



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 28, 2024 – 06:38 PM EDT

PDB ID : 1G23
Title : THE STRUCTURAL BASIS OF THE CATALYTIC MECHANISM AND REGULATION OF GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE (RMLA). GLUCOSE-1-PHOSPHATE COMPLEX.
Authors : Blankenfeldt, W.; Asuncion, M.; Lam, J.S.; Naismith, J.H.
Deposited on : 2000-10-16
Resolution : 2.80 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

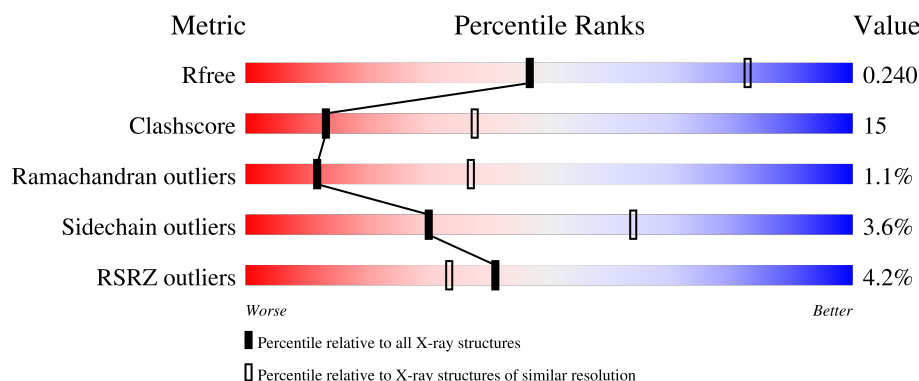
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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	293	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>24%</div> <div>.</div> </div> </div>
1	B	293	<div> <div>3%</div> <div> <div></div> <div>74%</div> <div>22%</div> <div>..</div> </div> </div>
1	C	293	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>24%</div> <div>..</div> </div> </div>
1	D	293	<div> <div>4%</div> <div> <div></div> <div>71%</div> <div>25%</div> <div>..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	E	293	<div><div>8%</div><div><div></div><div>71%</div><div>24%</div><div></div></div><div></div></div>
1	F	293	<div><div>7%</div><div><div></div><div>70%</div><div>26%</div><div></div></div><div></div></div>
1	G	293	<div><div>5%</div><div><div></div><div>71%</div><div>24%</div><div></div></div><div></div></div>
1	H	293	<div><div>2%</div><div><div></div><div>69%</div><div>27%</div><div></div></div><div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18473 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 GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	Se	0	0	0
			2285	1462	385	434	1	3			
1	B	292	Total	C	N	O	S	Se	0	0	0
			2285	1462	385	434	1	3			
1	C	292	Total	C	N	O	S	Se	0	0	0
			2285	1462	385	434	1	3			
1	D	292	Total	C	N	O	S	Se	0	0	0
			2285	1462	385	434	1	3			
1	E	292	Total	C	N	O	S	Se	0	0	0
			2285	1462	385	434	1	3			
1	F	292	Total	C	N	O	S	Se	0	0	0
			2285	1462	385	434	1	3			
1	G	292	Total	C	N	O	S	Se	0	0	0
			2285	1462	385	434	1	3			
1	H	292	Total	C	N	O	S	Se	0	0	0
			2285	1462	385	434	1	3			

There are 32 discrepancies between the modelled and reference sequences:

