



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:27 PM EDT

PDB ID : 3AXM / pdb_00003axm
Title : Structure of rice Rubisco in complex with 6PG
Authors : Matsumura, H.; Mizohata, E.; Ishida, H.; Kogami, A.; Ueno, T.; Makino, A.;
Inoue, T.; Yokota, A.; Mae, T.; Kai, Y.
Deposited on : 2011-04-11
Resolution : 1.65 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

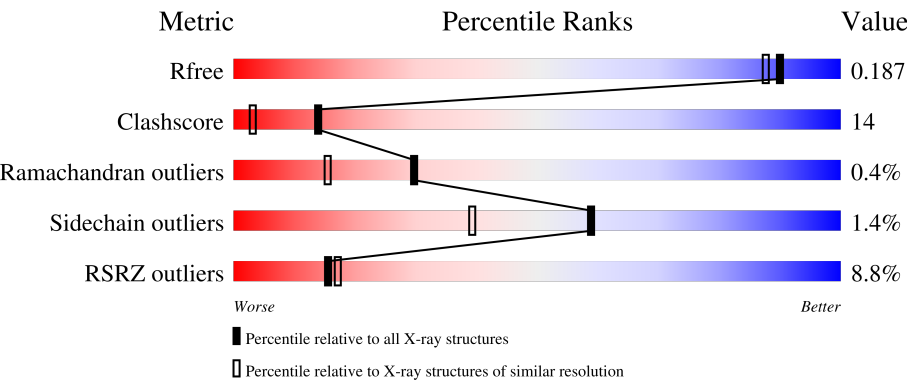
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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.



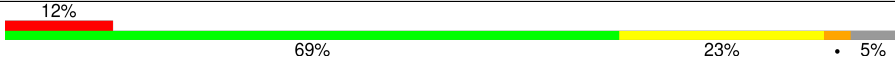
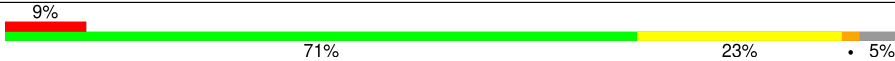
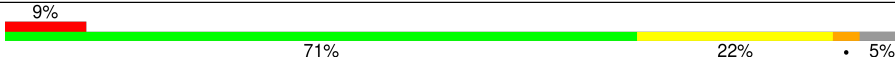
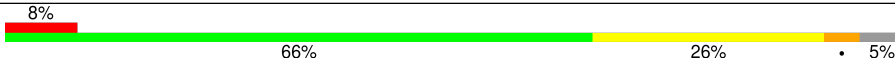
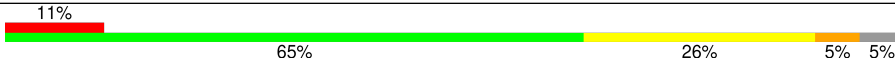
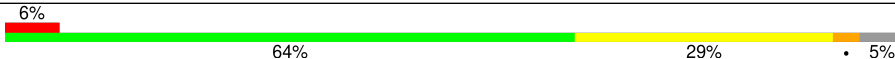
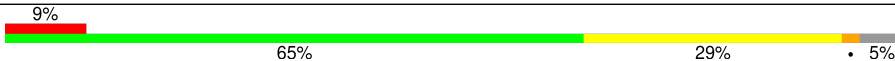
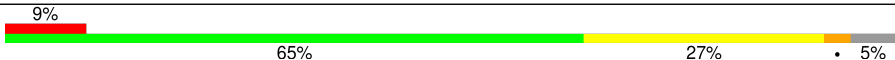
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	477	8% 72% 18% • 7%
1	B	477	8% 69% 22% • 7%
1	C	477	8% 71% 19% • 7%
1	D	477	7% 74% 17% • 7%
1	E	477	8% 73% 18% • 8%

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Mol	Chain	Length	Quality of chain
1	F	477	
1	G	477	
1	H	477	
2	S	129	
2	T	129	
2	U	129	
2	V	129	
2	W	129	
2	X	129	
2	Y	129	
2	Z	129	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 39557 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 Ribulose biphosphate carboxylase large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	0
			3464	2193	614	637	20			
1	B	443	Total	C	N	O	S	0	0	0
			3461	2192	613	636	20			
1	C	443	Total	C	N	O	S	0	0	0
			3459	2191	612	636	20			
1	D	444	Total	C	N	O	S	0	0	0
			3468	2197	614	637	20			
1	E	441	Total	C	N	O	S	0	0	0
			3445	2181	610	634	20			
1	F	444	Total	C	N	O	S	0	0	0
			3468	2197	614	637	20			
1	G	441	Total	C	N	O	S	0	0	0
			3445	2181	610	634	20			
1	H	444	Total	C	N	O	S	0	0	0
			3468	2197	614	637	20			

- Molecule 2 is a protein called Ribulose biphosphate carboxylase small chain, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S	123	Total	C	N	O	S	0	0	1
			1016	672	163	175	6			
2	T	123	Total	C	N	O	S	0	0	1
			1016	672	163	175	6			
2	U	123	Total	C	N	O	S	0	0	1
			1016	672	163	175	6			
2	V	123	Total	C	N	O	S	0	0	1
			1016	672	163	175	6			
2	W	123	Total	C	N	O	S	0	0	1
			1016	672	163	175	6			
2	X	123	Total	C	N	O	S	0	0	1
			1016	672	163	175	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	123	Total	C	N	O	S	0	0	1
			1016	672	163	175	6			
2	Z	123	Total	C	N	O	S	0	0	1
			1016	672	163	175	6			

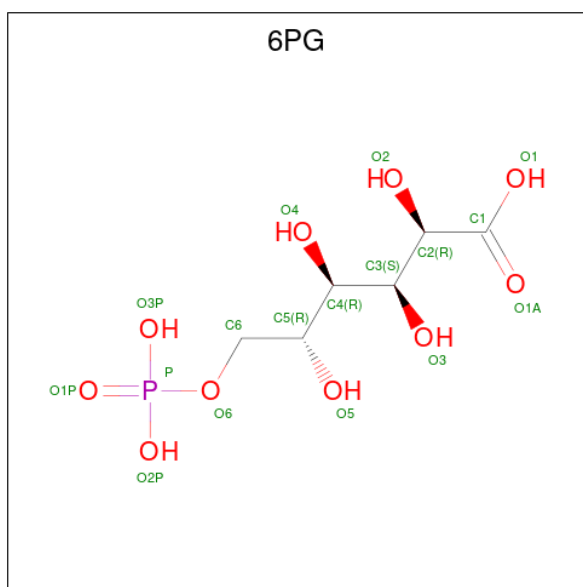
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	0	NME	-	amidation	UNP Q0INY7
T	0	NME	-	amidation	UNP Q0INY7
U	0	NME	-	amidation	UNP Q0INY7
V	0	NME	-	amidation	UNP Q0INY7
W	0	NME	-	amidation	UNP Q0INY7
X	0	NME	-	amidation	UNP Q0INY7
Y	0	NME	-	amidation	UNP Q0INY7
Z	0	NME	-	amidation	UNP Q0INY7

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		
3	G	1	Total	Mg	0	0
			1	1		
3	H	1	Total	Mg	0	0
			1	1		

- Molecule 4 is 6-PHOSPHOGLUCONIC ACID (CCD ID: 6PG) (formula: C₆H₁₃O₁₀P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			17	6	10	1		
4	B	1	Total	C	O	P	0	0
			17	6	10	1		
4	C	1	Total	C	O	P	0	0
			17	6	10	1		
4	D	1	Total	C	O	P	0	0
			17	6	10	1		
4	E	1	Total	C	O	P	0	0
			17	6	10	1		
4	F	1	Total	C	O	P	0	0
			17	6	10	1		
4	G	1	Total	C	O	P	0	0
			17	6	10	1		
4	H	1	Total	C	O	P	0	0
			17	6	10	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	309	Total	O	0	0
			309	309		
5	S	113	Total	O	0	0
			113	113		
5	B	345	Total	O	0	0
			345	345		
5	T	99	Total	O	0	0
			99	99		

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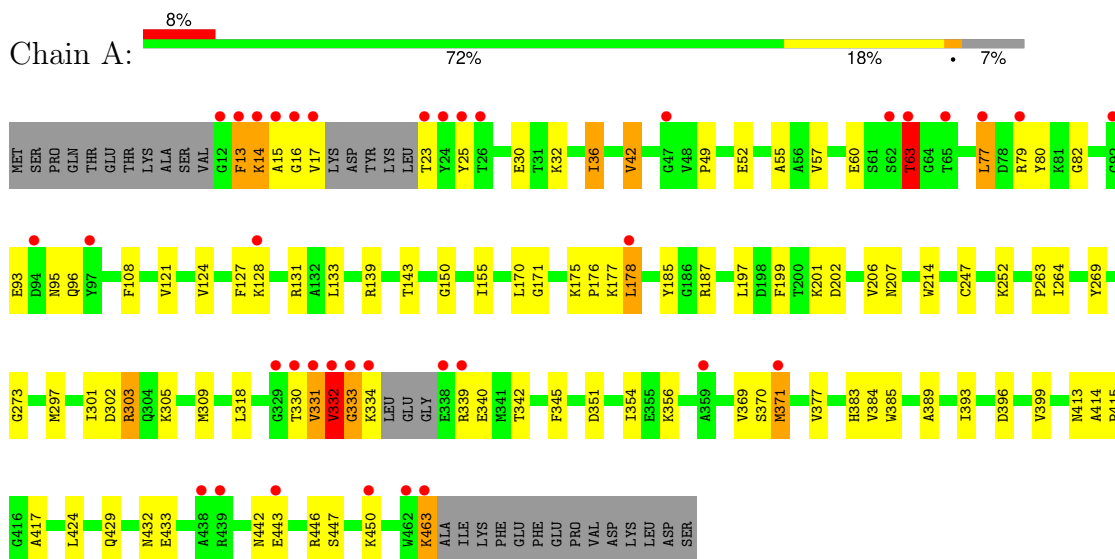
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	339	Total 339	O 339	0	0
5	U	125	Total 125	O 125	0	0
5	D	335	Total 335	O 335	0	0
5	V	123	Total 123	O 123	0	0
5	E	318	Total 318	O 318	0	0
5	W	122	Total 122	O 122	0	0
5	F	371	Total 371	O 371	0	0
5	X	115	Total 115	O 115	0	0
5	G	341	Total 341	O 341	0	0
5	Y	111	Total 111	O 111	0	0
5	H	326	Total 326	O 326	0	0
5	Z	115	Total 115	O 115	0	0

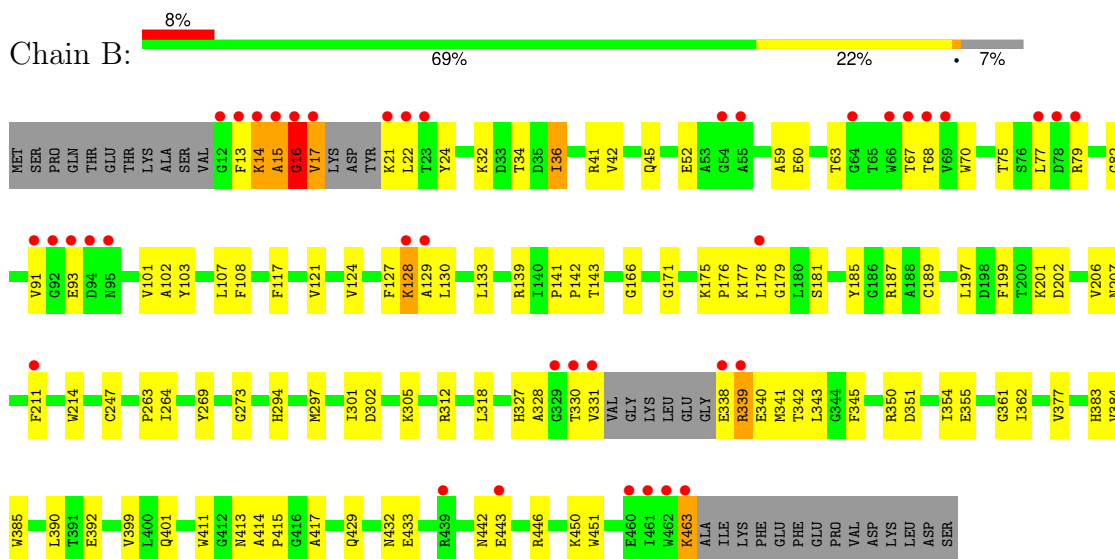
3 Residue-property plots [i](#)

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.

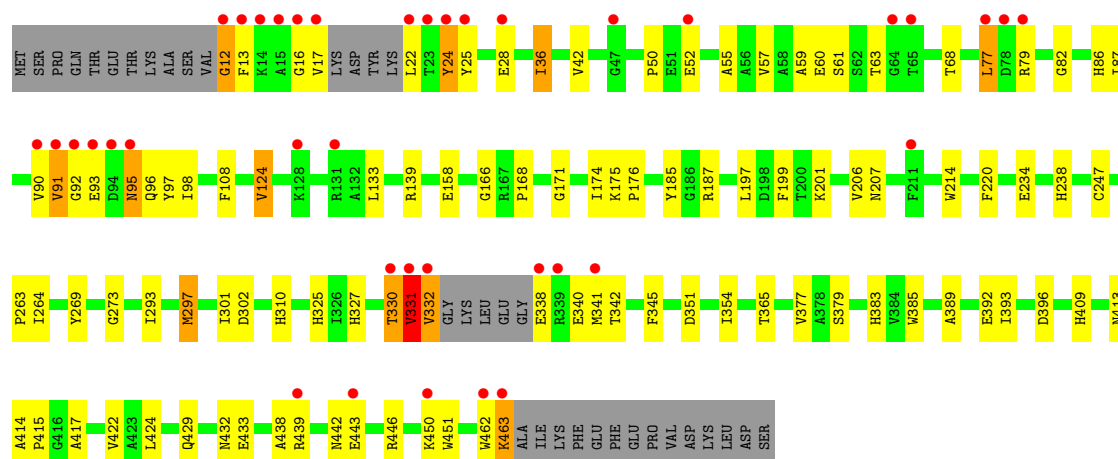
- Molecule 1: Ribulose biphosphate carboxylase large chain



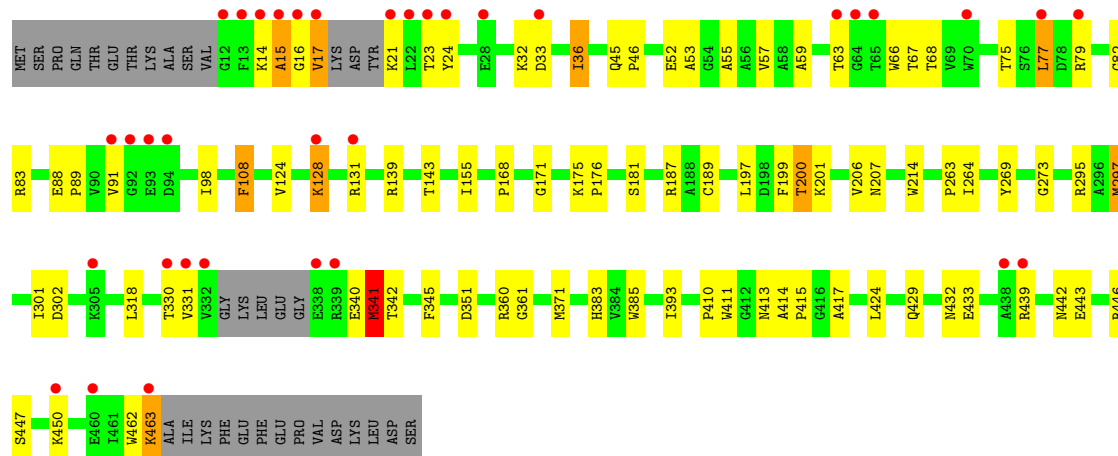
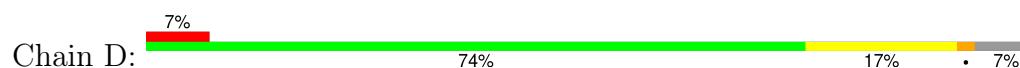
- Molecule 1: Ribulose biphosphate carboxylase large chain



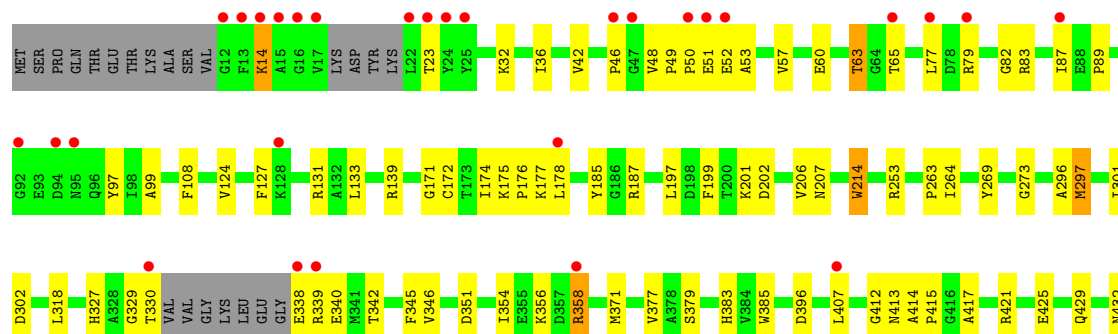
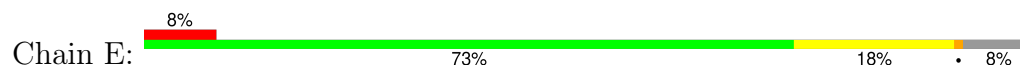
- Molecule 1: Ribulose biphosphate carboxylase large chain

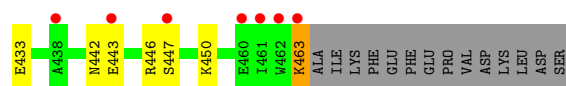


- Molecule 1: Ribulose biphosphate carboxylase large chain

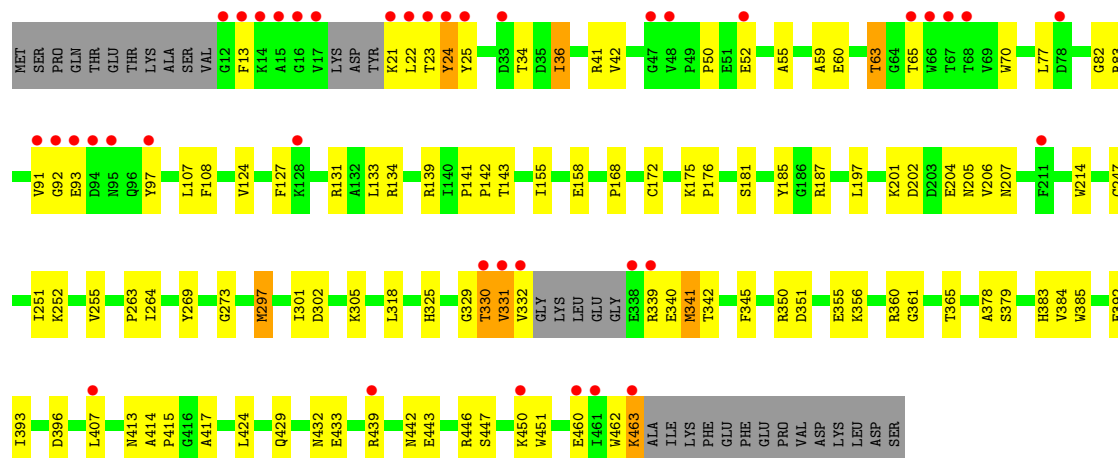


- Molecule 1: Ribulose biphosphate carboxylase large chain

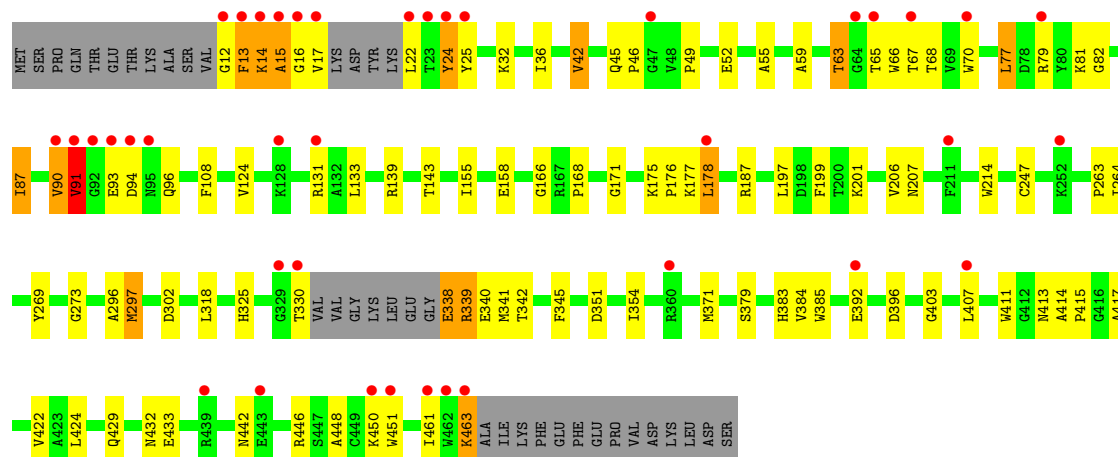




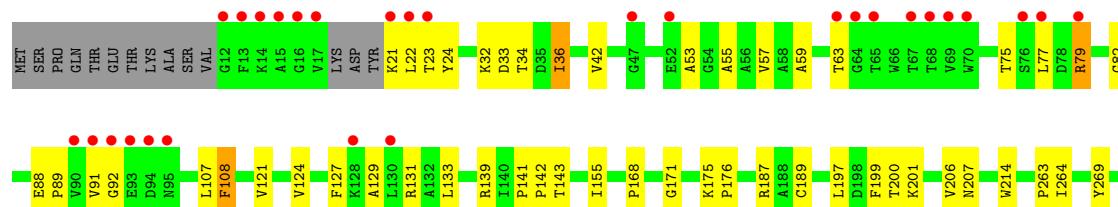
- Molecule 1: Ribulose biphosphate carboxylase large chain

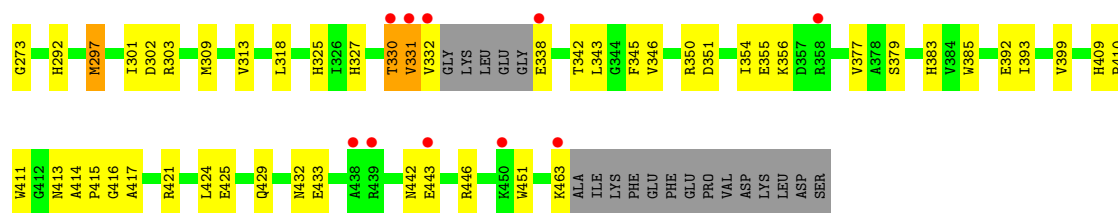


- Molecule 1: Ribulose biphosphate carboxylase large chain

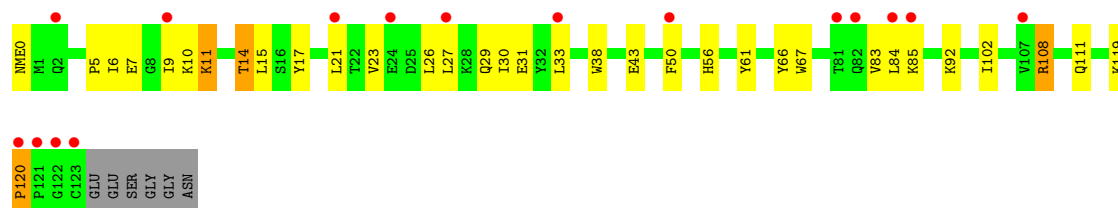


- Molecule 1: Ribulose biphosphate carboxylase large chain

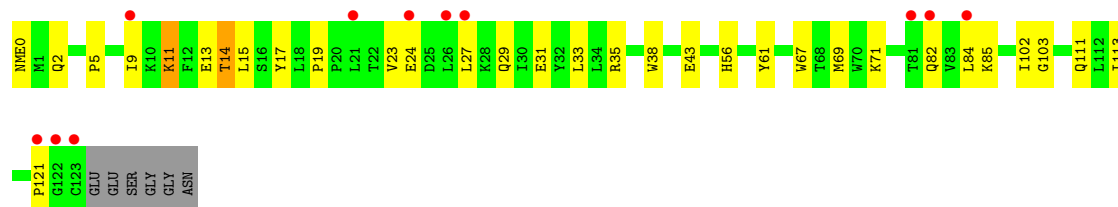




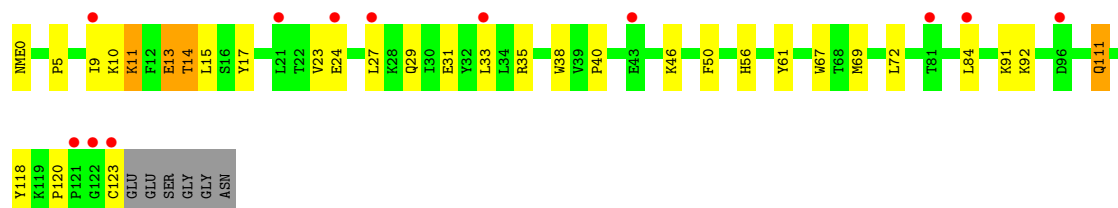
- Molecule 2: Ribulose biphosphate carboxylase small chain, chloroplastic



- Molecule 2: Ribulose biphosphate carboxylase small chain, chloroplastic



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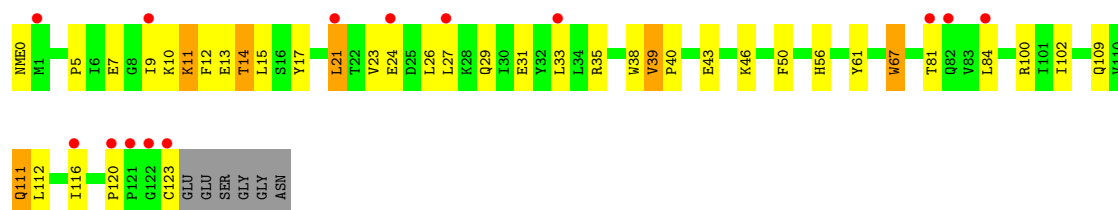


