



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 04:28 AM UTC

PDB ID : 4RKD / pdb_00004rkd
Title : Psychrophilic aromatic amino acids aminotransferase from Psychrobacter sp.
B6 cocrystalized with aspartic acid
Authors : Bujacz, A.; Rutkiewicz-Krotewicz, M.; Bujacz, G.; Nowakowska-Sapota, K.;
Turkiewicz, M.
Deposited on : 2014-10-12
Resolution : 2.76 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

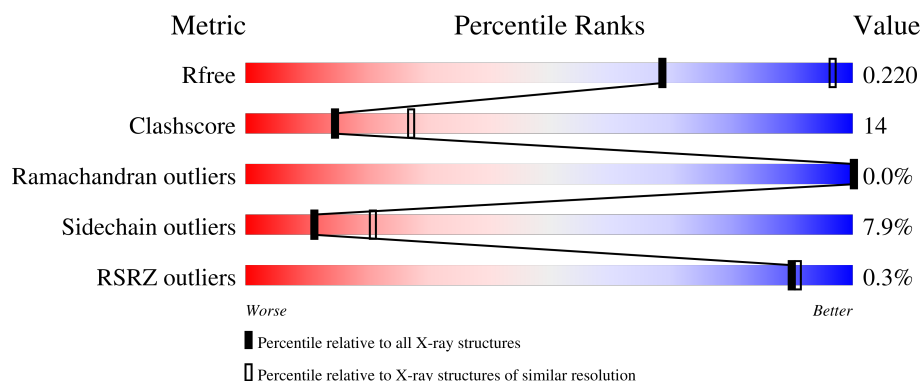
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.76 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	398	% 67% 29% .
1	B	398	% 67% 29% .
1	C	398	67% 28% 5%
1	D	398	63% 33% .

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Mol	Chain	Length	Quality of chain
1	E	398	 % 66% 30% •
1	F	398	 73% 23% •
1	G	398	 63% 33% •
1	H	398	 75% 22% •

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
3	PLP	B	401	-	X	-	-
4	KET	E	404[B]	-	-	X	-
6	PMP	D	401	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 25951 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.

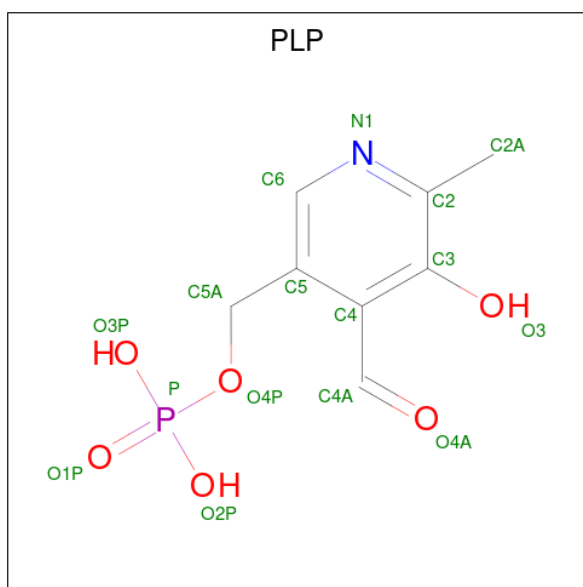
- Molecule 1 is a protein called Aromatic amino acid aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	S	0	2	0
			3115	1981	520	592	22			
1	B	398	Total	C	N	O	S	0	5	0
			3137	1994	524	597	22			
1	C	398	Total	C	N	O	S	0	2	0
			3110	1977	516	595	22			
1	D	398	Total	C	N	O	S	0	0	0
			3101	1971	516	592	22			
1	E	398	Total	C	N	O	S	0	3	0
			3121	1985	520	594	22			
1	F	398	Total	C	N	O	S	0	3	0
			3118	1981	517	598	22			
1	G	398	Total	C	N	O	S	0	2	0
			3117	1981	522	592	22			
1	H	398	Total	C	N	O	S	0	2	0
			3113	1979	518	594	22			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

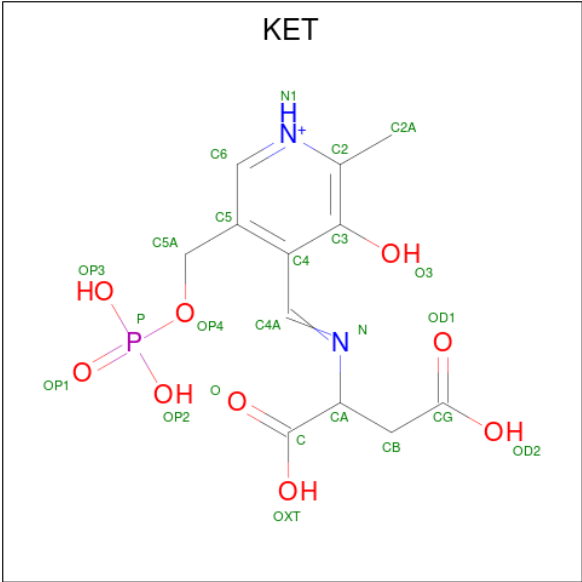
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	E	1	Total	Mg	0	0
			1	1		
2	G	1	Total	Mg	0	0
			1	1		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



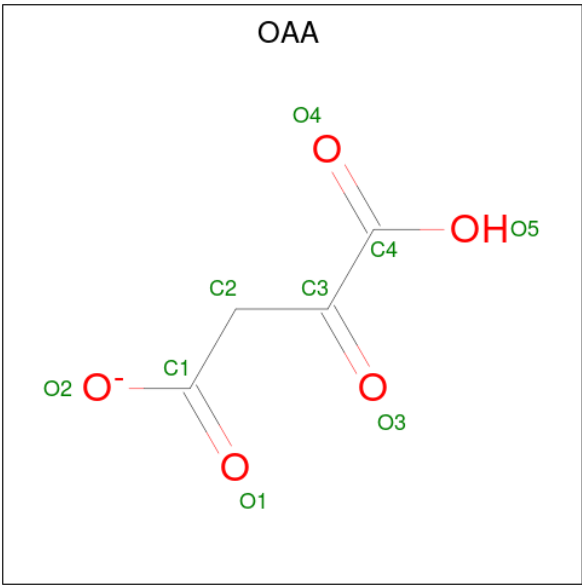
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	1
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	E	1	Total	C	N	O	P	0	1
			15	8	1	5	1		
3	F	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 4 is 2-[(3-HYDROXY-2-METHYL-5-PHOSPHONOXYMETHYL-PYRIDIN-4-YLMETHYLENE)-AMINO]-SUCCINIC ACID (CCD ID: KET) (formula: C₁₂H₁₆N₂O₉P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	1
			24	12	2	9	1		
4	E	1	Total	C	N	O	P	0	1
			24	12	2	9	1		
4	G	1	Total	C	N	O	P	0	0
			24	12	2	9	1		

- Molecule 5 is OXALOACETATE ION (CCD ID: OAA) (formula: C₄H₃O₅).



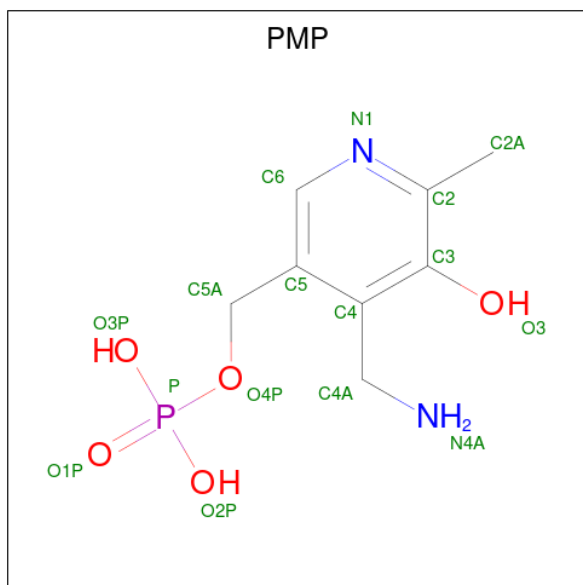
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			9	4	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	C	O	0	0
			9	4	5		

- Molecule 6 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (CCD ID: PMP) (formula: $C_8H_{13}N_2O_5P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	D	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
6	H	1	Total	C	N	O	P	0	0
			16	8	2	5	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	102	Total	O	0	0
			102	102		
7	B	142	Total	O	0	0
			142	142		
7	C	83	Total	O	0	0
			83	83		
7	D	119	Total	O	0	0
			119	119		
7	E	84	Total	O	0	0
			84	84		
7	F	96	Total	O	0	0
			96	96		

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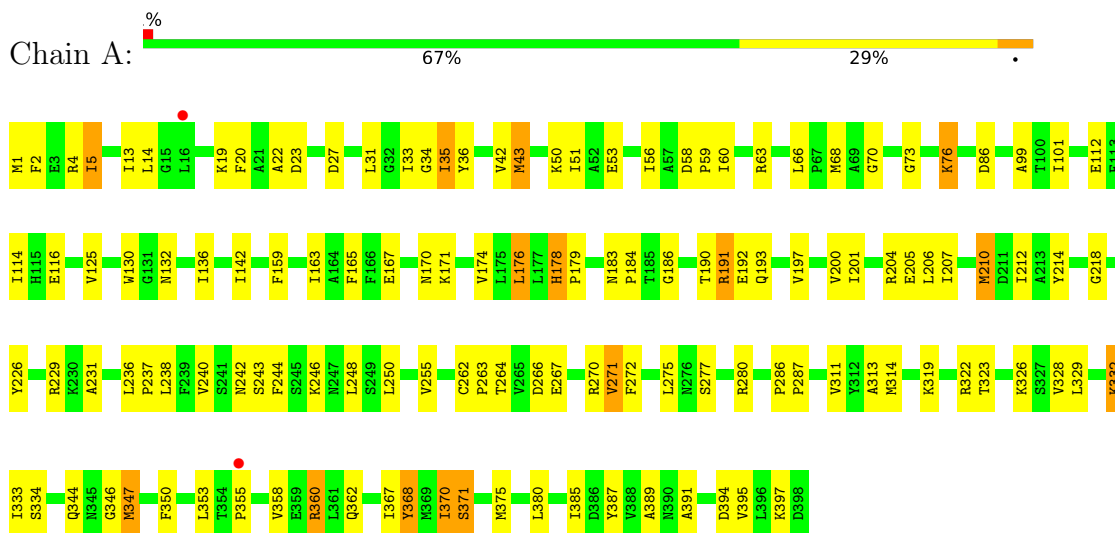
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	70	Total 70	O 70	0	0
7	H	122	Total 122	O 122	0	0

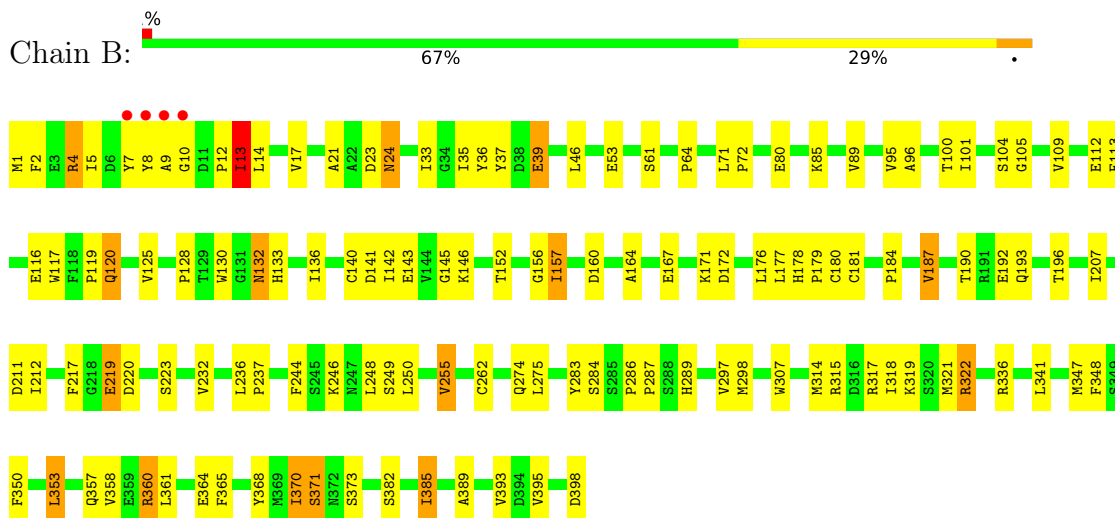
3 Residue-property plots

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: Aromatic amino acid aminotransferase

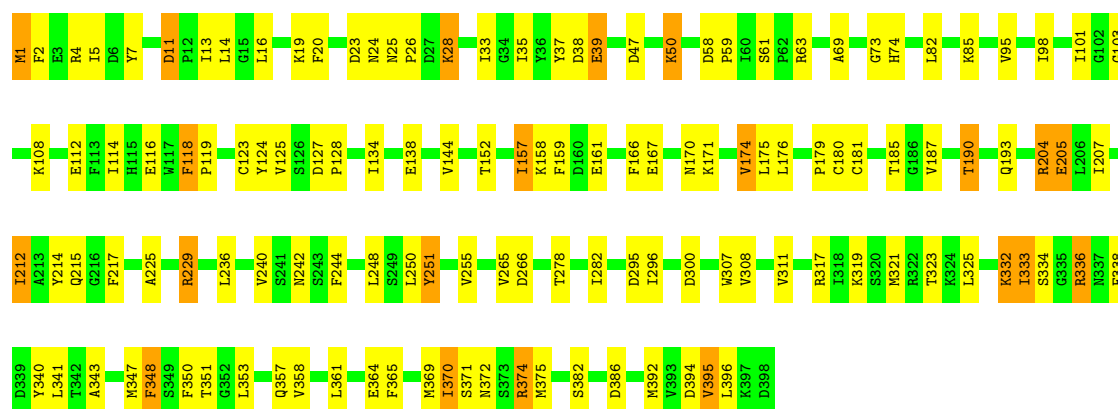


- Molecule 1: Aromatic amino acid aminotransferase



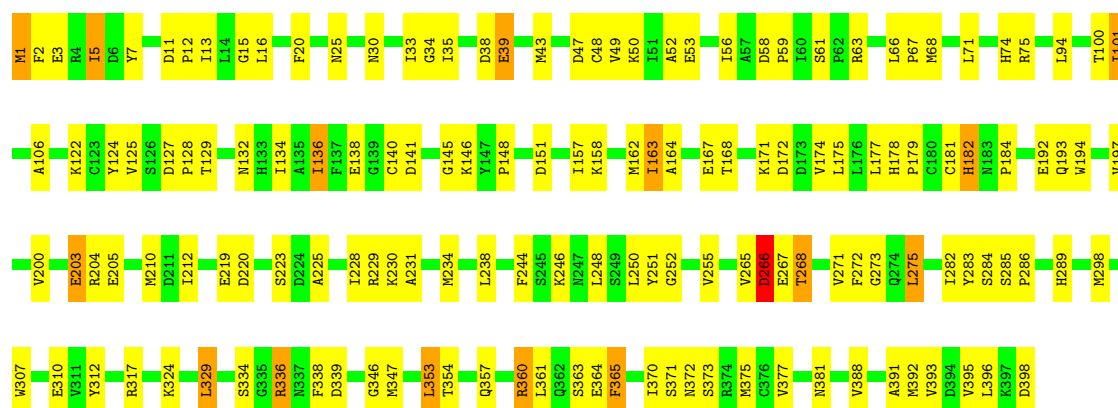
- Molecule 1: Aromatic amino acid aminotransferase





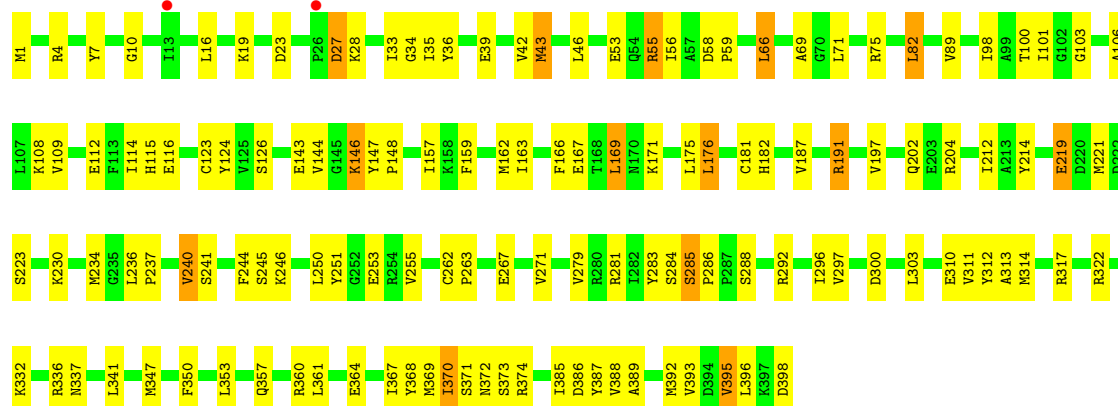
- Molecule 1: Aromatic amino acid aminotransferase

Chain D: 63% 33% .



