	1.79
4	D	1003	BEY	P-C17	2.81	1.82	1.79
4	F	1003	BEY	P-C17	2.65	1.82	1.79
4	L	1003	BEY	P-C17	2.40	1.82	1.79
4	I	1003	BEY	P-C17	2.19	1.81	1.79

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	1003	BEY	C1-C7-C8	4.18	121.69	113.74
4	K	1003	BEY	C7-C8-C9	3.77	119.79	110.91
4	C	1003	BEY	C7-C8-C9	-3.67	102.27	110.91
4	K	1003	BEY	C1-C7-C8	3.48	120.36	113.74
4	K	1003	BEY	O3-P-C19	-3.44	99.15	106.87
4	B	1003	BEY	O1-C9-C8	2.84	121.53	114.16
4	K	1003	BEY	O1-C9-C8	2.80	121.43	114.16
4	I	1003	BEY	C7-C8-C9	2.77	117.44	110.91
4	A	1003	BEY	O3-P-C19	-2.76	100.67	106.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1003	BEY	O3-P-C19	-2.68	100.84	106.87
4	A	1003	BEY	P-C19-C18	-2.46	106.28	111.17
4	E	1003	BEY	O1-C9-C8	2.37	120.31	114.16
4	B	1003	BEY	P-C19-C18	2.33	115.78	111.17
4	I	1003	BEY	O1-C9-C8	2.26	120.01	114.16
4	G	1003	BEY	C12-C11-C10	-2.25	117.47	120.24
4	A	1003	BEY	C13-C16-C10	2.23	121.55	118.23
4	C	1003	BEY	C1-C7-C8	-2.19	109.58	113.74
4	H	1003	BEY	O1-C9-C8	2.10	119.60	114.16
4	K	1003	BEY	P-C19-C18	2.10	115.32	111.17
4	B	1003	BEY	O1-C9-O2	-2.09	119.33	124.08
4	C	1003	BEY	C5-C1-C2	2.09	121.34	118.23
4	D	1003	BEY	O2-C9-C8	-2.07	117.36	122.86
4	K	1003	BEY	O1-C9-O2	-2.06	119.42	124.08
6	C	17	1PE	OH4-C24-C14	2.04	119.64	110.35
4	J	1003	BEY	P-C19-C18	2.03	115.19	111.17

There are no chirality outliers.

All (238) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1003	BEY	C18-C19-P-O4
4	A	1003	BEY	C8-C17-P-O3
4	A	1003	BEY	C8-C17-P-O4
4	A	1003	BEY	C16-C15-C18-C19
4	B	1003	BEY	C8-C17-P-O3
4	B	1003	BEY	C8-C17-P-O4
4	B	1003	BEY	C15-C18-C19-N
4	B	1003	BEY	P-C17-C8-C9
4	C	1003	BEY	C18-C19-P-O4
4	C	1003	BEY	C8-C17-P-O3
4	C	1003	BEY	C8-C17-P-O4
4	C	1003	BEY	C16-C15-C18-C19
4	C	1003	BEY	P-C17-C8-C9
4	C	1003	BEY	C1-C7-C8-C9
4	D	1003	BEY	C18-C19-P-O4
4	D	1003	BEY	C8-C17-P-O3
4	D	1003	BEY	C8-C17-P-O4
4	E	1003	BEY	C18-C19-P-O4
4	E	1003	BEY	C8-C17-P-O3
4	E	1003	BEY	C8-C17-P-O4
4	E	1003	BEY	C16-C15-C18-C19

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Mol	Chain	Res	Type	Atoms
4	F	1003	BEY	C18-C19-P-O4
4	F	1003	BEY	C8-C17-P-O3
4	F	1003	BEY	C8-C17-P-O4
4	F	1003	BEY	C16-C15-C18-C19
4	F	1003	BEY	P-C17-C8-C9
4	F	1003	BEY	C1-C7-C8-C9
4	G	1003	BEY	C18-C19-P-O4
4	G	1003	BEY	C8-C17-P-O3
4	G	1003	BEY	C8-C17-P-O4
4	G	1003	BEY	C16-C15-C18-C19
4	H	1003	BEY	C18-C19-P-O4
4	H	1003	BEY	C8-C17-P-O3
4	H	1003	BEY	C8-C17-P-O4
4	I	1003	BEY	C18-C19-P-O4
4	I	1003	BEY	C8-C17-P-O3
4	I	1003	BEY	C8-C17-P-O4
4	I	1003	BEY	C16-C15-C18-C19
4	I	1003	BEY	C1-C7-C8-C17
4	I	1003	BEY	C1-C7-C8-C9
4	J	1003	BEY	C18-C19-P-O4
4	J	1003	BEY	C8-C17-P-O3
4	J	1003	BEY	C8-C17-P-O4
4	J	1003	BEY	C15-C18-C19-N
4	K	1003	BEY	C18-C19-P-O4
4	K	1003	BEY	C8-C17-P-O3
4	K	1003	BEY	C8-C17-P-O4
4	K	1003	BEY	C16-C15-C18-C19
4	K	1003	BEY	C1-C7-C8-C17
4	K	1003	BEY	C1-C7-C8-C9
4	L	1003	BEY	C18-C19-P-O4
4	L	1003	BEY	C8-C17-P-O3
4	L	1003	BEY	C8-C17-P-O4
4	L	1003	BEY	C16-C15-C18-C19
4	L	1003	BEY	P-C17-C8-C7
6	B	62	1PE	OH4-C13-C23-OH3
6	D	67	1PE	OH5-C14-C24-OH4
6	I	22	1PE	OH5-C14-C24-OH4
6	I	21	1PE	OH5-C14-C24-OH4
6	L	56	1PE	OH5-C14-C24-OH4
4	A	1003	BEY	C2-C1-C7-C8
6	L	612	1PE	OH5-C14-C24-OH4
6	D	67	1PE	C14-C24-OH4-C13

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Mol	Chain	Res	Type	Atoms
6	G	12	1PE	OH5-C14-C24-OH4
4	A	1003	BEY	C5-C1-C7-C8
4	G	1003	BEY	C2-C1-C7-C8
6	B	62	1PE	OH5-C14-C24-OH4
4	B	1003	BEY	C2-C1-C7-C8
4	F	1003	BEY	C2-C1-C7-C8
4	G	1003	BEY	C5-C1-C7-C8
6	E	612	1PE	OH6-C15-C25-OH5
6	F	31	1PE	OH5-C14-C24-OH4
6	F	32	1PE	OH7-C16-C26-OH6
6	G	48	1PE	OH6-C15-C25-OH5
4	D	1003	BEY	C16-C15-C18-C19
4	H	1003	BEY	C16-C15-C18-C19
6	A	19	1PE	OH4-C13-C23-OH3
4	C	1003	BEY	C2-C1-C7-C8
6	B	61	1PE	OH4-C13-C23-OH3
6	L	56	1PE	OH6-C15-C25-OH5
4	F	1003	BEY	C5-C1-C7-C8
6	G	12	1PE	OH4-C13-C23-OH3
6	J	2	1PE	OH6-C15-C25-OH5
4	C	1003	BEY	C5-C1-C7-C8
4	B	1003	BEY	C5-C1-C7-C8
6	C	18	1PE	OH5-C14-C24-OH4
6	E	8	1PE	OH6-C15-C25-OH5
6	G	30	1PE	OH5-C14-C24-OH4
6	L	56	1PE	OH7-C16-C26-OH6
6	C	17	1PE	OH5-C14-C24-OH4
6	E	8	1PE	OH5-C14-C24-OH4
6	D	44	1PE	OH6-C15-C25-OH5
6	D	9	1PE	OH5-C14-C24-OH4
6	I	22	1PE	OH4-C13-C23-OH3
6	J	2	1PE	OH5-C14-C24-OH4
6	L	1	1PE	OH6-C15-C25-OH5
6	A	20	1PE	OH6-C15-C25-OH5
6	J	45	1PE	C14-C24-OH4-C13
6	E	8	1PE	OH4-C13-C23-OH3
6	A	19	1PE	OH5-C14-C24-OH4
4	H	1003	BEY	C2-C1-C7-C8
6	I	21	1PE	OH6-C15-C25-OH5
4	A	1003	BEY	C1-C7-C8-C9
4	G	1003	BEY	C1-C7-C8-C9
6	B	60	1PE	OH5-C14-C24-OH4