- Molecule 2: Ribulose biphosphate carboxylase small chain, chloroplastic



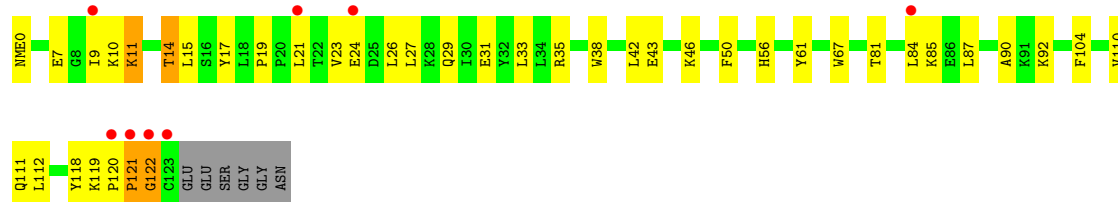
- Molecule 2: Ribulose biphosphate carboxylase small chain, chloroplastic

Chain W: 



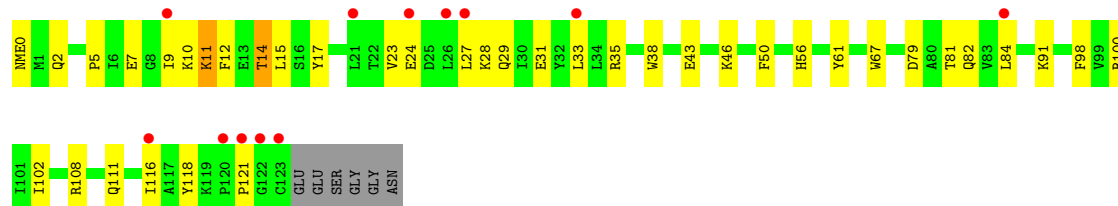
- Molecule 2: Ribulose biphosphate carboxylase small chain, chloroplastic

Chain X: 



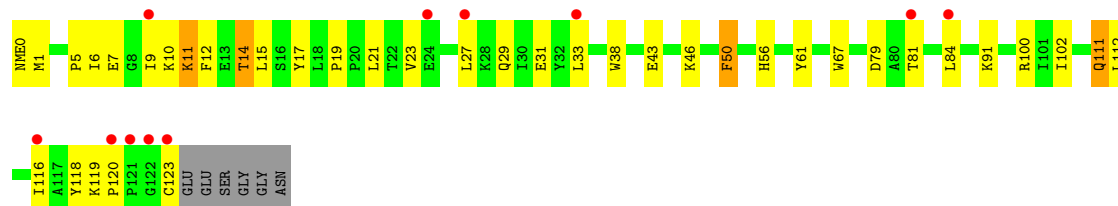
- Molecule 2: Ribulose biphosphate carboxylase small chain, chloroplastic

Chain Y: 



- Molecule 2: Ribulose biphosphate carboxylase small chain, chloroplastic

Chain Z: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	110.41Å 199.62Å 111.17Å 90.00° 91.45° 90.00°	Depositor
Resolution (Å)	74.26 – 1.65 74.26 – 1.65	Depositor EDS
% Data completeness (in resolution range)	85.2 (74.26-1.65) 85.2 (74.26-1.65)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 1.55Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.171 , 0.190 0.169 , 0.187	Depositor DCC
R_{free} test set	30599 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	10.3	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.033 for l,k,-h 0.028 for h,-k,-l 0.018 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	39557	wwPDB-VP
Average B, all atoms (Å ²)	15.0	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 40.91 % 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 2.5532e-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: 6PG, MG, KCX, NME

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	0.41	0/3536	0.96	25/4789 (0.5%)
1	B	0.41	0/3533	0.99	23/4785 (0.5%)
1	C	0.41	1/3531 (0.0%)	0.96	20/4784 (0.4%)
1	D	0.39	1/3540 (0.0%)	0.95	20/4795 (0.4%)
1	E	0.37	0/3517	0.94	20/4764 (0.4%)
1	F	0.36	0/3540	0.94	21/4795 (0.4%)
1	G	0.39	0/3517	1.00	26/4764 (0.5%)
1	H	0.36	0/3540	0.93	14/4795 (0.3%)
2	S	0.45	1/1048 (0.1%)	0.91	5/1421 (0.4%)
2	T	0.46	1/1048 (0.1%)	0.89	4/1421 (0.3%)
2	U	0.46	1/1048 (0.1%)	0.91	5/1421 (0.4%)
2	V	0.46	1/1048 (0.1%)	0.94	5/1421 (0.4%)
2	W	0.46	1/1048 (0.1%)	0.92	5/1421 (0.4%)
2	X	0.46	1/1048 (0.1%)	0.90	4/1421 (0.3%)
2	Y	0.45	1/1048 (0.1%)	0.90	4/1421 (0.3%)
2	Z	0.46	1/1048 (0.1%)	0.90	5/1421 (0.4%)
All	All	0.41	10/36638 (0.0%)	0.95	206/49639 (0.4%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	12	GLY	N-CA	10.35	1.62	1.45
2	S	0	NME	C-N	-10.10	1.33	1.43
2	Z	0	NME	C-N	-10.09	1.33	1.43
2	W	0	NME	C-N	-10.08	1.33	1.43
2	T	0	NME	C-N	-10.06	1.33	1.43
2	Y	0	NME	C-N	-10.02	1.33	1.43
2	X	0	NME	C-N	-10.01	1.33	1.43
2	V	0	NME	C-N	-9.97	1.33	1.43
2	U	0	NME	C-N	-9.96	1.33	1.43
1	D	341	MET	SD-CE	-6.71	1.62	1.79

All (206) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	15	ALA	N-CA-C	16.06	128.90	108.19
1	G	15	ALA	N-CA-C	11.04	126.89	108.90
1	C	124	VAL	N-CA-C	9.18	122.52	111.05
1	H	82	GLY	N-CA-C	-8.70	100.20	112.37
1	F	269	TYR	N-CA-C	8.54	120.59	111.28
1	A	332	VAL	N-CA-C	7.92	125.81	109.34
1	H	269	TYR	N-CA-C	7.83	120.71	111.71
1	G	13	PHE	N-CA-C	7.79	123.11	111.04
1	B	269	TYR	N-CA-C	7.74	120.61	111.71
1	D	462	TRP	N-CA-C	7.68	122.32	110.42
1	H	124	VAL	N-CA-C	7.66	120.62	111.05
1	D	124	VAL	N-CA-C	7.62	120.58	111.05
1	A	124	VAL	N-CA-C	7.62	120.57	111.05
1	E	269	TYR	N-CA-C	7.57	120.41	111.71
2	S	111	GLN	N-CA-C	-7.56	98.26	110.20
1	G	269	TYR	N-CA-C	7.42	120.24	111.71
1	G	124	VAL	N-CA-C	7.35	120.24	111.05
1	C	13	PHE	N-CA-C	-7.24	93.14	107.69
1	C	269	TYR	N-CA-C	7.23	120.02	111.71
1	D	269	TYR	N-CA-C	7.21	120.00	111.71
1	E	63	THR	N-CA-C	7.21	122.09	113.16
2	T	111	GLN	N-CA-C	-7.18	98.86	110.20
2	V	111	GLN	N-CA-C	-7.13	98.93	110.20
2	U	111	GLN	N-CA-C	-7.12	98.94	110.20
1	A	269	TYR	N-CA-C	7.11	119.89	111.71
1	G	302	ASP	N-CA-C	7.11	122.05	112.88
1	F	264	ILE	N-CA-C	7.08	117.69	108.35
1	C	91	VAL	N-CA-C	7.04	117.36	107.37
1	G	155	ILE	N-CA-C	7.01	117.52	110.23
1	B	124	VAL	N-CA-C	6.99	120.81	111.17
1	D	264	ILE	N-CA-C	6.92	117.48	108.35
2	Y	111	GLN	N-CA-C	-6.91	99.28	110.20
2	T	11	LYS	N-CA-C	6.86	120.22	110.14
1	F	155	ILE	N-CA-C	6.85	117.35	110.23
1	D	155	ILE	N-CA-C	6.83	117.33	110.23
2	W	111	GLN	N-CA-C	-6.82	99.42	110.20
1	G	91	VAL	N-CA-C	6.81	123.51	109.34
2	X	111	GLN	N-CA-C	-6.76	99.52	110.20
1	G	36	ILE	N-CA-C	-6.73	98.89	108.58
1	H	155	ILE	N-CA-C	6.71	117.21	110.23
2	X	11	LYS	N-CA-C	6.71	120.01	110.14
1	B	339	ARG	N-CA-C	6.68	118.45	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	339	ARG	N-CA-C	6.68	118.56	111.28
1	D	302	ASP	N-CA-C	6.66	121.11	112.92
1	G	264	ILE	N-CA-C	6.65	117.13	108.35
1	A	301	ILE	N-CA-C	6.65	117.29	111.90
2	Z	111	GLN	N-CA-C	-6.65	99.70	110.20
1	A	302	ASP	N-CA-C	6.60	121.03	112.92
2	S	11	LYS	N-CA-C	6.59	119.83	110.14
1	E	124	VAL	N-CA-C	6.59	120.27	111.17
1	F	302	ASP	N-CA-C	6.59	121.39	112.88
1	F	124	VAL	N-CA-C	6.59	120.27	111.17
2	Y	14	THR	N-CA-C	6.59	120.18	110.30
2	U	11	LYS	N-CA-C	6.58	119.81	110.14
1	B	14	LYS	CA-C-N	-6.55	110.02	122.08
1	B	14	LYS	C-N-CA	-6.55	110.02	122.08
2	Z	14	THR	N-CA-C	6.54	120.32	110.64
1	C	264	ILE	N-CA-C	6.51	116.95	108.35
1	C	36	ILE	N-CA-C	-6.50	99.06	108.36
1	B	82	GLY	N-CA-C	-6.48	100.95	112.54
1	E	264	ILE	N-CA-C	6.48	116.90	108.35
1	F	214	TRP	N-CA-C	6.46	118.33	111.28
1	H	301	ILE	N-CA-C	6.45	117.36	111.81
1	A	155	ILE	N-CA-C	6.45	116.93	110.23
1	B	63	THR	N-CA-C	6.44	120.75	113.02
1	H	302	ASP	N-CA-C	6.44	120.84	112.92
1	A	16	GLY	N-CA-C	6.43	119.64	111.09
1	C	302	ASP	N-CA-C	6.42	121.16	112.88
1	C	214	TRP	N-CA-C	6.41	118.27	111.28
1	H	264	ILE	N-CA-C	6.41	116.81	108.35
2	V	14	THR	N-CA-C	6.40	119.91	110.30
1	A	264	ILE	N-CA-C	6.39	116.78	108.35
1	D	82	GLY	N-CA-C	-6.39	100.31	111.62
2	W	14	THR	N-CA-C	6.37	119.85	110.30
1	H	263	PRO	N-CA-C	6.34	122.99	114.18
2	U	14	THR	N-CA-C	6.33	119.79	110.30
2	V	11	LYS	N-CA-C	6.32	119.43	110.14
2	S	14	THR	N-CA-C	6.28	119.73	110.30
1	H	36	ILE	N-CA-C	-6.28	99.38	108.36
1	H	108	PHE	N-CA-C	6.28	120.06	109.76
1	E	108	PHE	N-CA-C	6.27	120.05	109.76
1	C	413	ASN	N-CA-C	6.27	117.78	111.07
1	G	63	THR	N-CA-C	6.25	120.61	112.92
1	B	302	ASP	N-CA-C	6.23	120.58	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	351	ASP	N-CA-C	6.23	118.95	110.55
1	E	339	ARG	N-CA-C	6.23	117.76	110.97
1	A	384	VAL	N-CA-C	6.21	117.70	110.62
1	C	108	PHE	N-CA-C	6.21	119.94	109.76
1	E	82	GLY	N-CA-C	-6.19	101.45	112.54
1	E	301	ILE	N-CA-C	6.18	117.12	111.81
2	W	11	LYS	N-CA-C	6.18	119.22	110.14
1	A	82	GLY	N-CA-C	-6.17	101.50	112.54
1	A	214	TRP	N-CA-C	6.17	118.51	111.11
1	A	351	ASP	N-CA-C	6.15	118.46	110.53
1	F	36	ILE	N-CA-C	-6.13	99.60	108.36
2	T	14	THR	N-CA-C	6.10	119.67	110.64
1	G	384	VAL	N-CA-C	6.09	117.56	110.62
2	Y	11	LYS	N-CA-C	6.08	119.08	110.14
1	F	108	PHE	N-CA-C	6.08	119.73	109.76
1	B	384	VAL	N-CA-C	6.06	117.53	110.62
1	F	384	VAL	N-CA-C	6.06	117.53	110.62
1	A	263	PRO	N-CA-C	6.02	122.55	114.18
1	B	351	ASP	N-CA-C	6.01	118.29	110.53
1	G	351	ASP	N-CA-C	5.99	118.64	110.55
1	A	128	LYS	N-CA-C	5.99	118.58	111.33
1	E	214	TRP	N-CA-C	5.99	118.58	111.33
1	D	263	PRO	N-CA-C	5.98	122.49	114.18
1	G	108	PHE	N-CA-C	5.98	119.56	109.76
1	E	329	GLY	N-CA-C	5.96	117.58	111.56
2	Z	11	LYS	N-CA-C	5.95	118.89	110.14
1	G	413	ASN	N-CA-C	5.94	117.42	111.07
1	B	214	TRP	N-CA-C	5.94	118.23	111.11
1	E	302	ASP	N-CA-C	5.92	120.52	112.88
1	D	77	LEU	N-CA-C	5.91	118.20	111.11
1	G	82	GLY	N-CA-C	-5.90	101.99	112.54
1	C	263	PRO	N-CA-C	5.89	122.37	114.18
1	A	371	MET	N-CA-C	-5.88	102.36	109.83
1	F	351	ASP	N-CA-C	5.87	118.48	110.55
1	G	214	TRP	N-CA-C	5.87	118.15	111.11
1	A	413	ASN	N-CA-C	5.87	117.75	111.36
2	X	14	THR	N-CA-C	5.86	119.09	110.30
1	B	108	PHE	N-CA-C	5.82	119.31	109.76
1	F	263	PRO	N-CA-C	5.77	122.21	114.18
1	F	63	THR	N-CA-C	5.77	120.01	112.92
1	A	36	ILE	N-CA-C	-5.76	99.58	107.99
1	D	108	PHE	N-CA-C	5.74	119.17	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	301	ILE	N-CA-C	5.74	116.74	111.81
1	H	214	TRP	N-CA-C	5.71	117.97	111.11
1	E	263	PRO	N-CA-C	5.71	122.12	114.18
1	A	108	PHE	N-CA-C	5.71	119.12	109.76
1	F	396	ASP	N-CA-C	5.70	117.50	111.28
1	E	36	ILE	N-CA-C	-5.69	99.68	107.99
2	V	67	TRP	N-CA-C	-5.69	101.50	109.69
1	E	413	ASN	N-CA-C	5.68	117.14	111.07
1	F	82	GLY	N-CA-C	-5.67	102.38	112.54
1	D	351	ASP	N-CA-C	5.67	118.21	110.55
1	D	214	TRP	N-CA-C	5.67	117.92	111.11
1	D	36	ILE	N-CA-C	-5.67	100.25	108.36
1	D	63	THR	N-CA-C	5.66	119.18	112.72
1	G	94	ASP	N-CA-C	-5.66	106.25	114.12
1	G	42	VAL	N-CA-C	5.64	116.06	108.17
2	V	39	VAL	N-CA-C	5.59	114.03	107.77
1	C	13	PHE	N-CA-CB	5.58	119.91	110.69
1	F	413	ASN	N-CA-C	5.56	117.02	111.07
1	B	301	ILE	N-CA-C	5.55	116.59	111.81
1	H	413	ASN	N-CA-C	5.54	117.39	111.36
1	C	82	GLY	N-CA-C	-5.52	102.65	112.54
1	E	351	ASP	N-CA-C	5.48	117.95	110.55
1	B	263	PRO	N-CA-C	5.48	121.79	114.18
1	E	301	ILE	CB-CA-C	-5.47	105.26	111.55
1	A	339	ARG	N-CA-C	5.46	117.68	111.02
1	A	63	THR	N-CA-C	5.45	122.40	110.80
1	A	77	LEU	N-CA-C	5.44	117.91	111.33
2	Z	50	PHE	N-CA-C	5.42	117.22	109.14
1	E	396	ASP	N-CA-C	5.42	117.19	111.28
1	A	396	ASP	N-CA-C	5.38	117.23	111.36
1	G	263	PRO	N-CA-C	5.38	121.66	114.18
1	F	181	SER	N-CA-C	-5.37	103.30	110.55
2	X	67	TRP	N-CA-C	-5.36	101.29	109.65
1	F	301	ILE	N-CA-C	5.34	116.40	111.81
2	S	108	ARG	N-CA-C	-5.32	106.74	113.18
1	B	36	ILE	N-CA-C	-5.32	100.23	107.99
1	F	24	TYR	N-CA-C	5.32	119.46	112.92
2	Z	67	TRP	N-CA-C	-5.31	101.36	109.65
1	C	396	ASP	N-CA-C	5.31	117.82	111.71
1	G	90	VAL	N-CA-C	5.31	115.54	108.11
1	A	301	ILE	CB-CA-C	-5.30	106.21	111.30
1	B	264	ILE	N-CA-C	5.28	115.97	108.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	413	ASN	N-CA-C	5.26	117.01	111.28
1	C	24	TYR	N-CA-C	5.26	119.80	113.17
2	T	67	TRP	N-CA-C	-5.25	101.45	109.65
1	E	174	ILE	N-CA-C	5.25	115.87	109.30
2	U	67	TRP	N-CA-C	-5.25	101.46	109.65
1	C	365	THR	N-CA-C	-5.24	102.10	109.96
1	B	166	GLY	N-CA-C	5.24	122.96	114.90
1	B	16	GLY	CA-C-N	5.23	131.12	121.70
1	B	16	GLY	C-N-CA	5.23	131.12	121.70
1	G	24	TYR	N-CA-C	5.23	119.66	113.28
1	G	166	GLY	N-CA-C	5.20	122.91	114.90
2	S	67	TRP	N-CA-C	-5.20	101.54	109.65
1	D	181	SER	N-CA-C	-5.20	103.53	110.55
1	H	351	ASP	N-CA-C	5.20	117.56	110.55
1	E	371	MET	N-CA-C	-5.19	101.88	109.50
2	Y	67	TRP	N-CA-C	-5.17	101.58	109.65
1	B	413	ASN	N-CA-C	5.17	116.99	111.36
1	H	303	ARG	N-CA-C	5.15	117.68	111.40
1	D	128	LYS	N-CA-C	5.14	117.62	111.71
1	G	396	ASP	N-CA-C	5.13	116.95	111.36
1	C	301	ILE	N-CA-C	5.13	116.22	111.81
2	W	39	VAL	N-CA-C	5.12	113.51	107.77
2	W	67	TRP	N-CA-C	-5.11	101.68	109.65
1	A	42	VAL	N-CA-C	5.08	115.90	108.53
1	B	181	SER	N-CA-C	-5.08	103.70	110.55
1	F	365	THR	N-CA-C	-5.08	102.35	109.96
1	B	350	ARG	N-CA-C	5.07	119.45	113.12
1	G	461	ILE	N-CA-C	5.03	116.49	111.00
1	C	166	GLY	N-CA-C	5.03	122.54	115.30
1	D	371	MET	N-CA-C	-5.03	102.11	109.50
1	D	17	VAL	CA-C-O	-5.03	112.26	120.80
1	A	303	ARG	N-CA-C	5.02	117.53	111.40
1	F	462	TRP	N-CA-C	5.02	118.88	112.26
2	U	13	GLU	N-CA-C	5.02	115.42	108.00
1	G	371	MET	N-CA-C	-5.01	102.13	109.50
1	C	293	ILE	N-CA-C	5.01	115.19	108.17
1	E	346	VAL	N-CA-C	-5.00	105.67	110.72
1	F	350	ARG	N-CA-C	5.00	119.37	113.12