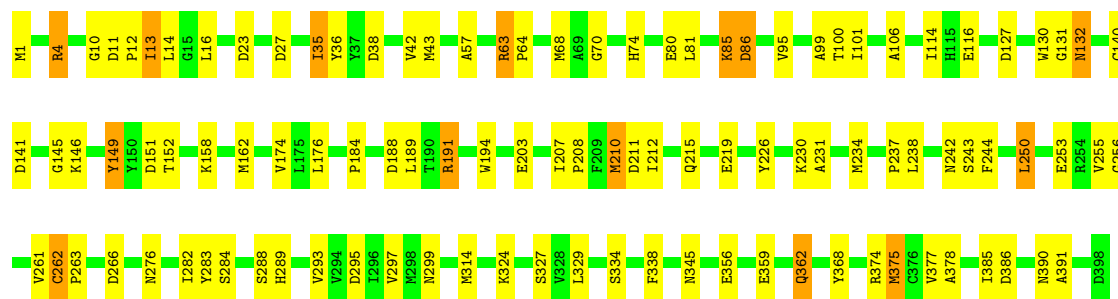
- Molecule 1: Aromatic amino acid aminotransferase

Chain E: 66% 30% .



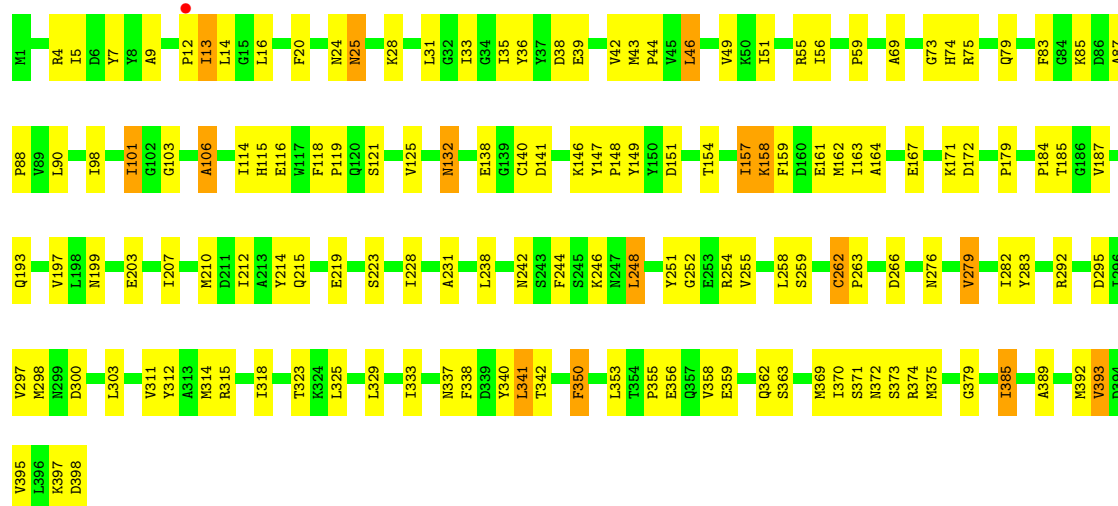
- Molecule 1: Aromatic amino acid aminotransferase

Chain F: 73% 23% .



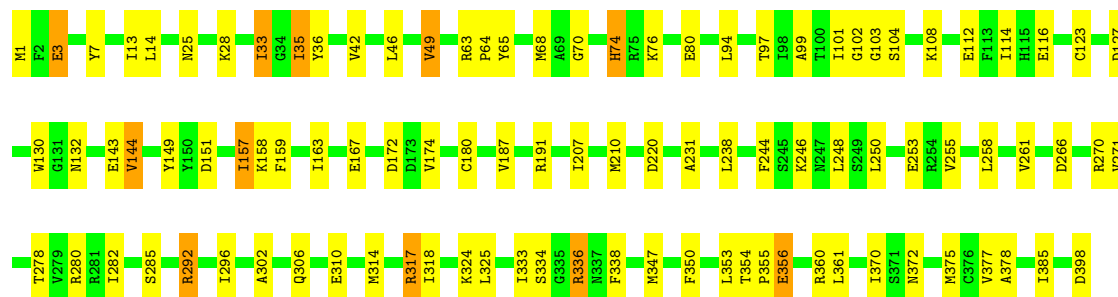
• Molecule 1: Aromatic amino acid aminotransferase

Chain G: 63% 33% .



• Molecule 1: Aromatic amino acid aminotransferase

Chain H: 75% 22% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.25Å 103.23Å 165.78Å 90.00° 98.58° 90.00°	Depositor
Resolution (Å)	45.74 – 2.76 45.74 – 2.76	Depositor EDS
% Data completeness (in resolution range)	97.4 (45.74-2.76) 97.4 (45.74-2.76)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.77Å)	Xtrriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.173 , 0.222 0.173 , 0.220	Depositor DCC
R_{free} test set	3862 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	31.5	Xtrriage
Anisotropy	0.094	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	25951	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.05 % 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 1.8670e-04. 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: PLP, PMP, KET, MG, OAA

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	1.09	0/3190	1.36	22/4321 (0.5%)
1	B	1.22	5/3218 (0.2%)	1.38	16/4358 (0.4%)
1	C	1.09	2/3185 (0.1%)	1.32	15/4316 (0.3%)
1	D	1.26	3/3170 (0.1%)	1.41	24/4296 (0.6%)
1	E	1.11	1/3199 (0.0%)	1.32	18/4333 (0.4%)
1	F	1.14	0/3193	1.34	16/4328 (0.4%)
1	G	1.03	0/3192	1.30	18/4324 (0.4%)
1	H	1.16	1/3185 (0.0%)	1.31	12/4315 (0.3%)
All	All	1.14	12/25532 (0.0%)	1.34	141/34591 (0.4%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	322	ARG	CA-C	6.59	1.61	1.52
1	C	236	LEU	CA-C	6.14	1.60	1.53
1	E	240	VAL	CA-C	-5.84	1.45	1.52
1	H	302	ALA	CA-C	5.75	1.60	1.52
1	B	145	GLY	N-CA	5.64	1.50	1.44
1	B	142	ILE	N-CA	-5.42	1.40	1.46
1	B	96	ALA	CA-C	5.30	1.59	1.52
1	D	67	PRO	N-CA	5.22	1.53	1.47
1	B	156	GLY	N-CA	5.14	1.50	1.44
1	D	219	GLU	CA-CB	-5.07	1.47	1.53
1	D	182	HIS	N-CA	-5.03	1.39	1.46
1	C	138	GLU	CA-C	-5.01	1.45	1.52

All (141) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	285	SER	CA-C-N	11.94	128.26	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	285	SER	C-N-CA	11.94	128.26	119.66
1	D	285	SER	CA-C-N	9.54	126.53	119.66
1	D	285	SER	C-N-CA	9.54	126.53	119.66
1	A	43	MET	CA-C-N	-9.46	110.63	120.85
1	A	43	MET	C-N-CA	-9.46	110.63	120.85
1	H	103	GLY	N-CA-C	-8.36	103.29	113.99
1	H	334	SER	N-CA-C	8.23	120.25	111.28
1	G	25	ASN	CA-C-N	-7.83	111.73	119.64
1	G	25	ASN	C-N-CA	-7.83	111.73	119.64
1	B	262	CYS	CA-C-N	7.54	127.42	119.05
1	B	262	CYS	C-N-CA	7.54	127.42	119.05
1	D	266	ASP	N-CA-C	7.43	119.02	111.07
1	C	61	SER	CA-C-N	-7.22	112.89	120.03
1	C	61	SER	C-N-CA	-7.22	112.89	120.03
1	D	275	LEU	N-CA-C	-7.12	103.59	111.36
1	F	114	ILE	N-CA-C	-7.12	103.53	110.72
1	B	232	VAL	N-CA-C	-7.07	103.89	110.53
1	G	207	ILE	N-CA-C	6.99	114.47	107.55
1	B	348	PHE	N-CA-C	6.97	120.94	110.14
1	A	207	ILE	N-CA-C	6.93	115.53	107.77
1	D	122	LYS	N-CA-C	-6.86	99.51	110.14
1	H	248	LEU	N-CA-C	-6.74	104.95	113.72
1	D	61	SER	N-CA-C	6.67	119.14	110.40
1	D	372	ASN	N-CA-C	-6.53	105.18	113.02
1	D	63	ARG	CA-C-N	-6.50	113.97	120.21
1	D	63	ARG	C-N-CA	-6.50	113.97	120.21
1	G	106	ALA	N-CA-C	-6.46	104.32	111.36
1	G	262	CYS	CA-C-N	6.45	126.95	119.47
1	G	262	CYS	C-N-CA	6.45	126.95	119.47
1	B	207	ILE	N-CA-C	6.41	114.95	107.77
1	A	368	TYR	N-CA-C	6.39	119.14	108.73
1	G	252	GLY	N-CA-C	6.38	121.88	114.16
1	F	345	ASN	N-CA-C	6.30	119.45	109.50
1	A	231	ALA	N-CA-C	-6.26	103.99	111.69
1	D	94	LEU	N-CA-C	6.25	120.94	112.88
1	H	191	ARG	N-CA-C	-6.19	104.61	111.36
1	C	190	THR	N-CA-C	-6.13	101.70	110.59
1	B	13	ILE	N-CA-C	6.10	116.26	110.53
1	G	279	VAL	N-CA-C	-6.09	104.57	110.72
1	F	262	CYS	CA-C-N	6.06	125.45	118.85
1	F	262	CYS	C-N-CA	6.06	125.45	118.85
1	A	286	PRO	N-CA-C	6.05	118.08	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	275	LEU	N-CA-C	-6.03	104.78	111.36
1	F	149	TYR	N-CA-C	6.02	120.30	111.34
1	A	272	PHE	N-CA-C	-6.01	104.72	111.28
1	D	347	MET	N-CA-C	6.00	118.78	111.82
1	A	332	LYS	N-CA-C	5.98	120.74	113.38
1	E	82	LEU	N-CA-C	5.93	117.55	111.14
1	A	334	SER	N-CA-C	5.92	117.81	111.36
1	D	15	GLY	N-CA-C	-5.89	107.36	114.66
1	B	12	PRO	CA-C-N	5.87	128.08	120.56
1	B	12	PRO	C-N-CA	5.87	128.08	120.56
1	E	10	GLY	N-CA-C	-5.86	106.39	111.95
1	G	121	SER	N-CA-C	5.82	118.69	109.96
1	C	95	VAL	N-CA-C	5.81	116.24	108.11
1	C	348	PHE	N-CA-C	5.78	119.14	109.95
1	A	313	ALA	N-CA-C	-5.78	104.98	111.28
1	C	395	VAL	N-CA-C	5.77	116.50	110.62
1	H	144	VAL	N-CA-C	5.76	116.18	108.11
1	C	296	ILE	N-CA-C	5.76	115.89	110.30
1	D	138	GLU	N-CA-C	-5.70	105.21	111.82
1	E	281	ARG	CA-C-N	-5.69	117.33	123.08
1	E	281	ARG	C-N-CA	-5.69	117.33	123.08
1	F	174	VAL	N-CA-C	5.69	116.50	108.36
1	G	363	SER	N-CA-C	5.66	118.55	111.24
1	D	252	GLY	N-CA-C	5.66	120.66	113.24
1	C	82	LEU	N-CA-C	5.65	118.29	111.40
1	F	145	GLY	N-CA-C	-5.64	102.72	111.12
1	G	74	HIS	N-CA-C	-5.63	105.04	111.07
1	B	219	GLU	N-CA-C	-5.62	104.42	112.13
1	F	391	ALA	N-CA-C	-5.62	105.16	111.28
1	D	136	ILE	N-CA-C	5.62	116.07	110.23
1	E	219	GLU	N-CA-C	-5.60	104.45	112.13
1	H	231	ALA	N-CA-C	-5.53	105.35	111.71
1	A	66	LEU	CA-C-N	-5.52	114.01	119.92
1	A	66	LEU	C-N-CA	-5.52	114.01	119.92
1	D	25	ASN	CA-C-N	-5.52	114.08	120.04
1	D	25	ASN	C-N-CA	-5.52	114.08	120.04
1	E	286	PRO	CB-CA-C	-5.50	106.00	111.17
1	H	361	LEU	N-CA-C	-5.49	104.93	111.69
1	A	73	GLY	N-CA-C	5.48	118.86	112.50
1	B	61	SER	N-CA-C	5.48	117.58	110.40
1	E	169	LEU	N-CA-C	5.47	118.61	110.52
1	F	10	GLY	CA-C-O	-5.46	118.52	122.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	46	LEU	N-CA-C	5.43	118.06	109.96
1	G	12	PRO	CA-C-N	5.42	127.49	120.56
1	G	12	PRO	C-N-CA	5.42	127.49	120.56
1	B	365	PHE	CB-CA-C	-5.41	101.09	109.80
1	D	174	VAL	N-CA-C	5.41	115.74	108.17
1	D	339	ASP	N-CA-C	-5.40	105.55	111.82
1	D	336	ARG	N-CA-C	5.39	117.87	108.76
1	E	159	PHE	N-CA-C	5.39	116.84	111.07
1	F	162	MET	N-CA-C	-5.37	104.84	111.40
1	C	204	ARG	N-CA-C	5.36	119.52	112.92
1	A	271	VAL	CB-CA-C	-5.35	105.12	111.97
1	C	103	GLY	N-CA-C	-5.34	106.24	113.24
1	D	391	ALA	N-CA-C	-5.34	104.89	111.40
1	B	24	ASN	N-CA-C	5.33	118.88	112.38
1	G	9	ALA	N-CA-C	5.32	117.50	111.11
1	F	256	GLY	N-CA-C	-5.30	101.86	110.55
1	C	185	THR	N-CA-C	5.30	119.84	112.90
1	E	66	LEU	CA-C-N	-5.28	114.34	119.78
1	E	66	LEU	C-N-CA	-5.28	114.34	119.78
1	C	205	GLU	N-CA-C	5.27	118.47	111.30
1	B	187	VAL	N-CA-CB	5.26	117.00	111.00
1	A	191	ARG	N-CA-C	5.26	116.70	111.07
1	H	220	ASP	N-CA-C	-5.25	101.49	108.74
1	B	217	PHE	N-CA-C	-5.24	106.83	113.18
1	H	271	VAL	N-CA-C	-5.23	105.61	110.53
1	F	375	MET	CA-C-N	-5.22	116.05	122.84
1	F	375	MET	C-N-CA	-5.22	116.05	122.84
1	G	197	VAL	N-CA-C	5.22	115.66	110.23
1	A	186	GLY	N-CA-C	-5.22	108.11	115.32
1	A	22	ALA	N-CA-C	5.19	116.94	111.28
1	C	118	PHE	CA-C-N	5.19	126.33	119.84
1	C	118	PHE	C-N-CA	5.19	126.33	119.84
1	A	355	PRO	CA-C-N	5.18	127.17	120.44
1	A	355	PRO	C-N-CA	5.18	127.17	120.44
1	B	336	ARG	N-CA-C	5.17	117.53	110.55
1	F	188	ASP	N-CA-C	5.15	118.12	110.14
1	E	55	ARG	N-CA-C	5.15	116.89	111.28
1	H	49	VAL	N-CA-C	-5.15	105.52	110.72
1	E	43	MET	CA-C-N	5.14	125.05	119.85
1	E	43	MET	C-N-CA	5.14	125.05	119.85
1	E	146	LYS	N-CA-C	5.14	117.97	109.85
1	H	317	ARG	N-CA-C	-5.13	105.77	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	149	TYR	N-CA-CB	-5.11	101.85	110.49
1	D	163	ILE	N-CA-C	-5.09	104.69	111.05
1	A	210	MET	CA-CB-CG	-5.05	104.00	114.10
1	F	38	ASP	N-CA-C	5.03	116.43	110.19
1	F	378	ALA	N-CA-C	-5.03	106.40	112.54
1	E	240	VAL	CB-CA-C	-5.03	103.28	110.12
1	C	240	VAL	N-CA-C	5.02	115.08	107.75
1	E	337	ASN	N-CA-CB	-5.02	102.24	110.42
1	D	134	ILE	CA-C-O	-5.02	115.85	121.17
1	A	142	ILE	CA-C-N	-5.01	115.53	122.30
1	A	142	ILE	C-N-CA	-5.01	115.53	122.30
1	G	248	LEU	N-CA-C	-5.01	106.58	113.30
1	H	74	HIS	N-CA-C	-5.01	105.73	111.14
1	D	361	LEU	N-CA-C	-5.00	105.91	111.36

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	3115	0	3059	93	0
1	B	3137	0	3081	98	0
1	C	3110	0	3044	93	0
1	D	3101	0	3036	100	0
1	E	3121	0	3065	110	0
1	F	3118	0	3047	67	0
1	G	3117	0	3062	97	0
1	H	3113	0	3053	63	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
2	E	1	0	0	0	0
2	G	1	0	0	0	0
3	A	15	0	7	1	0
3	B	15	0	6	2	0
3	C	15	0	7	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	15	0	6	1	0
3	F	15	0	6	2	0
4	A	24	0	12	5	0
4	E	24	0	11	12	0
4	G	24	0	12	3	0
5	C	9	0	2	1	0
5	E	9	0	2	0	0
6	D	16	0	11	8	0
6	H	16	0	11	3	0
7	A	102	0	0	6	0
7	B	142	0	0	16	0
7	C	83	0	0	6	0
7	D	119	0	0	6	0
7	E	84	0	0	13	0
7	F	96	0	0	4	0
7	G	70	0	0	5	0
7	H	122	0	0	5	0
All	All	25951	0	24540	689	0

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 14.