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Mol	Chain	Res	Type	Atoms
6	K	42	1PE	OH5-C14-C24-OH4
6	K	5	1PE	OH5-C14-C24-OH4
6	B	61	1PE	C23-C13-OH4-C24
6	D	44	1PE	OH5-C14-C24-OH4
6	E	43	1PE	OH5-C14-C24-OH4
4	H	1003	BEY	C5-C1-C7-C8
6	K	5	1PE	C12-C22-OH3-C23
6	G	58	1PE	C12-C22-OH3-C23
6	H	65	1PE	OH5-C14-C24-OH4
6	D	9	1PE	OH4-C13-C23-OH3
6	D	44	1PE	C16-C26-OH6-C15
6	L	612	1PE	C12-C22-OH3-C23
6	J	45	1PE	C16-C26-OH6-C15
6	I	22	1PE	C15-C25-OH5-C14
6	J	3	1PE	OH7-C16-C26-OH6
4	D	1003	BEY	C2-C1-C7-C8
6	D	63	1PE	OH4-C13-C23-OH3
6	H	64	1PE	C12-C22-OH3-C23
6	D	9	1PE	C24-C14-OH5-C25
6	K	50	1PE	C24-C14-OH5-C25
6	D	44	1PE	C25-C15-OH6-C26
6	H	64	1PE	C24-C14-OH5-C25
6	J	3	1PE	C24-C14-OH5-C25
6	K	42	1PE	C14-C24-OH4-C13
6	A	20	1PE	OH5-C14-C24-OH4
6	K	42	1PE	C24-C14-OH5-C25
6	J	45	1PE	OH5-C14-C24-OH4
6	K	50	1PE	C14-C24-OH4-C13
6	F	33	1PE	C16-C26-OH6-C15
4	J	1003	BEY	C2-C1-C7-C8
6	L	612	1PE	C23-C13-OH4-C24
6	H	64	1PE	OH5-C14-C24-OH4
6	L	612	1PE	C24-C14-OH5-C25
4	H	1003	BEY	C1-C7-C8-C9
6	E	43	1PE	C14-C24-OH4-C13
6	C	18	1PE	C23-C13-OH4-C24
6	H	64	1PE	C14-C24-OH4-C13
6	B	61	1PE	C12-C22-OH3-C23
6	H	65	1PE	C13-C23-OH3-C22
6	L	612	1PE	OH4-C13-C23-OH3
6	E	612	1PE	C12-C22-OH3-C23
6	L	612	1PE	C15-C25-OH5-C14

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Mol	Chain	Res	Type	Atoms
6	B	61	1PE	C24-C14-OH5-C25
6	G	48	1PE	C24-C14-OH5-C25
4	D	1003	BEY	C5-C1-C7-C8
6	F	31	1PE	OH7-C16-C26-OH6
6	I	21	1PE	C25-C15-OH6-C26
6	B	61	1PE	C14-C24-OH4-C13
6	L	1	1PE	C25-C15-OH6-C26
4	L	1003	BEY	C17-C8-C9-O2
4	L	1003	BEY	C17-C8-C9-O1
6	G	58	1PE	C24-C14-OH5-C25
6	B	62	1PE	C24-C14-OH5-C25
6	K	5	1PE	C15-C25-OH5-C14
6	E	8	1PE	C24-C14-OH5-C25
4	B	1003	BEY	P-C17-C8-C7
4	F	1003	BEY	P-C17-C8-C7
4	K	1003	BEY	P-C17-C8-C7
6	F	33	1PE	OH6-C15-C25-OH5
4	A	1003	BEY	P-C17-C8-C9
4	K	1003	BEY	P-C17-C8-C9
4	L	1003	BEY	P-C17-C8-C9
6	A	20	1PE	C15-C25-OH5-C14
4	J	1003	BEY	C5-C1-C7-C8
6	G	58	1PE	C13-C23-OH3-C22
6	G	47	1PE	C15-C25-OH5-C14
6	K	4	1PE	C12-C22-OH3-C23
6	E	43	1PE	C24-C14-OH5-C25
6	F	31	1PE	C15-C25-OH5-C14
6	G	30	1PE	C15-C25-OH5-C14
6	C	17	1PE	C14-C24-OH4-C13
6	L	1	1PE	C24-C14-OH5-C25
6	B	60	1PE	C14-C24-OH4-C13
6	G	58	1PE	C16-C26-OH6-C15
6	L	56	1PE	C25-C15-OH6-C26
6	K	42	1PE	C25-C15-OH6-C26
6	K	42	1PE	OH6-C15-C25-OH5
4	D	1003	BEY	C18-C15-C16-C10
4	K	1003	BEY	C18-C15-C16-C10
6	I	21	1PE	C14-C24-OH4-C13
6	G	58	1PE	OH6-C15-C25-OH5
6	I	21	1PE	C15-C25-OH5-C14
6	B	60	1PE	C13-C23-OH3-C22
4	D	1003	BEY	C18-C15-C16-C13

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Mol	Chain	Res	Type	Atoms
6	L	612	1PE	C14-C24-OH4-C13
6	G	12	1PE	C23-C13-OH4-C24
4	C	1003	BEY	C18-C15-C16-C10
6	I	21	1PE	C13-C23-OH3-C22
4	I	1003	BEY	C18-C15-C16-C10
6	L	56	1PE	C24-C14-OH5-C25
4	A	1003	BEY	C18-C15-C16-C10
4	H	1003	BEY	C18-C15-C16-C10
4	E	1003	BEY	C18-C15-C16-C10
4	I	1003	BEY	C18-C15-C16-C13
6	D	67	1PE	C24-C14-OH5-C25
4	K	1003	BEY	C18-C15-C16-C13
4	E	1003	BEY	C18-C15-C16-C13
4	A	1003	BEY	C18-C15-C16-C13
4	C	1003	BEY	C18-C15-C16-C13
4	H	1003	BEY	C18-C15-C16-C13
6	J	2	1PE	C15-C25-OH5-C14
6	I	66	1PE	C24-C14-OH5-C25
6	J	45	1PE	C25-C15-OH6-C26
6	J	2	1PE	C25-C15-OH6-C26
6	B	60	1PE	C12-C22-OH3-C23
6	C	18	1PE	C12-C22-OH3-C23
6	F	32	1PE	C25-C15-OH6-C26
6	F	32	1PE	OH5-C14-C24-OH4
6	C	17	1PE	C25-C15-OH6-C26
4	L	1003	BEY	C18-C15-C16-C10
6	I	21	1PE	C12-C22-OH3-C23
4	L	1003	BEY	C18-C15-C16-C13
6	L	1	1PE	C16-C26-OH6-C15
6	B	62	1PE	C23-C13-OH4-C24
4	B	1003	BEY	C18-C15-C16-C13
6	I	22	1PE	C14-C24-OH4-C13
6	F	33	1PE	OH5-C14-C24-OH4
6	G	12	1PE	C24-C14-OH5-C25
6	K	50	1PE	OH5-C14-C24-OH4
4	B	1003	BEY	C18-C15-C16-C10
4	C	1003	BEY	C1-C7-C8-C17
4	F	1003	BEY	C1-C7-C8-C17
6	I	66	1PE	OH5-C14-C24-OH4
6	J	3	1PE	C15-C25-OH5-C14
6	I	21	1PE	OH4-C13-C23-OH3
6	L	56	1PE	C15-C25-OH5-C14

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Mol	Chain	Res	Type	Atoms
6	H	64	1PE	OH4-C13-C23-OH3
4	A	1003	BEY	C15-C18-C19-N
6	L	1	1PE	OH7-C16-C26-OH6
4	A	1003	BEY	P-C17-C8-C7
4	E	1003	BEY	P-C17-C8-C7
4	J	1003	BEY	P-C17-C8-C7
4	J	1003	BEY	C18-C15-C16-C10

There are no ring outliers.

49 monomers are involved in 102 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1003	BEY	6	0
6	G	47	1PE	1	0
5	J	18	SO4	1	0
2	K	1002	CO3	2	0
6	E	43	1PE	2	0
6	K	50	1PE	1	0
6	G	30	1PE	1	0
2	H	1002	CO3	1	0
4	A	1003	BEY	4	0
4	F	1003	BEY	2	0
4	L	1003	BEY	2	0
2	I	1002	CO3	1	0
6	I	21	1PE	5	0
4	J	1003	BEY	3	0
4	I	1003	BEY	2	0
6	B	61	1PE	2	0
5	I	17	SO4	1	0
6	H	65	1PE	1	0
6	F	31	1PE	1	0
2	J	1002	CO3	1	0
4	C	1003	BEY	5	0
4	E	1003	BEY	2	0
5	J	20	SO4	1	0
6	D	44	1PE	4	0
6	I	22	1PE	1	0
6	J	2	1PE	2	0
5	E	7	SO4	2	0
6	J	45	1PE	2	0
6	E	612	1PE	2	0
4	B	1003	BEY	3	0