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	3464	0	3370	84	0
1	B	3461	0	3369	111	0
1	C	3459	0	3365	102	0
1	D	3468	0	3378	77	0
1	E	3445	0	3347	76	0
1	F	3468	0	3378	94	0
1	G	3445	0	3347	98	0
1	H	3468	0	3378	84	0
2	S	1016	0	1017	41	0
2	T	1016	0	1017	38	0
2	U	1016	0	1017	36	0
2	V	1016	0	1017	45	0
2	W	1016	0	1017	51	0
2	X	1016	0	1017	45	0
2	Y	1016	0	1017	50	0
2	Z	1016	0	1017	49	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	17	0	9	0	0
4	B	17	0	9	0	0
4	C	17	0	9	0	0
4	D	17	0	9	0	0
4	E	17	0	9	0	0
4	F	17	0	9	0	0
4	G	17	0	9	0	0
4	H	17	0	9	0	0
5	A	309	0	0	24	0
5	B	345	0	0	32	0
5	C	339	0	0	46	0
5	D	335	0	0	14	0
5	E	318	0	0	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	371	0	0	35	0
5	G	341	0	0	26	0
5	H	326	0	0	27	0
5	S	113	0	0	11	0
5	T	99	0	0	13	0
5	U	125	0	0	9	0
5	V	123	0	0	12	0
5	W	122	0	0	13	0
5	X	115	0	0	19	0
5	Y	111	0	0	14	0
5	Z	115	0	0	10	0
All	All	39557	0	35140	1016	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 (1016) 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:A:371:MET:HG2	5:A:480:HOH:O	1.42	1.16
1:B:312:ARG:HH21	1:B:341:MET:HE2	1.16	1.11
1:E:358:ARG:HH21	1:E:358:ARG:HG3	0.98	1.09
1:D:341:MET:HA	1:D:341:MET:HE2	1.32	1.09
1:D:16:GLY:HA2	1:D:68:THR:CB	1.83	1.08
1:B:341:MET:HE1	1:B:361:GLY:HA3	1.32	1.07
1:C:330:THR:HG23	1:C:379:SER:O	1.56	1.04
1:G:15:ALA:HB1	5:G:591:HOH:O	1.56	1.04
1:E:447:SER:HB3	5:E:2603:HOH:O	1.57	1.03
1:G:81:LYS:HB3	5:G:2366:HOH:O	1.59	1.02
1:C:61:SER:HB3	1:C:124:VAL:HG11	1.41	1.00
1:G:177:LYS:HG3	1:G:178:LEU:CD2	1.92	0.98
1:B:101:VAL:HG12	5:B:2531:HOH:O	1.59	0.98
2:V:31:GLU:HB3	5:V:2268:HOH:O	1.63	0.98
1:B:341:MET:HE3	1:B:341:MET:HA	1.43	0.98
2:S:26:LEU:HB3	5:S:2803:HOH:O	1.64	0.98
1:A:331:VAL:HG11	1:A:342:THR:HG21	1.45	0.96
1:A:150:GLY:HA3	1:A:371:MET:SD	2.06	0.95
1:F:330:THR:HG23	1:F:379:SER:O	1.65	0.95
1:D:16:GLY:HA2	1:D:68:THR:HB	1.46	0.94
1:A:177:LYS:HG3	1:A:178:LEU:HG	1.48	0.94
1:E:358:ARG:HG3	1:E:358:ARG:NH2	1.77	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:392:GLU:OE1	1:C:438:ALA:HB2	1.69	0.92
1:D:385:TRP:CB	1:D:463:LYS:HD3	1.99	0.92
2:V:24:GLU:HB3	5:V:2609:HOH:O	1.69	0.92
2:U:69:MET:HB2	5:E:2428:HOH:O	1.70	0.92
1:G:247:CYS:HB3	5:G:748:HOH:O	1.68	0.92
2:Y:100:ARG:HB3	2:Y:116:ILE:HD13	1.48	0.91
1:C:174:ILE:HG13	5:C:2812:HOH:O	1.71	0.91
1:F:247:CYS:HB3	5:F:1912:HOH:O	1.69	0.90
1:G:178:LEU:HB3	5:G:1816:HOH:O	1.71	0.89
1:G:338:GLU:OE1	1:G:340:GLU:HB2	1.72	0.89
1:H:346:VAL:HB	5:H:980:HOH:O	1.70	0.89
2:X:87:LEU:HA	5:X:2753:HOH:O	1.72	0.89
1:B:32:LYS:HD2	5:B:1147:HOH:O	1.73	0.88
1:G:77:LEU:HD23	5:G:2366:HOH:O	1.73	0.88
2:U:50:PHE:HB2	5:U:2324:HOH:O	1.73	0.88
1:F:52:GLU:HB2	5:F:2591:HOH:O	1.72	0.88
1:H:330:THR:HG22	5:H:1428:HOH:O	1.73	0.88
2:X:27:LEU:O	2:X:31:GLU:HG3	1.71	0.88
1:G:49:PRO:HG2	1:G:52:GLU:HG3	1.55	0.87
1:C:124:VAL:HB	5:C:1082:HOH:O	1.75	0.87
1:D:340:GLU:HG2	5:D:1946:HOH:O	1.75	0.86
2:V:27:LEU:HD11	2:V:84:LEU:HD11	1.56	0.86
1:C:247:CYS:HB3	5:C:516:HOH:O	1.75	0.86
1:B:312:ARG:HH21	1:B:341:MET:CE	1.88	0.86
1:B:392:GLU:HG2	5:B:2674:HOH:O	1.74	0.86
1:H:309:MET:HB3	5:H:1788:HOH:O	1.75	0.86
1:D:16:GLY:HA2	1:D:68:THR:OG1	1.75	0.85
1:E:340:GLU:HG2	5:E:2630:HOH:O	1.74	0.85
1:G:177:LYS:HG3	1:G:178:LEU:HD22	1.58	0.85
2:Z:27:LEU:O	2:Z:31:GLU:HG3	1.75	0.85
1:G:16:GLY:O	1:G:67:THR:HA	1.77	0.84
1:C:12:GLY:HA2	5:C:2352:HOH:O	1.76	0.84
2:W:24:GLU:HG2	5:W:2120:HOH:O	1.76	0.84
2:S:85:LYS:HE3	5:S:2189:HOH:O	1.76	0.84
1:B:93:GLU:HB2	5:B:2804:HOH:O	1.75	0.84
1:D:385:TRP:CG	1:D:463:LYS:HD3	2.13	0.84
2:Y:116:ILE:HB	5:Y:1394:HOH:O	1.76	0.84
2:T:24:GLU:HG2	5:T:1987:HOH:O	1.78	0.84
1:B:247:CYS:HB3	5:B:856:HOH:O	1.75	0.84
1:F:407:LEU:HD13	5:F:2471:HOH:O	1.78	0.83
2:W:27:LEU:HG	5:W:1268:HOH:O	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:439:ARG:HD3	5:C:2412:HOH:O	1.76	0.83
1:C:341:MET:HE2	5:C:2670:HOH:O	1.77	0.83
1:G:178:LEU:HD11	1:H:107:LEU:HD22	1.60	0.82
2:X:119:LYS:HD2	5:X:1959:HOH:O	1.78	0.82
2:V:27:LEU:O	2:V:31:GLU:HG3	1.80	0.82
1:H:309:MET:HE2	5:H:1788:HOH:O	1.78	0.82
2:Z:116:ILE:HD12	5:Z:142:HOH:O	1.80	0.82
1:G:32:LYS:HD2	5:G:2619:HOH:O	1.80	0.82
1:D:383:HIS:CE1	1:D:463:LYS:HB3	2.14	0.81
1:E:177:LYS:HG3	5:E:2185:HOH:O	1.79	0.81
1:B:312:ARG:NH2	1:B:341:MET:HE2	1.94	0.81
1:C:52:GLU:HG2	5:C:1591:HOH:O	1.80	0.81
1:G:13:PHE:CD1	1:G:70:TRP:HB3	2.15	0.81
1:H:79:ARG:HB2	5:H:2538:HOH:O	1.79	0.81
2:T:85:LYS:HG2	5:T:2552:HOH:O	1.80	0.81
2:U:27:LEU:HG	5:U:1472:HOH:O	1.80	0.81
2:V:27:LEU:HG	5:V:1389:HOH:O	1.79	0.81
1:F:187:ARG:HH22	2:Z:111:GLN:HE22	1.27	0.81
2:X:42:LEU:HD23	5:X:2753:HOH:O	1.80	0.81
2:Y:24:GLU:HG2	5:Y:1348:HOH:O	1.80	0.81
2:Y:27:LEU:HG	5:Y:1317:HOH:O	1.79	0.81
1:B:340:GLU:HG2	5:B:2043:HOH:O	1.79	0.81
1:C:90:VAL:HA	5:C:1746:HOH:O	1.78	0.81
2:U:24:GLU:HG2	5:U:1380:HOH:O	1.81	0.81
2:Z:81:THR:HA	2:Z:84:LEU:HD12	1.63	0.81
1:D:341:MET:HE1	1:D:361:GLY:N	1.96	0.81
2:U:35:ARG:HB3	5:U:2246:HOH:O	1.79	0.80
1:C:92:GLY:HA2	5:C:2651:HOH:O	1.80	0.80
1:A:247:CYS:HG	1:B:247:CYS:HG	0.81	0.79
1:D:385:TRP:HB3	1:D:463:LYS:HD3	1.63	0.79
1:B:189:CYS:HB3	5:B:2513:HOH:O	1.82	0.79
1:C:17:VAL:HG12	1:C:17:VAL:O	1.83	0.79
1:A:340:GLU:HG2	5:A:2166:HOH:O	1.81	0.79
1:D:45:GLN:HA	1:D:131:ARG:HG3	1.64	0.79
2:T:27:LEU:O	2:T:31:GLU:HG3	1.83	0.79
2:X:27:LEU:HG	5:X:1387:HOH:O	1.83	0.79
1:F:340:GLU:HG2	5:F:1616:HOH:O	1.83	0.79
1:D:16:GLY:O	1:D:17:VAL:HB	1.82	0.78
1:H:33:ASP:HB2	5:H:2435:HOH:O	1.83	0.78
1:D:17:VAL:HG12	1:D:17:VAL:O	1.81	0.78
2:Z:119:LYS:HD2	5:Z:2344:HOH:O	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:330:THR:HG22	5:F:1953:HOH:O	1.81	0.78
2:V:23:VAL:O	2:V:27:LEU:HD13	1.83	0.77
1:F:93:GLU:HB2	5:F:2556:HOH:O	1.83	0.77
1:D:33:ASP:HB2	5:D:1545:HOH:O	1.84	0.76
1:G:178:LEU:CD1	1:H:107:LEU:HD22	2.14	0.76
1:B:22:LEU:HB2	5:B:2763:HOH:O	1.84	0.76
1:A:178:LEU:HD12	1:B:107:LEU:HD22	1.65	0.76
1:A:371:MET:HE3	5:A:480:HOH:O	1.83	0.76
2:W:27:LEU:O	2:W:31:GLU:HG3	1.86	0.76
2:Y:23:VAL:O	2:Y:27:LEU:HD13	1.85	0.76
1:C:61:SER:HB3	1:C:124:VAL:CG1	2.16	0.76
1:B:414:ALA:HB3	1:B:415:PRO:HD3	1.68	0.76
2:X:24:GLU:HG2	5:X:936:HOH:O	1.86	0.76
1:D:341:MET:HA	1:D:341:MET:CE	2.14	0.76
2:X:9:ILE:HG22	2:X:11:LYS:HE2	1.67	0.75
1:G:330:THR:HG22	1:G:379:SER:O	1.87	0.75
2:Z:116:ILE:HG23	5:Z:142:HOH:O	1.87	0.75
1:G:178:LEU:HD21	5:H:1430:HOH:O	1.86	0.75
2:X:85:LYS:HE3	5:X:2348:HOH:O	1.87	0.75
1:B:15:ALA:O	1:B:68:THR:HB	1.87	0.75
1:G:177:LYS:HG3	1:G:178:LEU:HD23	1.68	0.74
1:E:358:ARG:HH21	1:E:358:ARG:CG	1.89	0.74
1:E:178:LEU:HD22	5:E:2605:HOH:O	1.87	0.74
1:G:175:LYS:HE3	5:H:2063:HOH:O	1.85	0.74
2:T:35:ARG:HB3	5:T:2677:HOH:O	1.85	0.74
1:G:463:LYS:NZ	1:G:463:LYS:HB2	2.02	0.74
2:W:12:PHE:CG	2:W:116:ILE:HG13	2.23	0.74
2:T:5:PRO:HB2	2:T:9:ILE:HG13	1.68	0.74
1:F:332:VAL:HA	5:F:2470:HOH:O	1.88	0.73
1:F:439:ARG:HD3	5:F:2626:HOH:O	1.87	0.73
1:B:463:LYS:NZ	1:B:463:LYS:HB2	2.04	0.73
1:E:50:PRO:HG2	5:E:2167:HOH:O	1.88	0.73
1:D:88:GLU:HG2	1:D:98:ILE:HB	1.70	0.73
1:G:45:GLN:HA	1:G:131:ARG:HG3	1.70	0.73
1:H:443:GLU:HG3	5:H:731:HOH:O	1.87	0.73
1:A:42:VAL:HG22	1:A:133:LEU:CD1	2.19	0.73
1:E:51:GLU:HG3	5:E:2167:HOH:O	1.88	0.72
2:Z:120:PRO:HG2	2:Z:123:CYS:SG	2.28	0.72
1:C:414:ALA:HB3	1:C:415:PRO:HD3	1.70	0.72
2:U:23:VAL:O	2:U:27:LEU:HD13	1.89	0.72
2:Y:9:ILE:HG22	2:Y:11:LYS:HE2	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:23:VAL:O	2:X:27:LEU:HD13	1.89	0.72
2:V:24:GLU:HG2	5:V:241:HOH:O	1.89	0.72
2:Y:116:ILE:HD12	5:Y:1304:HOH:O	1.89	0.72
1:B:14:LYS:HG3	1:B:15:ALA:N	2.02	0.72
1:C:238:HIS:HE1	5:C:2812:HOH:O	1.72	0.71
1:D:341:MET:HE1	1:D:361:GLY:CA	2.19	0.71
1:H:330:THR:HG23	1:H:379:SER:O	1.91	0.71
2:V:9:ILE:HG22	2:V:11:LYS:HE2	1.72	0.71
1:G:22:LEU:HA	5:G:2527:HOH:O	1.89	0.71
2:U:69:MET:HE3	5:E:2428:HOH:O	1.90	0.71
5:G:1666:HOH:O	1:H:77:LEU:HG	1.89	0.71
1:A:178:LEU:HD11	5:A:3283:HOH:O	1.91	0.70
2:U:111:GLN:HE22	1:E:187:ARG:HH22	1.39	0.70
1:B:339:ARG:HG2	5:B:2036:HOH:O	1.89	0.70
2:S:66:TYR:CE2	5:C:2509:HOH:O	2.44	0.70
2:Z:27:LEU:HG	2:Z:84:LEU:HD11	1.73	0.70
1:C:57:VAL:HA	5:C:1082:HOH:O	1.91	0.70
1:A:14:LYS:HE3	1:A:15:ALA:O	1.91	0.70
2:V:27:LEU:CD1	2:V:84:LEU:HD11	2.22	0.70
1:E:89:PRO:HG3	1:E:97:TYR:CE2	2.27	0.69
1:H:91:VAL:HG13	5:H:2177:HOH:O	1.92	0.69
1:A:331:VAL:HG11	1:A:342:THR:CG2	2.21	0.69
2:U:9:ILE:HG22	2:U:11:LYS:HE2	1.73	0.69
1:G:93:GLU:HG3	1:G:96:GLN:HB3	1.73	0.69
1:G:414:ALA:HB3	1:G:415:PRO:HD3	1.73	0.69
1:H:414:ALA:HB3	1:H:415:PRO:HD3	1.75	0.69
1:A:330:THR:C	1:A:332:VAL:H	1.99	0.69
1:C:93:GLU:HB3	5:C:854:HOH:O	1.92	0.69
2:V:43:GLU:CD	2:V:102:ILE:HD13	2.18	0.69
5:E:1726:HOH:O	1:F:70:TRP:HD1	1.75	0.69
2:W:9:ILE:HG22	2:W:11:LYS:HE2	1.73	0.69
1:F:355:GLU:HG3	5:F:2480:HOH:O	1.91	0.69
1:G:178:LEU:HD23	5:G:916:HOH:O	1.92	0.69
5:A:1861:HOH:O	1:B:70:TRP:HD1	1.76	0.69
1:H:79:ARG:HG3	5:H:2701:HOH:O	1.93	0.69
1:D:341:MET:HE1	1:D:360:ARG:C	2.18	0.68
1:A:42:VAL:HB	5:A:2346:HOH:O	1.94	0.68
1:A:332:VAL:HG13	1:A:333:GLY:N	2.07	0.68
1:B:93:GLU:HB3	5:B:2604:HOH:O	1.92	0.68
1:B:341:MET:HE1	1:B:361:GLY:CA	2.19	0.68
2:V:27:LEU:HD12	2:V:84:LEU:HD21	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:13:PHE:CD1	1:G:13:PHE:C	2.72	0.68
5:A:1861:HOH:O	1:B:13:PHE:CZ	2.45	0.68
1:G:46:PRO:HD3	1:G:131:ARG:HD2	1.76	0.68
1:A:371:MET:SD	5:A:483:HOH:O	2.51	0.67
2:W:120:PRO:HG2	2:W:123:CYS:SG	2.33	0.67
1:D:341:MET:HE1	1:D:361:GLY:HA3	1.76	0.67
2:Z:43:GLU:CD	2:Z:102:ILE:HD13	2.19	0.67
1:F:463:LYS:HB2	1:F:463:LYS:NZ	2.09	0.67
2:Y:81:THR:HA	2:Y:84:LEU:HD12	1.77	0.67
1:C:330:THR:CG2	1:C:379:SER:O	2.40	0.67
2:Z:12:PHE:CG	2:Z:116:ILE:HG13	2.29	0.67
1:B:463:LYS:HD2	5:B:2287:HOH:O	1.94	0.67
1:F:175:LYS:HB2	5:F:2471:HOH:O	1.93	0.67
1:A:334:LYS:HA	5:A:2620:HOH:O	1.94	0.67
1:A:432:ASN:HD22	2:S:29:GLN:HE22	1.43	0.67
1:G:338:GLU:OE2	1:G:341:MET:HG2	1.95	0.66
1:G:339:ARG:NH2	5:G:2358:HOH:O	2.27	0.66
1:B:330:THR:O	1:B:331:VAL:HB	1.94	0.66
2:W:43:GLU:CD	2:W:102:ILE:HD13	2.19	0.66
1:D:16:GLY:HA3	1:D:68:THR:H	1.61	0.66
1:E:432:ASN:HD22	2:W:29:GLN:HE22	1.42	0.66
1:F:414:ALA:HB3	1:F:415:PRO:HD3	1.78	0.66
1:G:340:GLU:HG2	5:G:2026:HOH:O	1.95	0.66
1:C:463:LYS:HB2	1:C:463:LYS:NZ	2.10	0.66
1:F:92:GLY:HA3	5:F:525:HOH:O	1.94	0.66
1:H:350:ARG:CZ	5:H:980:HOH:O	2.43	0.66
2:Y:12:PHE:CG	2:Y:116:ILE:HG13	2.30	0.66
5:A:1347:HOH:O	1:B:77:LEU:HG	1.95	0.66
2:V:27:LEU:HD11	2:V:84:LEU:CD1	2.25	0.66
1:D:16:GLY:CA	1:D:68:THR:H	2.09	0.66
2:W:26:LEU:HB3	5:W:2644:HOH:O	1.96	0.66
2:W:81:THR:HA	2:W:84:LEU:HD12	1.78	0.66
1:D:432:ASN:HD22	2:V:29:GLN:HE22	1.42	0.66
2:Y:5:PRO:HB2	2:Y:9:ILE:HG13	1.78	0.66
2:Y:82:GLN:HG2	5:Y:2500:HOH:O	1.95	0.66
2:T:33:LEU:HB2	5:T:928:HOH:O	1.94	0.66
2:V:121:PRO:O	2:V:123:CYS:N	2.27	0.66
1:F:172:CYS:SG	1:F:407:LEU:HD11	2.36	0.66
2:X:104:PHE:HD2	5:X:2758:HOH:O	1.78	0.66
1:A:414:ALA:HB3	1:A:415:PRO:HD3	1.77	0.65
1:A:330:THR:O	1:A:332:VAL:N	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:VAL:O	1:A:333:GLY:O	2.14	0.65
1:B:60:GLU:HG3	1:B:127:PHE:CD1	2.32	0.65
2:T:9:ILE:HG22	2:T:11:LYS:HE2	1.78	0.65
1:A:187:ARG:NH1	2:Y:43:GLU:OE2	2.30	0.65
1:B:16:GLY:HA2	5:B:898:HOH:O	1.96	0.65
1:E:52:GLU:HG2	5:E:2681:HOH:O	1.97	0.65
1:G:432:ASN:HD22	2:Y:29:GLN:HE22	1.44	0.65
1:G:17:VAL:HG22	1:G:66:TRP:O	1.97	0.65
1:G:330:THR:HG23	5:G:3585:HOH:O	1.95	0.64
1:E:414:ALA:HB3	1:E:415:PRO:HD3	1.78	0.64
1:B:93:GLU:HA	5:B:1609:HOH:O	1.96	0.64
1:F:432:ASN:HD22	2:X:29:GLN:HE22	1.43	0.64
1:G:22:LEU:HG	5:G:2134:HOH:O	1.97	0.64
2:Z:12:PHE:HB2	2:Z:116:ILE:HG12	1.78	0.64
1:A:252:LYS:HE2	5:A:2062:HOH:O	1.97	0.64
1:D:14:LYS:O	1:D:16:GLY:N	2.31	0.64
1:D:414:ALA:HB3	1:D:415:PRO:HD3	1.80	0.64
1:E:46:PRO:HG3	1:E:131:ARG:NH2	2.13	0.64
2:S:9:ILE:HG22	2:S:11:LYS:HE2	1.79	0.64
1:G:15:ALA:CB	5:G:591:HOH:O	2.27	0.64
1:G:45:GLN:OE1	1:G:131:ARG:HG2	1.97	0.64
1:B:442:ASN:HB3	1:B:446:ARG:HH12	1.62	0.64
1:B:341:MET:HE3	1:B:341:MET:CA	2.19	0.63
2:W:35:ARG:HD3	5:W:2228:HOH:O	1.99	0.63
1:A:371:MET:CE	5:A:480:HOH:O	2.44	0.63
1:C:238:HIS:CE1	5:C:2812:HOH:O	2.50	0.63
1:C:310:HIS:HE2	1:C:341:MET:HE3	1.64	0.63
1:H:75:THR:HG23	1:H:77:LEU:HD12	1.80	0.63
2:S:23:VAL:O	2:S:27:LEU:HD13	1.98	0.63
2:V:28:LYS:NZ	5:V:2609:HOH:O	2.31	0.63
2:Z:46:LYS:HD3	5:Z:2550:HOH:O	1.98	0.63
2:S:27:LEU:O	2:S:31:GLU:HG3	1.98	0.63
1:B:442:ASN:HB3	1:B:446:ARG:NH1	2.12	0.63
2:Z:12:PHE:CB	2:Z:116:ILE:CG1	2.76	0.63
1:B:331:VAL:HG21	1:B:390:LEU:HD23	1.81	0.63
2:Z:21:LEU:HD22	5:Z:2297:HOH:O	1.98	0.62
1:A:297:MET:HG3	1:B:121:VAL:HG23	1.81	0.62
2:T:35:ARG:HD3	5:T:2766:HOH:O	1.99	0.62
2:Z:27:LEU:CG	2:Z:84:LEU:HD11	2.30	0.62
1:B:41:ARG:NH1	1:B:305:LYS:HE2	2.14	0.62
1:F:21:LYS:HD3	1:F:52:GLU:OE1	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:407:LEU:HD22	5:F:2471:HOH:O	1.99	0.62
1:H:42:VAL:HG22	1:H:133:LEU:CD1	2.30	0.62
1:C:341:MET:SD	5:C:480:HOH:O	2.56	0.61
2:Z:11:LYS:HG3	2:Z:17:TYR:CE1	2.36	0.61
1:B:432:ASN:HD22	2:T:29:GLN:HE22	1.48	0.61
2:T:27:LEU:HD11	2:T:84:LEU:HD11	1.81	0.61
1:B:339:ARG:HB3	5:B:2663:HOH:O	1.99	0.61
1:F:93:GLU:HG2	5:F:1741:HOH:O	2.01	0.61
1:F:463:LYS:HD2	5:F:1063:HOH:O	2.00	0.61
2:X:90:ALA:HB3	5:X:2753:HOH:O	1.99	0.61
2:Z:9:ILE:HG22	2:Z:11:LYS:HE2	1.82	0.61
1:B:102:ALA:C	5:B:2531:HOH:O	2.43	0.61
2:T:84:LEU:HB3	5:T:2104:HOH:O	2.00	0.61
1:F:21:LYS:HD2	5:F:2326:HOH:O	2.01	0.61
1:A:63:THR:HG22	5:B:913:HOH:O	2.01	0.61
1:C:90:VAL:HG23	1:C:97:TYR:CA	2.30	0.61
1:F:460:GLU:HA	5:F:1063:HOH:O	2.00	0.61
1:A:429:GLN:O	1:A:433:GLU:HG3	2.01	0.61
2:U:27:LEU:O	2:U:31:GLU:HG3	2.01	0.60
2:W:109:GLN:HE22	1:H:79:ARG:HE	1.49	0.60
1:F:330:THR:O	1:F:331:VAL:HB	1.98	0.60
1:G:91:VAL:HG23	1:G:91:VAL:O	2.01	0.60
2:T:43:GLU:OE2	1:H:187:ARG:NH1	2.34	0.60
1:C:90:VAL:C	5:C:624:HOH:O	2.44	0.60
1:C:338:GLU:HB2	5:C:2670:HOH:O	2.01	0.60
1:C:338:GLU:HB3	1:C:341:MET:HG3	1.83	0.60
1:E:172:CYS:SG	1:E:407:LEU:HD11	2.42	0.60
1:E:338:GLU:HG3	5:E:2570:HOH:O	2.00	0.60
1:G:93:GLU:HG2	5:G:1391:HOH:O	2.00	0.60
1:B:17:VAL:O	1:B:17:VAL:HG13	2.01	0.60
5:E:1726:HOH:O	1:F:13:PHE:CZ	2.52	0.60
1:F:93:GLU:CD	5:F:2288:HOH:O	2.43	0.60
1:H:313:VAL:HB	5:H:1788:HOH:O	2.00	0.60
1:H:338:GLU:HB2	5:H:2717:HOH:O	2.02	0.60
1:E:463:LYS:HB2	1:E:463:LYS:NZ	2.17	0.60
2:U:33:LEU:HD23	2:U:38:TRP:O	2.02	0.60
1:D:341:MET:CE	1:D:360:ARG:C	2.75	0.60
2:W:26:LEU:HD22	5:W:2644:HOH:O	2.02	0.60
2:S:43:GLU:OE2	1:C:187:ARG:NH1	2.35	0.60
1:E:358:ARG:NH2	1:E:358:ARG:CG	2.58	0.60
2:W:9:ILE:HG22	2:W:9:ILE:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:23:VAL:O	2:Z:27:LEU:HD13	2.02	0.60
1:B:16:GLY:HA2	1:B:67:THR:OG1	2.02	0.59
1:D:383:HIS:HE1	1:D:463:LYS:HB3	1.64	0.59
2:W:21:LEU:HD23	2:W:26:LEU:HD23	1.83	0.59
2:Y:27:LEU:O	2:Y:31:GLU:HG3	2.02	0.59
2:S:27:LEU:HD11	2:S:84:LEU:HD11	1.82	0.59
1:C:340:GLU:HG2	5:C:1856:HOH:O	2.01	0.59
1:F:143:THR:HG23	5:F:488:HOH:O	2.01	0.59
1:C:432:ASN:HD22	2:U:29:GLN:HE22	1.51	0.59
1:F:341:MET:HE1	1:F:361:GLY:HA3	1.85	0.59
2:W:27:LEU:HG	2:W:84:LEU:HD11	1.83	0.59
1:F:341:MET:HA	1:F:341:MET:HE2	1.85	0.59
1:G:13:PHE:CG	1:G:70:TRP:HB3	2.38	0.59
2:Z:31:GLU:HG2	5:Z:2074:HOH:O	2.02	0.59
2:Z:100:ARG:HB3	2:Z:116:ILE:HD13	1.83	0.59
1:E:429:GLN:O	1:E:433:GLU:HG3	2.02	0.59
2:T:27:LEU:CD1	2:T:84:LEU:HD11	2.33	0.58
1:C:331:VAL:CG2	1:C:393:ILE:HD13	2.32	0.58
1:D:16:GLY:O	1:D:17:VAL:CB	2.51	0.58
2:S:5:PRO:HB2	2:S:9:ILE:HG13	1.84	0.58
2:W:5:PRO:HB2	2:W:9:ILE:HG13	1.84	0.58
1:F:339:ARG:NH1	1:F:393:ILE:HG12	2.17	0.58
1:A:25:TYR:HB3	5:A:1928:HOH:O	2.04	0.58
2:V:11:LYS:HG3	2:V:17:TYR:CE1	2.39	0.58
1:G:338:GLU:HG2	5:G:2026:HOH:O	2.03	0.58
1:F:360:ARG:NE	5:F:2240:HOH:O	2.36	0.58
1:H:79:ARG:HD2	5:H:808:HOH:O	2.02	0.58
2:T:27:LEU:CG	2:T:84:LEU:HD11	2.33	0.58
1:A:330:THR:C	1:A:332:VAL:N	2.61	0.58
2:U:35:ARG:HD3	5:U:1568:HOH:O	2.04	0.58
2:V:120:PRO:HB3	2:V:121:PRO:HD2	1.86	0.58
1:F:187:ARG:HH22	2:Z:111:GLN:NE2	2.00	0.58
1:C:197:LEU:HG	1:C:417:ALA:HB1	1.85	0.58
1:G:197:LEU:HG	1:G:417:ALA:HB1	1.85	0.58
2:Z:27:LEU:HD12	2:Z:84:LEU:HD21	1.86	0.58
1:A:443:GLU:HG3	5:A:1292:HOH:O	2.03	0.58
2:S:21:LEU:HD23	2:S:26:LEU:HD23	1.86	0.58
2:T:27:LEU:HG	2:T:84:LEU:HD11	1.86	0.58
1:D:443:GLU:HG3	5:D:1499:HOH:O	2.03	0.58
2:V:35:ARG:HD3	5:V:1306:HOH:O	2.04	0.57
2:X:9:ILE:HG22	2:X:9:ILE:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:110:VAL:C	5:X:2758:HOH:O	2.47	0.57
1:C:220:PHE:HA	5:C:2509:HOH:O	2.03	0.57
2:Y:27:LEU:CD1	2:Y:84:LEU:HD11	2.34	0.57
1:H:442:ASN:HB3	1:H:446:ARG:NH1	2.18	0.57
2:Z:12:PHE:CB	2:Z:116:ILE:HG12	2.34	0.57
2:V:105:ASP:OD2	2:V:108:ARG:HG3	2.04	0.57
1:F:339:ARG:NH2	1:F:392:GLU:OE1	2.32	0.57
1:F:197:LEU:HG	1:F:417:ALA:HB1	1.87	0.57
1:F:93:GLU:HA	5:F:1441:HOH:O	2.04	0.57
1:G:463:LYS:HB2	1:G:463:LYS:HZ2	1.67	0.57
2:Z:12:PHE:HB2	2:Z:116:ILE:CG1	2.35	0.57
1:A:143:THR:HG23	5:A:495:HOH:O	2.06	0.56
2:S:92:LYS:HE3	5:S:2034:HOH:O	2.05	0.56
1:D:429:GLN:O	1:D:433:GLU:HG3	2.05	0.56
2:Y:9:ILE:HG22	2:Y:9:ILE:O	2.05	0.56
1:B:429:GLN:O	1:B:433:GLU:HG3	2.04	0.56
1:E:443:GLU:HG3	5:E:1461:HOH:O	2.04	0.56
1:G:25:TYR:CE1	1:G:87:ILE:HD11	2.41	0.56
1:D:45:GLN:OE1	1:D:131:ARG:HG2	2.05	0.56
1:H:330:THR:O	1:H:331:VAL:HB	2.04	0.56
1:G:93:GLU:HG3	1:G:96:GLN:CB	2.35	0.56
1:H:22:LEU:HD12	5:H:1955:HOH:O	2.04	0.56
1:A:442:ASN:O	1:A:446:ARG:HG3	2.06	0.56
2:W:100:ARG:HB3	2:W:116:ILE:HD13	1.86	0.56
1:G:422:VAL:HG13	1:G:451:TRP:CH2	2.41	0.56
2:Z:5:PRO:HB2	2:Z:9:ILE:HG13	1.87	0.56
1:E:14:LYS:O	1:E:14:LYS:HG3	2.06	0.56
2:W:21:LEU:HG	5:W:1879:HOH:O	2.04	0.56
1:D:385:TRP:CB	1:D:463:LYS:CD	2.80	0.56
1:A:447:SER:HA	1:A:450:LYS:HD3	1.88	0.55
1:B:463:LYS:HB2	1:B:463:LYS:HZ2	1.71	0.55
2:T:9:ILE:HG22	2:T:9:ILE:O	2.05	0.55
1:E:63:THR:HG21	1:E:77:LEU:HD22	1.89	0.55
1:C:17:VAL:O	1:C:17:VAL:CG1	2.54	0.55
5:C:2133:HOH:O	1:D:77:LEU:HD23	2.05	0.55
2:U:9:ILE:HG22	2:U:9:ILE:O	2.05	0.55
2:W:11:LYS:HG3	2:W:17:TYR:CE1	2.41	0.55
2:W:39:VAL:HG22	5:W:2083:HOH:O	2.05	0.55
1:B:14:LYS:CG	1:B:15:ALA:N	2.69	0.55
1:D:75:THR:HG23	5:D:2656:HOH:O	2.07	0.55
1:F:175:LYS:HA	1:F:176:PRO:C	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:ALA:O	5:D:3479:HOH:O	2.18	0.55
1:H:356:LYS:HE3	5:H:1622:HOH:O	2.06	0.55
1:C:90:VAL:HG23	1:C:97:TYR:HA	1.88	0.55
2:X:92:LYS:HE3	5:X:1181:HOH:O	2.06	0.55
1:G:442:ASN:HB3	1:G:446:ARG:NH1	2.21	0.55
2:U:27:LEU:HD11	2:U:84:LEU:HD11	1.87	0.55
2:V:121:PRO:HA	5:V:1914:HOH:O	2.06	0.55
2:X:11:LYS:HG3	2:X:17:TYR:CE1	2.42	0.55
1:C:450:LYS:HE2	5:C:2549:HOH:O	2.07	0.54
1:H:432:ASN:HD22	2:Z:29:GLN:HE22	1.54	0.54
1:A:332:VAL:HG13	1:A:333:GLY:H	1.72	0.54
2:S:27:LEU:CD1	2:S:84:LEU:HD11	2.37	0.54
2:U:27:LEU:HD11	2:U:84:LEU:CD1	2.37	0.54
1:F:429:GLN:O	1:F:433:GLU:HG3	2.07	0.54
2:Y:27:LEU:HD11	2:Y:84:LEU:HD11	1.89	0.54
1:H:332:VAL:HG22	5:H:1428:HOH:O	2.06	0.54
1:C:60:GLU:C	1:C:124:VAL:HG12	2.32	0.54
2:U:27:LEU:HD12	2:U:84:LEU:HD21	1.90	0.54
1:E:296:ALA:O	1:E:297:MET:HB3	2.07	0.54
1:F:463:LYS:HB2	1:F:463:LYS:HZ2	1.72	0.54
2:X:81:THR:HA	2:X:84:LEU:HD12	1.89	0.54
2:Z:27:LEU:CD1	2:Z:84:LEU:HD11	2.37	0.54
1:D:89:PRO:HB2	5:D:2691:HOH:O	2.07	0.54
1:E:447:SER:HA	1:E:450:LYS:HD3	1.88	0.54
1:F:463:LYS:HB3	5:F:1063:HOH:O	2.06	0.54
1:B:16:GLY:C	1:B:67:THR:OG1	2.51	0.54
1:C:331:VAL:HG22	1:C:393:ILE:HD13	1.90	0.54
2:T:11:LYS:HG3	2:T:17:TYR:CE1	2.42	0.54
1:D:16:GLY:CA	1:D:68:THR:HB	2.28	0.54
2:V:7:GLU:CD	2:X:46:LYS:HD2	2.33	0.54
1:B:339:ARG:NH2	1:B:392:GLU:OE1	2.41	0.54
1:C:63:THR:HG22	5:D:793:HOH:O	2.08	0.54
1:E:42:VAL:HG22	1:E:133:LEU:CD1	2.38	0.54
2:S:27:LEU:CG	2:S:84:LEU:HD11	2.38	0.54
2:X:7:GLU:CD	2:Z:46:LYS:HD2	2.33	0.54
5:A:1861:HOH:O	1:B:70:TRP:CD1	2.55	0.53
1:D:21:LYS:HD3	1:D:52:GLU:HG2	1.89	0.53
1:F:21:LYS:HA	1:F:55:ALA:HB1	1.88	0.53
2:Y:116:ILE:HG23	5:Y:1304:HOH:O	2.09	0.53
1:A:93:GLU:HG3	1:A:96:GLN:OE1	2.08	0.53
1:G:49:PRO:HG2	1:G:52:GLU:CG	2.32	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:LEU:HD22	5:A:1830:HOH:O	2.08	0.53
2:X:27:LEU:HD12	2:X:84:LEU:HD21	1.89	0.53
2:S:27:LEU:HD11	2:S:84:LEU:CD1	2.38	0.53
2:S:30:ILE:HD13	2:S:83:VAL:HB	1.90	0.53
1:C:220:PHE:CA	5:C:2509:HOH:O	2.57	0.53
1:G:178:LEU:HD23	1:G:178:LEU:H	1.72	0.53
1:G:178:LEU:HD23	1:G:178:LEU:N	2.24	0.53
1:A:178:LEU:CD1	1:B:107:LEU:HD22	2.37	0.53
1:B:16:GLY:HA2	1:B:67:THR:HG1	1.74	0.53
2:X:90:ALA:CB	5:X:2753:HOH:O	2.56	0.53
1:D:385:TRP:CD1	1:D:463:LYS:HG2	2.44	0.53
1:C:462:TRP:HH2	5:C:2499:HOH:O	1.91	0.53
1:F:341:MET:HE1	1:F:361:GLY:CA	2.39	0.53
2:U:27:LEU:CD1	2:U:84:LEU:HD11	2.39	0.53
1:D:21:LYS:HA	1:D:55:ALA:HB1	1.90	0.53
1:D:341:MET:HE2	1:D:341:MET:CA	2.21	0.53
1:E:32:LYS:HE2	5:E:1178:HOH:O	2.08	0.53
2:W:33:LEU:HB2	5:W:708:HOH:O	2.08	0.53
1:C:42:VAL:HG22	1:C:133:LEU:CD1	2.38	0.53
2:Z:33:LEU:HB2	5:Z:820:HOH:O	2.09	0.53
1:A:175:LYS:HA	1:A:176:PRO:C	2.35	0.52
2:S:11:LYS:HG3	2:S:17:TYR:CE1	2.44	0.52
2:T:85:LYS:HE3	5:T:2584:HOH:O	2.09	0.52
1:G:32:LYS:HE2	5:G:2355:HOH:O	2.08	0.52
1:G:297:MET:O	1:G:297:MET:HG3	2.07	0.52
1:B:331:VAL:HA	5:B:2446:HOH:O	2.10	0.52
2:Y:14:THR:HG22	2:Y:15:LEU:HG	1.92	0.52
2:S:26:LEU:HD22	5:S:2004:HOH:O	2.09	0.52
2:X:27:LEU:HD11	2:X:84:LEU:CD1	2.39	0.52
1:B:143:THR:HG23	5:B:485:HOH:O	2.08	0.52
1:E:178:LEU:HD12	1:F:107:LEU:HD22	1.92	0.52
1:F:172:CYS:SG	1:F:407:LEU:CD1	2.97	0.52
1:F:393:ILE:HG13	5:F:2017:HOH:O	2.08	0.52
1:B:17:VAL:O	1:B:17:VAL:CG1	2.58	0.52
1:B:187:ARG:NH1	2:V:43:GLU:OE2	2.43	0.52
2:U:120:PRO:HG2	2:U:123:CYS:HB2	1.91	0.52
1:H:342:THR:HA	1:H:345:PHE:CE2	2.45	0.52
2:Z:9:ILE:HD11	5:Z:1925:HOH:O	2.10	0.52
1:E:83:ARG:NE	5:E:2311:HOH:O	2.43	0.52
2:W:43:GLU:OE2	1:G:187:ARG:NH1	2.43	0.52
1:A:23:THR:HG22	1:A:23:THR:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:PRO:O	1:C:87:ILE:HD13	2.09	0.52
1:C:93:GLU:HG3	1:C:96:GLN:HB3	1.91	0.52
1:B:128:LYS:HD3	1:B:129:ALA:N	2.25	0.51
2:T:27:LEU:HD11	2:T:84:LEU:CD1	2.40	0.51
2:X:104:PHE:CD2	5:X:2758:HOH:O	2.54	0.51
1:H:383:HIS:CE1	1:H:385:TRP:HB2	2.45	0.51
2:S:43:GLU:CD	2:S:102:ILE:HD13	2.35	0.51
1:C:185:TYR:CE2	5:C:2812:HOH:O	2.53	0.51
1:C:330:THR:C	1:C:332:VAL:H	2.17	0.51
1:C:341:MET:CG	5:C:480:HOH:O	2.57	0.51
2:V:31:GLU:HG2	5:V:1280:HOH:O	2.09	0.51
2:Y:12:PHE:CB	2:Y:116:ILE:HG12	2.40	0.51
2:Y:33:LEU:HD23	2:Y:38:TRP:O	2.09	0.51
1:A:463:LYS:HB2	1:A:463:LYS:NZ	2.25	0.51
2:S:9:ILE:HG22	2:S:9:ILE:O	2.10	0.51
1:H:355:GLU:HG3	5:H:2567:HOH:O	2.10	0.51
1:C:443:GLU:HG3	5:C:1665:HOH:O	2.09	0.51
1:D:197:LEU:HG	1:D:417:ALA:HB1	1.91	0.51
2:X:31:GLU:HG2	5:X:2338:HOH:O	2.10	0.51
2:Y:27:LEU:HD12	2:Y:84:LEU:HD21	1.91	0.51
1:H:197:LEU:HG	1:H:417:ALA:HB1	1.92	0.51