All (689) 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:D:246:LYS:HE3	6:D:401:PMP:N4A	1.44	1.29
1:D:246:LYS:CE	6:D:401:PMP:HNA2	1.56	1.17
1:G:246:LYS:HZ1	4:G:402:KET:H4A	1.15	1.09
1:D:33:ILE:HG13	1:D:35:ILE:HG12	1.37	1.07
1:C:11:ASP:HB2	1:C:14:LEU:HB2	1.32	1.06
1:E:39:GLU:HG2	1:E:317:ARG:HD2	1.38	1.05
1:G:13:ILE:HD12	1:G:14:LEU:H	1.16	1.04
1:F:210:MET:HG3	1:F:238:LEU:HD11	1.40	1.01
1:C:11:ASP:CB	1:C:14:LEU:HB2	1.97	0.95
5:C:403:OAA:H22	6:D:401:PMP:H4A1	1.50	0.94
1:A:167:GLU:HB3	1:A:204:ARG:HH12	1.28	0.94
1:E:221:MET:HB2	7:E:532:HOH:O	1.71	0.89
1:E:191:ARG:HG3	1:E:191:ARG:HH11	1.37	0.89
1:G:246:LYS:NZ	4:G:402:KET:H4A	1.88	0.88
1:G:311:VAL:HA	1:G:314:MET:HE3	1.53	0.87
1:A:244:PHE:HB2	1:A:255:VAL:HG23	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246:LYS:NZ	6:D:401:PMP:HNA2	1.72	0.87
1:C:23:ASP:O	1:C:28:LYS:HE3	1.74	0.86
1:D:246:LYS:CE	6:D:401:PMP:N4A	2.25	0.86
1:B:64:PRO:HA	7:B:606:HOH:O	1.74	0.86
1:E:39:GLU:HG2	1:E:317:ARG:CD	2.04	0.86
1:G:157:ILE:HD12	1:G:187:VAL:HG12	1.58	0.85
1:C:190:THR:OG1	1:C:193:GLN:HG3	1.77	0.85
1:C:357:GLN:HE22	1:C:396:LEU:HA	1.40	0.85
1:B:2:PHE:O	1:B:5:ILE:HG12	1.78	0.84
1:D:39:GLU:CD	1:D:39:GLU:H	1.83	0.84
1:A:33:ILE:HD12	1:A:34:GLY:H	1.41	0.84
1:E:4:ARG:HB2	7:E:501:HOH:O	1.77	0.83
1:H:246:LYS:HE2	6:H:401:PMP:H4A2	1.60	0.83
1:F:36:TYR:CD2	1:F:314:MET:HE2	2.15	0.82
1:G:157:ILE:CD1	1:G:187:VAL:HG12	2.09	0.82
1:B:119:PRO:HB3	7:B:566:HOH:O	1.77	0.82
1:B:132:ASN:O	1:B:136:ILE:HG13	1.79	0.82
1:E:157:ILE:CD1	1:E:187:VAL:HG12	2.10	0.81
1:G:157:ILE:HD12	1:G:187:VAL:CG1	2.10	0.81
1:G:13:ILE:CD1	1:G:14:LEU:H	1.94	0.81
1:A:190:THR:OG1	1:A:193:GLN:HG3	1.81	0.80
1:F:11[A]:ASP:OD1	1:F:12:PRO:HD2	1.81	0.80
1:A:167:GLU:HB3	1:A:204:ARG:NH1	1.95	0.80
1:G:246:LYS:HD3	1:G:251:TYR:HE1	1.45	0.79
1:C:353:LEU:HD11	1:C:361:LEU:HD12	1.64	0.79
1:E:1:MET:HE2	1:F:237:PRO:HG3	1.65	0.79
1:B:192[A]:GLU:HG2	7:B:543:HOH:O	1.82	0.79
1:G:13:ILE:HD12	1:G:14:LEU:N	1.94	0.79
1:A:167:GLU:HA	1:A:204:ARG:HH11	1.47	0.78
1:G:246:LYS:HD3	1:G:251:TYR:CE1	2.18	0.78
1:F:95:VAL:HG22	1:F:261:VAL:HG22	1.64	0.77
1:D:167:GLU:HA	1:D:167:GLU:OE1	1.85	0.76
1:G:159:PHE:CE2	1:G:193:GLN:HG2	2.20	0.76
1:G:355:PRO:O	1:G:359:GLU:HG3	1.85	0.75
1:B:64:PRO:CA	7:B:606:HOH:O	2.32	0.75
1:B:46:LEU:HD21	1:B:314:MET:HE3	1.69	0.74
1:A:14:LEU:HD22	7:A:586:HOH:O	1.85	0.74
1:D:246:LYS:HE3	6:D:401:PMP:HNA2	1.04	0.74
1:A:68:MET:HE2	1:A:280[B]:ARG:HD2	1.69	0.74
1:G:151:ASP:HB2	1:G:158:LYS:HG2	1.68	0.74
1:E:191:ARG:HH11	1:E:191:ARG:CG	2.01	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:VAL:HG22	1:C:207:ILE:HB	1.70	0.73
1:C:112:GLU:OE1	1:C:112:GLU:HA	1.88	0.73
1:B:389:ALA:O	1:B:393:VAL:HG23	1.89	0.73
1:C:357:GLN:NE2	1:C:396:LEU:HA	2.03	0.73
1:E:244:PHE:HB2	1:E:255:VAL:HG23	1.70	0.72
1:F:210:MET:CG	1:F:238:LEU:HD11	2.17	0.72
1:G:106:ALA:HB1	1:G:258:LEU:HB2	1.71	0.72
1:A:163:ILE:O	1:A:167:GLU:HG2	1.89	0.72
1:C:11:ASP:HB2	1:C:14:LEU:CB	2.17	0.72
1:D:171:LYS:O	1:D:172:ASP:HB2	1.90	0.71
1:D:360:ARG:NH2	1:D:364:GLU:OE2	2.23	0.71
1:H:33:ILE:HB	1:H:35:ILE:HD13	1.72	0.71
1:B:157:ILE:HD13	1:B:187:VAL:CG1	2.20	0.71
1:E:4:ARG:HG2	7:E:584:HOH:O	1.91	0.71
1:B:244:PHE:HB2	1:B:255:VAL:HG23	1.71	0.70
1:C:63:ARG:NH2	1:D:53:GLU:OE1	2.23	0.70
1:D:33:ILE:CG1	1:D:35:ILE:HG12	2.21	0.69
1:B:244:PHE:HB2	1:B:255:VAL:CG2	2.22	0.69
1:H:336:ARG:HD2	1:H:338:PHE:CZ	2.27	0.69
1:A:2:PHE:HB3	1:A:5:ILE:HG13	1.74	0.69
1:B:157:ILE:HD13	1:B:187:VAL:HG11	1.74	0.69
1:C:38:ASP:HB2	1:C:39:GLU:OE1	1.93	0.69
1:G:13:ILE:CD1	1:G:14:LEU:N	2.55	0.69
1:D:360:ARG:HG2	1:D:360:ARG:HH21	1.57	0.68
1:F:244:PHE:HB2	1:F:255:VAL:HG23	1.74	0.68
1:E:148:PRO:HG2	1:E:162:MET:HA	1.75	0.68
1:G:246:LYS:CD	1:G:251:TYR:HE1	2.06	0.68
1:E:157:ILE:CD1	1:E:187:VAL:CG1	2.72	0.67
1:A:33:ILE:CD1	1:A:34:GLY:H	2.07	0.67
1:C:25:ASN:OD1	1:C:26:PRO:HD2	1.93	0.67
1:B:220:ASP:OD2	1:B:223:SER:HB2	1.95	0.67
1:B:140:CYS:O	1:B:141:ASP:HB2	1.95	0.67
1:A:246[B]:LYS:NZ	4:A:403[B]:KET:O	2.25	0.66
1:A:101:ILE:HD13	1:B:101:ILE:HD12	1.77	0.66
1:D:375:MET:HE3	1:D:377:VAL:HG22	1.76	0.66
1:G:101:ILE:HD12	1:H:101:ILE:HD13	1.77	0.66
1:E:157:ILE:HD11	1:E:187:VAL:HG12	1.77	0.66
1:C:179:PRO:HG2	1:C:212:ILE:HB	1.76	0.66
1:E:53:GLU:OE2	1:F:63:ARG:NH1	2.29	0.65
1:E:246[B]:LYS:HE2	4:E:404[B]:KET:N	2.11	0.65
1:A:167:GLU:CA	1:A:204:ARG:HH11	2.10	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:VAL:HG12	1:A:201:ILE:HD12	1.78	0.64
1:B:17:VAL:HG13	7:B:554:HOH:O	1.96	0.64
1:G:370:ILE:HG13	7:G:552:HOH:O	1.95	0.64
1:E:27:ASP:O	1:E:387:TYR:HE2	1.81	0.64
1:G:358:VAL:HG12	7:G:545:HOH:O	1.96	0.64
1:H:28:LYS:HE2	7:H:561:HOH:O	1.98	0.64
1:B:297:VAL:HG12	1:B:298:MET:HE2	1.78	0.64
1:A:53:GLU:HA	1:A:56:ILE:HD12	1.79	0.64
1:H:375:MET:HE3	1:H:377:VAL:HG22	1.80	0.64
1:G:219:GLU:HG2	1:G:223:SER:CB	2.27	0.64
1:C:370:ILE:N	1:C:370:ILE:HD13	2.12	0.63
1:E:27:ASP:O	1:E:387:TYR:CE2	2.51	0.63
1:E:112:GLU:HA	1:E:112:GLU:OE1	1.97	0.63
1:H:246:LYS:HE2	6:H:401:PMP:C4A	2.28	0.63
1:A:171:LYS:HG3	1:A:205:GLU:HB2	1.79	0.63
1:G:214:TYR:CE1	1:G:246:LYS:HG3	2.34	0.63
1:A:370:ILE:N	1:A:370:ILE:HD13	2.14	0.63
1:B:120:GLN:HB2	7:B:628:HOH:O	1.99	0.62
1:A:112:GLU:OE1	1:A:112:GLU:HA	1.97	0.62
1:A:328:VAL:O	1:A:332:LYS:HG3	2.00	0.62
1:C:353:LEU:HD11	1:C:361:LEU:CD1	2.29	0.62
1:B:4[A]:ARG:HH11	1:B:4[A]:ARG:HB3	1.64	0.62
1:A:237:PRO:HB3	1:B:1:MET:HG2	1.82	0.62
1:B:322:ARG:HD3	1:B:341:LEU:O	2.00	0.62
1:E:33:ILE:HD12	1:E:34:GLY:H	1.65	0.62
1:E:367:ILE:HG12	1:E:388:VAL:HG22	1.82	0.62
7:C:506:HOH:O	1:D:289:HIS:HB2	1.99	0.62
1:D:38:ASP:HB2	1:D:39:GLU:OE1	2.00	0.61
1:B:157:ILE:CD1	1:B:187:VAL:CG1	2.77	0.61
1:A:59:PRO:HA	7:A:567:HOH:O	1.99	0.61
1:H:151:ASP:HB2	1:H:158:LYS:HG2	1.82	0.61
1:B:46:LEU:HD21	1:B:314:MET:CE	2.30	0.61
1:G:199:ASN:O	1:G:203:GLU:HG3	2.00	0.61
1:E:246[B]:LYS:HE2	4:E:404[B]:KET:C4A	2.30	0.61
1:E:360[B]:ARG:HE	1:E:395:VAL:HG23	1.64	0.61
1:A:63:ARG:NH2	1:B:53:GLU:OE1	2.25	0.60
1:D:35:ILE:CG2	1:D:43:MET:HE2	2.30	0.60
1:A:319:LYS:O	1:A:323:THR:HG23	2.01	0.60
1:E:148:PRO:O	1:E:162:MET:HB2	2.01	0.60
1:E:246[B]:LYS:CE	4:E:404[B]:KET:O	2.49	0.60
1:H:114:ILE:HD13	1:H:174:VAL:HG21	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:53:GLU:CD	1:F:63:ARG:HH12	2.09	0.60
1:B:157:ILE:CD1	1:B:187:VAL:HG12	2.32	0.60
1:G:325:LEU:HD12	1:G:389:ALA:HB2	1.83	0.60
1:C:101:ILE:HD13	1:D:101:ILE:HD12	1.84	0.59
1:F:68:MET:HE3	1:F:276:ASN:OD1	2.02	0.59
1:E:1:MET:HE2	1:F:237:PRO:CG	2.32	0.59
1:A:191:ARG:HD3	1:A:226:TYR:CE1	2.37	0.59
1:B:64:PRO:CB	7:B:606:HOH:O	2.50	0.59
1:F:211:ASP:OD2	3:F:401:PLP:N1	2.36	0.59
1:G:7:TYR:OH	1:H:266:ASP:OD1	2.20	0.59
1:E:246[B]:LYS:HZ3	4:E:404[B]:KET:CA	2.16	0.59
1:C:2:PHE:HB3	1:C:5:ILE:HD12	1.83	0.59
1:C:39:GLU:H	1:C:39:GLU:CD	2.11	0.59
1:B:360:ARG:NH1	1:B:395:VAL:HA	2.18	0.58
1:D:246:LYS:HZ2	6:D:401:PMP:HNA2	1.47	0.58
1:D:193:GLN:O	1:D:197:VAL:HG23	2.04	0.58
1:A:167:GLU:CB	1:A:204:ARG:NH1	2.65	0.58
1:C:212:ILE:HG23	1:C:212:ILE:O	2.03	0.58
1:E:66:LEU:CD1	1:E:288:SER:HB2	2.32	0.58
1:D:192:GLU:CD	1:D:192:GLU:H	2.11	0.58
1:D:230:LYS:O	1:D:234:MET:HG3	2.04	0.58
1:E:322:ARG:HD3	1:E:341:LEU:O	2.03	0.58
1:A:218:GLY:O	1:A:319:LYS:NZ	2.37	0.58
1:C:353:LEU:HD22	1:C:357:GLN:HB3	1.86	0.58
1:D:39:GLU:HG3	1:D:317:ARG:HD2	1.86	0.58
1:E:357:GLN:NE2	1:E:396:LEU:HA	2.19	0.58
1:G:184:PRO:HB3	1:G:374:ARG:HD3	1.84	0.58
1:A:311:VAL:HA	1:A:314:MET:HE3	1.86	0.58
1:F:130:TRP:CH2	1:F:132:ASN:HB3	2.39	0.58
1:H:76:LYS:O	1:H:80:GLU:HG3	2.04	0.58
1:D:124:TYR:HA	1:D:145:GLY:O	2.03	0.58
1:F:230:LYS:O	1:F:234:MET:HG3	2.04	0.58
1:G:297:VAL:HG12	1:G:298:MET:HE2	1.86	0.58
1:A:19:LYS:HD3	1:A:368:TYR:HE2	1.68	0.57
1:B:246:LYS:HG2	1:B:347:MET:HE1	1.86	0.57
1:D:184:PRO:HG3	7:D:578:HOH:O	2.03	0.57
1:E:246[B]:LYS:NZ	4:E:404[B]:KET:N	2.52	0.57
1:G:140:CYS:O	1:G:141:ASP:HB2	2.03	0.57
1:G:340:TYR:CE1	1:G:341:LEU:HD23	2.39	0.57
1:B:196:THR:HA	7:B:550:HOH:O	2.05	0.57
1:F:151:ASP:HB2	1:F:158:LYS:HG2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:LEU:HA	1:C:19:LYS:HB3	1.86	0.57
1:C:124:TYR:HB2	1:C:175:LEU:CD2	2.34	0.57
1:C:158:LYS:HB3	1:C:161[B]:GLU:HB2	1.85	0.57
1:G:56:ILE:HD11	1:G:292:ARG:HB2	1.86	0.57
1:E:300:ASP:HB3	1:E:303:LEU:HB2	1.87	0.57
1:G:333:ILE:HG12	1:G:397:LYS:HD3	1.87	0.57
1:H:36:TYR:CZ	1:H:314:MET:HG2	2.39	0.57
1:A:159:PHE:CE2	1:A:193:GLN:HB3	2.40	0.57
1:A:167:GLU:CA	1:A:204:ARG:NH1	2.68	0.57
1:D:329:LEU:HD12	1:D:393:VAL:HG23	1.87	0.56
1:E:372:ASN:O	1:E:373:SER:OG	2.16	0.56
7:G:567:HOH:O	1:H:132:ASN:HB2	2.05	0.56
1:B:220:ASP:OD2	1:B:223:SER:CB	2.52	0.56
1:E:370:ILE:HD13	1:E:370:ILE:N	2.20	0.56
1:G:87:ALA:HB1	1:G:88:PRO:HD2	1.87	0.56
1:H:296:ILE:HA	7:H:588:HOH:O	2.06	0.56
1:A:322:ARG:NH1	1:A:346:GLY:O	2.39	0.56
1:E:46:LEU:HD21	1:E:314:MET:CE	2.36	0.56
1:G:75:ARG:O	1:G:79:GLN:HG3	2.06	0.56
1:A:179:PRO:HG2	1:A:212:ILE:HB	1.87	0.56
1:C:353:LEU:HD23	1:C:396:LEU:HD21	1.87	0.56
1:A:167:GLU:HA	1:A:204:ARG:NH1	2.20	0.56
1:C:16:LEU:O	1:C:20:PHE:N	2.38	0.56
1:G:163:ILE:O	1:G:167:GLU:HG2	2.06	0.56
1:C:35:ILE:HG12	1:C:251:TYR:CE1	2.41	0.55
1:D:171:LYS:HD2	1:D:205:GLU:OE1	2.06	0.55
1:D:273:GLY:HA3	7:D:582:HOH:O	2.07	0.55
1:E:176:LEU:HB3	7:E:508:HOH:O	2.06	0.55
1:H:3:GLU:CD	1:H:3:GLU:H	2.15	0.55
1:E:389:ALA:O	1:E:393:VAL:HG23	2.06	0.55
1:A:244:PHE:HB3	1:A:248:LEU:HD12	1.89	0.55
1:E:1:MET:HG2	1:F:237:PRO:HB3	1.87	0.55
1:A:326:LYS:CE	7:A:580:HOH:O	2.53	0.55
1:G:103:GLY:N	4:G:402:KET:OP1	2.40	0.55
1:G:148:PRO:O	1:G:162:MET:HB2	2.05	0.55
1:B:371:SER:C	1:B:373:SER:H	2.14	0.55
1:C:321:MET:HE2	1:C:321:MET:HA	1.89	0.55
1:G:258:LEU:HD12	1:G:259:SER:H	1.71	0.55
1:C:244:PHE:HB3	1:C:248:LEU:HD12	1.89	0.55
1:G:159:PHE:O	1:G:163:ILE:HG12	2.07	0.55
1:G:369:MET:HG2	1:G:375:MET:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:GLN:HB3	1:B:395:VAL:CG1	2.36	0.54
1:E:55:ARG:NH1	7:E:517:HOH:O	2.26	0.54
1:E:245:SER:HB3	1:E:251:TYR:HA	1.89	0.54
1:E:246[B]:LYS:NZ	4:E:404[B]:KET:CA	2.70	0.54
1:A:367:ILE:CD1	1:A:391:ALA:CB	2.85	0.54
1:B:10:GLY:HA2	7:B:598:HOH:O	2.06	0.54
1:C:134:ILE:HG12	1:C:144:VAL:HG11	1.89	0.54
1:G:39:GLU:CD	1:G:39:GLU:H	2.14	0.54
1:G:266:ASP:OD1	1:H:7:TYR:OH	2.22	0.54