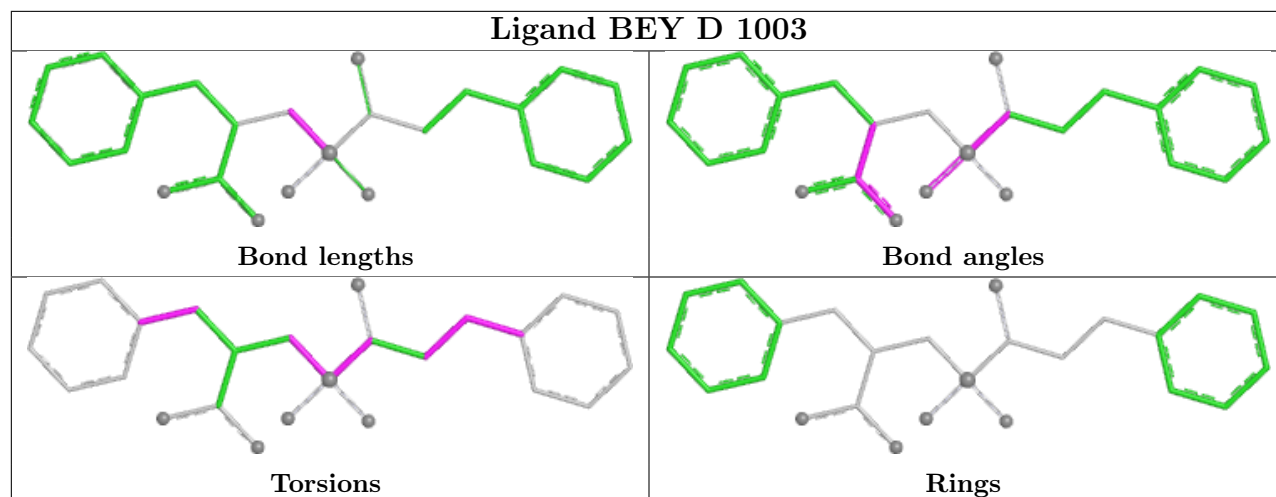
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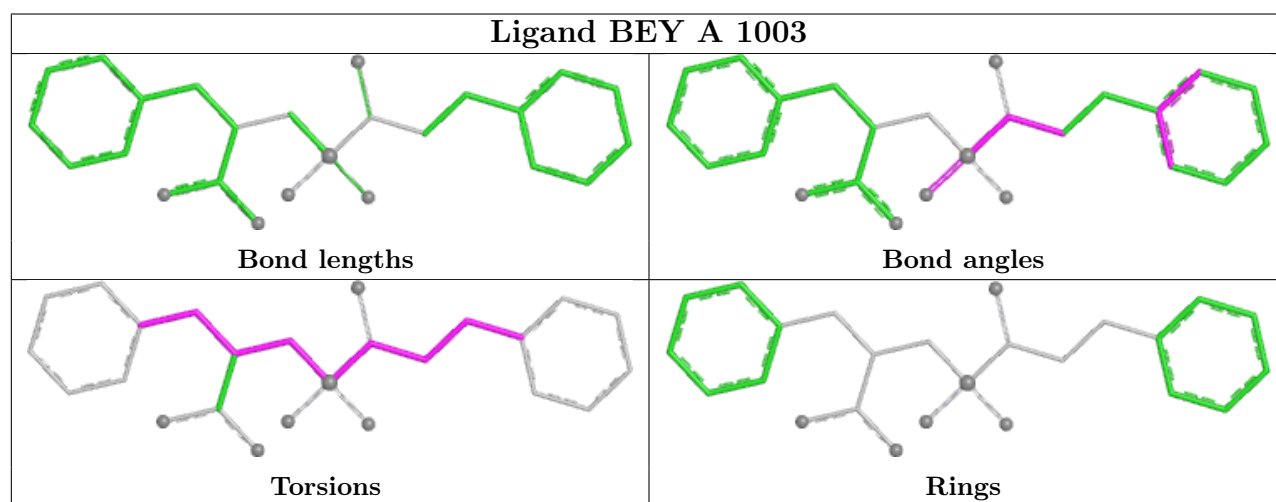
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1003	BEY	3	0
6	A	20	1PE	2	0
6	K	42	1PE	3	0
6	G	58	1PE	2	0
2	D	1002	CO3	2	0
5	C	3	SO4	1	0
2	L	1002	CO3	1	0
6	B	60	1PE	1	0
4	K	1003	BEY	3	0
6	J	3	1PE	5	0
5	E	22	SO4	1	0
6	K	4	1PE	1	0
6	L	612	1PE	3	0
6	D	63	1PE	1	0
4	H	1003	BEY	7	0
6	K	5	1PE	3	0
6	L	1	1PE	2	0
5	F	21	SO4	1	0
6	C	17	1PE	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

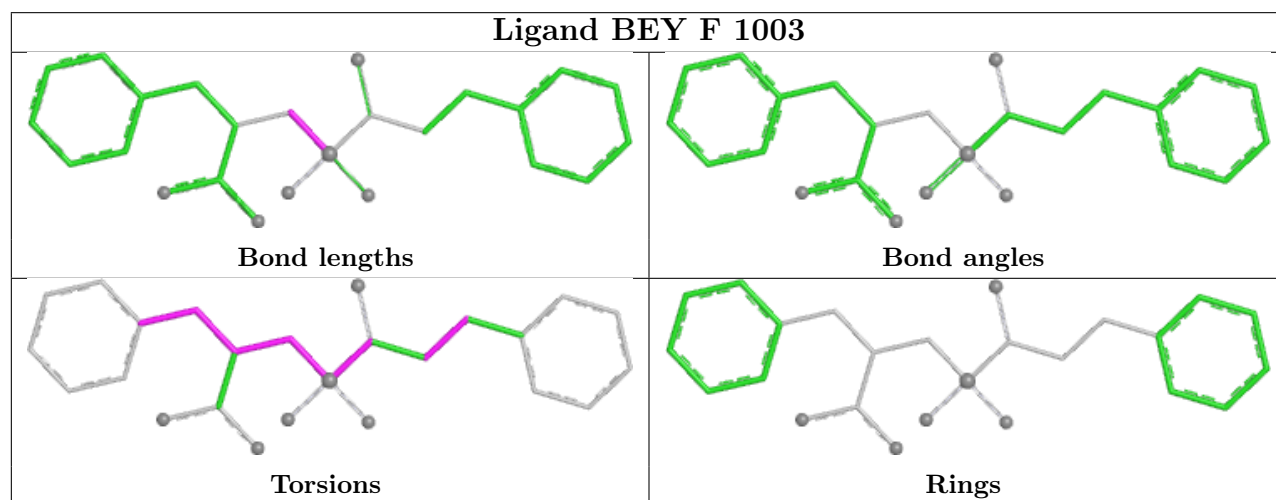
Ligand BEY D 1003

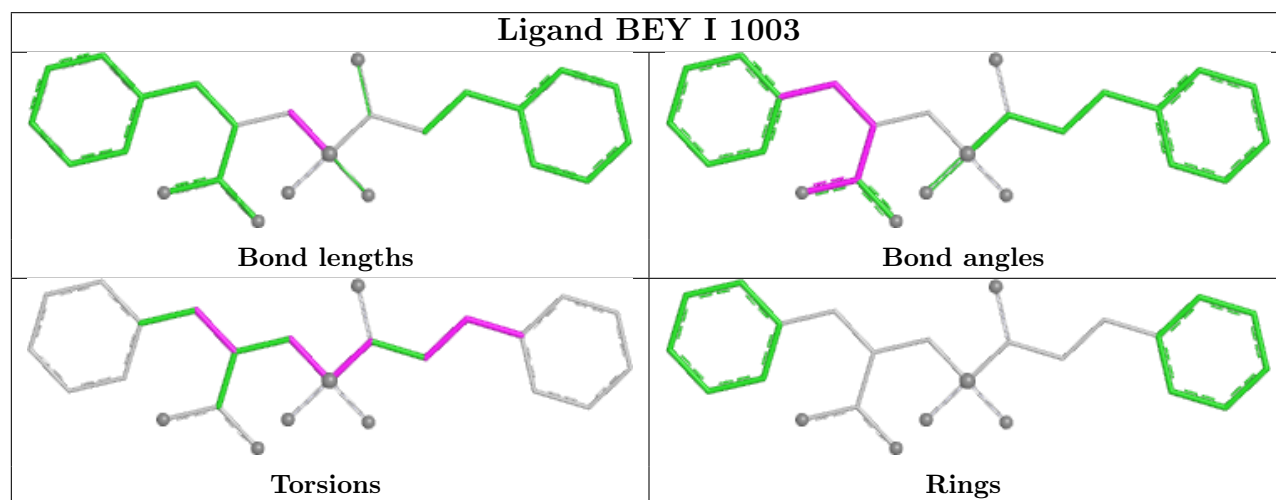
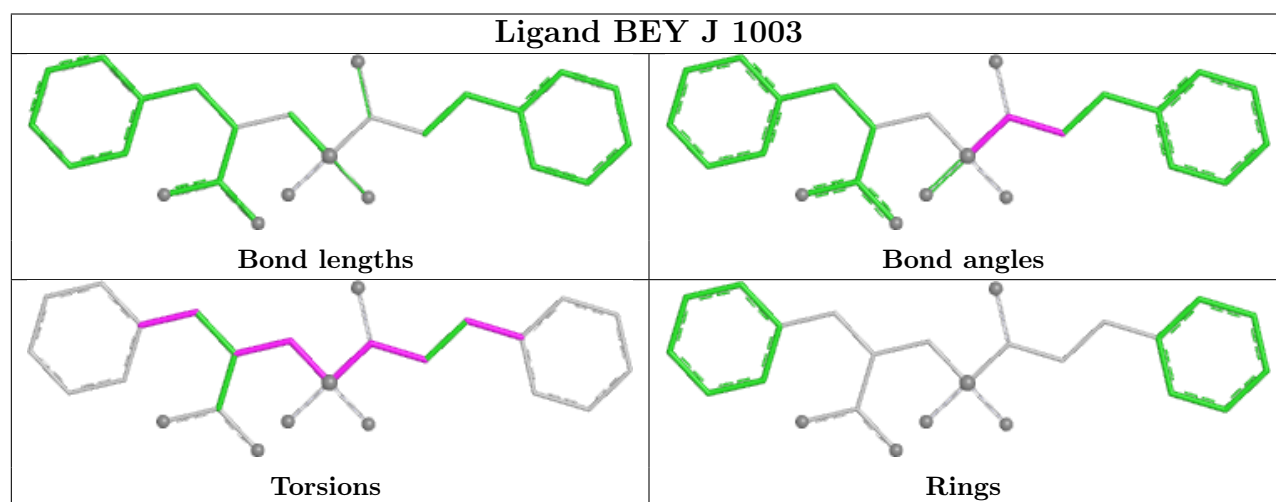
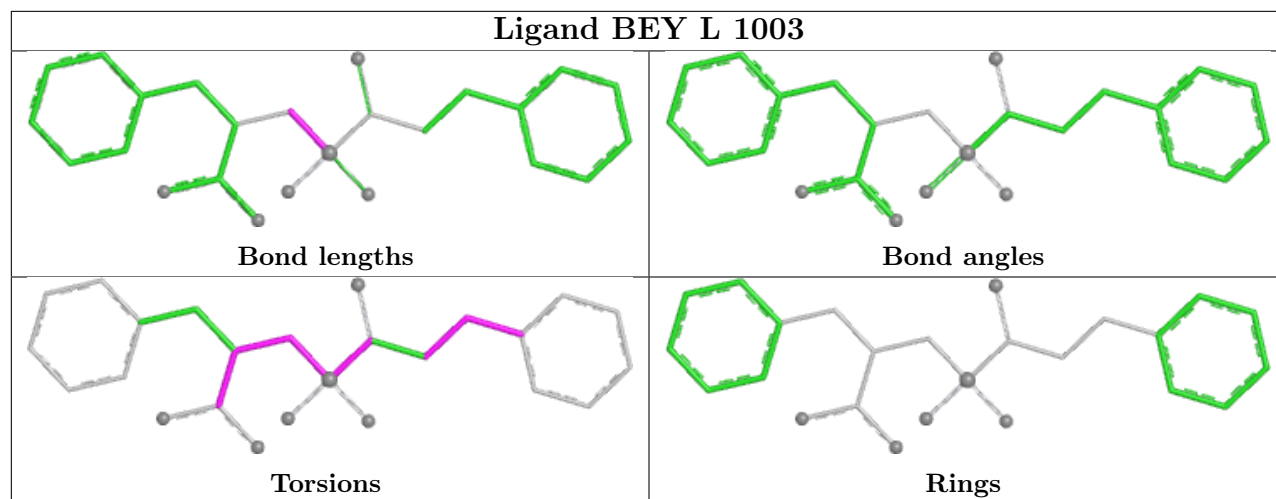