1:D:342:THR:HA	1:D:345:PHE:CE2	2.45	0.51
2:V:33:LEU:HB2	5:V:1558:HOH:O	2.09	0.51
1:E:49:PRO:HG2	1:E:52:GLU:HB3	1.91	0.51
1:F:331:VAL:HG11	1:F:393:ILE:HD13	1.92	0.51
1:F:463:LYS:HD2	5:F:1798:HOH:O	2.08	0.51
1:B:101:VAL:C	5:B:2531:HOH:O	2.53	0.51
2:T:121:PRO:HA	5:T:2317:HOH:O	2.10	0.51
2:V:108:ARG:NH1	5:V:2396:HOH:O	2.43	0.51
1:H:21:LYS:HA	1:H:55:ALA:HB1	1.92	0.51
1:G:42:VAL:HG22	1:G:133:LEU:CD1	2.41	0.51
1:H:297:MET:HG3	1:H:297:MET:O	2.09	0.51
2:S:9:ILE:HD11	5:S:2675:HOH:O	2.10	0.51
2:T:23:VAL:O	2:T:27:LEU:HD13	2.11	0.51
1:C:93:GLU:HG2	5:C:624:HOH:O	2.11	0.51
1:A:371:MET:CG	5:A:480:HOH:O	2.23	0.51
1:E:175:LYS:HA	1:E:176:PRO:C	2.36	0.51
1:B:128:LYS:HD2	5:B:819:HOH:O	2.11	0.51
1:C:93:GLU:HG3	1:C:96:GLN:CB	2.41	0.51
1:D:143:THR:HG23	5:D:3374:HOH:O	2.10	0.51
2:V:120:PRO:CB	2:V:121:PRO:HD2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:343:LEU:HA	1:H:346:VAL:CG2	2.41	0.51
1:H:343:LEU:HA	1:H:346:VAL:HG22	1.91	0.51
1:B:42:VAL:HG22	1:B:133:LEU:CD1	2.41	0.50
1:E:49:PRO:HG2	1:E:52:GLU:CB	2.41	0.50
1:B:139:ARG:HD2	1:B:139:ARG:C	2.36	0.50
2:U:46:LYS:HD2	2:W:7:GLU:CD	2.37	0.50
1:H:143:THR:HG23	5:H:513:HOH:O	2.10	0.50
1:B:197:LEU:HG	1:B:417:ALA:HB1	1.93	0.50
1:F:22:LEU:C	5:F:1917:HOH:O	2.54	0.50
2:X:27:LEU:HD11	2:X:84:LEU:HD11	1.94	0.50
2:Y:43:GLU:CD	2:Y:102:ILE:HD13	2.37	0.50
1:H:139:ARG:HD2	1:H:139:ARG:C	2.36	0.50
1:H:332:VAL:CG2	5:H:1428:HOH:O	2.59	0.50
1:A:49:PRO:HG2	1:A:52:GLU:HB3	1.93	0.50
1:A:197:LEU:HG	1:A:417:ALA:HB1	1.92	0.50
2:T:33:LEU:HD23	2:T:38:TRP:O	2.12	0.50
2:U:11:LYS:HG3	2:U:17:TYR:CE1	2.46	0.50
1:G:392:GLU:HG3	5:G:2262:HOH:O	2.12	0.50
2:Y:12:PHE:CB	2:Y:116:ILE:CG1	2.89	0.50
1:B:103:TYR:CD2	5:B:2531:HOH:O	2.55	0.50
1:B:342:THR:HA	1:B:345:PHE:CE2	2.46	0.50
2:Z:43:GLU:OE2	2:Z:102:ILE:HD13	2.12	0.50
1:B:312:ARG:NH2	1:B:341:MET:CE	2.61	0.50
1:E:197:LEU:HG	1:E:417:ALA:HB1	1.94	0.50
1:F:297:MET:O	1:F:297:MET:HG3	2.12	0.50
1:A:187:ARG:CZ	2:Y:43:GLU:OE2	2.60	0.50
1:A:450:LYS:HG3	5:A:2308:HOH:O	2.12	0.50
2:V:5:PRO:HB2	2:V:9:ILE:HG13	1.93	0.50
1:F:342:THR:HA	1:F:345:PHE:CE2	2.46	0.50
1:A:303:ARG:HH22	1:B:128:LYS:HA	1.77	0.50
2:S:27:LEU:HG	2:S:84:LEU:HD11	1.92	0.50
1:C:429:GLN:O	1:C:433:GLU:HG3	2.11	0.50
1:E:358:ARG:NH1	5:E:2622:HOH:O	2.45	0.50
1:F:63:THR:HG21	1:F:77:LEU:HD22	1.93	0.50
1:F:91:VAL:HG22	5:F:2463:HOH:O	2.12	0.50
1:A:79:ARG:NH1	5:A:2147:HOH:O	2.44	0.49
1:B:75:THR:HG23	1:B:77:LEU:HD12	1.94	0.49
2:W:46:LYS:HD2	2:Y:7:GLU:CD	2.36	0.49
1:F:42:VAL:HG22	1:F:133:LEU:CD1	2.41	0.49
1:G:429:GLN:O	1:G:433:GLU:HG3	2.12	0.49
2:Y:91:LYS:HE3	2:Y:118:TYR:CD1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ASN:ND2	1:A:131:ARG:HH21	2.11	0.49
1:A:13:PHE:O	1:A:14:LYS:HB3	2.12	0.49
1:C:354:ILE:N	1:C:354:ILE:HD12	2.27	0.49
1:E:46:PRO:HG3	1:E:131:ARG:HH22	1.75	0.49
1:C:16:GLY:O	1:C:68:THR:HG23	2.12	0.49
1:D:83:ARG:NE	5:D:2218:HOH:O	2.42	0.49
1:G:93:GLU:HB3	5:G:1670:HOH:O	2.11	0.49
1:D:32:LYS:HE2	5:D:1370:HOH:O	2.12	0.49
2:V:33:LEU:HD12	5:V:1558:HOH:O	2.11	0.49
1:A:332:VAL:CG1	1:A:333:GLY:N	2.75	0.49
1:D:463:LYS:O	1:D:463:LYS:HG3	2.12	0.49
1:E:50:PRO:HB3	1:E:97:TYR:CE2	2.47	0.49
1:G:65:THR:HG22	5:G:1898:HOH:O	2.12	0.49
2:Z:10:LYS:HB3	2:Z:50:PHE:CE1	2.48	0.49
2:Y:35:ARG:HD3	5:Y:1838:HOH:O	2.12	0.49
1:C:79:ARG:CZ	5:C:2230:HOH:O	2.60	0.49
1:E:139:ARG:HD2	1:E:139:ARG:C	2.38	0.49
2:W:43:GLU:CD	5:W:1911:HOH:O	2.55	0.49
1:G:139:ARG:HD2	1:G:139:ARG:C	2.38	0.49
2:Y:100:ARG:HB3	2:Y:116:ILE:CD1	2.32	0.49
2:V:10:LYS:HB3	2:V:50:PHE:CE1	2.48	0.49
1:H:377:VAL:HG22	1:H:399:VAL:HB	1.94	0.49
2:Z:23:VAL:O	2:Z:27:LEU:CD1	2.61	0.49
1:A:42:VAL:HG21	1:A:57:VAL:HG21	1.94	0.49
2:S:43:GLU:OE2	1:C:187:ARG:CZ	2.61	0.49
1:B:34:THR:HG22	1:B:143:THR:HG21	1.94	0.49
1:E:89:PRO:HG3	1:E:97:TYR:HE2	1.76	0.49
1:E:297:MET:HG3	1:E:297:MET:O	2.13	0.49
2:X:27:LEU:HG	2:X:84:LEU:HD11	1.95	0.49
1:A:177:LYS:C	1:A:178:LEU:HD23	2.38	0.48
1:F:187:ARG:NE	5:F:1422:HOH:O	2.46	0.48
1:G:45:GLN:CD	1:G:131:ARG:HG2	2.38	0.48
2:Z:12:PHE:CB	2:Z:116:ILE:HG13	2.42	0.48
1:C:90:VAL:HG12	5:C:1289:HOH:O	2.13	0.48
1:C:90:VAL:HG12	1:C:91:VAL:N	2.28	0.48
1:C:175:LYS:HA	1:C:176:PRO:C	2.38	0.48
1:D:297:MET:O	1:D:297:MET:HG3	2.12	0.48
1:G:206:VAL:C	1:G:207:ASN:HD22	2.21	0.48
1:C:22:LEU:N	5:C:2229:HOH:O	2.46	0.48
2:U:14:THR:HG22	2:U:15:LEU:HG	1.95	0.48
2:V:14:THR:HG22	2:V:15:LEU:HG	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:GLU:HG2	5:C:1289:HOH:O	2.13	0.48
2:U:23:VAL:O	2:U:27:LEU:CD1	2.60	0.48
2:V:9:ILE:HG22	2:V:9:ILE:O	2.13	0.48
2:W:111:GLN:HE22	1:G:187:ARG:HH21	1.61	0.48
1:G:15:ALA:HA	1:G:68:THR:HB	1.94	0.48
1:H:168:PRO:HD2	1:H:424:LEU:HD11	1.96	0.48
1:B:211:PHE:CZ	2:V:109:GLN:HB2	2.49	0.48
1:F:92:GLY:C	5:F:2288:HOH:O	2.56	0.48
1:G:383:HIS:CE1	1:G:385:TRP:HB2	2.49	0.48
1:C:22:LEU:N	5:C:1654:HOH:O	2.46	0.48
2:W:23:VAL:O	2:W:27:LEU:HD13	2.14	0.48
1:G:24:TYR:CD2	1:G:59:ALA:HB2	2.49	0.48
1:C:139:ARG:HD2	1:C:139:ARG:C	2.39	0.48
1:E:178:LEU:HB2	5:E:2185:HOH:O	2.13	0.48
2:W:12:PHE:CB	2:W:116:ILE:CG1	2.92	0.48
2:X:120:PRO:O	2:X:122:GLY:N	2.47	0.48
1:B:16:GLY:CA	1:B:67:THR:OG1	2.62	0.48
1:B:451:TRP:CH2	2:T:19:PRO:HD3	2.48	0.48
2:U:33:LEU:HB2	5:U:1274:HOH:O	2.13	0.48
1:E:51:GLU:N	5:E:2167:HOH:O	2.46	0.48
2:X:10:LYS:HB3	2:X:50:PHE:CE1	2.49	0.48
2:Z:43:GLU:CD	5:Z:749:HOH:O	2.57	0.48
2:U:91:LYS:HE3	2:U:118:TYR:CD1	2.49	0.47
2:X:33:LEU:HD23	2:X:38:TRP:O	2.14	0.47
2:Z:27:LEU:HD11	2:Z:84:LEU:HD11	1.94	0.47
1:C:93:GLU:CB	5:C:624:HOH:O	2.62	0.47
1:C:422:VAL:HG13	1:C:451:TRP:CH2	2.50	0.47
2:X:104:PHE:HA	5:X:2758:HOH:O	2.14	0.47
2:T:14:THR:HG22	2:T:15:LEU:HG	1.96	0.47
1:G:12:GLY:HA2	5:G:2771:HOH:O	2.14	0.47
1:H:34:THR:HG23	5:H:2435:HOH:O	2.14	0.47
1:A:121:VAL:HG11	1:A:309:MET:HE3	1.95	0.47
1:C:91:VAL:O	1:C:91:VAL:HG23	2.14	0.47
2:W:12:PHE:CB	2:W:116:ILE:HG13	2.45	0.47
1:D:139:ARG:C	1:D:139:ARG:HD2	2.40	0.47
1:D:175:LYS:HA	1:D:176:PRO:C	2.38	0.47
1:E:463:LYS:HB2	1:E:463:LYS:HZ2	1.78	0.47
1:G:22:LEU:N	5:G:2134:HOH:O	2.46	0.47
1:G:450:LYS:HD2	1:G:450:LYS:N	2.30	0.47
1:A:80:TYR:CE2	1:B:179:GLY:HA2	2.49	0.47
2:S:21:LEU:HD13	5:S:1722:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:GLU:HB2	5:C:624:HOH:O	2.13	0.47
1:C:463:LYS:HB2	1:C:463:LYS:HZ2	1.78	0.47
2:U:10:LYS:HB3	2:U:50:PHE:CE1	2.50	0.47
1:E:178:LEU:HG	5:E:2185:HOH:O	2.15	0.47
1:H:32:LYS:HE2	5:H:1771:HOH:O	2.15	0.47
1:H:53:ALA:O	1:H:57:VAL:HG23	2.14	0.47
1:H:442:ASN:O	1:H:446:ARG:HG3	2.14	0.47
1:B:175:LYS:HA	1:B:176:PRO:C	2.39	0.47
2:T:69:MET:HG2	2:T:71:LYS:O	2.15	0.47
2:V:23:VAL:O	2:V:27:LEU:CD1	2.57	0.47
1:E:172:CYS:SG	1:E:407:LEU:CD1	3.03	0.47
1:F:83:ARG:NH2	5:F:1720:HOH:O	2.47	0.47
2:X:27:LEU:CD1	2:X:84:LEU:HD11	2.44	0.47
1:G:175:LYS:HA	1:G:176:PRO:C	2.40	0.47
2:Y:23:VAL:O	2:Y:27:LEU:CD1	2.60	0.47
2:Y:27:LEU:HD11	2:Y:84:LEU:CD1	2.44	0.47
1:B:341:MET:CE	1:B:361:GLY:HA3	2.22	0.47
2:T:84:LEU:HD22	5:T:2104:HOH:O	2.13	0.47
1:F:50:PRO:HB3	1:F:97:TYR:CE2	2.50	0.47
1:B:102:ALA:N	5:B:2531:HOH:O	2.47	0.47
2:V:43:GLU:CD	5:V:837:HOH:O	2.58	0.47
2:Y:33:LEU:HB2	5:Y:789:HOH:O	2.13	0.47
2:Z:9:ILE:HG22	2:Z:9:ILE:O	2.15	0.47
1:C:220:PHE:HD1	5:C:2509:HOH:O	1.98	0.47
2:W:109:GLN:NE2	1:H:79:ARG:HE	2.13	0.47
1:G:90:VAL:HG22	1:G:91:VAL:HG22	1.96	0.47
1:A:389:ALA:O	1:A:393:ILE:HG13	2.15	0.46
2:T:43:GLU:OE2	1:H:187:ARG:NH2	2.48	0.46
1:C:90:VAL:HB	5:C:624:HOH:O	2.14	0.46
1:F:330:THR:O	1:F:331:VAL:CB	2.63	0.46
1:H:385:TRP:NE1	1:H:463:LYS:HA	2.30	0.46
2:Z:61:TYR:CD1	2:Z:61:TYR:C	2.93	0.46
1:B:45:GLN:HG3	1:B:128:LYS:O	2.15	0.46
1:D:439:ARG:HH21	1:D:439:ARG:HG3	1.80	0.46
2:W:10:LYS:HB3	2:W:50:PHE:CE1	2.50	0.46
2:W:43:GLU:OE2	1:G:187:ARG:CZ	2.63	0.46
2:X:23:VAL:O	2:X:27:LEU:CD1	2.61	0.46
1:G:273:GLY:HA3	1:H:273:GLY:HA3	1.96	0.46
1:C:331:VAL:HG21	1:C:393:ILE:HD13	1.95	0.46
2:V:91:LYS:HE3	2:V:118:TYR:CD1	2.51	0.46
1:G:354:ILE:HD12	1:G:354:ILE:N	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:LYS:HE2	5:B:2135:HOH:O	2.15	0.46
1:C:273:GLY:HA3	1:D:273:GLY:HA3	1.97	0.46
2:V:33:LEU:HD23	2:V:38:TRP:O	2.15	0.46
2:W:27:LEU:CG	2:W:84:LEU:HD11	2.46	0.46
1:F:383:HIS:CE1	1:F:385:TRP:HB2	2.51	0.46
1:G:463:LYS:HB2	1:G:463:LYS:HZ3	1.80	0.46
1:H:175:LYS:HA	1:H:176:PRO:C	2.39	0.46
1:A:331:VAL:HG11	1:A:342:THR:CB	2.46	0.46
2:S:33:LEU:HB2	5:S:882:HOH:O	2.16	0.46
2:T:23:VAL:O	2:T:27:LEU:CD1	2.64	0.46
1:C:310:HIS:HE2	1:C:341:MET:CE	2.29	0.46
2:U:92:LYS:HE3	5:U:1583:HOH:O	2.15	0.46
1:H:92:GLY:HA3	5:H:2561:HOH:O	2.14	0.46
1:A:273:GLY:HA3	1:B:273:GLY:HA3	1.97	0.46
2:Y:79:ASP:OD2	2:Y:81:THR:HB	2.16	0.46
1:B:338:GLU:CD	5:B:2663:HOH:O	2.58	0.46
2:U:35:ARG:HD2	5:U:2246:HOH:O	2.15	0.46
2:W:46:LYS:HD3	5:W:1675:HOH:O	2.15	0.46
2:Y:61:TYR:C	2:Y:61:TYR:CD1	2.94	0.46
1:H:79:ARG:NH2	5:H:2489:HOH:O	2.48	0.46
2:S:30:ILE:CD1	5:S:2803:HOH:O	2.63	0.46
1:F:329:GLY:O	1:F:378:ALA:HA	2.16	0.46
1:G:45:GLN:HA	1:G:131:ARG:CG	2.43	0.46
2:Z:14:THR:HG22	2:Z:15:LEU:HG	1.97	0.46
1:A:77:LEU:C	1:A:79:ARG:H	2.23	0.46
1:B:32:LYS:HE2	5:B:1760:HOH:O	2.15	0.46
1:B:187:ARG:HH21	2:V:111:GLN:HE22	1.63	0.46
1:B:463:LYS:HB2	1:B:463:LYS:HZ3	1.81	0.46
1:C:297:MET:O	1:C:297:MET:HG3	2.15	0.46
1:D:88:GLU:O	1:D:88:GLU:HG3	2.16	0.46
1:E:87:ILE:HD12	1:E:99:ALA:HB2	1.97	0.46
1:H:343:LEU:C	1:H:346:VAL:HG22	2.41	0.46
2:S:61:TYR:CD1	2:S:61:TYR:C	2.94	0.46
1:C:409:HIS:N	5:C:2499:HOH:O	2.48	0.46
1:F:34:THR:HG22	1:F:143:THR:HG21	1.97	0.46
1:G:442:ASN:HB3	1:G:446:ARG:HH12	1.81	0.46
1:H:131:ARG:HD3	5:H:2101:HOH:O	2.15	0.46
2:S:10:LYS:HB3	2:S:50:PHE:CE1	2.50	0.45
1:D:53:ALA:O	1:D:57:VAL:HG23	2.16	0.45
2:Z:27:LEU:HD11	2:Z:84:LEU:CD1	2.46	0.45
1:A:139:ARG:C	1:A:139:ARG:HD2	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:33:LEU:HD23	2:S:38:TRP:O	2.16	0.45
1:B:318:LEU:C	1:B:318:LEU:HD13	2.42	0.45
1:C:171:GLY:HA2	1:C:199:PHE:O	2.17	0.45
1:B:24:TYR:CD2	1:B:59:ALA:HB2	2.51	0.45
1:F:187:ARG:NH2	2:Z:111:GLN:NE2	2.64	0.45
1:D:45:GLN:CA	1:D:131:ARG:HG3	2.42	0.45
1:D:411:TRP:CD1	2:V:1:MET:HG3	2.52	0.45
1:G:178:LEU:HD12	1:H:107:LEU:HD22	1.96	0.45
1:A:331:VAL:CG1	1:A:342:THR:HG21	2.32	0.45
2:S:23:VAL:O	2:S:27:LEU:CD1	2.63	0.45
1:C:25:TYR:HB3	5:C:1550:HOH:O	2.16	0.45
1:C:95:ASN:N	5:C:854:HOH:O	2.48	0.45
2:X:118:TYR:OH	2:X:121:PRO:HD2	2.15	0.45
1:G:168:PRO:HD2	1:G:424:LEU:HD11	1.97	0.45
2:S:7:GLU:CD	2:Y:46:LYS:HD2	2.41	0.45
1:B:206:VAL:C	1:B:207:ASN:HD22	2.25	0.45
1:B:343:LEU:HD12	5:B:2036:HOH:O	2.17	0.45
1:D:91:VAL:HG23	1:D:91:VAL:O	2.17	0.45
1:E:177:LYS:HG3	1:E:178:LEU:HG	1.99	0.45
2:X:14:THR:HG22	2:X:15:LEU:HG	1.98	0.45
1:H:318:LEU:HD13	1:H:318:LEU:C	2.42	0.45
2:Z:33:LEU:HD23	2:Z:38:TRP:O	2.16	0.45
1:C:450:LYS:HE3	5:C:2608:HOH:O	2.17	0.45
2:U:5:PRO:HB2	2:U:9:ILE:HG13	1.99	0.45
1:G:392:GLU:CG	5:G:2262:HOH:O	2.65	0.45
1:G:450:LYS:HE2	5:G:2422:HOH:O	2.17	0.45
1:H:354:ILE:N	1:H:354:ILE:HD12	2.32	0.45
1:C:61:SER:CB	1:C:124:VAL:HG11	2.28	0.45
1:C:206:VAL:C	1:C:207:ASN:HD22	2.25	0.45
2:V:27:LEU:CD1	2:V:84:LEU:HD21	2.47	0.45
1:E:206:VAL:C	1:E:207:ASN:HD22	2.25	0.45
2:Y:11:LYS:HG3	2:Y:17:TYR:CE1	2.52	0.45
2:S:7:GLU:OE1	2:Y:46:LYS:HD2	2.17	0.45
1:B:383:HIS:CE1	1:B:385:TRP:HB2	2.52	0.44
2:W:33:LEU:HD12	5:W:708:HOH:O	2.16	0.44
1:F:158:GLU:CD	1:F:325:HIS:HE2	2.23	0.44
1:H:206:VAL:C	1:H:207:ASN:HD22	2.25	0.44
2:S:14:THR:HG22	2:S:15:LEU:HG	1.99	0.44
1:D:36:ILE:HD12	1:D:108:PHE:CE2	2.52	0.44
1:D:447:SER:HA	1:D:450:LYS:HD3	1.98	0.44
1:E:178:LEU:CB	5:E:2185:HOH:O	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:330:THR:HG23	1:E:379:SER:O	2.18	0.44
2:W:120:PRO:HG2	2:W:123:CYS:HB2	1.99	0.44
1:F:443:GLU:HG3	5:F:602:HOH:O	2.17	0.44
1:C:98:ILE:HG12	5:C:1746:HOH:O	2.17	0.44
1:E:171:GLY:HA2	1:E:199:PHE:O	2.16	0.44
1:E:354:ILE:HD12	1:E:354:ILE:N	2.33	0.44
2:W:9:ILE:HD11	5:W:1905:HOH:O	2.18	0.44
1:F:24:TYR:CD2	1:F:59:ALA:HB2	2.53	0.44
1:F:442:ASN:O	1:F:446:ARG:HG3	2.17	0.44
1:A:60:GLU:HG3	1:A:127:PHE:CD2	2.53	0.44
1:B:331:VAL:HB	5:B:2473:HOH:O	2.16	0.44
5:T:1836:HOH:O	1:G:79:ARG:HD2	2.16	0.44
1:E:318:LEU:HD13	1:E:318:LEU:C	2.42	0.44
1:D:206:VAL:C	1:D:207:ASN:HD22	2.25	0.44
1:E:178:LEU:CG	5:E:2185:HOH:O	2.65	0.44
1:E:442:ASN:HB3	1:E:446:ARG:NH1	2.32	0.44
2:X:35:ARG:HD3	5:X:1872:HOH:O	2.16	0.44
1:H:343:LEU:CA	1:H:346:VAL:HG22	2.47	0.44
1:B:354:ILE:HD12	1:B:354:ILE:N	2.32	0.44
2:T:43:GLU:CD	2:T:102:ILE:HD13	2.42	0.44
2:T:61:TYR:CD1	2:T:61:TYR:C	2.94	0.44
2:Z:79:ASP:OD2	2:Z:81:THR:HB	2.17	0.44
1:B:15:ALA:HB1	1:B:16:GLY:H	1.45	0.44
1:D:89:PRO:HD2	5:D:2691:HOH:O	2.18	0.44
2:W:14:THR:HG22	2:W:15:LEU:HG	2.00	0.44
1:G:158:GLU:CD	1:G:325:HIS:HE2	2.23	0.44
1:G:450:LYS:HD2	1:G:450:LYS:H	1.82	0.44
1:C:383:HIS:CE1	1:C:385:TRP:HB2	2.53	0.44
2:U:10:LYS:NZ	5:U:2761:HOH:O	2.51	0.44
1:D:23:THR:HG22	1:D:23:THR:O	2.17	0.44
1:G:171:GLY:HA2	1:G:199:PHE:O	2.17	0.44
2:Y:10:LYS:HB3	2:Y:50:PHE:CE1	2.53	0.44
1:H:342:THR:O	1:H:346:VAL:HG13	2.18	0.44
1:A:25:TYR:HB2	1:A:55:ALA:HB2	2.00	0.44
1:A:377:VAL:HG22	1:A:399:VAL:HB	1.99	0.44
2:S:66:TYR:HE2	5:C:2509:HOH:O	1.89	0.44
1:C:28:GLU:OE2	1:C:28:GLU:N	2.46	0.44
1:D:330:THR:O	1:D:331:VAL:HB	2.16	0.44
2:V:14:THR:O	2:V:15:LEU:HB2	2.18	0.44
1:E:342:THR:HA	1:E:345:PHE:CE2	2.53	0.44
1:G:338:GLU:OE2	1:G:341:MET:CG	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:448:ALA:HA	1:G:451:TRP:NE1	2.33	0.44
2:Z:33:LEU:HD12	5:Z:820:HOH:O	2.18	0.44
1:D:171:GLY:HA2	1:D:199:PHE:O	2.17	0.43
1:D:189:CYS:HA	1:D:200:THR:HG21	1.99	0.43
2:W:120:PRO:HG2	2:W:123:CYS:CB	2.48	0.43
1:G:383:HIS:HE1	1:G:385:TRP:HB2	1.83	0.43
1:H:392:GLU:C	1:H:392:GLU:CD	2.86	0.43
1:B:185:TYR:OH	1:B:202:ASP:HA	2.19	0.43
1:E:383:HIS:CE1	1:E:385:TRP:HB2	2.53	0.43
1:F:25:TYR:HB2	1:F:55:ALA:HB2	2.00	0.43
1:F:36:ILE:N	1:F:36:ILE:HD12	2.33	0.43
1:F:206:VAL:C	1:F:207:ASN:HD22	2.26	0.43
2:X:21:LEU:HD23	2:X:26:LEU:HD23	1.99	0.43
2:X:121:PRO:HA	5:X:2016:HOH:O	2.18	0.43
1:D:187:ARG:NH1	2:X:43:GLU:OE2	2.45	0.43
1:E:79:ARG:NH1	5:E:2064:HOH:O	2.49	0.43
1:F:318:LEU:C	1:F:318:LEU:HD13	2.44	0.43
1:F:251:ILE:O	1:F:255:VAL:HG23	2.17	0.43
1:F:339:ARG:HH12	1:F:393:ILE:CG1	2.31	0.43
1:G:403:GLY:O	1:G:407:LEU:HD12	2.17	0.43
1:G:442:ASN:O	1:G:446:ARG:HG3	2.18	0.43
2:Y:23:VAL:HG23	5:Y:1672:HOH:O	2.19	0.43
2:Y:28:LYS:HA	2:Y:31:GLU:OE1	2.19	0.43
1:A:206:VAL:C	1:A:207:ASN:HD22	2.26	0.43
2:S:6:ILE:HG13	2:S:7:GLU:HG3	2.00	0.43
1:B:79:ARG:HD3	5:Y:2071:HOH:O	2.18	0.43
2:T:43:GLU:OE2	1:H:187:ARG:CZ	2.66	0.43
1:F:21:LYS:C	1:F:23:THR:H	2.26	0.43
1:F:60:GLU:HG3	1:F:127:PHE:CD1	2.54	0.43
1:H:21:LYS:C	1:H:23:THR:H	2.25	0.43
1:H:171:GLY:HA2	1:H:199:PHE:O	2.18	0.43
1:A:303:ARG:NH2	1:B:128:LYS:HA	2.33	0.43
2:S:33:LEU:HD12	5:S:882:HOH:O	2.19	0.43
1:B:187:ARG:CZ	2:V:43:GLU:OE2	2.67	0.43
1:B:377:VAL:HG22	1:B:399:VAL:HB	1.99	0.43
1:B:443:GLU:HG3	5:B:739:HOH:O	2.17	0.43
1:C:25:TYR:HB2	1:C:55:ALA:HB2	2.00	0.43
1:C:342:THR:HA	1:C:345:PHE:CE2	2.54	0.43
2:W:33:LEU:HD23	2:W:38:TRP:O	2.19	0.43
1:H:189:CYS:HA	1:H:200:THR:HG21	1.99	0.43
1:A:305:LYS:HB2	5:A:2523:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:ARG:NH1	5:D:2049:HOH:O	2.50	0.43
2:Y:14:THR:O	2:Y:15:LEU:HB2	2.19	0.43
1:D:442:ASN:O	1:D:446:ARG:HG3	2.19	0.43
1:F:447:SER:HA	1:F:450:LYS:HD3	2.00	0.43
1:H:42:VAL:HG21	1:H:57:VAL:HG21	2.01	0.43
1:B:294:HIS:CE1	5:B:1425:HOH:O	2.71	0.43
1:C:158:GLU:CD	1:C:325:HIS:HE2	2.26	0.43
1:C:442:ASN:O	1:C:446:ARG:HG3	2.19	0.43
1:D:318:LEU:C	1:D:318:LEU:HD13	2.44	0.43
1:D:331:VAL:HG11	1:D:393:ILE:HD13	2.01	0.43
1:D:410:PRO:O	2:V:1:MET:HE2	2.18	0.43
1:E:214:TRP:CD2	1:E:253:ARG:HG2	2.54	0.43
1:G:296:ALA:O	1:G:297:MET:HB3	2.17	0.43
1:G:411:TRP:CZ3	2:Y:2:GLN:HB2	2.54	0.43
1:A:185:TYR:OH	1:A:202:ASP:HA	2.18	0.43
1:B:21:LYS:HD3	1:B:52:GLU:HG3	2.01	0.43
1:B:328:ALA:HB1	1:B:345:PHE:HE1	1.84	0.43
1:B:339:ARG:NH1	1:B:343:LEU:HD11	2.34	0.43
1:D:46:PRO:HD3	1:D:131:ARG:HD2	2.00	0.43
1:E:442:ASN:O	1:E:446:ARG:HG3	2.19	0.43
1:G:197:LEU:HG	1:G:417:ALA:CB	2.49	0.43
1:H:410:PRO:O	2:Z:1:MET:HE2	2.19	0.43
1:A:342:THR:HA	1:A:345:PHE:CE2	2.54	0.42
1:F:360:ARG:CZ	5:F:2240:HOH:O	2.66	0.42
1:E:65:THR:HG22	1:F:175:LYS:HD3	2.00	0.42
2:W:61:TYR:CD1	2:W:61:TYR:C	2.96	0.42
1:F:330:THR:C	5:F:1953:HOH:O	2.62	0.42
2:X:27:LEU:CG	2:X:84:LEU:HD11	2.48	0.42
1:G:318:LEU:HD13	1:G:318:LEU:C	2.44	0.42
1:H:451:TRP:CH2	2:Z:19:PRO:HD3	2.54	0.42
1:A:171:GLY:HA2	1:A:199:PHE:O	2.19	0.42
2:V:61:TYR:CD1	2:V:61:TYR:C	2.97	0.42
1:E:46:PRO:CD	1:E:131:ARG:HH21	2.33	0.42
2:W:67:TRP:HB2	5:W:1911:HOH:O	2.19	0.42
1:F:65:THR:HG22	5:F:3590:HOH:O	2.18	0.42
1:F:185:TYR:OH	1:F:202:ASP:HA	2.18	0.42
1:A:383:HIS:CE1	1:A:385:TRP:HB2	2.55	0.42
2:T:33:LEU:HD12	5:T:928:HOH:O	2.18	0.42
1:E:23:THR:O	1:E:23:THR:HG22	2.20	0.42
2:W:23:VAL:O	2:W:27:LEU:CD1	2.68	0.42
5:G:916:HOH:O	1:H:63:THR:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:108:ARG:NH1	5:S:1227:HOH:O	2.52	0.42
2:T:82:GLN:HG3	5:T:2712:HOH:O	2.18	0.42
1:C:327:HIS:HA	1:C:377:VAL:HB	2.01	0.42
2:V:43:GLU:OE2	2:V:102:ILE:HD13	2.19	0.42
1:E:273:GLY:HA3	1:F:273:GLY:HA3	2.00	0.42
2:W:12:PHE:CB	2:W:116:ILE:HG12	2.49	0.42
1:G:63:THR:HG22	5:H:1099:HOH:O	2.19	0.42
2:U:27:LEU:HG	2:U:84:LEU:HD11	2.01	0.42
1:D:168:PRO:HD2	1:D:424:LEU:HD11	2.01	0.42
1:E:327:HIS:HA	1:E:377:VAL:HB	2.01	0.42
1:G:342:THR:HA	1:G:345:PHE:CE2	2.55	0.42
1:H:292:HIS:HA	1:H:325:HIS:HB2	2.01	0.42
1:H:421:ARG:O	1:H:425:GLU:HG3	2.19	0.42
1:A:318:LEU:HD13	1:A:318:LEU:C	2.44	0.42
1:C:197:LEU:HG	1:C:417:ALA:CB	2.49	0.42
1:D:295:ARG:HG2	5:D:1060:HOH:O	2.20	0.42
1:F:168:PRO:HD2	1:F:424:LEU:HD11	2.01	0.42
1:B:36:ILE:HD12	1:B:36:ILE:N	2.35	0.42
2:U:33:LEU:HD22	2:U:40:PRO:HD3	2.02	0.42
1:E:185:TYR:OH	1:E:202:ASP:HA	2.20	0.42
2:X:61:TYR:CD1	2:X:61:TYR:C	2.97	0.42
1:H:331:VAL:HG11	1:H:393:ILE:HD13	2.01	0.42
1:A:42:VAL:HG22	1:A:133:LEU:HD12	2.01	0.42
2:S:43:GLU:OE2	1:C:187:ARG:NH2	2.53	0.42
1:B:463:LYS:CD	5:B:2287:HOH:O	2.63	0.42
1:H:330:THR:O	1:H:331:VAL:CB	2.67	0.42
2:T:103:GLY:N	2:T:113:ILE:HB	2.34	0.42
1:C:442:ASN:HB3	1:C:446:ARG:NH1	2.35	0.42
1:E:46:PRO:CD	1:E:131:ARG:NH2	2.83	0.42
2:W:23:VAL:HG12	2:W:27:LEU:CD1	2.49	0.42
1:F:139:ARG:C	1:F:139:ARG:HD2	2.43	0.42
2:Z:6:ILE:HG13	2:Z:7:GLU:HG3	2.02	0.42
1:A:463:LYS:NZ	1:A:463:LYS:CB	2.83	0.41
1:B:14:LYS:HE3	1:B:14:LYS:HB2	1.72	0.41
2:U:61:TYR:CD1	2:U:61:TYR:C	2.98	0.41
2:W:12:PHE:HB3	2:W:116:ILE:HG12	2.01	0.41
1:H:36:ILE:HD12	1:H:108:PHE:CE2	2.55	0.41
1:F:134:ARG:HD2	1:F:305:LYS:O	2.20	0.41
1:F:197:LEU:HG	1:F:417:ALA:CB	2.49	0.41
1:F:356:LYS:HE3	5:F:1098:HOH:O	2.20	0.41
1:A:332:VAL:CG1	1:A:333:GLY:H	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:TRP:CZ3	2:T:2:GLN:HB2	2.54	0.41
1:C:77:LEU:HG	5:D:1101:HOH:O	2.21	0.41
1:E:356:LYS:HE3	5:E:948:HOH:O	2.20	0.41
1:F:204:GLU:HG2	1:F:205:ASN:N	2.35	0.41
1:H:88:GLU:HA	1:H:89:PRO:HD3	1.91	0.41
1:H:127:PHE:CE2	1:H:129:ALA:HB3	2.55	0.41
1:A:356:LYS:HE3	5:A:1279:HOH:O	2.20	0.41
1:A:450:LYS:HE3	5:A:2308:HOH:O	2.20	0.41
1:B:339:ARG:CB	5:B:2663:HOH:O	2.64	0.41
2:T:13:GLU:HB3	2:T:14:THR:H	1.70	0.41
1:C:79:ARG:CZ	5:C:2685:HOH:O	2.68	0.41
1:C:90:VAL:CG1	1:C:91:VAL:N	2.82	0.41
2:V:27:LEU:CG	2:V:84:LEU:HD11	2.51	0.41
1:E:407:LEU:HD12	1:E:407:LEU:H	1.85	0.41
1:E:463:LYS:NZ	1:E:463:LYS:CB	2.84	0.41
2:W:27:LEU:CD1	2:W:84:LEU:HD11	2.50	0.41
2:Y:100:ARG:CB	2:Y:116:ILE:HD13	2.35	0.41
1:H:411:TRP:CD1	2:Z:1:MET:HG3	2.55	0.41
1:H:429:GLN:O	1:H:433:GLU:HG3	2.20	0.41
1:C:124:VAL:HG13	5:C:2944:HOH:O	2.20	0.41
2:Y:12:PHE:HB3	2:Y:116:ILE:HG12	2.03	0.41
1:D:14:LYS:O	1:D:14:LYS:HG3	2.20	0.41
1:D:45:GLN:HG3	1:D:128:LYS:O	2.21	0.41
1:D:66:TRP:CE3	1:D:67:THR:HB	2.55	0.41
1:G:178:LEU:CD2	1:G:178:LEU:N	2.84	0.41
1:H:141:PRO:HA	1:H:142:PRO:HD3	1.97	0.41
1:A:77:LEU:C	1:A:79:ARG:N	2.79	0.41
1:B:354:ILE:CG2	1:B:362:ILE:HD13	2.51	0.41
1:C:24:TYR:CD2	1:C:59:ALA:HB2	2.55	0.41
1:C:86:HIS:CD2	5:C:2589:HOH:O	2.73	0.41
2:U:14:THR:O	2:U:15:LEU:HB2	2.20	0.41
1:F:451:TRP:CH2	2:X:19:PRO:HD3	2.55	0.41
1:B:117:PHE:O	1:B:121:VAL:HG22	2.20	0.41
1:B:171:GLY:HA3	1:B:401:GLN:NE2	2.36	0.41
1:C:36:ILE:N	1:C:36:ILE:HD12	2.36	0.41
1:E:46:PRO:CG	1:E:131:ARG:NH2	2.82	0.41
2:W:33:LEU:HD22	2:W:40:PRO:HD3	2.03	0.41
1:F:252:LYS:HG3	5:F:501:HOH:O	2.21	0.41
2:X:85:LYS:HD2	5:X:1900:HOH:O	2.20	0.41
1:G:45:GLN:CA	1:G:131:ARG:HG3	2.47	0.41
1:C:168:PRO:HD2	1:C:424:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:TYR:CD2	1:D:59:ALA:HB2	2.56	0.41
1:E:46:PRO:HD3	1:E:131:ARG:NH2	2.36	0.41
1:E:421:ARG:O	1:E:425:GLU:HG3	2.21	0.41
2:Y:9:ILE:HG21	5:Y:2600:HOH:O	2.20	0.41
2:Y:98:PHE:HB3	5:Y:1304:HOH:O	2.20	0.41
1:H:383:HIS:HE1	1:H:385:TRP:HB2	1.84	0.41
2:Z:91:LYS:HE3	2:Z:118:TYR:CD1	2.56	0.41
1:B:177:LYS:C	1:B:178:LEU:HD22	2.46	0.41
1:E:48:VAL:HA	1:E:49:PRO:HD2	1.96	0.41
2:X:33:LEU:HD12	5:X:398:HOH:O	2.21	0.41
1:A:32:LYS:HE2	5:A:2155:HOH:O	2.21	0.40
1:A:303:ARG:NH2	1:B:130:LEU:O	2.54	0.40
1:A:354:ILE:HD12	1:A:354:ILE:N	2.37	0.40
1:A:369:VAL:O	1:A:370:SER:HB2	2.21	0.40
2:S:27:LEU:HD12	2:S:84:LEU:HD21	2.03	0.40
2:S:119:LYS:O	2:S:120:PRO:O	2.38	0.40
1:B:355:GLU:HG3	5:B:2378:HOH:O	2.21	0.40
2:T:14:THR:O	2:T:15:LEU:HB2	2.21	0.40
1:E:53:ALA:O	1:E:57:VAL:HG23	2.20	0.40
2:W:46:LYS:HD2	2:Y:7:GLU:OE1	2.20	0.40
1:F:97:TYR:CD1	1:F:97:TYR:N	2.89	0.40
1:G:25:TYR:HB2	1:G:55:ALA:HB2	2.02	0.40
2:Y:108:ARG:HG2	5:Y:1314:HOH:O	2.21	0.40
1:H:24:TYR:CD2	1:H:59:ALA:HB2	2.56	0.40
1:H:121:VAL:HG11	1:H:309:MET:HE3	2.02	0.40
2:S:85:LYS:HD2	5:S:2497:HOH:O	2.20	0.40
1:B:141:PRO:HA	1:B:142:PRO:HD3	1.98	0.40
1:E:60:GLU:HG3	1:E:127:PHE:CD1	2.56	0.40
2:W:13:GLU:HB3	2:W:14:THR:H	1.70	0.40
1:F:339:ARG:NH1	1:F:393:ILE:CG1	2.84	0.40
1:A:330:THR:OG1	1:A:332:VAL:HB	2.22	0.40
2:T:121:PRO:HD3	5:T:1302:HOH:O	2.20	0.40
1:F:41:ARG:NH1	1:F:305:LYS:HE2	2.37	0.40
1:H:327:HIS:HA	1:H:377:VAL:HB	2.03	0.40
1:A:170:LEU:HD21	1:A:424:LEU:HD22	2.03	0.40
1:B:171:GLY:HA2	1:B:199:PHE:O	2.21	0.40
1:F:21:LYS:HB2	5:F:1395:HOH:O	2.20	0.40
1:F:141:PRO:HA	1:F:142:PRO:HD3	1.94	0.40
2:Y:116:ILE:HD13	2:Y:116:ILE:HA	1.91	0.40
2:Y:121:PRO:HD3	5:Y:1859:HOH:O	2.21	0.40
1:H:409:HIS:CD2	1:H:416:GLY:HA2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ILE:HD12	1:A:36:ILE:N	2.36	0.40
1:B:327:HIS:HA	1:B:377:VAL:HB	2.02	0.40
1:C:93:GLU:CG	5:C:624:HOH:O	2.69	0.40
1:C:234:GLU:OE2	2:U:13:GLU:HA	2.21	0.40
1:C:389:ALA:O	1:C:393:ILE:HG13	2.21	0.40
2:U:72:LEU:HD21	1:E:412:GLY:HA2	2.02	0.40
2:X:14:THR:O	2:X:15:LEU:HB2	2.21	0.40
2:X:33:LEU:HB2	5:X:398:HOH:O	2.20	0.40
1:G:143:THR:HG23	5:G:495:HOH:O	2.21	0.40
1:G:338:GLU:CD	1:G:341:MET:H	2.29	0.40