1:B:184:PRO:HB2	1:B:350:PHE:HE2	1.72	0.54
1:H:210:MET:HE3	1:H:238:LEU:CD1	2.37	0.54
1:C:69:ALA:CB	1:C:98:ILE:HG22	2.37	0.54
1:F:127:ASP:O	1:F:149:TYR:HB3	2.08	0.54
1:C:73:GLY:HA3	1:C:295:ASP:OD1	2.08	0.54
1:D:265:VAL:O	1:D:268:THR:HB	2.08	0.54
1:D:371:SER:C	1:D:373:SER:H	2.15	0.54
1:E:253:GLU:OE1	1:F:63:ARG:HD2	2.08	0.54
1:G:69:ALA:CB	1:G:98:ILE:HG22	2.38	0.54
1:E:191:ARG:HG3	1:E:191:ARG:NH1	2.16	0.54
1:G:69:ALA:O	1:G:75:ARG:HD2	2.07	0.53
1:G:312:TYR:HB3	1:G:315:ARG:NH2	2.22	0.53
1:B:184:PRO:HB2	1:B:350:PHE:CE2	2.43	0.53
1:D:52:ALA:O	1:D:56:ILE:HG13	2.08	0.53
1:E:246[B]:LYS:CE	4:E:404[B]:KET:N	2.72	0.53
1:H:255:VAL:HG12	7:H:621:HOH:O	2.08	0.53
1:E:221:MET:HE1	1:E:311:VAL:HG11	1.90	0.53
1:G:244:PHE:O	1:G:248:LEU:HB2	2.08	0.53
1:A:362:GLN:HB3	1:A:368:TYR:CZ	2.44	0.53
7:E:577:HOH:O	1:F:1:MET:HE1	2.07	0.53
1:C:125:VAL:HG12	1:C:176:LEU:HD23	1.91	0.53
1:G:5:ILE:O	1:H:270:ARG:HD3	2.08	0.53
1:B:180:CYS:HG	1:B:181:CYS:HG	1.55	0.53
1:B:360:ARG:NH2	1:B:364:GLU:OE2	2.42	0.53
1:D:11:ASP:OD1	1:D:12:PRO:HD2	2.08	0.53
1:D:388:VAL:O	1:D:392:MET:HG3	2.08	0.53
1:C:174:VAL:CG2	1:C:207:ILE:HB	2.38	0.53
1:A:27:ASP:HB3	1:A:387:TYR:CE2	2.44	0.53
1:B:4[A]:ARG:HB3	1:B:4[A]:ARG:NH1	2.24	0.53
1:C:180:CYS:SG	1:C:181:CYS:SG	3.05	0.53
1:E:7:TYR:OH	1:F:266:ASP:OD1	2.20	0.53
1:F:386:ASP:O	1:F:390:ASN:ND2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:LEU:HD21	1:A:380:LEU:HD23	1.91	0.52
1:B:80:GLU:OE1	1:B:85[B]:LYS:HE2	2.09	0.52
1:E:357:GLN:HE22	1:E:396:LEU:HD23	1.74	0.52
1:B:100:THR:HB	7:B:505:HOH:O	2.09	0.52
1:D:364:GLU:HB2	1:D:365:PHE:CD2	2.44	0.52
1:E:66:LEU:HD11	1:E:288:SER:HB2	1.90	0.52
1:C:212:ILE:CD1	1:C:215:GLN:HB2	2.39	0.52
1:G:161:GLU:O	1:G:164:ALA:HB3	2.09	0.52
1:B:8:TYR:CD1	1:B:9:ALA:N	2.78	0.52
1:B:13:ILE:HG13	1:B:14:LEU:N	2.24	0.52
1:D:164:ALA:O	1:D:167:GLU:HB2	2.10	0.52
1:E:163:ILE:O	1:E:167:GLU:HG2	2.09	0.52
1:F:212:ILE:CD1	1:F:215:GLN:HB2	2.40	0.52
1:D:360:ARG:NH2	1:D:360:ARG:HG2	2.25	0.52
1:F:375:MET:HE3	1:F:377:VAL:HG22	1.92	0.52
1:B:157:ILE:HD13	1:B:187:VAL:HG12	1.91	0.52
1:B:315:ARG:O	1:B:319:LYS:HG3	2.09	0.52
1:C:124:TYR:HB2	1:C:175:LEU:HD23	1.92	0.52
1:D:49:VAL:O	1:D:53:GLU:HG3	2.09	0.52
1:D:181:CYS:HB3	1:D:346:GLY:HA3	1.92	0.52
1:F:189:LEU:HD12	1:F:194:TRP:CZ2	2.45	0.52
1:H:70:GLY:HA3	1:H:99:ALA:HB3	1.92	0.52
1:E:246[B]:LYS:HZ3	4:E:404[B]:KET:HA	1.75	0.51
1:H:354:THR:HB	1:H:355:PRO:HD2	1.92	0.51
1:A:266:ASP:OD1	1:B:7:TYR:OH	2.26	0.51
1:A:19:LYS:HD3	1:A:368:TYR:CE2	2.45	0.51
1:B:21:ALA:HB2	7:B:554:HOH:O	2.11	0.51
1:C:317:ARG:HD2	7:C:535:HOH:O	2.10	0.51
1:B:64:PRO:HB3	7:B:606:HOH:O	2.11	0.51
1:H:333:ILE:HG22	1:H:333:ILE:O	2.09	0.51
1:H:97:THR:HA	1:H:258:LEU:O	2.10	0.51
1:H:127:ASP:O	1:H:149:TYR:HB3	2.09	0.51
1:C:157:ILE:HD11	1:C:187:VAL:HG12	1.91	0.51
1:E:296:ILE:HG22	1:E:297:VAL:N	2.24	0.51
1:E:191:ARG:CG	1:E:191:ARG:NH1	2.71	0.51
1:E:283:TYR:O	1:E:284:SER:HB2	2.09	0.51
1:F:130:TRP:CZ3	1:F:132:ASN:HB3	2.46	0.51
1:B:184:PRO:HG3	7:B:544:HOH:O	2.10	0.51
1:G:333:ILE:HG22	1:G:333:ILE:O	2.11	0.50
1:D:47:ASP:N	1:D:310:GLU:OE1	2.44	0.50
1:E:171:LYS:HE2	7:E:563:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:ARG:O	1:B:364:GLU:HB2	2.10	0.50
1:C:167:GLU:HA	1:C:204:ARG:HE	1.76	0.50
1:F:329:LEU:HD23	1:F:338:PHE:CE1	2.47	0.50
1:G:31:LEU:HD13	1:G:375:MET:HG3	1.94	0.50
1:C:47:ASP:HA	1:C:50:LYS:HE2	1.93	0.50
1:C:336:ARG:HG2	1:C:338:PHE:CZ	2.46	0.50
1:D:181:CYS:HB3	7:D:508:HOH:O	2.12	0.50
1:E:360[B]:ARG:NH2	1:E:364:GLU:OE2	2.44	0.50
1:F:4:ARG:HG2	7:F:578:HOH:O	2.11	0.50
1:G:385:ILE:HG13	1:G:385:ILE:O	2.11	0.50
1:A:171:LYS:HE3	1:A:205:GLU:OE2	2.12	0.50
1:C:348:PHE:CD2	1:C:374:ARG:HD2	2.47	0.50
1:G:20:PHE:CZ	1:G:28:LYS:HG3	2.47	0.50
1:A:114:ILE:HD13	1:A:174:VAL:HG21	1.94	0.50
1:C:158:LYS:HB3	1:C:161[A]:GLU:HB2	1.93	0.50
1:C:214:TYR:N	7:C:518:HOH:O	2.43	0.50
1:H:46:LEU:HB2	1:H:49:VAL:HG23	1.93	0.50
1:C:336:ARG:CG	1:C:338:PHE:CZ	2.95	0.49
1:C:217:PHE:CE1	1:C:347:MET:HE2	2.47	0.49
1:C:319:LYS:O	1:C:323:THR:HG23	2.12	0.49
1:D:39:GLU:HB3	7:D:529:HOH:O	2.11	0.49
1:H:360:ARG:HH12	1:H:398:ASP:HA	1.78	0.49
1:G:244:PHE:HB2	1:G:255:VAL:HG23	1.93	0.49
1:C:370:ILE:HB	1:C:372:ASN:OD1	2.11	0.49
1:G:46:LEU:O	1:G:49:VAL:N	2.38	0.49
1:H:123:CYS:O	1:H:144:VAL:HA	2.12	0.49
1:H:292:ARG:O	1:H:296:ILE:HG13	2.12	0.49
1:C:1:MET:N	1:D:267:GLU:OE1	2.46	0.49
1:F:191:ARG:HD3	7:F:568:HOH:O	2.13	0.49
1:F:250:LEU:HD13	1:F:253:GLU:HB2	1.94	0.49
1:H:130:TRP:CZ2	1:H:132:ASN:HB3	2.48	0.49
1:D:212:ILE:HG23	1:D:212:ILE:O	2.13	0.49
1:C:7:TYR:OH	1:D:266:ASP:OD2	2.27	0.49
1:D:192:GLU:CD	1:D:192:GLU:N	2.70	0.49
1:E:361:LEU:HG	1:E:367:ILE:HB	1.95	0.49
1:G:159:PHE:CZ	1:G:193:GLN:HG2	2.48	0.49
1:H:13:ILE:HG12	1:H:370:ILE:HD12	1.94	0.49
1:A:243:SER:OG	4:A:403[B]:KET:OP3	2.25	0.48
1:E:221:MET:CE	1:E:311:VAL:HG11	2.43	0.48
1:F:80:GLU:OE2	1:F:85:LYS:HG3	2.13	0.48
1:H:157:ILE:HG22	1:H:159:PHE:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:TRP:NE1	4:A:403[B]:KET:HB2	2.28	0.48
1:E:360[B]:ARG:CZ	1:E:364:GLU:OE2	2.60	0.48
1:H:25:ASN:O	1:H:28:LYS:HG2	2.12	0.48
1:D:220:ASP:HB2	1:D:312:TYR:OH	2.13	0.48
1:E:46:LEU:HD21	1:E:314:MET:HE1	1.95	0.48
1:F:140:CYS:O	1:F:141:ASP:HB2	2.13	0.48
1:C:278:THR:O	1:C:282:ILE:HG13	2.13	0.48
1:A:125:VAL:HG12	1:A:176:LEU:HD23	1.96	0.48
1:D:231:ALA:HB3	1:D:238:LEU:HD22	1.96	0.48
1:F:68:MET:HG2	1:F:284:SER:O	2.13	0.48
1:A:192:GLU:CD	1:A:192:GLU:H	2.22	0.48
1:E:279:VAL:HG13	1:E:283:TYR:CE2	2.49	0.48
1:C:39:GLU:HB3	7:C:577:HOH:O	2.13	0.48
1:D:151:ASP:HB2	1:D:158:LYS:HG2	1.95	0.48
1:D:364:GLU:HB2	1:D:365:PHE:CE2	2.49	0.48
1:E:246[B]:LYS:HE3	4:E:404[B]:KET:O	2.14	0.48
1:H:306:GLN:O	1:H:310:GLU:HG3	2.14	0.48
1:B:180:CYS:SG	1:B:181:CYS:SG	3.10	0.48
1:B:246:LYS:CG	1:B:347:MET:HE1	2.42	0.48
1:E:392:MET:O	1:E:396:LEU:HB2	2.13	0.48
1:G:337:ASN:OD1	1:G:338:PHE:N	2.47	0.48
1:H:163:ILE:O	1:H:167:GLU:HG2	2.14	0.48
1:G:114:ILE:O	1:G:115:HIS:C	2.56	0.48
1:A:33:ILE:CG1	1:A:34:GLY:N	2.76	0.47
1:A:353:LEU:HB3	1:A:358:VAL:HG23	1.95	0.47
1:A:367:ILE:CD1	1:A:391:ALA:HB3	2.44	0.47
1:E:237:PRO:HB3	1:F:1:MET:HE3	1.96	0.47
1:C:190:THR:HG1	1:C:193:GLN:HG3	1.76	0.47
1:C:225:ALA:O	1:C:229:ARG:HG3	2.14	0.47
1:D:100:THR:HG21	1:D:106:ALA:HA	1.97	0.47
1:D:171:LYS:HG3	1:D:205:GLU:HB2	1.97	0.47
1:D:282:ILE:HG22	1:D:283:TYR:HD1	1.79	0.47
1:E:353:LEU:HD21	1:E:396:LEU:HG	1.96	0.47
1:G:282:ILE:HG23	1:H:108:LYS:HG2	1.95	0.47
1:D:203:GLU:HG3	1:D:204:ARG:HG2	1.96	0.47
1:B:249:SER:HB3	7:B:525:HOH:O	2.14	0.47
1:C:20:PHE:CE1	1:C:28:LYS:HB2	2.49	0.47
1:C:69:ALA:HB1	1:C:98:ILE:HG22	1.96	0.47
3:C:402:PLP:H5A1	7:C:574:HOH:O	2.14	0.47
1:B:157:ILE:HD11	1:B:187:VAL:HG12	1.95	0.47
1:A:35:ILE:HG23	1:A:43:MET:HE2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:LEU:HA	1:B:72:PRO:HD2	1.77	0.47
1:C:212:ILE:HD13	1:C:215:GLN:HB2	1.97	0.47
1:C:244:PHE:HB2	1:C:255:VAL:HG23	1.96	0.47
1:C:251:TYR:CD2	1:C:251:TYR:N	2.80	0.47
1:C:351:THR:HG21	1:C:375:MET:HE3	1.97	0.47
1:D:244:PHE:O	1:D:248:LEU:HB2	2.15	0.47
1:E:347:MET:HE3	1:E:347:MET:HB2	1.80	0.47
1:G:36:TYR:C	1:G:36:TYR:CD2	2.92	0.47
1:D:39:GLU:CD	1:D:39:GLU:N	2.58	0.47
1:E:16:LEU:HA	1:E:16:LEU:HD12	1.75	0.47
1:H:244:PHE:HB2	1:H:255:VAL:HG23	1.97	0.47
1:D:20:PHE:CE1	1:D:30:ASN:HB2	2.49	0.47
1:H:112:GLU:OE1	1:H:112:GLU:HA	2.15	0.47
1:D:177:LEU:HB2	1:D:210:MET:HG2	1.97	0.47
1:E:369:MET:HB3	1:E:374:ARG:O	2.14	0.47
1:H:370:ILE:HB	1:H:372:ASN:OD1	2.14	0.47
1:F:212:ILE:HD11	1:F:215:GLN:HB2	1.96	0.46
1:A:132:ASN:O	1:A:136:ILE:HG13	2.15	0.46
1:C:58:ASP:HA	1:C:59:PRO:HA	1.86	0.46
1:H:46:LEU:HB2	1:H:49:VAL:CG2	2.45	0.46
1:B:157:ILE:HD13	1:B:157:ILE:N	2.31	0.46
1:D:244:PHE:HB3	1:D:248:LEU:HB2	1.96	0.46
1:G:31:LEU:HD23	1:G:379:GLY:HA3	1.96	0.46
1:G:228:ILE:O	1:G:231:ALA:HB3	2.16	0.46
1:E:157:ILE:HD12	1:E:187:VAL:HG11	1.97	0.46
1:A:270:ARG:HD3	1:B:5:ILE:O	2.15	0.46
1:H:36:TYR:C	1:H:36:TYR:CD2	2.93	0.46
1:H:278:THR:O	1:H:282:ILE:HG13	2.16	0.46
1:A:171:LYS:HG3	1:A:205:GLU:CB	2.46	0.46
1:D:71:LEU:O	1:D:75:ARG:HG3	2.15	0.46
1:A:33:ILE:HG13	1:A:34:GLY:N	2.30	0.46
1:C:357:GLN:NE2	1:C:395:VAL:O	2.41	0.46
1:F:36:TYR:CE2	1:F:314:MET:HG2	2.51	0.46
1:G:159:PHE:CD2	1:G:193:GLN:HG2	2.50	0.46
1:G:171:LYS:O	1:G:172:ASP:HB2	2.16	0.46
1:A:214:TYR:CE1	1:A:246[B]:LYS:HG2	2.51	0.46
1:G:69:ALA:HB1	1:G:98:ILE:HG22	1.97	0.46
1:A:322:ARG:HH21	1:A:344:GLN:HB2	1.81	0.46
1:A:360:ARG:HE	1:A:360:ARG:HB2	1.48	0.46
1:B:286:PRO:HG3	7:B:504:HOH:O	2.15	0.46
1:E:246[B]:LYS:NZ	4:E:404[B]:KET:HA	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:179:PRO:HG3	1:G:210:MET:HG2	1.98	0.46
1:A:5:ILE:HD12	1:B:113:PHE:CZ	2.51	0.46
1:A:370:ILE:HG22	1:A:371:SER:N	2.31	0.46
1:G:38:ASP:HB2	1:G:39:GLU:OE1	2.16	0.46
1:G:79:GLN:O	1:G:83:PHE:HD2	1.99	0.46
1:H:250:LEU:HA	1:H:250:LEU:HD12	1.53	0.46
1:A:237:PRO:CB	1:B:1:MET:HG2	2.46	0.45
1:D:74:HIS:C	1:D:74:HIS:CD2	2.94	0.45
1:D:194:TRP:HA	1:D:194:TRP:CE3	2.51	0.45
6:D:401:PMP:H4A2	6:D:401:PMP:O4P	2.16	0.45
1:F:36:TYR:CE2	1:F:314:MET:HE2	2.51	0.45
1:G:392:MET:HE2	1:G:392:MET:HB3	1.83	0.45
7:E:571:HOH:O	1:F:57:ALA:HB2	2.16	0.45
1:F:295:ASP:OD1	1:F:299:ASN:ND2	2.47	0.45
1:B:39:GLU:HB3	1:B:317:ARG:HD2	1.96	0.45
1:B:248:LEU:HD23	1:B:307:TRP:CD1	2.51	0.45
1:D:182:HIS:HE1	1:D:184:PRO:HD2	1.80	0.45
1:D:354:THR:HG23	1:D:357:GLN:OE1	2.16	0.45
1:E:123:CYS:O	1:E:144:VAL:HA	2.15	0.45
1:F:288:SER:O	1:F:289:HIS:C	2.58	0.45
1:B:212:ILE:HG23	1:B:212:ILE:O	2.15	0.45
1:C:214:TYR:HB2	7:C:518:HOH:O	2.14	0.45
1:C:361:LEU:HG	1:C:395:VAL:HG21	1.98	0.45
1:A:328:VAL:HG11	1:A:389:ALA:HB1	1.99	0.45
1:B:104:SER:OG	3:B:401:PLP:O3P	2.22	0.45
1:D:2:PHE:O	1:D:5:ILE:HB	2.17	0.45
1:D:66:LEU:HD22	1:D:286:PRO:O	2.16	0.45
1:F:74:HIS:C	1:F:74:HIS:CD2	2.94	0.45
1:H:149:TYR:O	1:H:157:ILE:HA	2.17	0.45
1:A:347:MET:HE3	1:A:347:MET:HB2	1.67	0.45
1:B:36:TYR:CE2	1:B:314:MET:HG2	2.52	0.45
1:D:365:PHE:CD2	1:D:365:PHE:N	2.84	0.45
1:G:51:ILE:O	1:G:55:ARG:HG3	2.17	0.45
1:A:163:ILE:HG23	1:A:200:VAL:HG21	1.98	0.45
1:C:266:ASP:OD1	1:D:7:TYR:OH	2.28	0.45
1:D:35:ILE:HG21	1:D:43:MET:CE	2.46	0.45
1:D:127:ASP:HA	1:D:128:PRO:HA	1.84	0.45
1:E:115:HIS:ND1	7:E:506:HOH:O	2.34	0.45