Ligand BEY A 1003

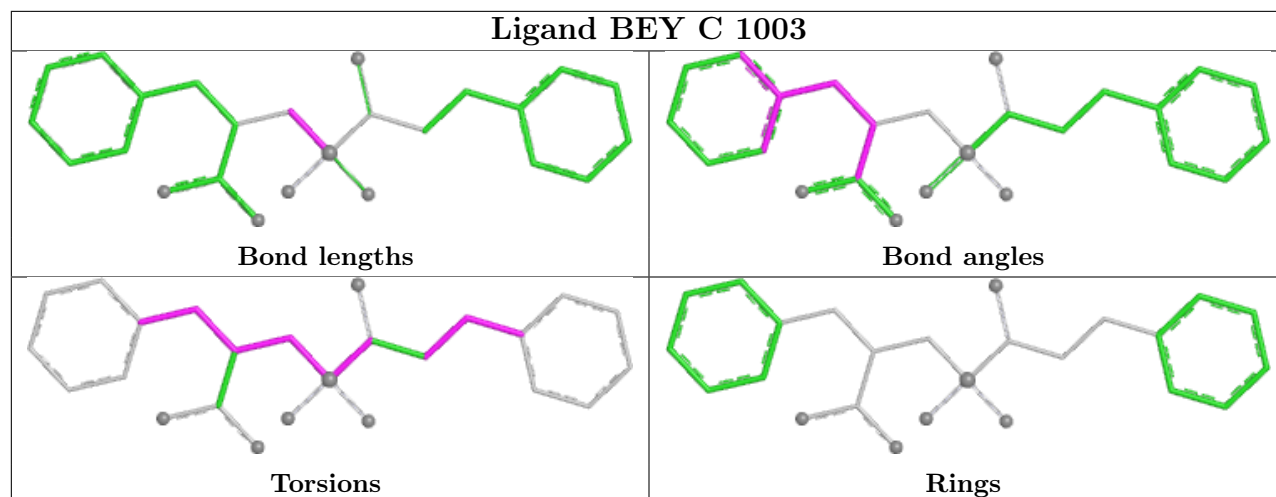


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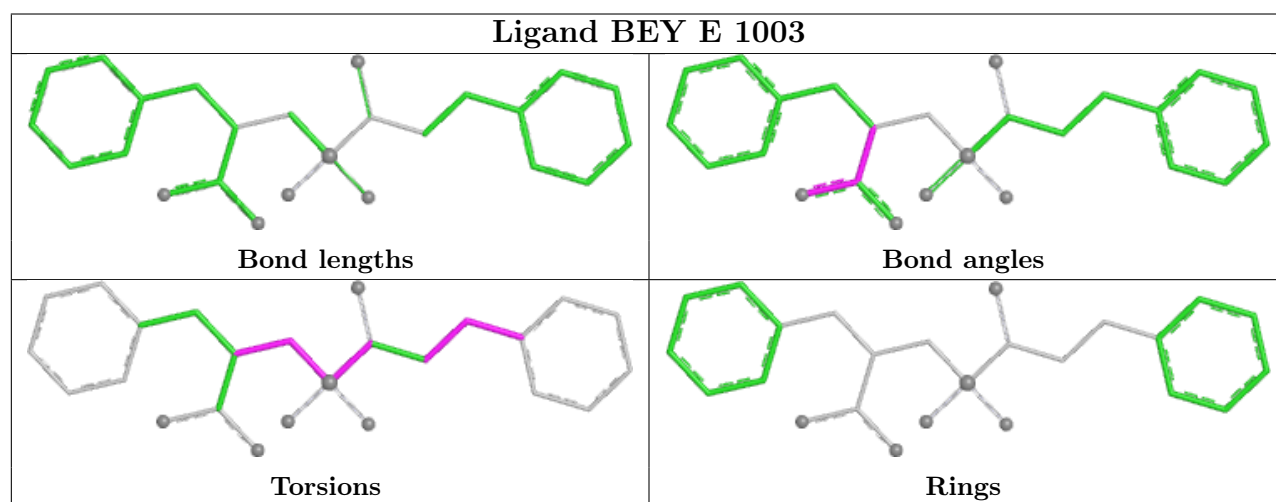