There are no symmetry-related clashes.

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	437/477 (92%)	412 (94%)	20 (5%)	5 (1%)	11	2
1	B	436/477 (91%)	416 (95%)	18 (4%)	2 (0%)	24	10
1	C	436/477 (91%)	417 (96%)	17 (4%)	2 (0%)	24	10
1	D	437/477 (92%)	416 (95%)	20 (5%)	1 (0%)	43	27
1	E	434/477 (91%)	419 (96%)	15 (4%)	0	100	100
1	F	437/477 (92%)	415 (95%)	21 (5%)	1 (0%)	43	27
1	G	434/477 (91%)	415 (96%)	17 (4%)	2 (0%)	24	10
1	H	437/477 (92%)	415 (95%)	21 (5%)	1 (0%)	43	27
2	S	121/129 (94%)	113 (93%)	7 (6%)	1 (1%)	16	4
2	T	121/129 (94%)	114 (94%)	7 (6%)	0	100	100
2	U	121/129 (94%)	113 (93%)	8 (7%)	0	100	100
2	V	121/129 (94%)	112 (93%)	6 (5%)	3 (2%)	4	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	W	121/129 (94%)	116 (96%)	5 (4%)	0	100	100
2	X	121/129 (94%)	111 (92%)	8 (7%)	2 (2%)	7	1
2	Y	121/129 (94%)	116 (96%)	5 (4%)	0	100	100
2	Z	121/129 (94%)	116 (96%)	5 (4%)	0	100	100
All	All	4456/4848 (92%)	4236 (95%)	200 (4%)	20 (0%)	30	15