1:B:358:VAL:HA	1:B:361:LEU:HD12	1.98	0.45
1:C:74:HIS:C	1:C:74:HIS:CD2	2.95	0.45
1:C:1:MET:HE2	1:D:172:ASP:OD1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:262:CYS:HA	1:G:263:PRO:HD2	1.79	0.45
7:G:548:HOH:O	1:H:116:GLU:HG3	2.16	0.45
1:A:238:LEU:HG	1:A:240:VAL:HG23	1.99	0.45
1:B:89:VAL:HG22	1:B:95:VAL:HG23	1.98	0.45
1:F:207:ILE:HA	1:F:208:PRO:HD3	1.76	0.45
1:G:219:GLU:HG2	1:G:223:SER:HB3	1.98	0.45
1:D:225:ALA:O	1:D:229:ARG:HG3	2.17	0.44
1:H:1:MET:N	1:H:3:GLU:OE1	2.40	0.44
1:A:214:TYR:OH	3:A:402[A]:PLP:O3	2.33	0.44
1:B:157:ILE:CD1	1:B:157:ILE:N	2.80	0.44
1:C:123:CYS:O	1:C:144:VAL:HA	2.16	0.44
1:C:340:TYR:HA	1:C:343:ALA:HB3	1.99	0.44
1:E:43:MET:HE1	1:F:64:PRO:HB3	2.00	0.44
1:G:79:GLN:HB3	1:G:90:LEU:HD21	1.99	0.44
1:H:360:ARG:HD3	7:H:613:HOH:O	2.16	0.44
1:E:56:ILE:HA	1:E:292:ARG:NH1	2.32	0.44
4:A:403[B]:KET:OP4	4:A:403[B]:KET:H4A	2.18	0.44
1:F:324:LYS:O	1:F:327:SER:HB2	2.17	0.44
1:H:210:MET:HE3	1:H:238:LEU:HD13	1.99	0.44
1:A:130:TRP:CH2	1:A:132:ASN:HB3	2.52	0.44
1:B:128:PRO:HG2	1:B:184:PRO:HG2	1.99	0.44
1:D:20:PHE:CZ	1:D:30:ASN:HB2	2.53	0.44
1:D:370:ILE:HD13	1:D:370:ILE:N	2.31	0.44
1:E:100:THR:HG21	1:E:106:ALA:HA	2.00	0.44
1:E:112:GLU:O	1:E:116[B]:GLU:HG2	2.18	0.44
1:E:124:TYR:CE2	1:E:169:LEU:HD22	2.52	0.44
1:G:212:ILE:HD11	1:G:215:GLN:HG3	2.00	0.44
1:C:157:ILE:HG22	1:C:159:PHE:N	2.32	0.44
1:F:13:ILE:HD11	7:F:591:HOH:O	2.16	0.44
1:H:130:TRP:CH2	1:H:132:ASN:HB3	2.53	0.44
1:A:183:ASN:OD1	1:A:184:PRO:HA	2.17	0.44
1:C:325:LEU:HD11	1:C:392:MET:CE	2.48	0.44
1:G:300:ASP:HB3	1:G:303:LEU:HB2	2.00	0.44
1:H:246:LYS:HE2	6:H:401:PMP:N4A	2.32	0.44
1:A:263:PRO:HB2	1:A:264:THR:HG23	2.00	0.44
1:A:326:LYS:HE3	7:A:580:HOH:O	2.14	0.44
1:F:289:HIS:O	1:F:293:VAL:HG23	2.18	0.44
1:A:191:ARG:HD3	1:A:226:TYR:CZ	2.53	0.44
1:C:244:PHE:O	1:C:248:LEU:HB2	2.17	0.44
1:D:33:ILE:HD12	1:D:34:GLY:H	1.83	0.44
1:D:171:LYS:HG3	1:D:205:GLU:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:19:LYS:HD3	1:E:368:TYR:HE2	1.83	0.43
1:E:23:ASP:O	1:E:28:LYS:HE2	2.18	0.43
1:E:370:ILE:HG22	1:E:371:SER:N	2.33	0.43
1:F:243:SER:OG	3:F:401:PLP:O3P	2.22	0.43
1:D:298:MET:HE1	1:D:307:TRP:CZ3	2.53	0.43
1:E:46:LEU:HD21	1:E:314:MET:HE2	2.00	0.43
1:G:43:MET:HE1	1:H:64:PRO:HA	2.01	0.43
1:A:271:VAL:O	1:A:275:LEU:HG	2.18	0.43
1:B:171:LYS:O	1:B:172:ASP:HB2	2.19	0.43
1:B:371:SER:C	1:B:373:SER:N	2.76	0.43
1:C:127:ASP:HA	1:C:128:PRO:HA	1.75	0.43
1:D:35:ILE:CG2	1:D:43:MET:CE	2.95	0.43
1:E:143:GLU:HG2	7:E:562:HOH:O	2.18	0.43
1:E:166:PHE:CE1	1:E:175:LEU:HD22	2.54	0.43
1:E:263:PRO:HD3	7:E:554:HOH:O	2.18	0.43
1:F:262:CYS:HA	1:F:263:PRO:HD3	1.85	0.43
1:C:108:LYS:HE2	1:D:282:ILE:HG12	2.00	0.43
1:C:171:LYS:HE3	1:C:205:GLU:HB3	1.99	0.43
1:D:336:ARG:HB3	1:D:338:PHE:CE2	2.53	0.43
1:B:190:THR:HG23	1:B:193:GLN:OE1	2.19	0.43
1:C:364:GLU:HG2	1:C:365:PHE:CD2	2.54	0.43
1:E:126:SER:HA	1:E:147:TYR:CE2	2.54	0.43
1:A:1:MET:HE2	1:B:237:PRO:CB	2.48	0.43
1:A:27:ASP:O	1:A:387:TYR:HE2	2.02	0.43
1:D:68:MET:HG2	1:D:284:SER:O	2.18	0.43
1:E:58:ASP:HA	1:E:59:PRO:HA	1.72	0.43
1:H:324:LYS:O	1:H:325:LEU:C	2.59	0.43
1:A:36:TYR:CZ	1:A:314:MET:HG2	2.54	0.43
1:D:163:ILE:HG23	1:D:200:VAL:HG21	2.01	0.43
1:G:20:PHE:CE1	1:G:28:LYS:HG3	2.53	0.43
1:D:1:MET:HE2	1:D:1:MET:HB2	1.83	0.43
1:E:263:PRO:HB2	1:E:267:GLU:OE2	2.18	0.43
1:F:11[A]:ASP:OD1	1:F:12:PRO:CD	2.62	0.43
1:G:258:LEU:HD12	1:G:259:SER:N	2.34	0.43
1:A:170:ASN:O	1:A:206:LEU:HD23	2.19	0.43
1:E:230:LYS:O	1:E:234:MET:HG3	2.18	0.43
1:G:51:ILE:HG21	1:G:303:LEU:HD21	2.01	0.43
1:A:130:TRP:HE1	4:A:403[B]:KET:HB2	1.84	0.42
1:B:23:ASP:OD1	1:B:368:TYR:OH	2.25	0.42
1:B:283:TYR:O	1:B:284:SER:HB2	2.18	0.42
1:C:175:LEU:HD23	1:C:175:LEU:HA	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307:TRP:O	1:C:311:VAL:HG23	2.19	0.42
1:D:353:LEU:HD12	1:D:396:LEU:HD21	2.01	0.42
1:E:250:LEU:HD12	1:E:250:LEU:HA	1.88	0.42
1:G:279:VAL:HG13	1:G:283:TYR:CE2	2.54	0.42
1:H:253:GLU:HA	1:H:253:GLU:OE2	2.19	0.42
1:B:37:TYR:O	1:B:317:ARG:NH2	2.52	0.42
1:G:323:THR:HG22	1:G:342:THR:HG21	2.01	0.42
1:H:261:VAL:HG12	7:H:597:HOH:O	2.18	0.42
1:H:318:ILE:HD11	1:H:378:ALA:HB2	2.00	0.42
1:B:130:TRP:O	1:B:133:HIS:HB2	2.19	0.42
1:B:236:LEU:HD23	1:B:236:LEU:HA	1.78	0.42
1:C:118:PHE:N	1:C:119:PRO:CD	2.81	0.42
1:E:103:GLY:HA3	3:E:402[A]:PLP:H5A2	2.01	0.42
1:E:332:LYS:HD3	7:E:525:HOH:O	2.18	0.42
1:F:231:ALA:HB3	1:F:238:LEU:HD22	2.01	0.42
1:B:116:GLU:HB3	1:B:117:TRP:CD1	2.55	0.42
1:B:164:ALA:O	1:B:167:GLU:HB2	2.19	0.42
1:C:250:LEU:O	1:C:251:TYR:C	2.62	0.42
1:D:140:CYS:O	1:D:141:ASP:HB2	2.19	0.42
1:E:157:ILE:HD12	1:E:187:VAL:CG1	2.49	0.42
1:F:35:ILE:CG2	1:F:43:MET:HE2	2.50	0.42
1:F:385:ILE:HG23	1:F:386:ASP:N	2.34	0.42
1:H:356:GLU:CD	1:H:356:GLU:H	2.27	0.42
1:C:24:ASN:ND2	1:F:86:ASP:OD1	2.53	0.42
1:G:43:MET:HA	1:G:44:PRO:HD3	1.91	0.42
1:B:370:ILE:H	1:B:370:ILE:HG12	1.70	0.42
1:C:332:LYS:C	1:C:333:ILE:HG13	2.45	0.42
1:E:221:MET:HG2	1:E:312:TYR:OH	2.20	0.42
1:F:184:PRO:CB	1:F:374:ARG:HD3	2.49	0.42
1:G:118:PHE:N	1:G:119:PRO:HD3	2.35	0.42
1:G:147:TYR:HA	1:G:148:PRO:HD3	1.88	0.42
1:G:353:LEU:HD11	1:G:392:MET:HE3	2.02	0.42
1:A:35:ILE:CG2	1:A:43:MET:HE2	2.49	0.42
1:B:321:MET:CE	7:B:605:HOH:O	2.67	0.42
1:E:36:TYR:CD2	1:E:36:TYR:C	2.97	0.42
4:E:404[B]:KET:C4A	4:E:404[B]:KET:OP4	2.67	0.42
1:B:157:ILE:CD1	1:B:187:VAL:HG11	2.46	0.42
1:G:276:ASN:HD22	1:G:276:ASN:H	1.68	0.42
1:B:382:SER:HA	1:B:385:ILE:HG22	2.02	0.42
1:D:71:LEU:HA	1:D:71:LEU:HD23	1.77	0.42
1:E:214:TYR:OH	4:E:404[B]:KET:O3	2.29	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4[A]:ARG:NH1	1:G:4[A]:ARG:HB2	2.35	0.42
1:B:192[A]:GLU:HA	1:B:192[A]:GLU:OE1	2.20	0.42
1:D:148:PRO:O	1:D:162:MET:HB2	2.20	0.42
1:D:168:THR:C	7:D:536:HOH:O	2.63	0.42
1:F:191:ARG:HH21	1:F:226:TYR:HB2	1.85	0.42
1:D:132:ASN:O	1:D:136:ILE:HG13	2.20	0.41
1:A:58:ASP:HA	1:A:59:PRO:HA	1.82	0.41
1:A:179:PRO:HG3	1:A:210:MET:HB3	2.02	0.41
1:C:166:PHE:CE1	1:C:175:LEU:HD13	2.55	0.41
1:F:184:PRO:HB3	1:F:374:ARG:HD3	2.02	0.41
1:G:132:ASN:HD22	1:G:132:ASN:HA	1.75	0.41
1:H:172:ASP:O	1:H:207:ILE:HD12	2.19	0.41
1:B:353:LEU:HD23	1:B:361:LEU:HD11	2.02	0.41
1:C:25:ASN:OD1	1:C:26:PRO:CD	2.67	0.41
1:E:357:GLN:HE21	1:E:396:LEU:HA	1.85	0.41
1:F:131:GLY:HA2	7:F:575:HOH:O	2.19	0.41
1:H:74:HIS:CD2	1:H:74:HIS:C	2.98	0.41
1:A:178:HIS:N	1:A:178:HIS:CD2	2.88	0.41
1:C:50:LYS:HE2	1:C:50:LYS:HB2	1.67	0.41
1:E:267:GLU:O	1:E:271:VAL:HG23	2.20	0.41
1:F:132:ASN:HD22	1:F:132:ASN:HA	1.64	0.41
1:G:138:GLU:HG2	7:G:528:HOH:O	2.20	0.41
1:G:151:ASP:CB	1:G:158:LYS:HG2	2.45	0.41
1:G:248:LEU:HD23	1:G:248:LEU:HA	1.88	0.41
1:A:27:ASP:O	1:A:387:TYR:CE2	2.73	0.41
1:F:23:ASP:OD1	1:F:368:TYR:OH	2.37	0.41
1:A:165:PHE:CD2	1:A:165:PHE:C	2.98	0.41
1:C:114:ILE:HD13	1:C:174:VAL:HG21	2.03	0.41
1:D:58:ASP:HA	1:D:59:PRO:HA	1.96	0.41
1:G:372:ASN:O	1:G:373:SER:OG	2.34	0.41
1:H:102:GLY:C	1:H:104:SER:N	2.78	0.41
1:A:287:PRO:HG3	1:B:287:PRO:HG3	2.01	0.41
1:B:179:PRO:HG2	1:B:212:ILE:HB	2.03	0.41
1:D:246:LYS:HD3	1:D:251:TYR:HE1	1.86	0.41
1:E:98:ILE:HD11	1:E:109:VAL:HG11	2.03	0.41
1:E:181:CYS:O	1:E:182:HIS:C	2.64	0.41
1:E:310:GLU:O	1:E:313:ALA:HB3	2.20	0.41
1:A:159:PHE:HE2	1:A:193:GLN:HB3	1.84	0.41
1:C:2:PHE:CB	1:C:5:ILE:HD12	2.49	0.41
1:F:70:GLY:HA3	1:F:99:ALA:HB3	2.02	0.41
1:H:36:TYR:CE2	1:H:314:MET:HG2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:ILE:CG2	1:B:274:GLN:HG3	2.51	0.41
1:A:277:SER:HB2	1:B:8:TYR:CD1	2.55	0.41
1:A:326:LYS:NZ	7:A:580:HOH:O	2.39	0.41
1:B:39:GLU:H	1:B:39:GLU:CD	2.28	0.41
1:B:105:GLY:O	1:B:109:VAL:HG23	2.21	0.41
1:B:176:LEU:HA	1:B:176:LEU:HD12	1.76	0.41
1:D:275:LEU:HD23	1:D:275:LEU:HA	1.96	0.41
1:E:69:ALA:O	1:E:75:ARG:HD2	2.21	0.41
1:E:71:LEU:O	1:E:75:ARG:HG3	2.21	0.41
1:E:108:LYS:HE2	1:F:282:ILE:HG12	2.02	0.41
1:E:157:ILE:CD1	1:E:187:VAL:HG11	2.51	0.41
1:E:236:LEU:HD23	1:E:236:LEU:HA	1.89	0.41
1:F:81:LEU:HA	1:F:81:LEU:HD12	1.87	0.41
1:F:356:GLU:O	1:F:359[B]:GLU:HG3	2.21	0.41
1:H:385:ILE:HD12	1:H:385:ILE:HA	1.72	0.41
1:A:76:LYS:HE3	7:A:540:HOH:O	2.21	0.41
1:C:353:LEU:CD1	1:C:361:LEU:HD12	2.44	0.41
1:D:48:CYS:SG	1:D:307:TRP:HB2	2.61	0.41
1:D:125:VAL:HB	1:D:129:THR:HG21	2.03	0.41
1:D:381:ASN:OD1	1:D:381:ASN:C	2.64	0.41
1:E:244:PHE:HB2	1:E:255:VAL:CG2	2.46	0.41
1:G:333:ILE:HD12	1:G:393:VAL:HG22	2.02	0.41
1:B:53:GLU:OE2	1:B:289:HIS:NE2	2.39	0.40
1:B:125:VAL:HG12	1:B:176:LEU:HD23	2.03	0.40
1:D:68:MET:HE3	1:D:68:MET:HB2	1.90	0.40
1:E:82:LEU:HD23	1:E:82:LEU:HA	1.72	0.40
1:A:267:GLU:OE1	1:B:2:PHE:N	2.50	0.40
1:E:19:LYS:HD3	1:E:368:TYR:CE2	2.56	0.40
1:E:284:SER:HB3	7:E:550:HOH:O	2.20	0.40
1:F:283:TYR:O	1:F:284:SER:HB2	2.19	0.40
1:G:375:MET:HE2	1:G:375:MET:HB3	1.88	0.40
1:H:157:ILE:CD1	1:H:187:VAL:HG12	2.50	0.40
1:B:112:GLU:HG2	1:B:140:CYS:SG	2.61	0.40
1:D:177:LEU:O	1:D:179:PRO:HD3	2.21	0.40
1:D:271:VAL:O	1:D:272:PHE:C	2.65	0.40
1:D:317:ARG:HH11	1:D:317:ARG:HG2	1.86	0.40
1:F:100:THR:HG21	1:F:106:ALA:HA	2.02	0.40
1:G:254:ARG:NH1	1:H:65:TYR:HE2	2.18	0.40
1:A:70:GLY:HA3	1:A:99:ALA:HB3	2.04	0.40
1:B:211:ASP:OD2	3:B:401:PLP:H2A3	2.22	0.40
1:C:300:ASP:OD2	1:C:300:ASP:C	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:ARG:HG3	1:C:338:PHE:CZ	2.57	0.40
1:D:100:THR:HB	7:D:503:HOH:O	2.22	0.40
1:F:293:VAL:O	1:F:297:VAL:HG23	2.21	0.40
1:G:24:ASN:HD22	1:G:24:ASN:HA	1.72	0.40
1:G:25:ASN:O	1:G:28:LYS:HD3	2.20	0.40
1:C:37:TYR:O	1:C:317:ARG:NH2	2.54	0.40
1:D:255:VAL:HG23	1:D:255:VAL:O	2.22	0.40
1:E:106:ALA:HB3	1:E:241:SER:HB2	2.03	0.40
1:E:246[A]:LYS:HG3	1:E:251:TYR:HE1	1.86	0.40
1:G:73:GLY:HA3	1:G:295:ASP:OD1	2.22	0.40
1:G:185:THR:HA	1:G:350:PHE:CD2	2.57	0.40
1:H:68:MET:HE3	1:H:68:MET:HB2	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	398/398 (100%)	377 (95%)	21 (5%)	0	100	100
1	B	401/398 (101%)	383 (96%)	18 (4%)	0	100	100
1	C	398/398 (100%)	374 (94%)	23 (6%)	1 (0%)	36	56
1	D	396/398 (100%)	377 (95%)	19 (5%)	0	100	100
1	E	399/398 (100%)	373 (94%)	26 (6%)	0	100	100
1	F	399/398 (100%)	380 (95%)	19 (5%)	0	100	100
1	G	398/398 (100%)	372 (94%)	26 (6%)	0	100	100
1	H	398/398 (100%)	371 (93%)	27 (7%)	0	100	100
All	All	3187/3184 (100%)	3007 (94%)	179 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	333	ILE