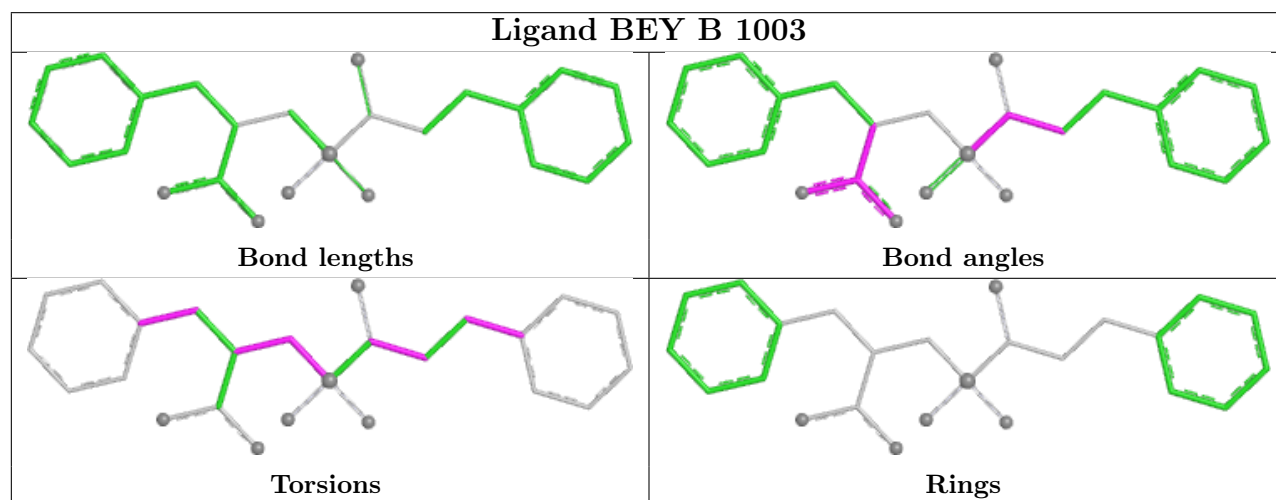
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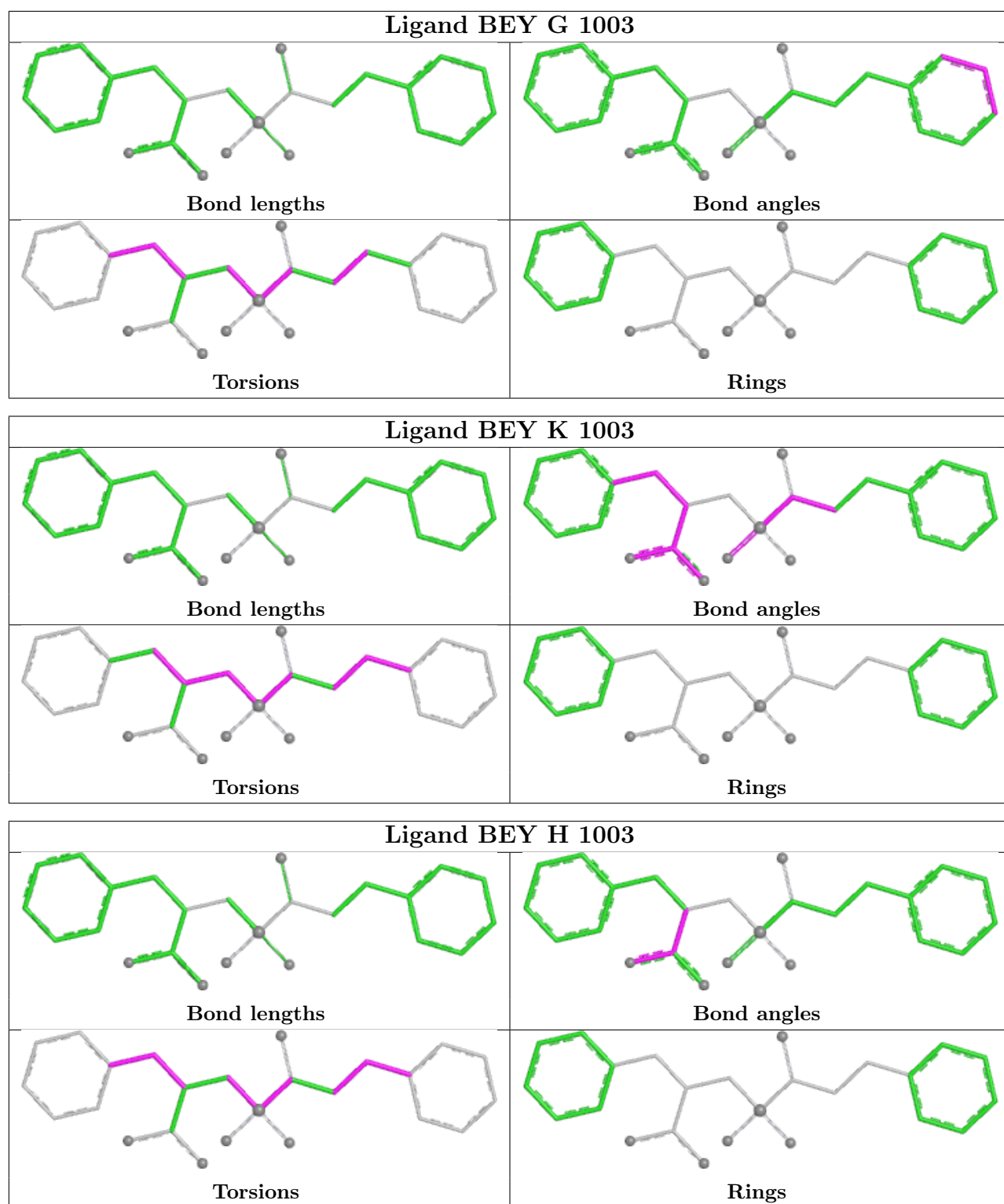


Ligand BEY E 1003



Ligand BEY B 1003





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	518/528 (98%)	-0.02	5 (0%) 79 81	13, 25, 45, 61	1 (0%)
1	B	518/528 (98%)	0.23	12 (2%) 61 62	13, 29, 64, 77	0
1	C	518/528 (98%)	0.02	4 (0%) 82 85	11, 26, 49, 59	0
1	D	513/528 (97%)	-0.04	5 (0%) 79 81	15, 25, 44, 66	0
1	E	510/528 (96%)	-0.06	4 (0%) 82 85	11, 24, 40, 59	0
1	F	510/528 (96%)	0.30	15 (2%) 53 55	18, 30, 60, 72	0
1	G	516/528 (97%)	0.01	3 (0%) 85 88	13, 25, 44, 62	0
1	H	509/528 (96%)	0.18	14 (2%) 55 56	14, 28, 60, 72	0
1	I	518/528 (98%)	0.03	4 (0%) 82 85	15, 26, 52, 64	0
1	J	513/528 (97%)	0.04	6 (1%) 76 78	12, 25, 46, 69	0
1	K	509/528 (96%)	-0.07	3 (0%) 85 88	13, 24, 42, 58	0
1	L	513/528 (97%)	0.15	8 (1%) 70 72	16, 28, 55, 63	0
All	All	6165/6336 (97%)	0.06	83 (1%) 75 76	11, 26, 53, 77	1 (0%)