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	PHE
1	A	333	GLY
2	S	120	PRO
1	C	331	VAL
1	D	15	ALA
2	V	120	PRO
2	V	121	PRO
1	F	331	VAL
1	G	14	LYS
1	G	91	VAL
1	A	331	VAL
1	A	332	VAL
1	C	95	ASN
2	V	122	GLY
1	A	63	THR
1	B	16	GLY
1	B	91	VAL
1	H	331	VAL
2	X	122	GLY
2	X	121	PRO

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	355/385 (92%)	350 (99%)	5 (1%)	59	39
1	B	355/385 (92%)	351 (99%)	4 (1%)	65	48
1	C	355/385 (92%)	349 (98%)	6 (2%)	53	32
1	D	356/385 (92%)	352 (99%)	4 (1%)	65	48
1	E	353/385 (92%)	349 (99%)	4 (1%)	65	48
1	F	356/385 (92%)	351 (99%)	5 (1%)	59	39
1	G	353/385 (92%)	346 (98%)	7 (2%)	48	26
1	H	356/385 (92%)	353 (99%)	3 (1%)	73	60
2	S	110/114 (96%)	109 (99%)	1 (1%)	70	56
2	T	110/114 (96%)	109 (99%)	1 (1%)	70	56
2	U	110/114 (96%)	109 (99%)	1 (1%)	70	56
2	V	110/114 (96%)	108 (98%)	2 (2%)	51	30
2	W	110/114 (96%)	107 (97%)	3 (3%)	39	16
2	X	110/114 (96%)	108 (98%)	2 (2%)	51	30
2	Y	110/114 (96%)	109 (99%)	1 (1%)	70	56
2	Z	110/114 (96%)	108 (98%)	2 (2%)	51	30
All	All	3719/3992 (93%)	3668 (99%)	51 (1%)	59	39

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LYS
1	A	17	VAL
1	A	30	GLU
1	A	178	LEU
1	A	463	LYS
2	S	56	HIS
1	B	17	VAL
1	B	128	LYS
1	B	297	MET
1	B	463	LYS
2	T	56	HIS
1	C	77	LEU
1	C	297	MET
1	C	330	THR
1	C	331	VAL
1	C	332	VAL

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Mol	Chain	Res	Type
1	C	463	LYS
2	U	56	HIS
1	D	200	THR
1	D	297	MET
1	D	341	MET
1	D	463	LYS
2	V	56	HIS
2	V	112	LEU
1	E	14	LYS
1	E	297	MET
1	E	358	ARG
1	E	463	LYS
2	W	21	LEU
2	W	56	HIS
2	W	112	LEU
1	F	131	ARG
1	F	297	MET
1	F	330	THR
1	F	341	MET
1	F	463	LYS
2	X	56	HIS
2	X	112	LEU
1	G	14	LYS
1	G	77	LEU
1	G	87	ILE
1	G	178	LEU
1	G	297	MET
1	G	338	GLU
1	G	463	LYS
2	Y	56	HIS
1	H	79	ARG
1	H	297	MET
1	H	330	THR
2	Z	56	HIS
2	Z	112	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	95	ASN
1	A	163	ASN

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Mol	Chain	Res	Type
1	A	207	ASN
1	A	277	ASN
2	S	2	GLN
2	S	29	GLN
2	S	111	GLN
1	B	163	ASN
1	B	207	ASN
1	B	401	GLN
1	B	429	GLN
2	T	29	GLN
2	T	55	ASN
2	T	109	GLN
2	T	111	GLN
1	C	123	ASN
1	C	207	ASN
2	U	29	GLN
2	U	109	GLN
2	U	111	GLN
1	D	156	GLN
1	D	207	ASN
1	D	277	ASN
2	V	29	GLN
2	V	111	GLN
1	E	95	ASN
1	E	207	ASN
1	E	277	ASN
1	E	401	GLN
2	W	29	GLN
2	W	109	GLN
2	W	111	GLN
1	F	184	ASN
1	F	207	ASN
1	F	401	GLN
2	X	2	GLN
2	X	29	GLN
2	X	109	GLN
2	X	111	GLN
1	G	207	ASN
1	G	277	ASN
2	Y	29	GLN
2	Y	109	GLN
2	Y	111	GLN

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Mol	Chain	Res	Type
1	H	207	ASN
1	H	277	ASN
1	H	429	GLN
2	Z	29	GLN
2	Z	111	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	KCX	B	201	3,1	10,11,12	0.92	0	6,12,14	1.46	1 (16%)
1	KCX	F	201	3,1	10,11,12	0.94	0	6,12,14	1.49	2 (33%)
1	KCX	G	201	3,1	10,11,12	0.92	0	6,12,14	1.34	1 (16%)
1	KCX	H	201	3,1	10,11,12	0.99	0	6,12,14	1.44	1 (16%)
1	KCX	A	201	3,1	10,11,12	1.10	1 (10%)	6,12,14	1.31	1 (16%)
1	KCX	E	201	3,1	10,11,12	1.03	1 (10%)	6,12,14	1.29	1 (16%)
1	KCX	C	201	3,1	10,11,12	1.02	1 (10%)	6,12,14	1.29	1 (16%)
1	KCX	D	201	3,1	10,11,12	0.93	0	6,12,14	1.44	1 (16%)

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
1	KCX	B	201	3,1	-	0/9/10/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	F	201	3,1	-	0/9/10/12	-
1	KCX	G	201	3,1	-	0/9/10/12	-
1	KCX	H	201	3,1	-	1/9/10/12	-
1	KCX	A	201	3,1	-	0/9/10/12	-
1	KCX	E	201	3,1	-	0/9/10/12	-
1	KCX	C	201	3,1	-	1/9/10/12	-
1	KCX	D	201	3,1	-	1/9/10/12	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	201	KCX	OQ1-CX	2.21	1.25	1.21
1	C	201	KCX	OQ1-CX	2.18	1.25	1.21
1	E	201	KCX	OQ1-CX	2.03	1.25	1.21

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	201	KCX	OQ1-CX-NZ	-2.95	120.43	124.92
1	B	201	KCX	OQ1-CX-NZ	-2.95	120.45	124.92
1	H	201	KCX	OQ1-CX-NZ	-2.92	120.49	124.92
1	F	201	KCX	OQ1-CX-NZ	-2.91	120.50	124.92
1	G	201	KCX	OQ1-CX-NZ	-2.76	120.73	124.92
1	C	201	KCX	OQ1-CX-NZ	-2.65	120.89	124.92
1	E	201	KCX	OQ1-CX-NZ	-2.64	120.91	124.92
1	A	201	KCX	OQ1-CX-NZ	-2.59	120.98	124.92
1	F	201	KCX	CE-NZ-CX	2.05	125.46	121.98

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	H	201	KCX	C-CA-CB-CG
1	C	201	KCX	C-CA-CB-CG
1	D	201	KCX	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	6PG	D	479	3	16,16,16	1.64	2 (12%)	21,23,23	1.93	6 (28%)
4	6PG	E	479	3	16,16,16	1.67	3 (18%)	21,23,23	1.87	5 (23%)
4	6PG	F	479	3	16,16,16	1.50	3 (18%)	21,23,23	1.59	4 (19%)
4	6PG	A	479	3	16,16,16	1.46	3 (18%)	21,23,23	1.67	6 (28%)
4	6PG	G	479	3	16,16,16	1.45	3 (18%)	21,23,23	1.49	4 (19%)
4	6PG	B	479	3	16,16,16	1.71	2 (12%)	21,23,23	2.11	10 (47%)
4	6PG	H	479	3	16,16,16	1.74	3 (18%)	21,23,23	1.84	6 (28%)
4	6PG	C	479	3	16,16,16	1.38	3 (18%)	21,23,23	1.52	5 (23%)

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	6PG	D	479	3	-	3/22/22/22	-
4	6PG	E	479	3	-	5/22/22/22	-
4	6PG	F	479	3	-	1/22/22/22	-
4	6PG	A	479	3	-	2/22/22/22	-
4	6PG	G	479	3	-	3/22/22/22	-
4	6PG	B	479	3	-	3/22/22/22	-
4	6PG	H	479	3	-	3/22/22/22	-
4	6PG	C	479	3	-	2/22/22/22	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	479	6PG	O1-C1	-5.02	1.14	1.30
4	H	479	6PG	O1-C1	-4.64	1.15	1.30
4	B	479	6PG	O1-C1	-4.07	1.17	1.30
4	F	479	6PG	O1-C1	-3.96	1.18	1.30
4	A	479	6PG	O1-C1	-3.92	1.18	1.30
4	D	479	6PG	O1-C1	-3.85	1.18	1.30
4	G	479	6PG	O1-C1	-3.67	1.18	1.30
4	C	479	6PG	O1-C1	-3.65	1.19	1.30
4	B	479	6PG	P-O2P	-3.14	1.43	1.54
4	E	479	6PG	P-O3P	-2.72	1.44	1.54
4	D	479	6PG	P-O2P	-2.57	1.45	1.54
4	H	479	6PG	P-O2P	-2.55	1.45	1.54
4	F	479	6PG	P-O3P	-2.49	1.45	1.54
4	G	479	6PG	P-O2P	-2.47	1.45	1.54
4	C	479	6PG	P-O3P	-2.47	1.45	1.54
4	A	479	6PG	P-O3P	-2.32	1.46	1.54
4	G	479	6PG	P-O3P	-2.25	1.46	1.54
4	E	479	6PG	P-O2P	-2.25	1.46	1.54
4	A	479	6PG	P-O2P	-2.21	1.46	1.54
4	F	479	6PG	P-O2P	-2.21	1.46	1.54
4	C	479	6PG	P-O2P	-2.21	1.46	1.54
4	H	479	6PG	C4-C3	2.01	1.57	1.53

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	479	6PG	O4-C4-C3	-3.82	100.53	109.46
4	H	479	6PG	O2P-P-O6	3.77	116.49	106.67
4	D	479	6PG	O2P-P-O6	3.65	116.18	106.67
4	E	479	6PG	C4-C3-C2	3.65	120.06	113.62
4	B	479	6PG	O2P-P-O6	3.56	115.94	106.67
4	H	479	6PG	O4-C4-C3	-3.55	101.18	109.46
4	B	479	6PG	C6-C5-C4	3.52	118.86	112.22
4	A	479	6PG	C4-C3-C2	3.34	119.52	113.62
4	G	479	6PG	C4-C3-C2	3.29	119.43	113.62
4	E	479	6PG	O2P-P-O6	3.27	115.20	106.67
4	D	479	6PG	C4-C3-C2	3.15	119.19	113.62
4	E	479	6PG	O6-P-O1P	-3.15	97.93	106.44
4	F	479	6PG	O2P-P-O6	3.12	114.81	106.67
4	B	479	6PG	C4-C3-C2	3.07	119.04	113.62
4	C	479	6PG	O2P-P-O6	3.01	114.52	106.67
4	F	479	6PG	C4-C3-C2	2.96	118.86	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	479	6PG	O2P-P-O6	2.94	114.34	106.67
4	C	479	6PG	C4-C3-C2	2.92	118.78	113.62
4	H	479	6PG	O6-P-O1P	-2.89	98.62	106.44
4	B	479	6PG	O3P-P-O6	-2.88	99.17	106.67
4	A	479	6PG	O6-P-O1P	-2.87	98.68	106.44
4	F	479	6PG	O6-P-O1P	-2.85	98.74	106.44
4	B	479	6PG	O2-C2-C1	-2.84	104.62	110.69
4	D	479	6PG	O6-P-O1P	-2.83	98.78	106.44
4	D	479	6PG	O1-C1-C2	2.70	120.82	113.31
4	B	479	6PG	O1A-C1-C2	-2.57	114.76	121.62
4	G	479	6PG	O4-C4-C3	-2.55	103.51	109.46
4	H	479	6PG	O1-C1-C2	2.51	120.28	113.31
4	E	479	6PG	O4-C4-C3	-2.48	103.67	109.46
4	E	479	6PG	O1-C1-C2	2.47	120.18	113.31
4	B	479	6PG	O3-C3-C4	-2.45	103.73	109.46
4	A	479	6PG	O1-C1-C2	2.43	120.05	113.31
4	H	479	6PG	O3-C3-C2	2.40	113.59	109.29
4	B	479	6PG	O4-C4-C3	-2.39	103.88	109.46
4	C	479	6PG	O6-P-O1P	-2.38	100.02	106.44
4	B	479	6PG	O1-C1-C2	2.29	119.67	113.31
4	A	479	6PG	O4-C4-C3	-2.27	104.16	109.46
4	F	479	6PG	O1-C1-C2	2.25	119.57	113.31
4	A	479	6PG	O2-C2-C1	-2.19	106.00	110.69
4	B	479	6PG	O6-P-O1P	-2.16	100.59	106.44
4	H	479	6PG	O3P-P-O6	-2.15	101.05	106.67
4	C	479	6PG	O4-C4-C3	-2.13	104.48	109.46
4	G	479	6PG	O6-P-O1P	-2.12	100.70	106.44
4	G	479	6PG	O1-C1-C2	2.06	119.05	113.31
4	C	479	6PG	O1-C1-C2	2.06	119.03	113.31
4	D	479	6PG	O1A-C1-C2	-2.04	116.17	121.62

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	479	6PG	C6-O6-P-O2P
4	B	479	6PG	C6-O6-P-O3P
4	D	479	6PG	C6-O6-P-O2P
4	D	479	6PG	C6-O6-P-O3P
4	E	479	6PG	C6-O6-P-O1P
4	E	479	6PG	C6-O6-P-O2P
4	G	479	6PG	C4-C5-C6-O6

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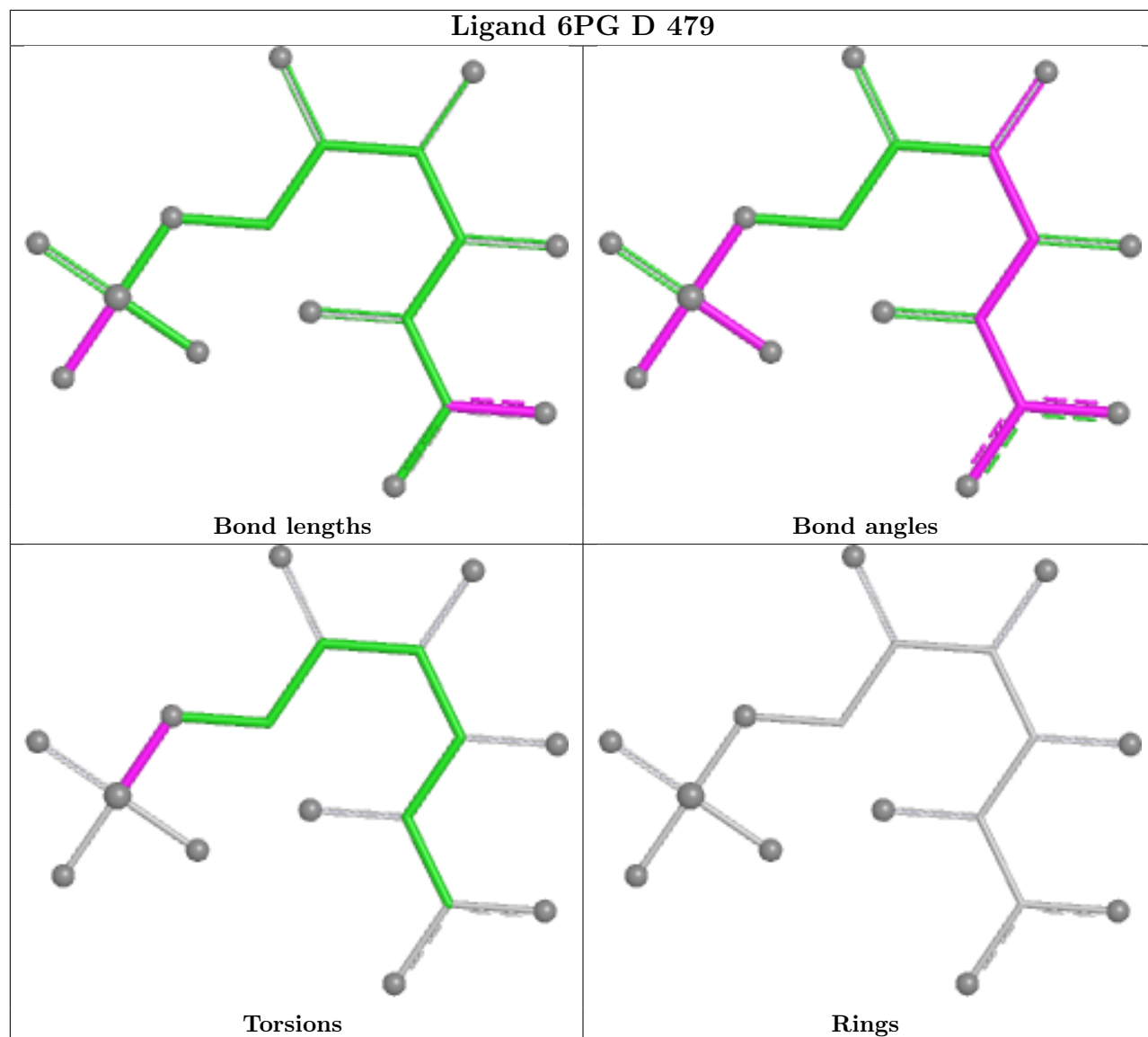
Mol	Chain	Res	Type	Atoms
4	H	479	6PG	C6-O6-P-O2P
4	H	479	6PG	C6-O6-P-O3P
4	B	479	6PG	C6-O6-P-O1P
4	D	479	6PG	C6-O6-P-O1P
4	A	479	6PG	C4-C5-C6-O6
4	C	479	6PG	C4-C5-C6-O6
4	E	479	6PG	C4-C5-C6-O6
4	G	479	6PG	C6-O6-P-O1P
4	H	479	6PG	C6-O6-P-O1P
4	G	479	6PG	O5-C5-C6-O6
4	C	479	6PG	C6-O6-P-O2P
4	E	479	6PG	C6-O6-P-O3P
4	F	479	6PG	C6-O6-P-O2P
4	A	479	6PG	C2-C3-C4-C5
4	E	479	6PG	O3-C3-C4-C5

There are no ring outliers.

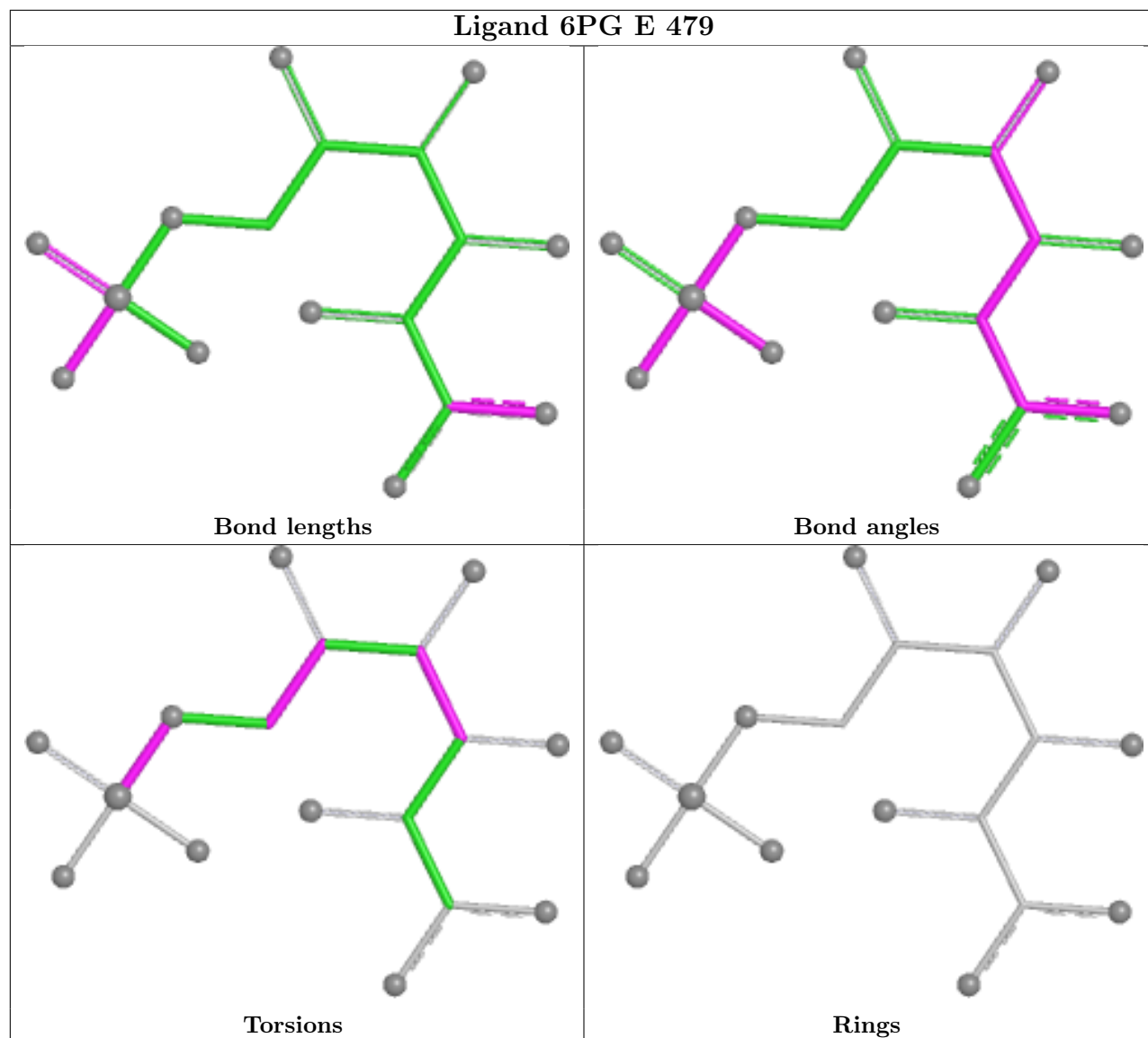
No monomer is involved in short contacts.

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.