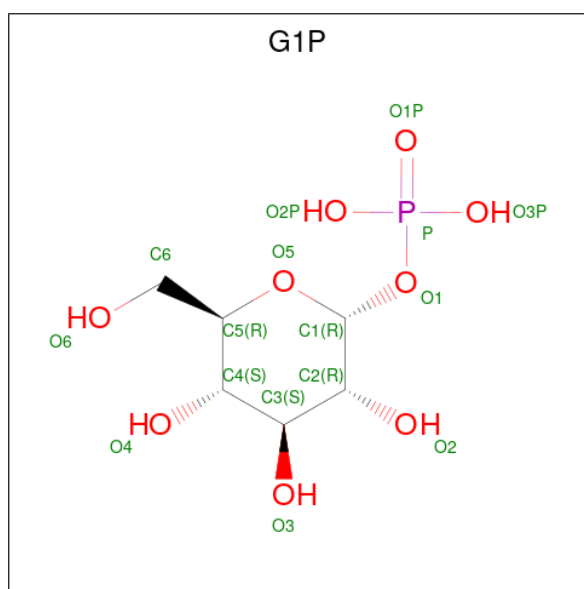
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q9HU22
A	35	MSE	MET	modified residue	UNP Q9HU22
A	44	MSE	MET	modified residue	UNP Q9HU22
A	217	MSE	MET	modified residue	UNP Q9HU22
B	1	MSE	MET	modified residue	UNP Q9HU22
B	35	MSE	MET	modified residue	UNP Q9HU22
B	44	MSE	MET	modified residue	UNP Q9HU22
B	217	MSE	MET	modified residue	UNP Q9HU22
C	1	MSE	MET	modified residue	UNP Q9HU22
C	35	MSE	MET	modified residue	UNP Q9HU22
C	44	MSE	MET	modified residue	UNP Q9HU22
C	217	MSE	MET	modified residue	UNP Q9HU22

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MSE	MET	modified residue	UNP Q9HU22
D	35	MSE	MET	modified residue	UNP Q9HU22
D	44	MSE	MET	modified residue	UNP Q9HU22
D	217	MSE	MET	modified residue	UNP Q9HU22
E	1	MSE	MET	modified residue	UNP Q9HU22
E	35	MSE	MET	modified residue	UNP Q9HU22
E	44	MSE	MET	modified residue	UNP Q9HU22
E	217	MSE	MET	modified residue	UNP Q9HU22
F	1	MSE	MET	modified residue	UNP Q9HU22
F	35	MSE	MET	modified residue	UNP Q9HU22
F	44	MSE	MET	modified residue	UNP Q9HU22
F	217	MSE	MET	modified residue	UNP Q9HU22
G	1	MSE	MET	modified residue	UNP Q9HU22
G	35	MSE	MET	modified residue	UNP Q9HU22
G	44	MSE	MET	modified residue	UNP Q9HU22
G	217	MSE	MET	modified residue	UNP Q9HU22
H	1	MSE	MET	modified residue	UNP Q9HU22
H	35	MSE	MET	modified residue	UNP Q9HU22
H	44	MSE	MET	modified residue	UNP Q9HU22
H	217	MSE	MET	modified residue	UNP Q9HU22

- Molecule 2 is 1-O-phosphono-alpha-D-glucopyranose (three-letter code: G1P) (formula: $C_6H_{13}O_9P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			16	6	9	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	O	P	0	0
			16	6	9	1		
2	C	1	Total	C	O	P	0	0
			16	6	9	1		
2	D	1	Total	C	O	P	0	0
			16	6	9	1		
2	E	1	Total	C	O	P	0	0
			16	6	9	1		
2	F	1	Total	C	O	P	0	0
			16	6	9	1		
2	G	1	Total	C	O	P	0	0
			16	6	9	1		
2	H	1	Total	C	O	P	0	0
			16	6	9	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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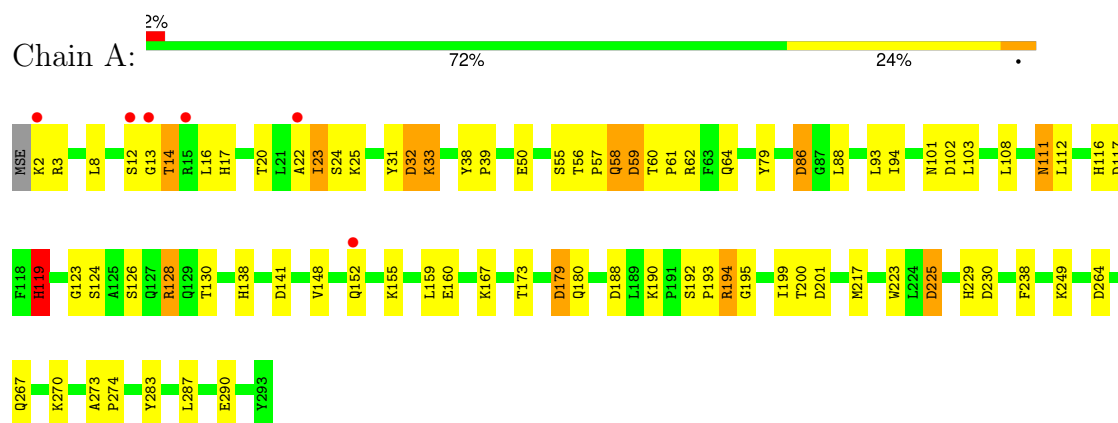
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		