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	260	ASN	5.7
1	B	259	VAL	4.7
1	G	183	ASN	4.3
1	F	362	LYS	4.3
1	F	363	GLY	3.9
1	A	364	ASP	3.8
1	L	605	LEU	3.3
1	K	161	ASN	3.1
1	D	603	ASP	3.0
1	E	602	ASN	2.9
1	D	219	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	603	ASP	2.9
1	B	198	LEU	2.9
1	F	156	PHE	2.9
1	H	178	PHE	2.9
1	B	257	LYS	2.9
1	F	603	ASP	2.9
1	F	152	GLN	2.8
1	G	364	ASP	2.8
1	J	183	ASN	2.8
1	B	258	ASN	2.8
1	B	196	ALA	2.8
1	B	197	ASP	2.8
1	B	364	ASP	2.7
1	K	603	ASP	2.7
1	A	603	ASP	2.7
1	H	364	ASP	2.7
1	I	196	ALA	2.7
1	B	549	SER	2.6
1	F	139	ASN	2.6
1	L	104	ASN	2.6
1	J	603	ASP	2.6
1	L	140	GLY	2.6
1	I	195	VAL	2.6
1	F	549	SER	2.6
1	D	364	ASP	2.5
1	F	160	GLU	2.5
1	H	195	VAL	2.5
1	L	604	ALA	2.5
1	J	136	GLY	2.5
1	H	196	ALA	2.5
1	D	85	ALA	2.4
1	B	550	SER	2.4
1	E	456	GLY	2.4
1	F	364	ASP	2.4
1	H	549	SER	2.4
1	A	259	VAL	2.4
1	B	603	ASP	2.4
1	H	142	VAL	2.4
1	L	362	LYS	2.4
1	J	137	LYS	2.3
1	G	602	ASN	2.3
1	C	196	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	363	GLY	2.3
1	F	195	VAL	2.3
1	F	217	ASN	2.3
1	H	217	ASN	2.3
1	L	420	ASN	2.3
1	B	109	ASP	2.3
1	K	550	SER	2.2
1	H	109	ASP	2.2
1	C	260	ASN	2.2
1	F	196	ALA	2.2
1	H	194	SER	2.2
1	F	114	VAL	2.2
1	H	153	VAL	2.2
1	I	363	GLY	2.2
1	L	363	GLY	2.2
1	E	549	SER	2.2
1	L	165	PHE	2.1
1	E	217	ASN	2.1
1	H	104	ASN	2.1
1	A	498	SER	2.1
1	F	197	ASP	2.1
1	J	549	SER	2.1
1	C	602	ASN	2.1
1	H	550	SER	2.1
1	A	261	MET	2.1
1	D	261	MET	2.1
1	B	160	GLU	2.0
1	F	130	PHE	2.0
1	C	277	TYR	2.0
1	I	549	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	1PE	B	62	10/16	0.62	0.35	74,89,91,92	0
6	1PE	J	45	10/16	0.70	0.28	50,68,73,75	0
6	1PE	B	61	10/16	0.73	0.16	34,46,48,51	0
5	SO4	A	2	5/5	0.77	0.16	60,62,74,74	0
6	1PE	D	44	11/16	0.79	0.20	37,51,60,63	0
6	1PE	D	67	7/16	0.81	0.22	30,41,53,54	0
6	1PE	K	4	12/16	0.83	0.13	27,44,55,55	0
6	1PE	L	56	11/16	0.83	0.14	30,44,50,50	0
6	1PE	G	58	15/16	0.84	0.15	43,47,56,56	0
6	1PE	D	63	10/16	0.84	0.13	37,42,46,53	0
5	SO4	E	22	5/5	0.84	0.17	90,90,94,97	0
6	1PE	K	50	6/16	0.84	0.17	11,25,55,55	0
6	1PE	F	31	10/16	0.84	0.16	36,44,74,74	0
6	1PE	L	612	12/16	0.85	0.18	41,59,63,64	0
6	1PE	I	66	7/16	0.85	0.14	26,35,44,46	0
6	1PE	H	64	10/16	0.86	0.16	43,47,52,53	0
6	1PE	I	22	11/16	0.86	0.17	30,47,62,67	0
5	SO4	A	24	5/5	0.87	0.13	53,57,63,64	0
6	1PE	F	33	10/16	0.87	0.15	33,61,63,64	0
6	1PE	K	42	11/16	0.87	0.13	30,44,49,51	0
6	1PE	D	9	10/16	0.88	0.14	27,38,45,48	0
6	1PE	A	20	12/16	0.88	0.15	49,54,58,58	0
6	1PE	B	60	10/16	0.88	0.17	33,48,74,75	0
5	SO4	J	20	5/5	0.88	0.24	72,74,78,81	0
5	SO4	L	25	5/5	0.88	0.14	68,71,75,76	0
6	1PE	J	3	10/16	0.88	0.12	33,50,53,54	0
6	1PE	E	43	8/16	0.89	0.14	43,45,55,55	0
5	SO4	K	19	5/5	0.89	0.25	71,71,76,77	0
5	SO4	F	21	5/5	0.89	0.12	69,70,71,75	0
6	1PE	C	17	13/16	0.89	0.12	15,36,43,43	0
6	1PE	C	18	9/16	0.89	0.12	27,36,38,45	0
6	1PE	H	65	10/16	0.89	0.14	42,49,54,55	0
6	1PE	I	21	15/16	0.89	0.12	25,34,53,54	0
6	1PE	E	612	12/16	0.89	0.12	31,46,54,55	0
6	1PE	G	30	7/16	0.90	0.12	24,39,53,57	0
5	SO4	D	5	5/5	0.90	0.14	92,94,97,97	0
6	1PE	A	19	9/16	0.91	0.10	20,25,34,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	1PE	G	12	9/16	0.91	0.11	20,25,41,44	0
5	SO4	A	1	5/5	0.91	0.14	61,62,66,66	0
6	1PE	F	32	10/16	0.91	0.09	33,42,45,46	0
6	1PE	K	5	12/16	0.92	0.10	23,35,52,53	0
5	SO4	G	26	5/5	0.93	0.28	30,30,30,30	0
4	BEY	D	1003	25/25	0.93	0.12	20,40,59,61	0
4	BEY	E	1003	25/25	0.93	0.12	22,42,59,61	0
4	BEY	F	1003	25/25	0.93	0.11	23,35,51,55	0
4	BEY	H	1003	25/25	0.93	0.10	26,38,46,50	0
4	BEY	K	1003	25/25	0.93	0.11	19,30,45,54	0
4	BEY	L	1003	25/25	0.93	0.14	36,57,69,71	0
6	1PE	J	2	11/16	0.93	0.11	12,25,44,48	0
2	CO3	F	1002	4/4	0.94	0.10	35,38,39,44	0
2	CO3	K	1002	4/4	0.94	0.12	25,30,31,37	0
4	BEY	I	1003	25/25	0.94	0.10	21,33,40,50	0
2	CO3	L	1002	4/4	0.94	0.08	27,27,28,33	0
2	CO3	A	1002	4/4	0.94	0.10	39,42,43,46	0
2	CO3	E	1002	4/4	0.94	0.08	31,33,34,34	0
6	1PE	G	47	6/16	0.95	0.08	15,22,28,39	0
6	1PE	E	8	12/16	0.95	0.11	18,34,63,63	0
4	BEY	C	1003	25/25	0.95	0.09	16,33,43,47	0
5	SO4	G	23	5/5	0.95	0.16	45,45,49,50	0
2	CO3	H	1002	4/4	0.95	0.07	15,23,23,28	0
4	BEY	J	1003	25/25	0.95	0.10	28,42,55,57	0
6	1PE	L	1	10/16	0.95	0.07	15,23,33,35	0
4	BEY	A	1003	25/25	0.95	0.11	17,33,63,65	0
4	BEY	B	1003	25/25	0.95	0.09	26,38,48,50	0
2	CO3	G	1002	4/4	0.96	0.09	19,20,22,26	0
2	CO3	C	1002	4/4	0.96	0.09	13,21,22,28	0
4	BEY	G	1003	25/25	0.96	0.09	13,29,59,61	0
6	1PE	G	48	6/16	0.96	0.07	16,22,26,26	0
2	CO3	J	1002	4/4	0.97	0.09	27,27,29,31	0
2	CO3	B	1002	4/4	0.98	0.06	11,14,16,19	0
2	CO3	D	1002	4/4	0.98	0.06	22,24,25,27	0
2	CO3	I	1002	4/4	0.98	0.06	18,19,22,23	0
3	ZN	C	1004	1/1	0.98	0.06	42,42,42,42	0
3	ZN	I	1004	1/1	0.98	0.06	35,35,35,35	0
3	ZN	L	1001	1/1	0.99	0.02	29,29,29,29	0
3	ZN	L	1004	1/1	0.99	0.04	39,39,39,39	0
3	ZN	B	1004	1/1	0.99	0.04	36,36,36,36	0
5	SO4	J	18	5/5	0.99	0.05	22,28,36,37	0
3	ZN	C	1001	1/1	0.99	0.02	26,26,26,26	0

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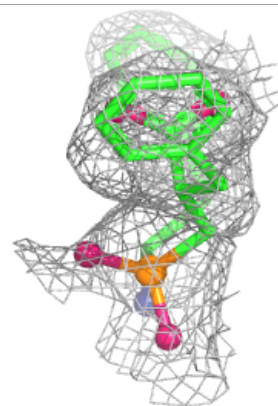
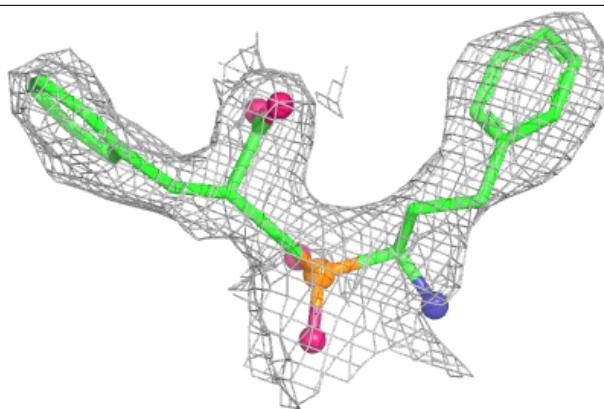
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	A	1004	1/1	0.99	0.03	37,37,37,37	0
3	ZN	D	1001	1/1	0.99	0.03	41,41,41,41	0
3	ZN	D	1004	1/1	0.99	0.03	39,39,39,39	0
3	ZN	E	1001	1/1	0.99	0.02	30,30,30,30	0
3	ZN	E	1004	1/1	0.99	0.05	45,45,45,45	0
3	ZN	F	1001	1/1	0.99	0.03	29,29,29,29	0
3	ZN	F	1004	1/1	0.99	0.03	37,37,37,37	0
3	ZN	G	1001	1/1	0.99	0.02	28,28,28,28	0
3	ZN	G	1004	1/1	0.99	0.03	35,35,35,35	0
3	ZN	H	1001	1/1	0.99	0.02	39,39,39,39	0
3	ZN	H	1004	1/1	0.99	0.05	32,32,32,32	0
3	ZN	A	1001	1/1	0.99	0.02	30,30,30,30	0
3	ZN	I	1001	1/1	0.99	0.01	26,26,26,26	0
5	SO4	C	3	5/5	0.99	0.06	17,18,25,26	0
3	ZN	J	1004	1/1	0.99	0.04	46,46,46,46	0
5	SO4	E	7	5/5	0.99	0.05	16,24,35,37	0
3	ZN	K	1004	1/1	0.99	0.05	39,39,39,39	0
3	ZN	K	1001	1/1	1.00	0.03	23,23,23,23	0
3	ZN	J	1001	1/1	1.00	0.02	39,39,39,39	0
5	SO4	I	17	5/5	1.00	0.02	8,10,15,22	0
3	ZN	B	1001	1/1	1.00	0.02	35,35,35,35	0

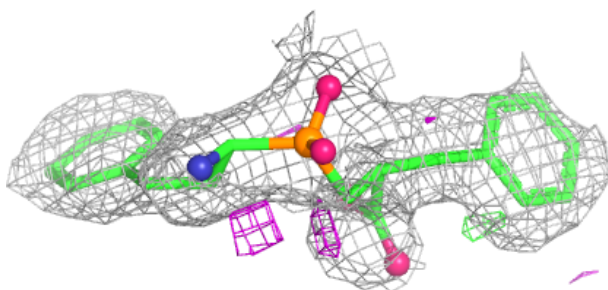
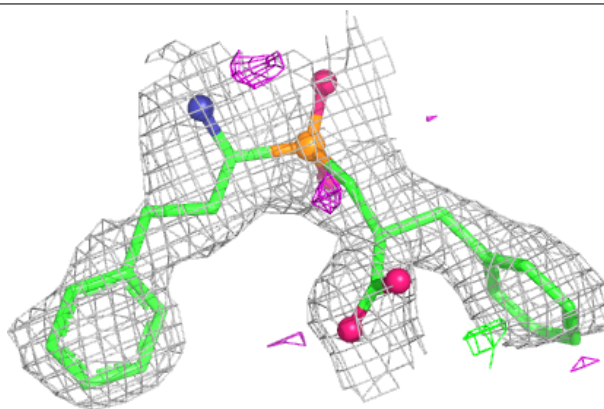
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around BEY D 1003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