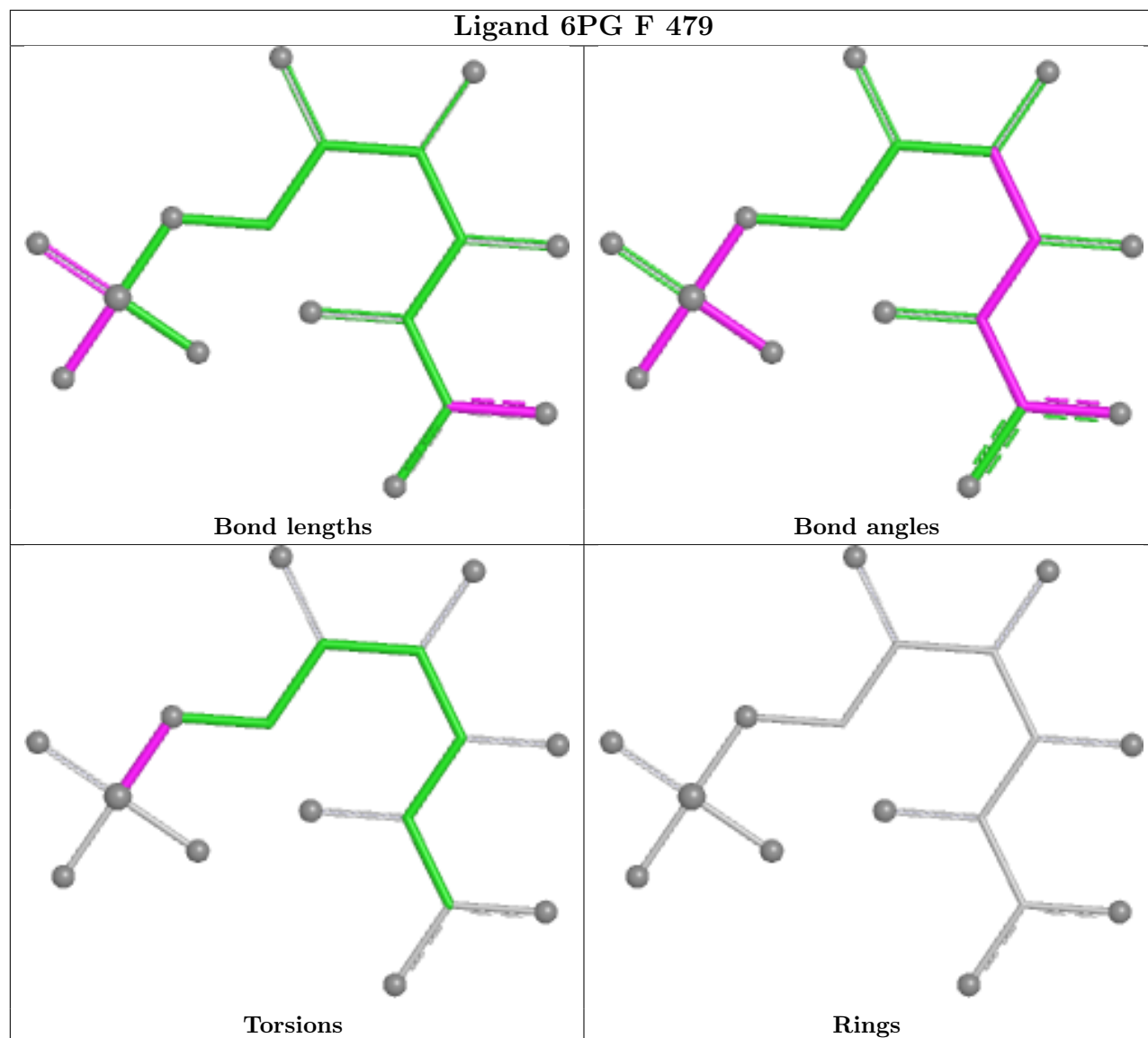
Ligand 6PG D 479



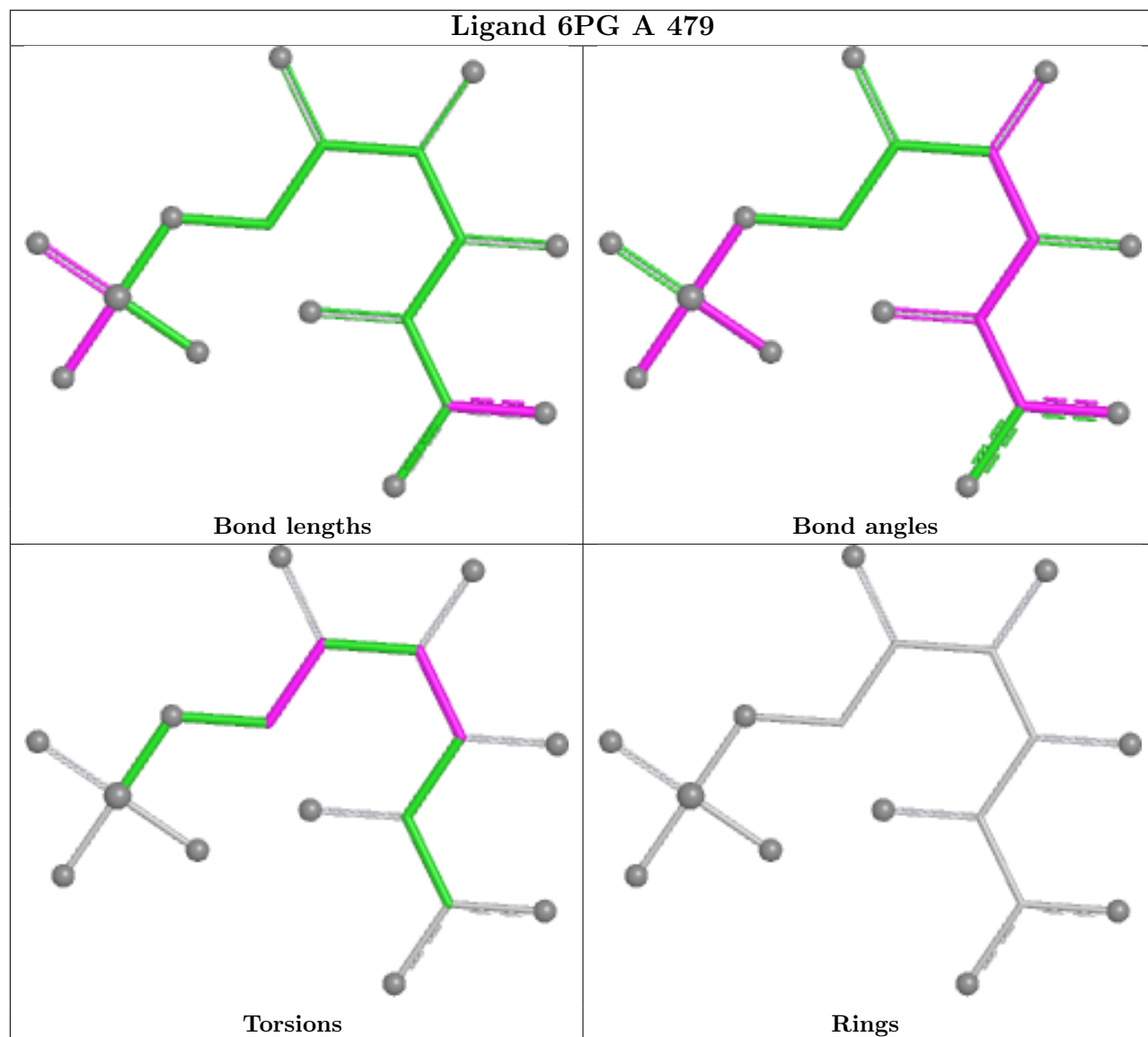
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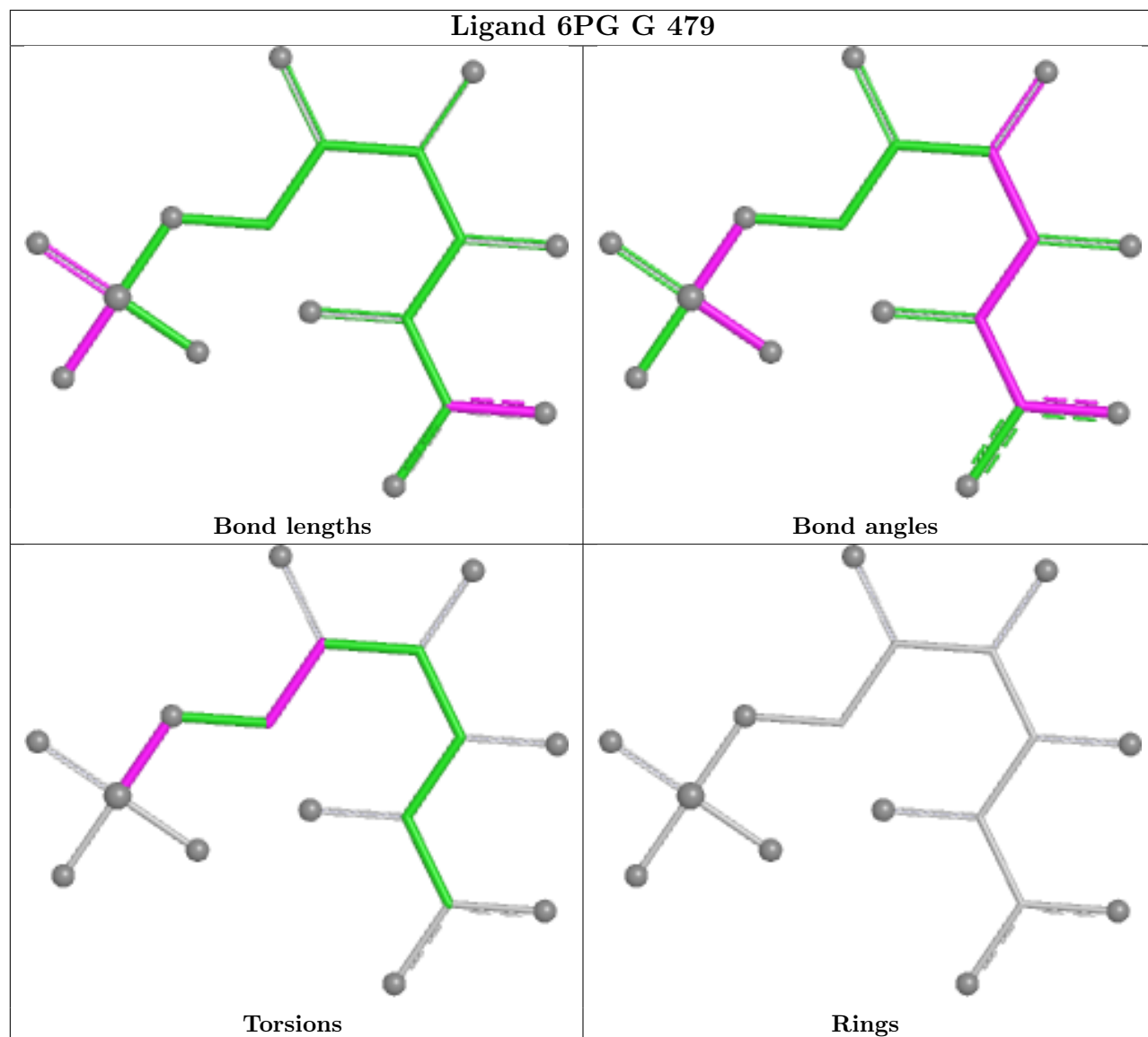
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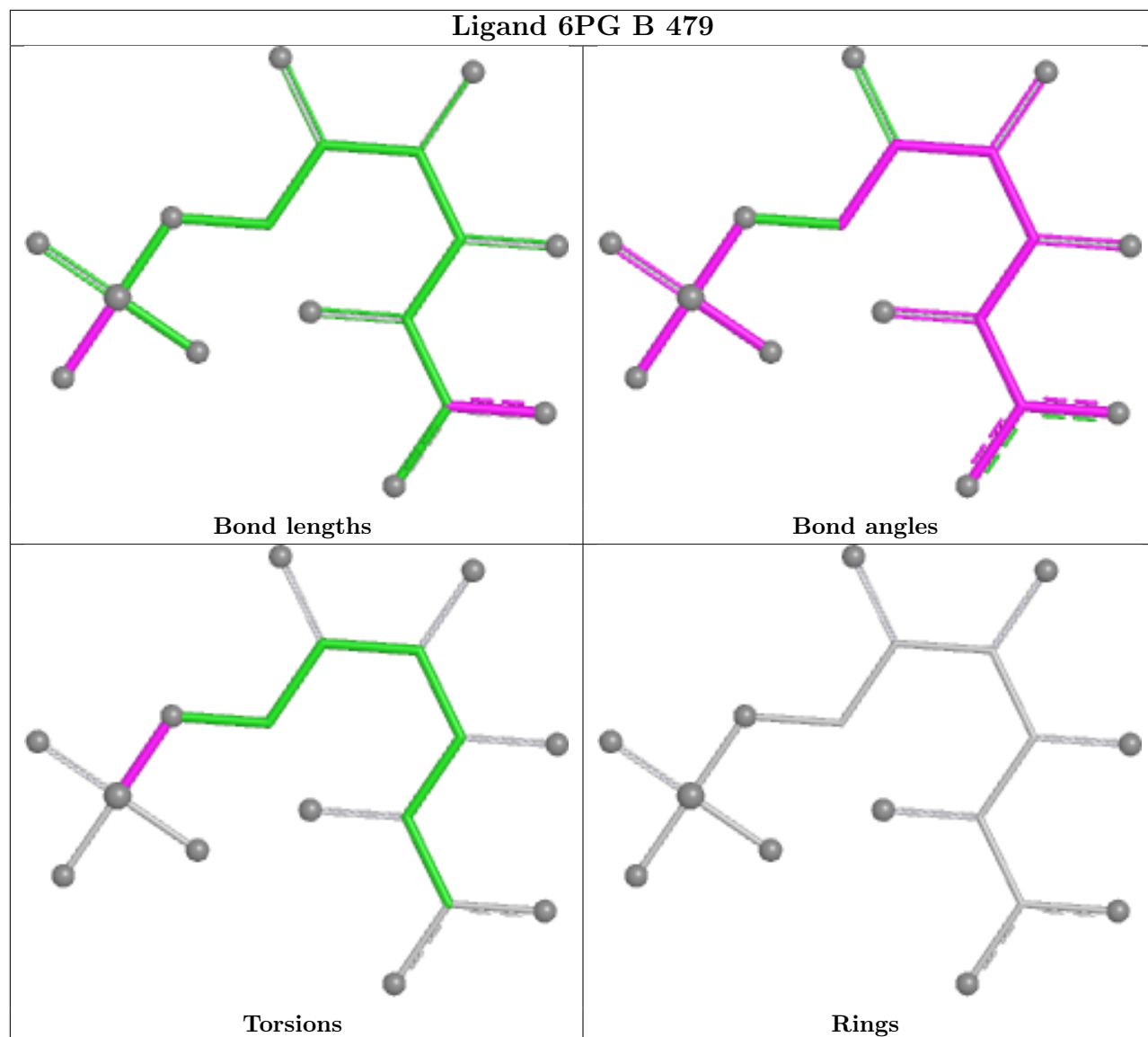
Ligand 6PG A 479



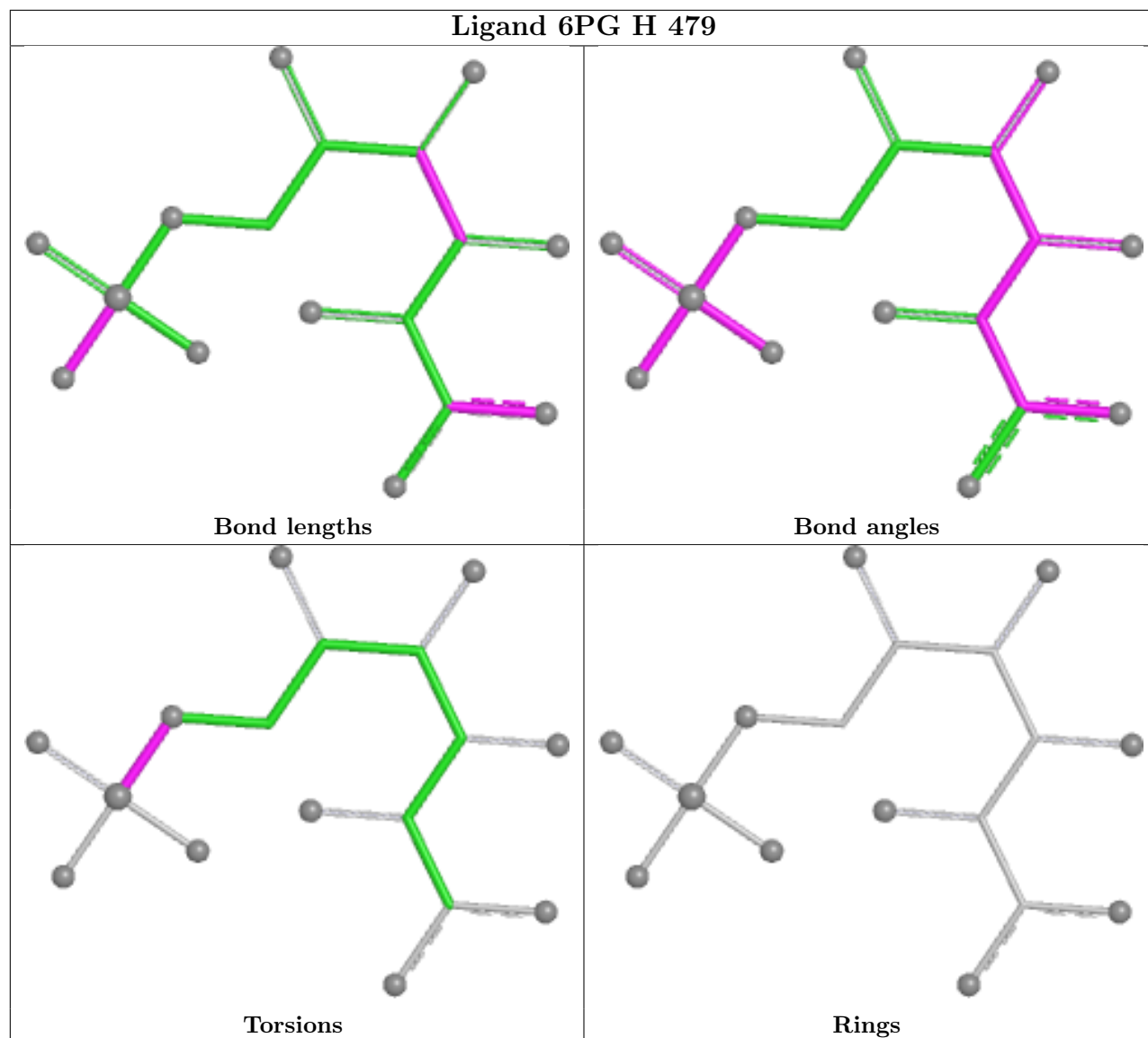
Ligand 6PG G 479

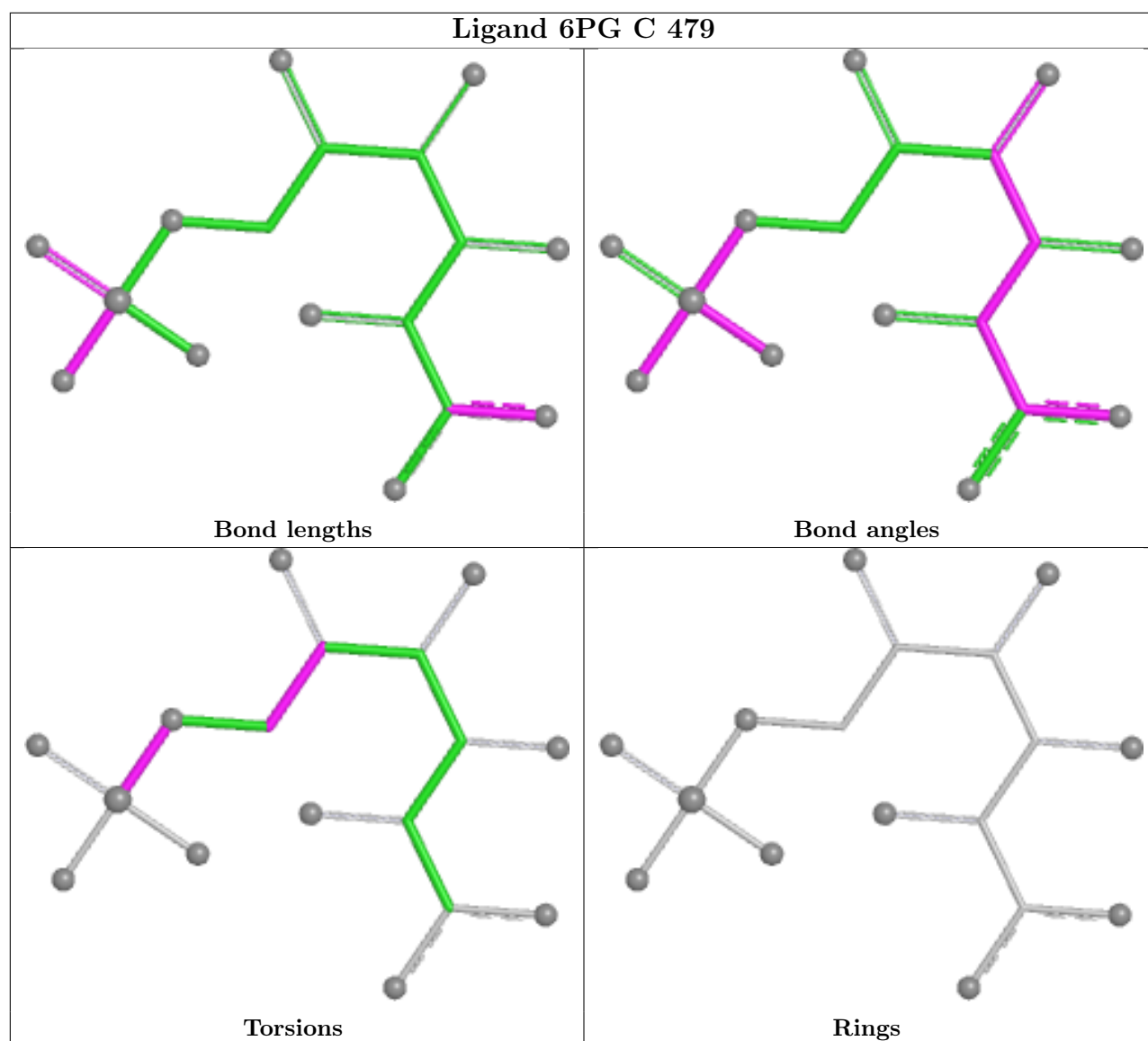


Ligand 6PG B 479



Ligand 6PG H 479





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

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	443/477 (92%)	0.22	37 (8%) 17 19	7, 12, 29, 63	0
1	B	442/477 (92%)	0.18	39 (8%) 15 17	7, 11, 29, 66	0
1	C	442/477 (92%)	0.11	38 (8%) 16 18	7, 11, 29, 63	0
1	D	443/477 (92%)	0.15	35 (7%) 18 21	6, 11, 30, 67	0
1	E	440/477 (92%)	0.12	36 (8%) 17 19	6, 11, 29, 62	0
1	F	443/477 (92%)	0.16	39 (8%) 15 17	7, 11, 30, 65	0
1	G	440/477 (92%)	0.16	39 (8%) 15 17	7, 11, 27, 67	0
1	H	443/477 (92%)	0.20	39 (8%) 15 17	7, 12, 30, 64	0
2	S	122/129 (94%)	0.61	16 (13%) 7 8	9, 15, 27, 59	0
2	T	122/129 (94%)	0.57	11 (9%) 15 16	8, 15, 28, 55	0
2	U	122/129 (94%)	0.45	12 (9%) 13 14	8, 14, 25, 53	0
2	V	122/129 (94%)	0.50	10 (8%) 17 19	8, 15, 25, 61	0
2	W	122/129 (94%)	0.62	14 (11%) 9 10	8, 15, 28, 55	0
2	X	122/129 (94%)	0.41	8 (6%) 24 27	8, 15, 26, 55	0
2	Y	122/129 (94%)	0.60	12 (9%) 13 14	9, 15, 27, 55	0
2	Z	122/129 (94%)	0.49	11 (9%) 15 16	9, 15, 27, 56	0
All	All	4512/4848 (93%)	0.24	396 (8%) 15 17	6, 12, 29, 67	0

All (396) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	90	VAL	11.6
1	F	92	GLY	11.1
1	E	22	LEU	10.9
1	D	16	GLY	10.7
1	D	15	ALA	10.5

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Mol	Chain	Res	Type	RSRZ
1	G	17	VAL	10.2
1	F	331	VAL	9.9
2	S	123	CYS	9.9
1	B	331	VAL	9.9
1	G	16	GLY	9.8
1	G	91	VAL	9.8
1	G	13	PHE	9.4
1	B	15	ALA	9.3
1	G	15	ALA	9.2
1	F	22	LEU	9.1
1	A	16	GLY	9.0
2	W	123	CYS	9.0
1	C	22	LEU	8.9
1	G	92	GLY	8.7
1	H	22	LEU	8.6
1	D	22	LEU	8.6
1	C	92	GLY	8.4
1	B	92	GLY	8.4
1	D	17	VAL	8.3
1	F	332	VAL	8.3
1	G	94	ASP	8.3
1	A	13	PHE	8.2
1	E	17	VAL	8.1
1	A	17	VAL	8.0
1	C	94	ASP	7.9
1	H	331	VAL	7.9
1	G	22	LEU	7.8
1	D	23	THR	7.8
1	H	332	VAL	7.8
1	D	332	VAL	7.7
1	H	91	VAL	7.7
1	B	22	LEU	7.6
1	C	91	VAL	7.6
1	H	17	VAL	7.5
1	D	77	LEU	7.4
2	Z	123	CYS	7.4
1	D	331	VAL	7.4
1	B	17	VAL	7.3
2	Y	123	CYS	7.3
2	U	123	CYS	7.1
1	A	332	VAL	7.0
1	C	13	PHE	7.0

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Mol	Chain	Res	Type	RSRZ
1	D	21	LYS	7.0
1	D	463	LYS	7.0
1	F	463	LYS	6.8
1	E	23	THR	6.8
1	B	94	ASP	6.7
1	C	17	VAL	6.6
2	X	122	GLY	6.6
1	B	16	GLY	6.6
1	A	15	ALA	6.4
1	F	17	VAL	6.4
1	B	93	GLU	6.4
1	B	463	LYS	6.4
2	S	121	PRO	6.3
2	X	123	CYS	6.3
1	F	94	ASP	6.3
1	E	15	ALA	6.2
1	C	332	VAL	6.2
1	H	15	ALA	6.2
2	V	123	CYS	6.1
1	F	21	LYS	6.1
1	F	24	TYR	6.1
1	A	92	GLY	6.1
1	D	92	GLY	6.0
1	E	16	GLY	6.0
1	F	15	ALA	6.0
1	H	21	LYS	6.0
1	E	13	PHE	6.0
1	F	25	TYR	5.9
1	C	16	GLY	5.9
1	H	16	GLY	5.9
1	A	333	GLY	5.9
2	V	121	PRO	5.7
1	A	331	VAL	5.7
1	G	23	THR	5.7
1	F	91	VAL	5.7
1	C	15	ALA	5.7
2	T	121	PRO	5.6
1	F	16	GLY	5.5
2	X	121	PRO	5.5
1	H	12	GLY	5.5
1	F	66	TRP	5.5
1	D	91	VAL	5.4