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	339/337 (101%)	307 (91%)	32 (9%)	8	16
1	B	342/337 (102%)	317 (93%)	25 (7%)	13	24
1	C	339/337 (101%)	305 (90%)	34 (10%)	7	14
1	D	337/337 (100%)	310 (92%)	27 (8%)	11	20
1	E	340/337 (101%)	315 (93%)	25 (7%)	13	24
1	F	340/337 (101%)	316 (93%)	24 (7%)	13	25
1	G	339/337 (101%)	311 (92%)	28 (8%)	10	19
1	H	339/337 (101%)	320 (94%)	19 (6%)	19	36
All	All	2715/2696 (101%)	2501 (92%)	214 (8%)	11	21

All (214) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	5	ILE
1	A	13	ILE
1	A	20	PHE
1	A	23	ASP
1	A	35	ILE
1	A	42	VAL
1	A	50	LYS
1	A	51	ILE
1	A	60	ILE
1	A	76	LYS
1	A	86	ASP
1	A	116	GLU
1	A	176	LEU
1	A	178	HIS

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Mol	Chain	Res	Type
1	A	229	ARG
1	A	236	LEU
1	A	242	ASN
1	A	250	LEU
1	A	262	CYS
1	A	329	LEU
1	A	333	ILE
1	A	347	MET
1	A	350	PHE
1	A	360	ARG
1	A	370	ILE
1	A	371	SER
1	A	375	MET
1	A	385	ILE
1	A	394	ASP
1	A	395	VAL
1	A	397	LYS
1	B	4[A]	ARG
1	B	4[B]	ARG
1	B	13	ILE
1	B	24	ASN
1	B	33	ILE
1	B	35	ILE
1	B	39	GLU
1	B	120	GLN
1	B	132	ASN
1	B	143	GLU
1	B	146	LYS
1	B	152	THR
1	B	157	ILE
1	B	177	LEU
1	B	178	HIS
1	B	219	GLU
1	B	250	LEU
1	B	255	VAL
1	B	318	ILE
1	B	353	LEU
1	B	360	ARG
1	B	370	ILE
1	B	371	SER
1	B	385	ILE
1	B	398	ASP

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Mol	Chain	Res	Type
1	C	1	MET
1	C	4	ARG
1	C	11	ASP
1	C	13	ILE
1	C	28	LYS
1	C	33	ILE
1	C	39	GLU
1	C	50	LYS
1	C	85	LYS
1	C	116	GLU
1	C	152	THR
1	C	157	ILE
1	C	170	ASN
1	C	174	VAL
1	C	212	ILE
1	C	229	ARG
1	C	242	ASN
1	C	251	TYR
1	C	265	VAL
1	C	308	VAL
1	C	332	LYS
1	C	334	SER
1	C	336	ARG
1	C	341	LEU
1	C	350	PHE
1	C	358	VAL
1	C	369	MET
1	C	370	ILE
1	C	371	SER
1	C	374	ARG
1	C	382[A]	SER
1	C	382[B]	SER
1	C	386	ASP
1	C	394	ASP
1	D	1	MET
1	D	3	GLU
1	D	5	ILE
1	D	13	ILE
1	D	16	LEU
1	D	39	GLU
1	D	50	LYS
1	D	101	ILE

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Mol	Chain	Res	Type
1	D	146	LYS
1	D	157	ILE
1	D	175	LEU
1	D	178	HIS
1	D	203	GLU
1	D	223	SER
1	D	228	ILE
1	D	250	LEU
1	D	266	ASP
1	D	268	THR
1	D	324	LYS
1	D	329	LEU
1	D	334	SER
1	D	353	LEU
1	D	360	ARG
1	D	363	SER
1	D	365	PHE
1	D	395	VAL
1	D	398	ASP
1	E	27	ASP
1	E	35	ILE
1	E	42	VAL
1	E	89	VAL
1	E	101	ILE
1	E	114	ILE
1	E	146	LYS
1	E	176	LEU
1	E	191	ARG
1	E	197	VAL
1	E	202	GLN
1	E	204	ARG
1	E	212	ILE
1	E	219	GLU
1	E	223	SER
1	E	240	VAL
1	E	262	CYS
1	E	285	SER
1	E	336	ARG
1	E	350	PHE
1	E	370	ILE
1	E	385	ILE
1	E	386	ASP

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Mol	Chain	Res	Type
1	E	395	VAL
1	E	398	ASP
1	F	4	ARG
1	F	13	ILE
1	F	14	LEU
1	F	16	LEU
1	F	27	ASP
1	F	35	ILE
1	F	42	VAL
1	F	63	ARG
1	F	85	LYS
1	F	86	ASP
1	F	101	ILE
1	F	116	GLU
1	F	132	ASN
1	F	146	LYS
1	F	152	THR
1	F	176	LEU
1	F	191	ARG
1	F	203	GLU
1	F	210	MET
1	F	219	GLU
1	F	242	ASN
1	F	250	LEU
1	F	334	SER
1	F	362	GLN
1	G	13	ILE
1	G	16	LEU
1	G	33	ILE
1	G	35	ILE
1	G	42	VAL
1	G	59	PRO
1	G	85	LYS
1	G	101	ILE
1	G	116	GLU
1	G	125	VAL
1	G	132	ASN
1	G	146	LYS
1	G	154	THR
1	G	157	ILE
1	G	158	LYS
1	G	238	LEU

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Mol	Chain	Res	Type
1	G	242	ASN
1	G	318	ILE
1	G	329	LEU
1	G	341	LEU
1	G	350	PHE
1	G	356	GLU
1	G	362	GLN
1	G	371	SER
1	G	385	ILE
1	G	393	VAL
1	G	395	VAL
1	G	398	ASP
1	H	3	GLU
1	H	14	LEU
1	H	33	ILE
1	H	35	ILE
1	H	42	VAL
1	H	63	ARG
1	H	94	LEU
1	H	143	GLU
1	H	157	ILE
1	H	180	CYS
1	H	280	ARG
1	H	285	SER
1	H	292	ARG
1	H	317	ARG
1	H	336	ARG
1	H	347	MET
1	H	350	PHE
1	H	353	LEU
1	H	356	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	178	HIS
1	A	345	ASN
1	B	24	ASN
1	B	132	ASN
1	B	202	GLN
1	B	304	HIS

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Mol	Chain	Res	Type
1	B	345	ASN
1	C	132	ASN
1	C	242	ASN
1	C	304	HIS
1	C	337	ASN
1	C	345	ASN
1	C	357	GLN
1	C	362	GLN
1	D	24	ASN
1	D	170	ASN
1	D	242	ASN
1	D	306	GLN
1	D	362	GLN
1	E	120	GLN
1	E	199	ASN
1	E	304	HIS
1	E	345	ASN
1	E	390	ASN
1	F	24	ASN
1	F	132	ASN
1	F	345	ASN
1	G	24	ASN
1	G	74	HIS
1	G	132	ASN
1	G	202	GLN
1	G	276	ASN
1	G	304	HIS
1	G	306	GLN
1	G	345	ASN
1	G	390	ASN
1	H	24	ASN
1	H	132	ASN
1	H	274	GLN
1	H	306	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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$
3	PLP	C	402	1	15,15,16	4.12	4 (26%)	21,22,23	2.75	9 (42%)
3	PLP	B	401	1	15,15,16	3.34	4 (26%)	21,22,23	2.93	11 (52%)
5	OAA	E	403	-	8,8,8	2.47	2 (25%)	8,10,10	1.74	3 (37%)
3	PLP	E	402[A]	1	15,15,16	3.29	4 (26%)	21,22,23	1.71	3 (14%)
4	KET	E	404[B]	-	22,24,24	1.28	1 (4%)	21,34,34	2.76	5 (23%)
6	PMP	D	401	-	16,16,16	2.86	3 (18%)	22,23,23	1.79	4 (18%)
4	KET	A	403[B]	-	22,24,24	1.32	3 (13%)	21,34,34	1.90	5 (23%)
6	PMP	H	401	-	16,16,16	3.87	4 (25%)	22,23,23	1.91	6 (27%)
4	KET	G	402	-	22,24,24	1.50	5 (22%)	21,34,34	2.83	9 (42%)
3	PLP	A	402[A]	1	15,15,16	3.43	3 (20%)	21,22,23	1.73	7 (33%)
5	OAA	C	403	-	8,8,8	2.26	1 (12%)	8,10,10	1.82	3 (37%)
3	PLP	F	401	1	15,15,16	4.01	3 (20%)	21,22,23	2.22	6 (28%)