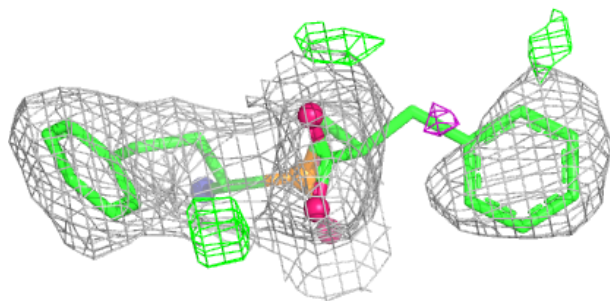
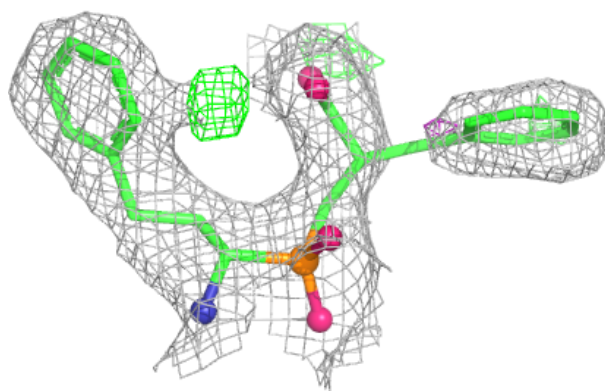
**Electron density around BEY E 1003:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



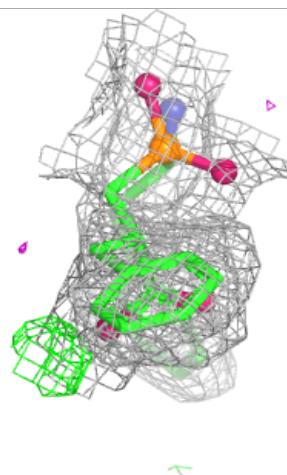
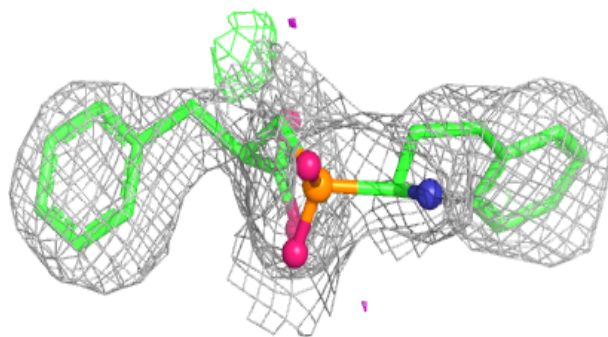
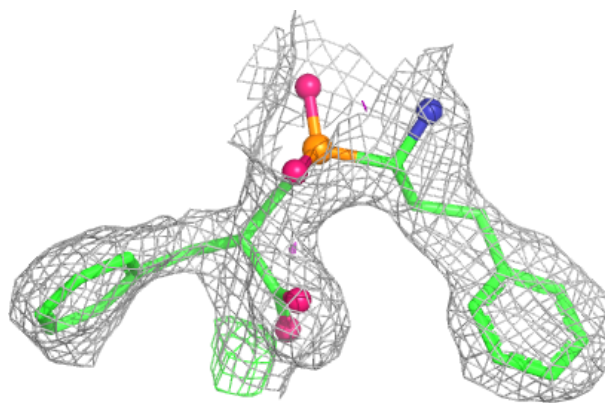
Electron density around BEY F 1003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



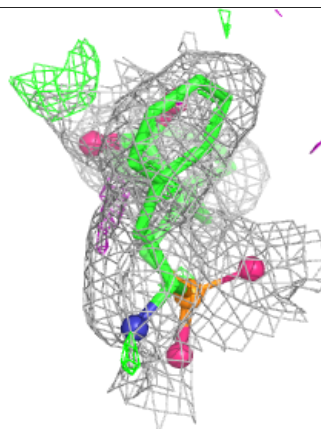
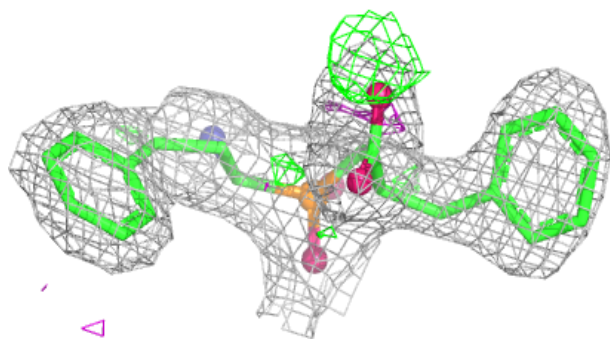
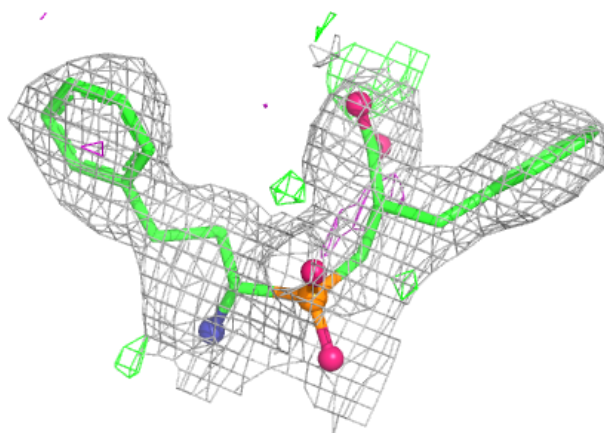
Electron density around BEY H 1003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



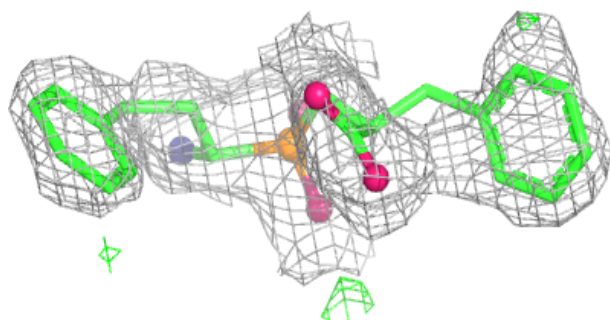
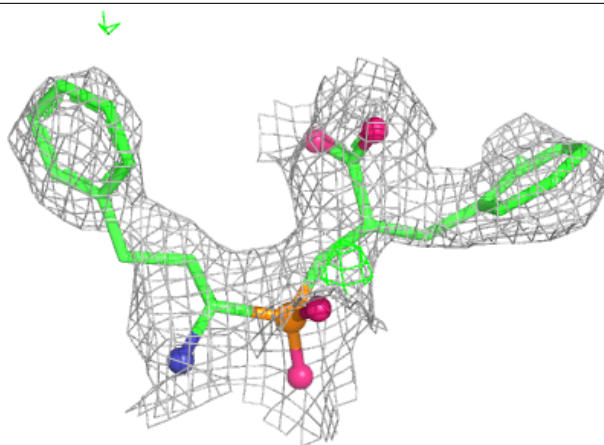
Electron density around BEY K 1003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

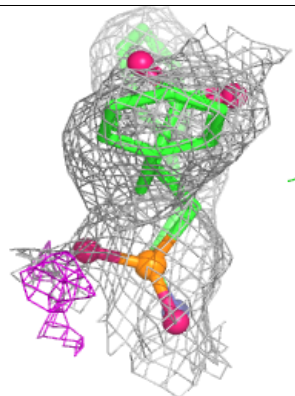
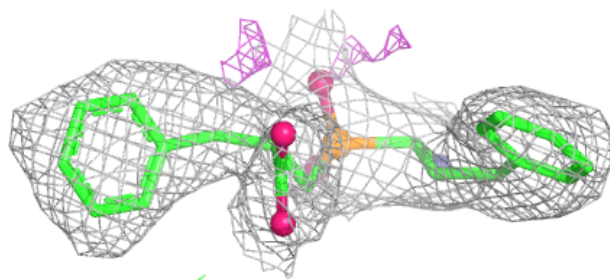
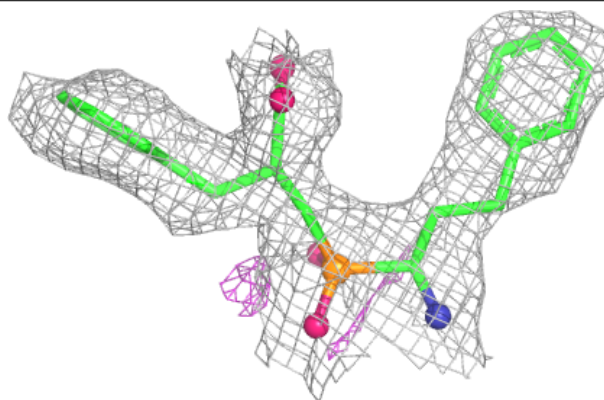