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Mol	Chain	Res	Type	RSRZ
1	D	13	PHE	5.4
1	A	12	GLY	5.4
1	D	94	ASP	5.4
1	A	23	THR	5.3
1	H	94	ASP	5.3
1	B	95	ASN	5.3
1	F	23	THR	5.3
2	Y	116	ILE	5.2
2	S	122	GLY	5.2
2	W	9	ILE	5.2
1	F	13	PHE	5.2
2	Y	121	PRO	5.2
1	C	12	GLY	5.1
2	T	123	CYS	5.1
1	B	21	LYS	5.0
1	A	77	LEU	5.0
2	W	116	ILE	5.0
1	C	331	VAL	5.0
1	D	12	GLY	5.0
2	W	121	PRO	5.0
2	Z	9	ILE	5.0
2	U	122	GLY	4.9
1	G	463	LYS	4.9
2	W	122	GLY	4.9
1	B	13	PHE	4.9
1	F	93	GLU	4.8
1	D	79	ARG	4.8
2	U	121	PRO	4.8
1	F	95	ASN	4.8
1	G	12	GLY	4.8
2	V	122	GLY	4.8
2	S	9	ILE	4.8
1	H	13	PHE	4.8
2	S	84	LEU	4.8
2	U	9	ILE	4.7
1	E	463	LYS	4.7
1	G	95	ASN	4.7
1	C	93	GLU	4.7
1	H	92	GLY	4.7
1	E	14	LYS	4.6
2	Z	116	ILE	4.5
1	H	23	THR	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	95	ASN	4.5
2	Y	9	ILE	4.5
2	T	122	GLY	4.4
1	A	463	LYS	4.4
2	Y	122	GLY	4.4
1	G	70	TRP	4.4
1	D	14	LYS	4.4
2	T	21	LEU	4.4
1	G	330	THR	4.4
2	V	9	ILE	4.4
1	G	93	GLU	4.4
2	Z	121	PRO	4.3
2	T	9	ILE	4.3
1	C	23	THR	4.2
1	B	91	VAL	4.2
1	E	462	TRP	4.2
1	B	66	TRP	4.2
1	C	463	LYS	4.1
2	Z	122	GLY	4.1
2	Y	24	GLU	4.1
1	F	14	LYS	4.0
1	G	14	LYS	4.0
1	C	25	TYR	3.9
1	B	12	GLY	3.9
1	B	338	GLU	3.9
2	X	9	ILE	3.9
1	C	330	THR	3.9
2	W	84	LEU	3.9
1	A	79	ARG	3.8
1	E	79	ARG	3.8
1	H	77	LEU	3.8
1	C	65	THR	3.8
1	E	52	GLU	3.8
1	B	54	GLY	3.7
1	B	14	LYS	3.7
1	A	14	LYS	3.6
1	F	128	LYS	3.6
2	V	120	PRO	3.6
1	G	90	VAL	3.6
2	X	24	GLU	3.6
1	B	23	THR	3.5
1	F	330	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	50	PRO	3.5
1	H	93	GLU	3.5
1	H	463	LYS	3.5
1	F	12	GLY	3.5
2	T	82	GLN	3.4
1	F	48	VAL	3.4
1	D	63	THR	3.4
1	A	334	LYS	3.4
1	E	338	GLU	3.4
1	A	94	ASP	3.4
1	B	64	GLY	3.4
1	H	63	THR	3.4
2	V	84	LEU	3.4
1	A	462	TRP	3.4
1	E	94	ASP	3.3
1	G	65	THR	3.3
1	E	407	LEU	3.3
1	C	52	GLU	3.3
1	B	330	THR	3.3
1	H	67	THR	3.3
1	C	24	TYR	3.2
1	G	451	TRP	3.2
1	G	24	TYR	3.2
2	Y	120	PRO	3.2
1	B	55	ALA	3.2
1	D	438	ALA	3.2
1	F	65	THR	3.2
2	S	24	GLU	3.2
2	U	24	GLU	3.1
1	A	63	THR	3.1
1	C	443	GLU	3.1
1	D	93	GLU	3.1
2	Y	26	LEU	3.1
1	E	95	ASN	3.1
1	H	128	LYS	3.1
2	Z	33	LEU	3.1
2	S	21	LEU	3.0
1	A	24	TYR	3.0
1	C	28	GLU	3.0
2	X	21	LEU	3.0
1	G	450	LYS	3.0
1	F	338	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	H	52	GLU	3.0
1	H	68	THR	3.0
2	T	84	LEU	3.0
2	W	21	LEU	3.0
1	F	68	THR	2.9
1	B	78	ASP	2.9
1	E	339	ARG	2.9
1	C	341	MET	2.9
1	E	128	LYS	2.9
2	T	27	LEU	2.9
1	E	12	GLY	2.9
1	C	131	ARG	2.9
1	G	392	GLU	2.9
1	B	68	THR	2.9
1	A	97	TYR	2.9
2	Y	27	LEU	2.9
1	B	128	LYS	2.9
1	D	70	TRP	2.9
2	V	24	GLU	2.8
1	E	461	ILE	2.8
1	E	358	ARG	2.8
1	F	67	THR	2.8
1	C	338	GLU	2.8
1	F	460	GLU	2.8
1	A	371	MET	2.8
1	F	97	TYR	2.8
1	H	79	ARG	2.8
1	E	330	THR	2.8
1	B	460	GLU	2.8
2	Z	84	LEU	2.8
1	F	78	ASP	2.8
1	H	64	GLY	2.8
1	C	439	ARG	2.7
2	X	84	LEU	2.7
1	C	47	GLY	2.7
1	D	131	ARG	2.7
1	G	211	PHE	2.7
2	S	82	GLN	2.7
1	C	128	LYS	2.7
1	G	439	ARG	2.7
1	G	462	TRP	2.7
1	C	77	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	24	TYR	2.7
1	A	439	ARG	2.6
1	D	460	GLU	2.6
1	H	76	SER	2.6
2	U	81	THR	2.6
2	S	27	LEU	2.6
2	Y	21	LEU	2.6
1	A	338	GLU	2.6
1	D	28	GLU	2.6
1	E	438	ALA	2.6
1	C	462	TRP	2.6
1	D	450	LYS	2.6
1	H	14	LYS	2.6
1	A	330	THR	2.6
2	T	24	GLU	2.6
2	U	27	LEU	2.6
1	F	439	ARG	2.6
1	D	330	THR	2.5
1	F	407	LEU	2.5
1	F	450	LYS	2.5
2	U	84	LEU	2.5
1	H	95	ASN	2.5
1	C	79	ARG	2.5
1	F	52	GLU	2.5
1	G	461	ILE	2.5
1	F	47	GLY	2.5
1	H	47	GLY	2.5
1	B	462	TRP	2.5
1	E	447	SER	2.5
1	H	443	GLU	2.5
2	Z	24	GLU	2.5
1	E	77	LEU	2.5
2	U	21	LEU	2.5
1	C	78	ASP	2.5
1	A	438	ALA	2.5
1	C	64	GLY	2.5
1	A	65	THR	2.5
2	V	27	LEU	2.5
1	E	25	TYR	2.5
1	B	69	VAL	2.5
1	D	65	THR	2.5
1	D	439	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
2	U	43	GLU	2.5
2	T	81	THR	2.5
2	W	82	GLN	2.4
1	H	70	TRP	2.4
1	F	211	PHE	2.4
2	T	26	LEU	2.4
2	Y	33	LEU	2.4
1	D	338	GLU	2.4
1	H	338	GLU	2.4
1	D	64	GLY	2.4
1	H	330	THR	2.4
2	S	81	THR	2.4
1	H	90	VAL	2.4
1	H	439	ARG	2.4
2	U	33	LEU	2.4
2	W	33	LEU	2.4
2	Z	27	LEU	2.4
2	Z	81	THR	2.4
1	A	339	ARG	2.4
1	C	14	LYS	2.4
1	A	47	GLY	2.3
1	E	92	GLY	2.3
2	S	120	PRO	2.3
1	E	178	LEU	2.3
1	H	65	THR	2.3
1	A	128	LYS	2.3
1	E	87	ILE	2.3
1	E	47	GLY	2.3
1	E	443	GLU	2.3
1	B	129	ALA	2.3
2	W	1	MET	2.3
1	A	178	LEU	2.3
1	B	178	LEU	2.3
2	W	27	LEU	2.3
1	A	25	TYR	2.3
1	G	131	ARG	2.3
1	H	358	ARG	2.3
1	A	329	GLY	2.3
1	G	67	THR	2.3
2	S	2	GLN	2.3
2	W	24	GLU	2.3
1	C	211	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	360	ARG	2.3
1	H	450	LYS	2.3
1	G	47	GLY	2.3
1	B	79	ARG	2.2
1	D	339	ARG	2.2
1	H	130	LEU	2.2
2	S	33	LEU	2.2
1	D	128	LYS	2.2
1	B	211	PHE	2.2
1	D	24	TYR	2.2
1	B	461	ILE	2.2
1	B	443	GLU	2.2
1	E	46	PRO	2.2
2	W	120	PRO	2.2
1	B	67	THR	2.2
1	C	339	ARG	2.2
1	B	439	ARG	2.2
1	E	65	THR	2.2
2	S	85	LYS	2.2
1	B	329	GLY	2.2
2	Y	84	LEU	2.2
1	D	305	LYS	2.2
1	G	128	LYS	2.2
1	A	26	THR	2.2
1	A	62	SER	2.2
1	F	33	ASP	2.1
1	H	69	VAL	2.1
1	G	252	LYS	2.1
2	S	50	PHE	2.1
1	E	460	GLU	2.1
2	V	31	GLU	2.1
1	H	438	ALA	2.1
1	G	64	GLY	2.1
1	G	407	LEU	2.1
1	F	339	ARG	2.1
1	G	79	ARG	2.1
2	X	120	PRO	2.1
1	G	443	GLU	2.1
1	D	33	ASP	2.1
1	B	339	ARG	2.1
1	G	178	LEU	2.1
2	W	81	THR	2.1

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Mol	Chain	Res	Type	RSRZ
2	Z	120	PRO	2.1
1	F	461	ILE	2.1
1	A	359	ALA	2.0
1	A	443	GLU	2.0
1	E	51	GLU	2.0
2	S	107	VAL	2.0
1	B	77	LEU	2.0
1	C	450	LYS	2.0
1	G	329	GLY	2.0
2	V	1	MET	2.0
1	G	25	TYR	2.0
2	U	96	ASP	2.0
1	A	450	LYS	2.0

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

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
1	KCX	B	201	12/13	0.96	0.06	9,10,11,11	0
1	KCX	D	201	12/13	0.96	0.06	7,8,10,11	0
1	KCX	E	201	12/13	0.96	0.06	8,9,11,12	0
1	KCX	G	201	12/13	0.96	0.06	7,9,11,11	0
1	KCX	H	201	12/13	0.96	0.06	7,9,11,12	0
1	KCX	F	201	12/13	0.97	0.05	7,9,11,11	0
1	KCX	A	201	12/13	0.97	0.06	7,9,10,11	0
1	KCX	C	201	12/13	0.97	0.06	7,8,11,12	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

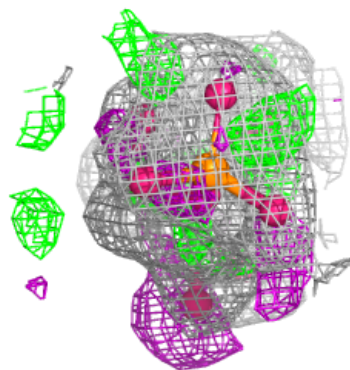
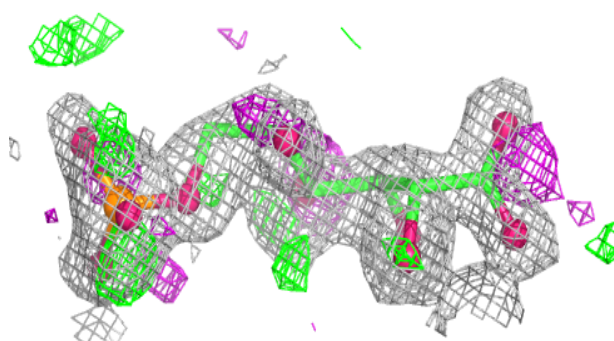
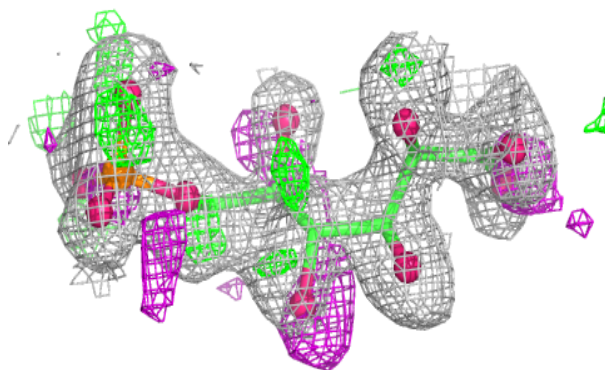
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	6PG	B	479	17/17	0.88	0.13	12,21,27,27	0
4	6PG	E	479	17/17	0.91	0.10	12,20,29,30	0
4	6PG	D	479	17/17	0.92	0.10	10,20,29,30	0
4	6PG	H	479	17/17	0.92	0.10	11,20,31,33	0
4	6PG	C	479	17/17	0.94	0.09	11,17,23,24	0
4	6PG	F	479	17/17	0.94	0.10	12,21,26,27	0
4	6PG	G	479	17/17	0.94	0.09	11,19,25,26	0
4	6PG	A	479	17/17	0.94	0.08	12,17,29,30	0
3	MG	A	478	1/1	0.98	0.05	11,11,11,11	0
3	MG	C	478	1/1	0.98	0.03	10,10,10,10	0
3	MG	G	478	1/1	0.99	0.02	10,10,10,10	0
3	MG	H	478	1/1	0.99	0.03	11,11,11,11	0
3	MG	B	478	1/1	0.99	0.03	10,10,10,10	0
3	MG	E	478	1/1	0.99	0.03	11,11,11,11	0
3	MG	F	478	1/1	0.99	0.02	9,9,9,9	0
3	MG	D	478	1/1	1.00	0.02	10,10,10,10	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.

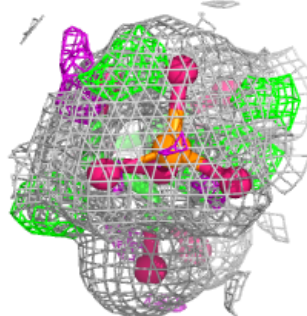
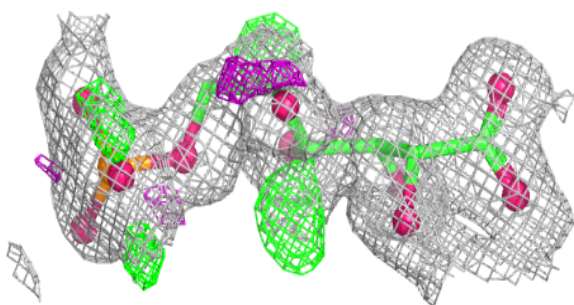
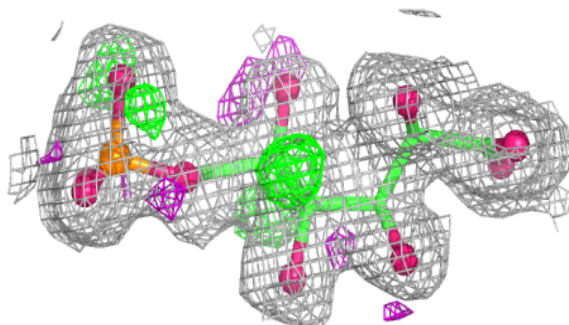
Electron density around 6PG B 479:

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mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

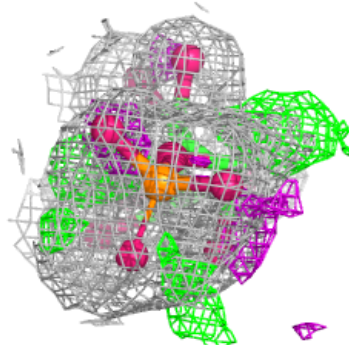
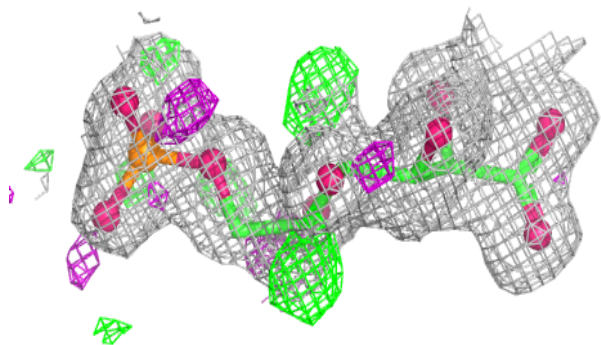
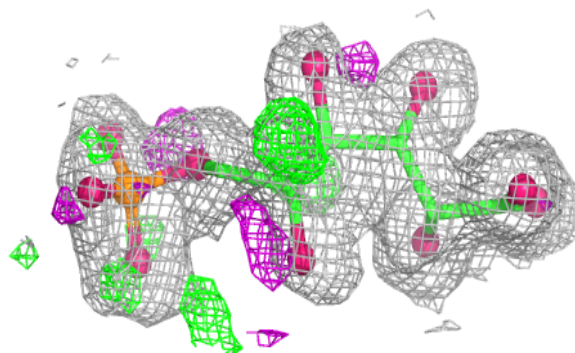


Electron density around 6PG E 479:

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

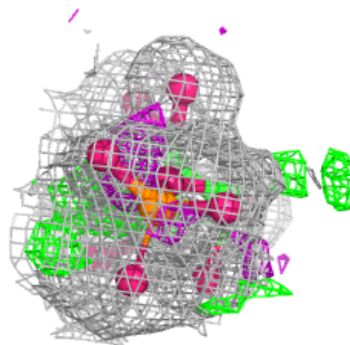
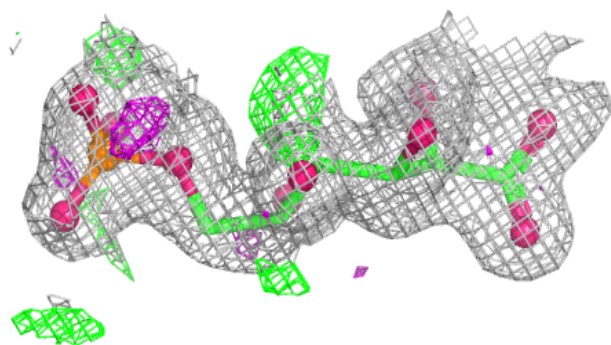
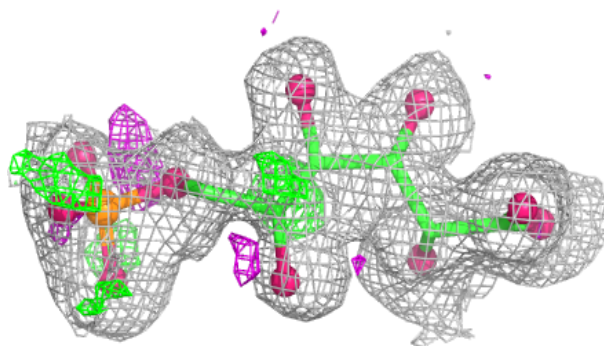
**Electron density around 6PG D 479:**

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

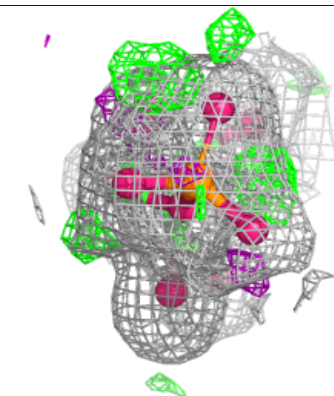
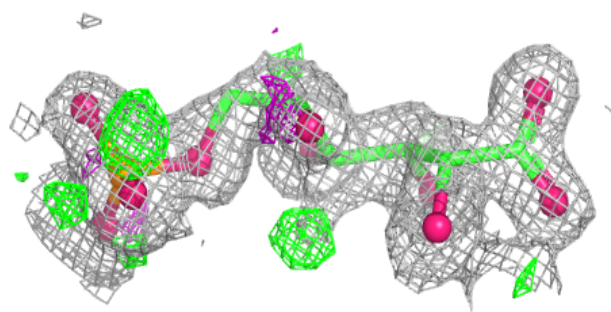
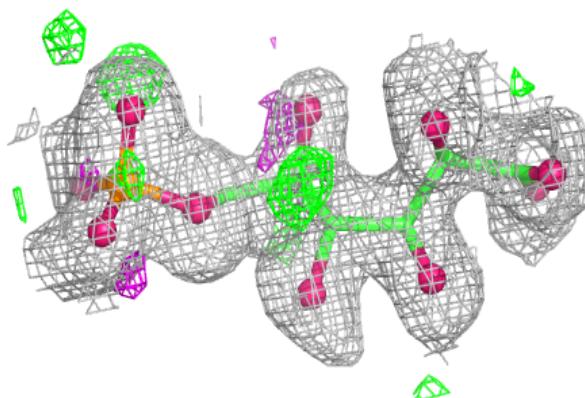


Electron density around 6PG H 479:

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

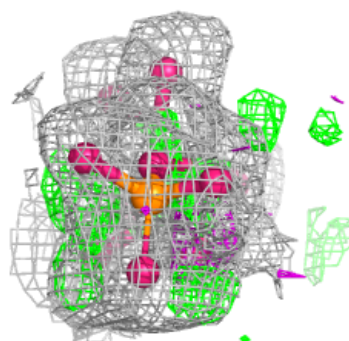
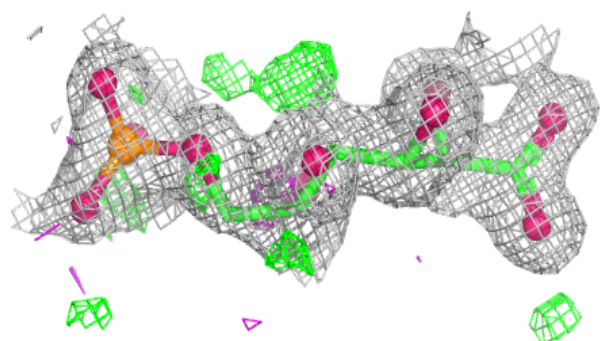
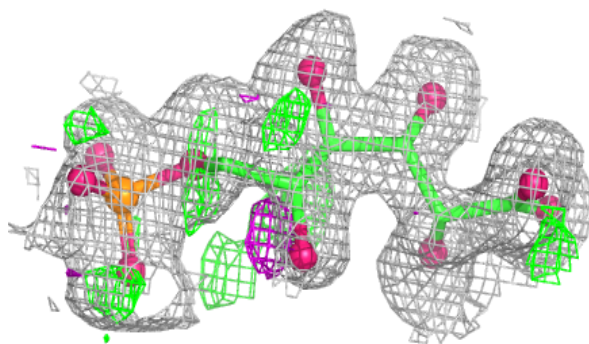
**Electron density around 6PG C 479:**

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

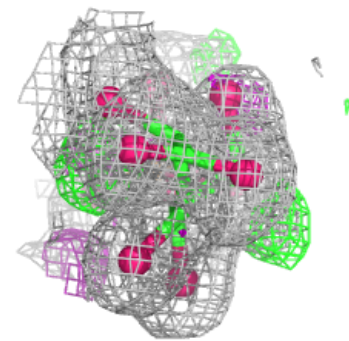
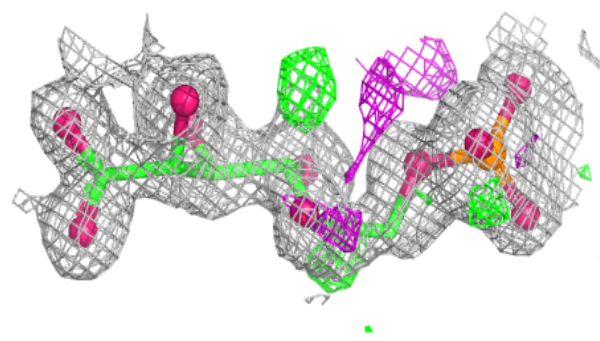
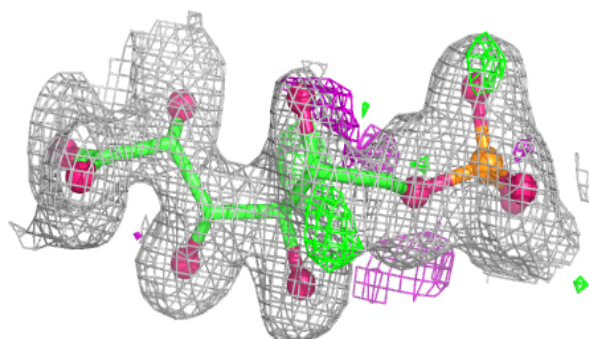


Electron density around 6PG F 479:

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

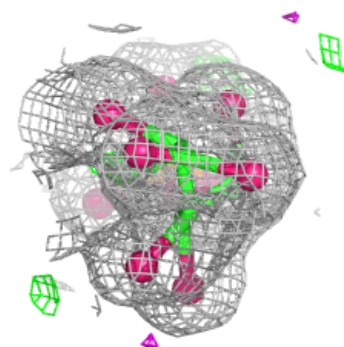
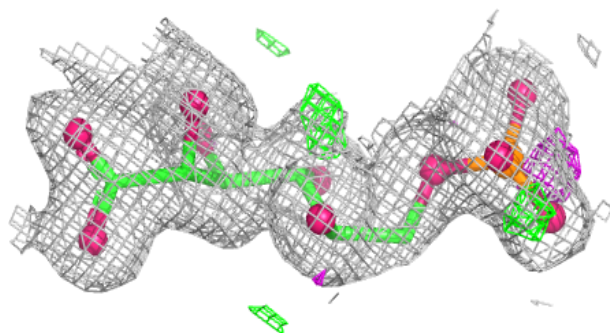
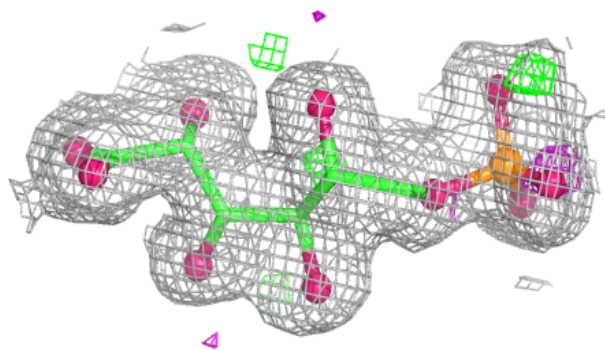
**Electron density around 6PG G 479:**

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



Electron density around 6PG A 479:

$2mF_o-DF_c$ (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.