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
3	PLP	C	402	1	-	3/6/6/8	0/1/1/1
3	PLP	B	401	1	-	3/6/6/8	0/1/1/1
5	OAA	E	403	-	-	3/8/8/8	-
3	PLP	E	402[A]	1	-	5/6/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	KET	E	404[B]	-	-	11/18/19/19	0/1/1/1
6	PMP	D	401	-	-	4/8/8/8	0/1/1/1
4	KET	A	403[B]	-	-	7/18/19/19	0/1/1/1
6	PMP	H	401	-	-	7/8/8/8	0/1/1/1
4	KET	G	402	-	-	6/18/19/19	0/1/1/1
3	PLP	A	402[A]	1	-	2/6/6/8	0/1/1/1
5	OAA	C	403	-	-	5/8/8/8	-
3	PLP	F	401	1	-	2/6/6/8	0/1/1/1

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	401	PLP	C5-C4	11.70	1.53	1.40
6	H	401	PMP	C3-C2	11.62	1.53	1.41
3	B	401	PLP	C3-C2	10.35	1.51	1.41
3	C	402	PLP	C3-C2	9.74	1.51	1.41
3	C	402	PLP	C5-C4	9.32	1.51	1.40
3	A	402[A]	PLP	C3-C2	8.71	1.50	1.41
3	A	402[A]	PLP	C5-C4	8.41	1.50	1.40
3	E	402[A]	PLP	C5-C4	8.19	1.49	1.40
3	E	402[A]	PLP	C3-C2	7.97	1.49	1.41
3	F	401	PLP	C3-C2	7.62	1.48	1.41
3	C	402	PLP	C3-C4	7.59	1.54	1.40
6	D	401	PMP	C3-C4	7.39	1.50	1.40
6	H	401	PMP	C3-C4	6.99	1.50	1.40
6	H	401	PMP	C5-C4	6.81	1.50	1.40
6	D	401	PMP	C5-C4	6.51	1.49	1.40
3	F	401	PLP	C3-C4	6.19	1.51	1.40
5	E	403	OAA	C3-C4	-6.14	1.44	1.53
5	C	403	OAA	C3-C4	-5.59	1.45	1.53
6	D	401	PMP	C3-C2	5.49	1.46	1.41
3	B	401	PLP	C5-C4	5.47	1.46	1.40
3	A	402[A]	PLP	C3-C4	5.12	1.49	1.40
3	E	402[A]	PLP	C3-C4	4.46	1.48	1.40
3	B	401	PLP	C3-C4	3.91	1.47	1.40
4	G	402	KET	CA-C	-3.02	1.48	1.52
4	E	404[B]	KET	C4A-C4	2.98	1.50	1.45
4	A	403[B]	KET	CA-C	-2.95	1.48	1.52
4	G	402	KET	OP4-C5A	-2.74	1.40	1.43
4	A	403[B]	KET	C4A-C4	2.54	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	PLP	C2-N1	2.47	1.38	1.33
3	E	402[A]	PLP	P-O3P	-2.32	1.46	1.54
4	A	403[B]	KET	C2-N1	-2.30	1.34	1.39
4	G	402	KET	OD2-CG	-2.19	1.23	1.30
4	G	402	KET	C4A-N	-2.15	1.24	1.27
4	G	402	KET	C4A-C4	2.12	1.49	1.45
5	E	403	OAA	O5-C4	-2.11	1.24	1.30
3	B	401	PLP	C6-C5	2.09	1.41	1.37
6	H	401	PMP	C2-N1	2.01	1.37	1.33

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	404[B]	KET	CA-N-C4A	10.26	139.33	117.01
4	G	402	KET	CA-N-C4A	7.61	133.57	117.01
3	B	401	PLP	C6-C5-C4	6.57	123.48	118.10
3	C	402	PLP	C6-C5-C4	6.45	123.38	118.10
3	B	401	PLP	C5A-C5-C4	-6.06	110.68	122.64
4	G	402	KET	OP4-P-OP1	-5.73	90.96	106.44
3	F	401	PLP	O4P-C5A-C5	5.69	120.02	109.36
4	A	403[B]	KET	CB-CA-C	-5.28	99.62	110.35
6	D	401	PMP	O4P-C5A-C5	5.09	118.89	109.36
3	B	401	PLP	O3P-P-O4P	-4.97	93.71	106.67
3	C	402	PLP	O2P-P-O4P	-4.55	94.79	106.67
4	G	402	KET	C2A-C2-N1	4.37	119.02	112.46
6	H	401	PMP	C2A-C2-C3	4.35	125.89	120.80
3	C	402	PLP	C4A-C4-C3	4.35	127.77	120.52
3	C	402	PLP	C3-C4-C5	-4.17	113.58	118.59
3	F	401	PLP	C3-C4-C5	-4.08	113.69	118.59
3	B	401	PLP	C5A-C5-C6	3.97	125.83	119.36
3	E	402[A]	PLP	C4A-C4-C5	3.90	124.97	120.94
4	G	402	KET	C2A-C2-C3	-3.72	119.71	125.54
4	E	404[B]	KET	C2A-C2-N1	3.59	117.85	112.46
3	B	401	PLP	C3-C4-C5	-3.57	114.31	118.59
3	F	401	PLP	C5A-C5-C6	-3.51	113.64	119.36
3	A	402[A]	PLP	C5A-C5-C6	-3.47	113.71	119.36
3	F	401	PLP	O3P-P-O2P	3.37	120.44	107.80
4	G	402	KET	O3-C3-C2	3.35	121.60	118.29
3	C	402	PLP	O3-C3-C4	3.21	126.48	118.10
6	H	401	PMP	C6-C5-C4	3.19	120.47	118.06
6	H	401	PMP	O3-C3-C2	3.12	124.04	117.58
4	E	404[B]	KET	C2A-C2-C3	-3.12	120.66	125.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	403	OAA	O1-C1-C2	-3.03	113.48	122.11
6	H	401	PMP	O3P-P-O2P	2.99	119.01	107.80
6	D	401	PMP	C6-N1-C2	2.87	124.41	119.20
6	D	401	PMP	C3-C4-C5	-2.81	116.18	118.73
3	F	401	PLP	C5A-C5-C4	2.80	128.16	122.64
3	F	401	PLP	O3-C3-C4	2.79	125.38	118.10
6	H	401	PMP	C6-N1-C2	2.79	124.25	119.20
4	E	404[B]	KET	C-CA-N	2.79	115.09	108.22
3	B	401	PLP	C4A-C4-C3	2.78	125.16	120.52
5	C	403	OAA	O4-C4-C3	-2.71	118.44	121.81
4	A	403[B]	KET	CA-N-C4A	2.71	122.91	117.01
3	E	402[A]	PLP	C5A-C5-C6	-2.71	114.94	119.36
3	B	401	PLP	O3P-P-O2P	2.69	117.89	107.80
4	E	404[B]	KET	OP3-P-OP4	-2.69	99.67	106.67
5	E	403	OAA	O3-C3-C2	2.66	124.51	120.41
3	A	402[A]	PLP	C3-C4-C5	-2.63	115.44	118.59
6	D	401	PMP	O2P-P-O4P	-2.55	100.02	106.67
3	B	401	PLP	O3-C3-C2	2.53	122.83	117.58
3	C	402	PLP	C6-N1-C2	2.50	123.73	119.20
5	E	403	OAA	O4-C4-C3	-2.48	118.72	121.81
4	A	403[B]	KET	C2A-C2-N1	2.45	116.15	112.46
3	C	402	PLP	C5A-C5-C4	-2.45	117.80	122.64
3	C	402	PLP	O2P-P-O1P	2.43	120.32	110.83
3	A	402[A]	PLP	C4A-C4-C5	2.39	123.40	120.94
3	A	402[A]	PLP	C6-C5-C4	2.38	120.04	118.10
4	G	402	KET	C-CA-N	2.36	114.04	108.22
3	B	401	PLP	O3P-P-O1P	2.34	119.95	110.83
6	H	401	PMP	C3-C4-C5	-2.33	116.62	118.73
3	E	402[A]	PLP	C6-N1-C2	2.32	123.41	119.20
4	A	403[B]	KET	OD1-CG-CB	-2.31	115.75	122.84
3	B	401	PLP	C2A-C2-C3	-2.31	118.10	120.80
4	G	402	KET	OP3-P-OP2	2.29	116.39	107.80
4	G	402	KET	OP3-P-OP1	2.29	119.74	110.83
3	A	402[A]	PLP	O4P-C5A-C5	2.24	113.55	109.36
3	C	402	PLP	C4A-C4-C5	-2.23	118.64	120.94
3	A	402[A]	PLP	C6-N1-C2	2.20	123.19	119.20
3	A	402[A]	PLP	C2A-C2-C3	2.20	123.37	120.80
3	B	401	PLP	O4P-P-O1P	-2.15	100.62	106.44
4	G	402	KET	CB-CA-N	2.14	112.81	109.56
4	A	403[B]	KET	CB-CA-N	-2.08	106.42	109.56
5	C	403	OAA	O5-C4-C3	2.05	119.29	113.59
5	E	403	OAA	O2-C1-C2	2.01	120.73	114.51

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402[A]	PLP	C4-C5-C5A-O4P
3	A	402[A]	PLP	C6-C5-C5A-O4P
3	B	401	PLP	C5A-O4P-P-O1P
3	B	401	PLP	C5A-O4P-P-O2P
3	B	401	PLP	C5A-O4P-P-O3P
3	C	402	PLP	C5A-O4P-P-O1P
3	C	402	PLP	C5A-O4P-P-O2P
3	C	402	PLP	C5A-O4P-P-O3P
3	E	402[A]	PLP	C4-C5-C5A-O4P
3	E	402[A]	PLP	C6-C5-C5A-O4P
3	E	402[A]	PLP	C5A-O4P-P-O2P
3	E	402[A]	PLP	C5A-O4P-P-O3P
3	F	401	PLP	C4-C5-C5A-O4P
3	F	401	PLP	C6-C5-C5A-O4P
4	A	403[B]	KET	C5A-OP4-P-OP2
4	A	403[B]	KET	C5A-OP4-P-OP3
4	A	403[B]	KET	N-CA-CB-CG
4	A	403[B]	KET	C-CA-CB-CG
4	E	404[B]	KET	C3-C4-C4A-N
4	E	404[B]	KET	C5-C4-C4A-N
4	E	404[B]	KET	C4-C4A-N-CA
4	E	404[B]	KET	C5A-OP4-P-OP1
4	E	404[B]	KET	C5A-OP4-P-OP3
4	E	404[B]	KET	CB-CA-N-C4A
4	E	404[B]	KET	C-CA-N-C4A
4	G	402	KET	C-CA-N-C4A
4	G	402	KET	N-CA-CB-CG
4	G	402	KET	C-CA-CB-CG
5	C	403	OAA	C2-C3-C4-O5
5	E	403	OAA	C2-C3-C4-O5
6	D	401	PMP	C4-C5-C5A-O4P
6	D	401	PMP	C6-C5-C5A-O4P
6	H	401	PMP	C3-C4-C4A-N4A
6	H	401	PMP	C5-C4-C4A-N4A
6	H	401	PMP	C4-C5-C5A-O4P
6	H	401	PMP	C6-C5-C5A-O4P
6	H	401	PMP	C5A-O4P-P-O2P
6	H	401	PMP	C5A-O4P-P-O3P
3	E	402[A]	PLP	C5A-O4P-P-O1P
4	A	403[B]	KET	C5A-OP4-P-OP1

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Mol	Chain	Res	Type	Atoms
6	H	401	PMP	C5A-O4P-P-O1P
4	G	402	KET	OXT-C-CA-N
4	G	402	KET	O-C-CA-N
5	C	403	OAA	C1-C2-C3-O3
5	C	403	OAA	O3-C3-C4-O4
5	E	403	OAA	C1-C2-C3-O3
5	C	403	OAA	C2-C3-C4-O4
4	A	403[B]	KET	C4-C5-C5A-OP4
4	E	404[B]	KET	C4-C5-C5A-OP4
4	E	404[B]	KET	CA-CB-CG-OD1
4	E	404[B]	KET	CA-CB-CG-OD2
4	A	403[B]	KET	OXT-C-CA-N
5	C	403	OAA	O3-C3-C4-O5
4	G	402	KET	C3-C4-C4A-N
4	E	404[B]	KET	C5A-OP4-P-OP2
5	E	403	OAA	O1-C1-C2-C3
6	D	401	PMP	C3-C4-C4A-N4A
6	D	401	PMP	C5-C4-C4A-N4A

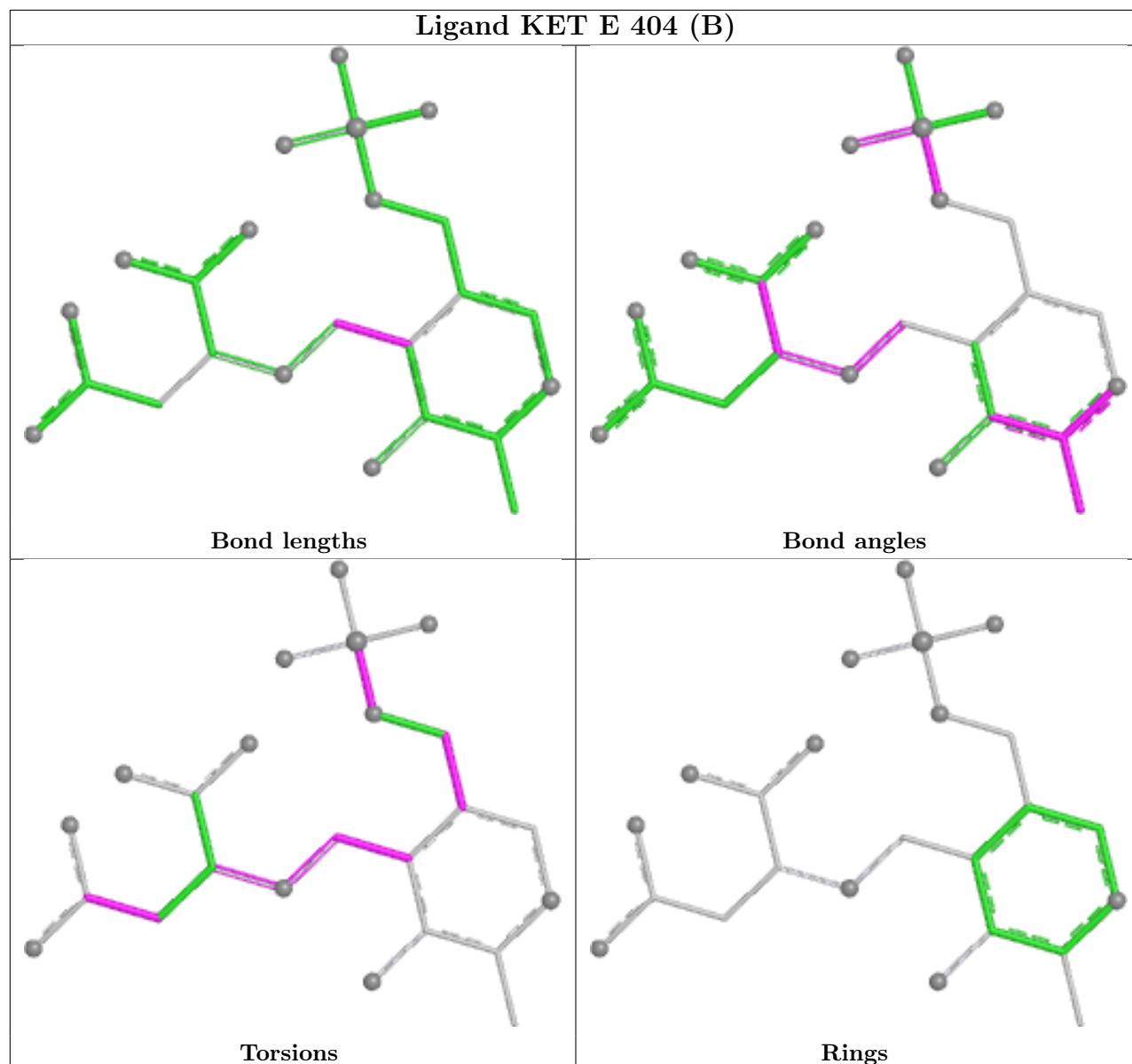
There are no ring outliers.