Electron density around BEY L 1003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

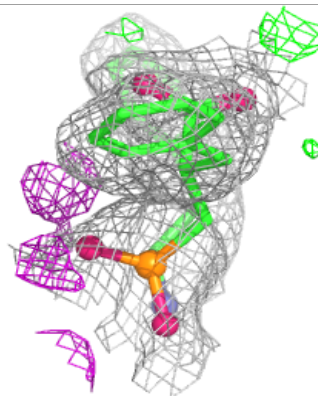
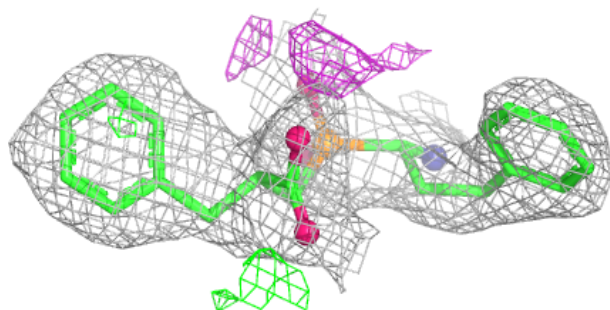
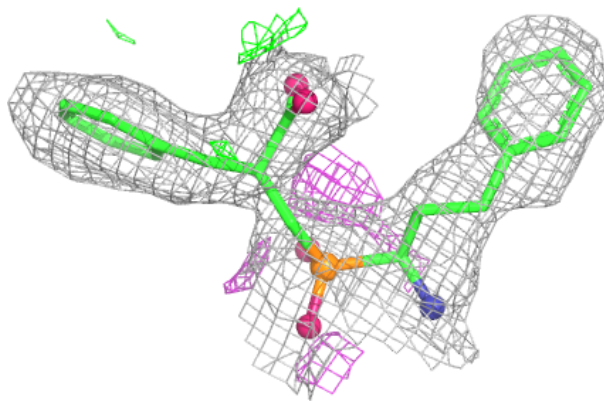
**Electron density around BEY I 1003:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

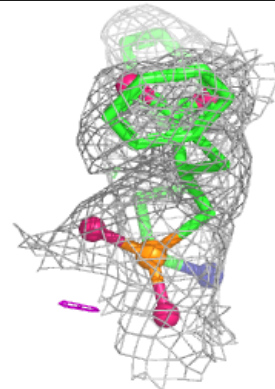
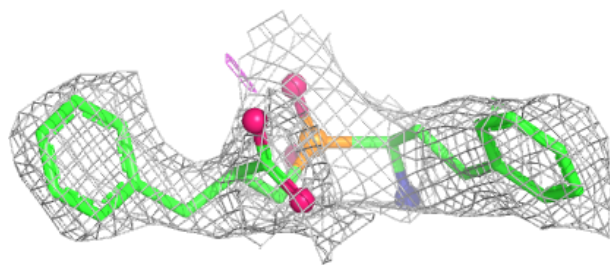
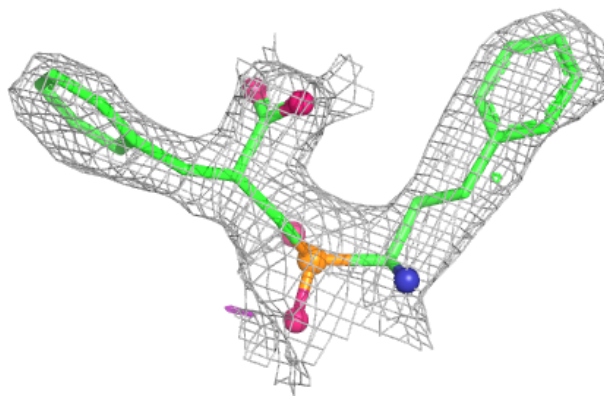


Electron density around BEY C 1003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

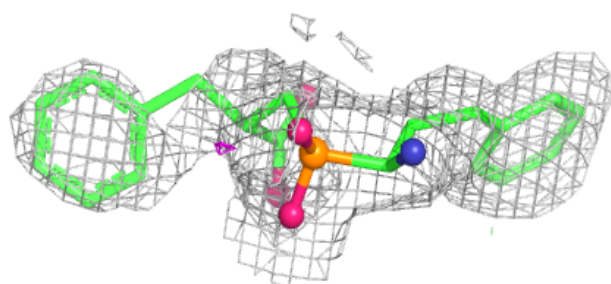
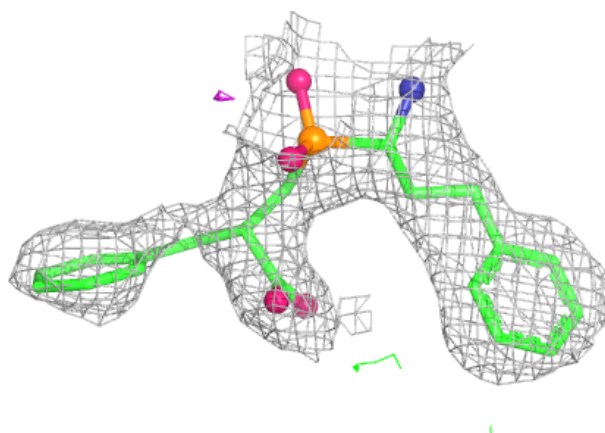
**Electron density around BEY J 1003:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

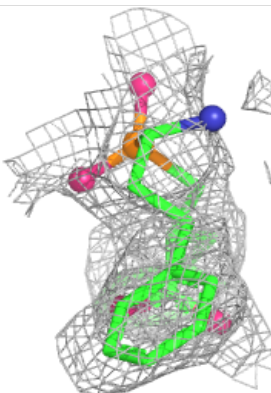
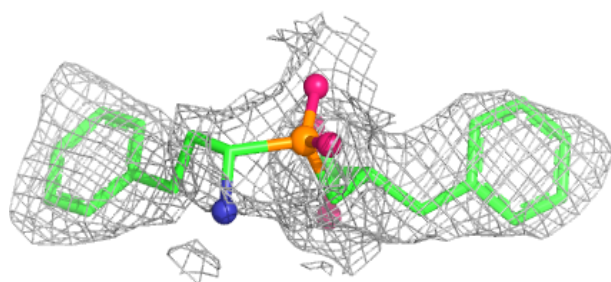
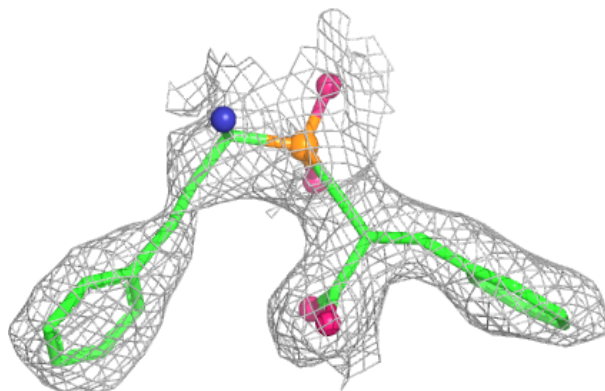


Electron density around BEY A 1003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

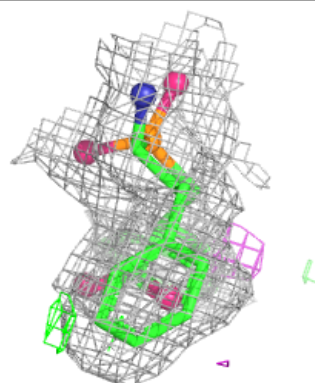
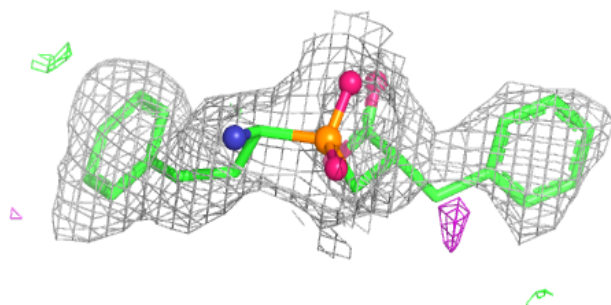
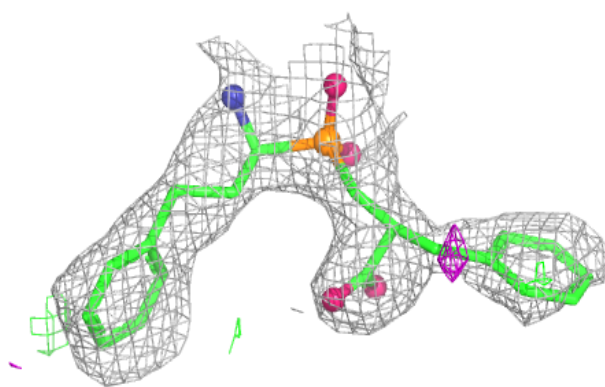
**Electron density around BEY B 1003:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around BEY G 1003:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.