11 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	402	PLP	1	0
3	B	401	PLP	2	0
3	E	402[A]	PLP	1	0
4	E	404[B]	KET	12	0
6	D	401	PMP	8	0
4	A	403[B]	KET	5	0
6	H	401	PMP	3	0
4	G	402	KET	3	0
3	A	402[A]	PLP	1	0
5	C	403	OAA	1	0
3	F	401	PLP	2	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.



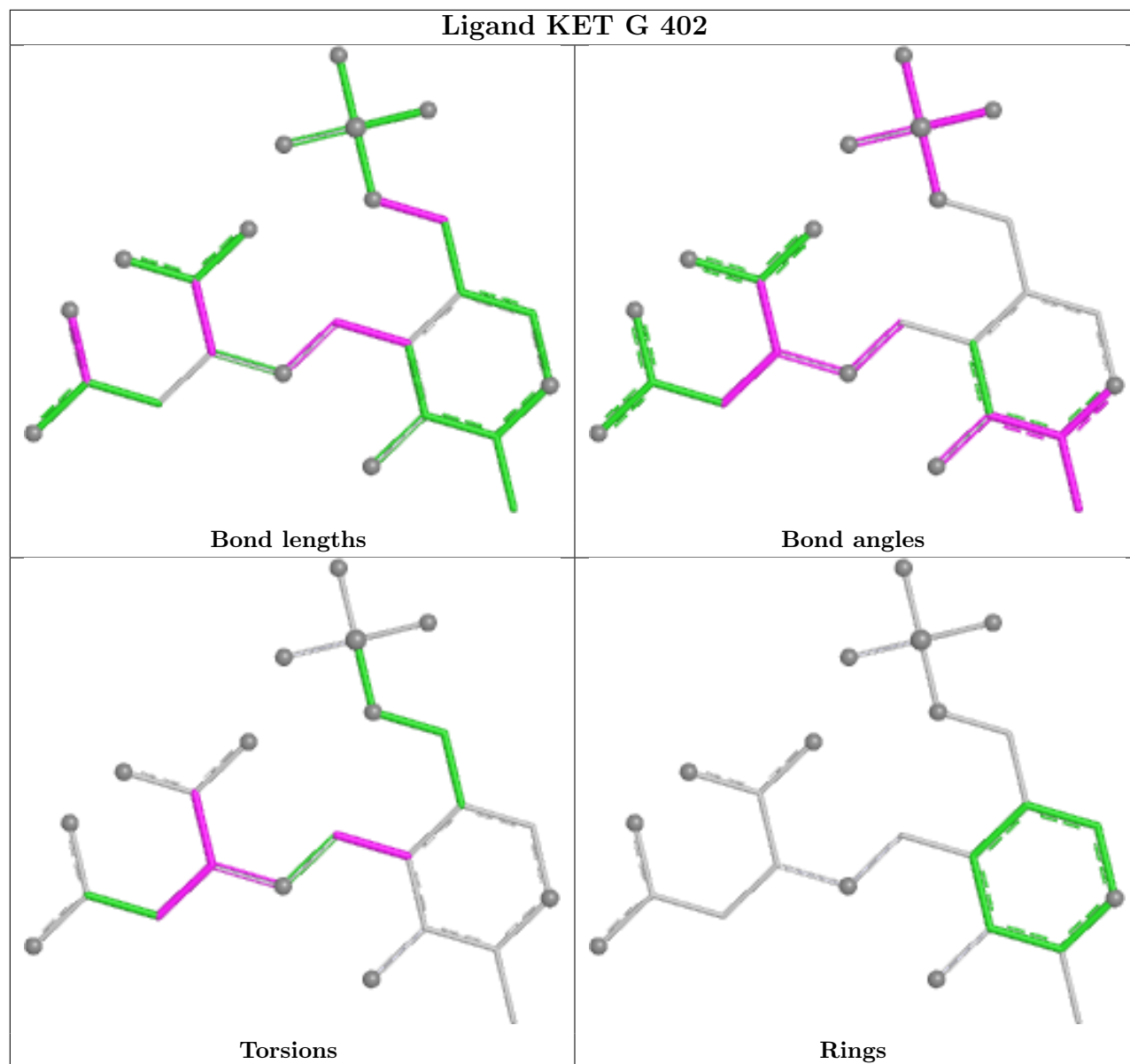
Ligand KET A 403 (B)

Bond lengths

Bond angles

Torsions

Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	398/398 (100%)	-0.34	2 (0%) 87 87	13, 36, 94, 128	2 (0%)
1	B	398/398 (100%)	-0.55	4 (1%) 79 79	13, 31, 64, 114	5 (1%)
1	C	398/398 (100%)	-0.31	0 100 100	22, 42, 86, 130	2 (0%)
1	D	398/398 (100%)	-0.63	0 100 100	17, 29, 55, 99	0
1	E	398/398 (100%)	-0.35	2 (0%) 87 87	18, 37, 89, 123	3 (0%)
1	F	398/398 (100%)	-0.53	0 100 100	17, 34, 61, 94	3 (0%)
1	G	398/398 (100%)	-0.25	1 (0%) 90 91	19, 45, 85, 112	2 (0%)
1	H	398/398 (100%)	-0.58	0 100 100	15, 31, 66, 93	2 (0%)
All	All	3184/3184 (100%)	-0.44	9 (0%) 90 91	13, 35, 78, 130	19 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	12	PRO	3.0
1	B	7	TYR	2.8
1	B	9	ALA	2.7
1	A	16	LEU	2.7
1	B	8	TYR	2.1
1	A	355	PRO	2.1
1	E	26	PRO	2.1
1	E	13	ILE	2.1
1	B	10	GLY	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

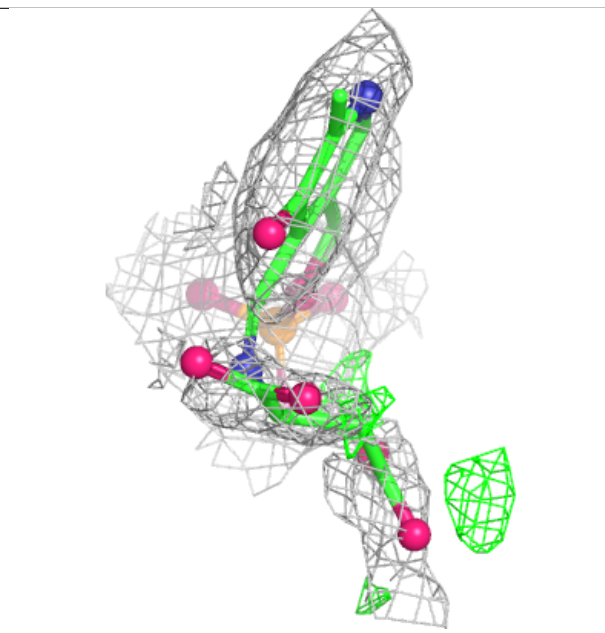
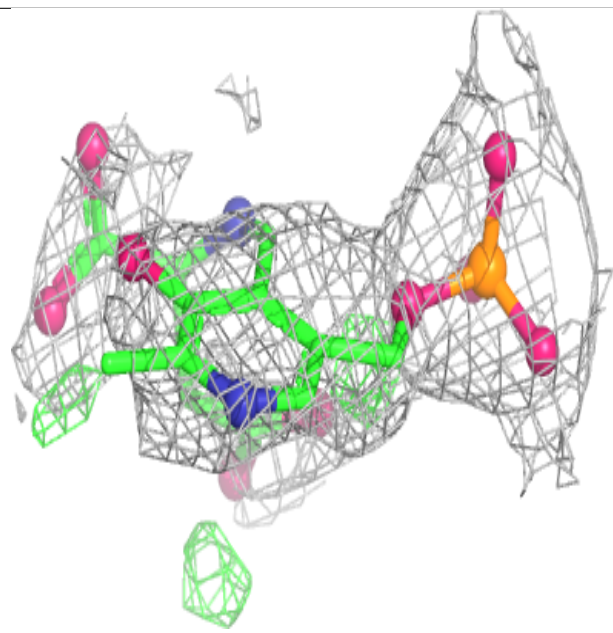
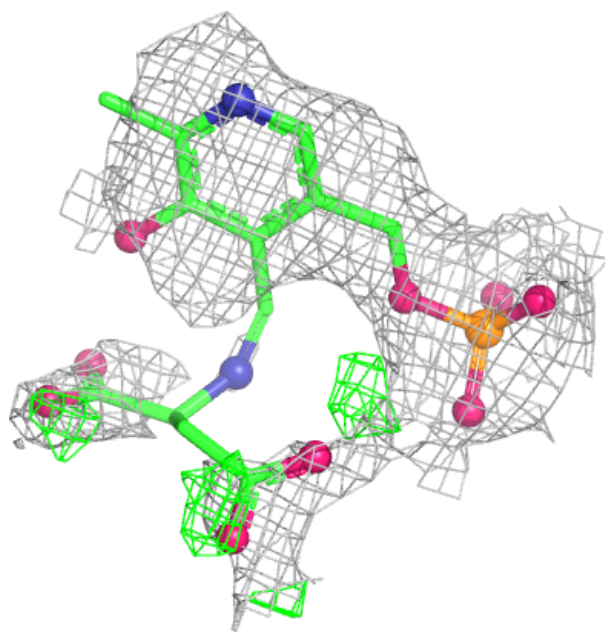
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	OAA	C	403	9/9	0.85	0.14	26,28,31,32	9
4	KET	E	404[B]	24/24	0.87	0.15	24,38,42,44	24
5	OAA	E	403	9/9	0.90	0.12	20,24,27,27	9
4	KET	A	403[B]	24/24	0.95	0.09	9,12,13,14	24
3	PLP	E	402[A]	15/16	0.96	0.11	30,61,71,71	15
3	PLP	A	402[A]	15/16	0.97	0.07	34,39,43,50	15
4	KET	G	402	24/24	0.97	0.08	27,45,90,102	0
3	PLP	C	402	15/16	0.98	0.07	21,35,46,48	0
2	MG	C	401	1/1	0.98	0.03	25,25,25,25	0
3	PLP	F	401	15/16	0.98	0.06	21,25,30,30	0
3	PLP	B	401	15/16	0.98	0.06	18,26,35,38	0
6	PMP	D	401	16/16	0.98	0.06	19,28,34,35	0
6	PMP	H	401	16/16	0.98	0.05	22,29,35,36	0
2	MG	A	401	1/1	0.99	0.05	15,15,15,15	0
2	MG	E	401	1/1	0.99	0.03	13,13,13,13	0
2	MG	G	401	1/1	1.00	0.01	19,19,19,19	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.

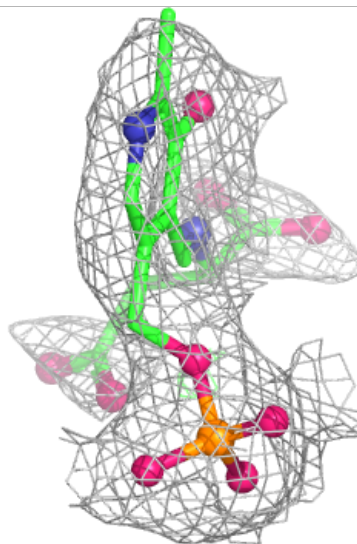
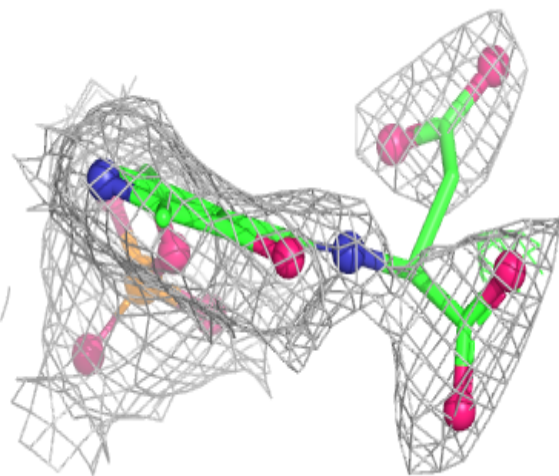
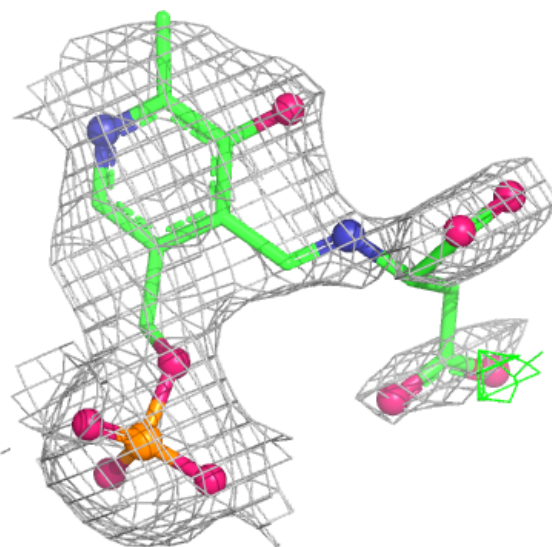
Electron density around KET E 404 (B):

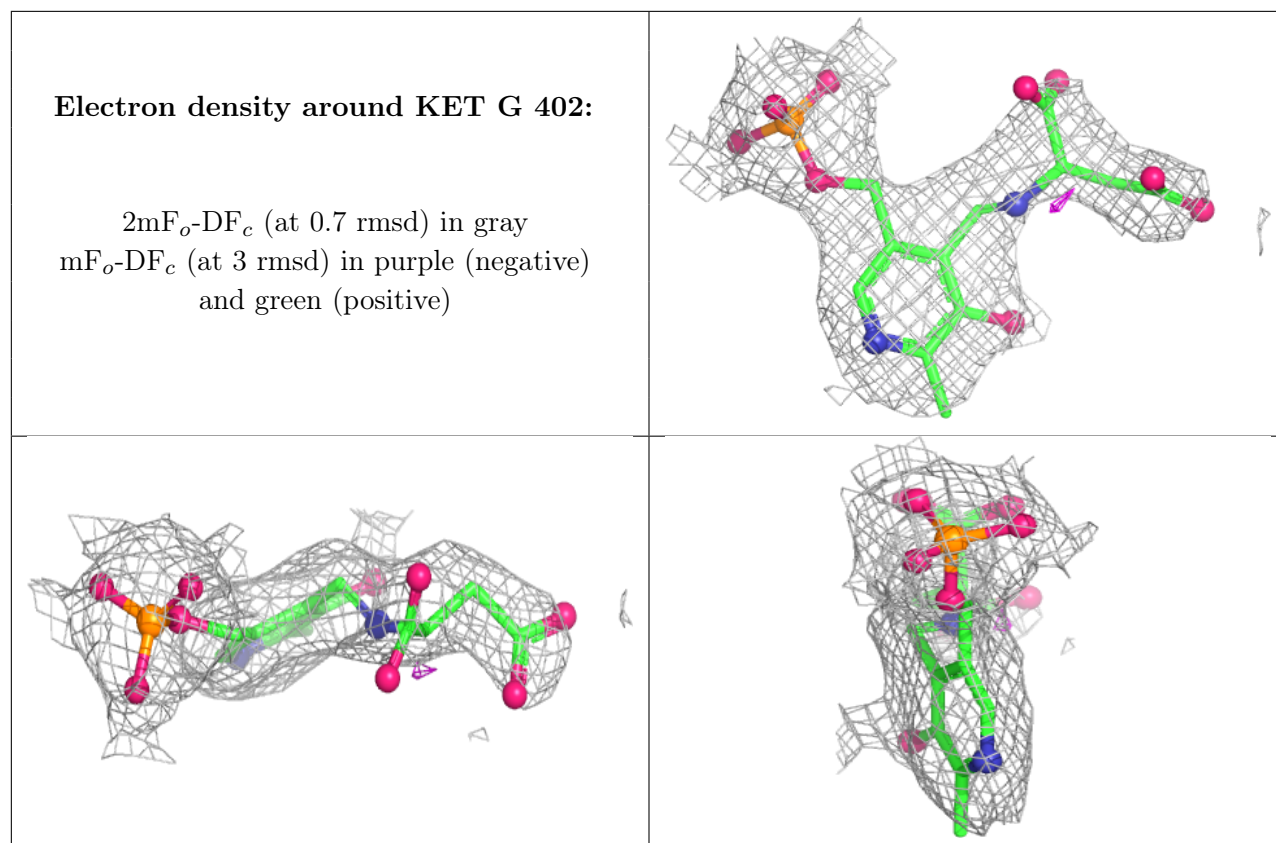
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around KET A 403 (B):

$2mF_o-DF_c$ (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.