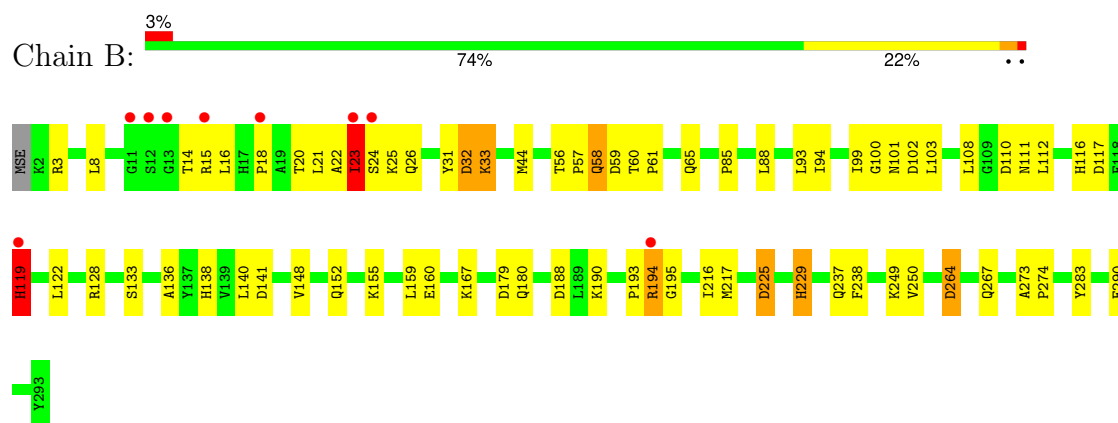
3 Residue-property plots [i](#)

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.

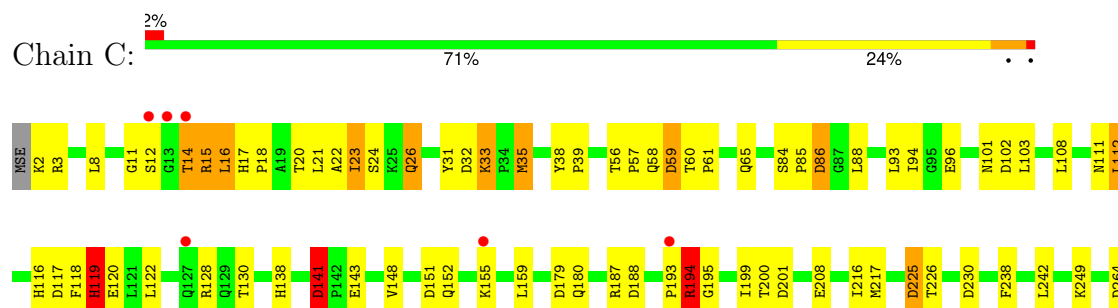
• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

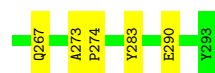


• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

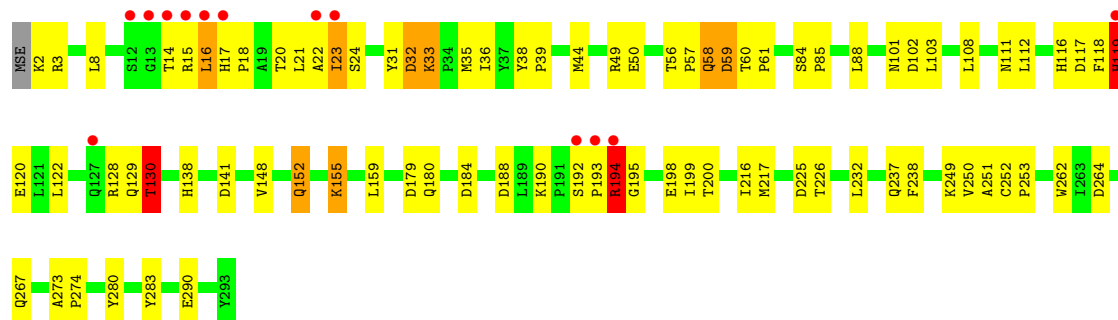


• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

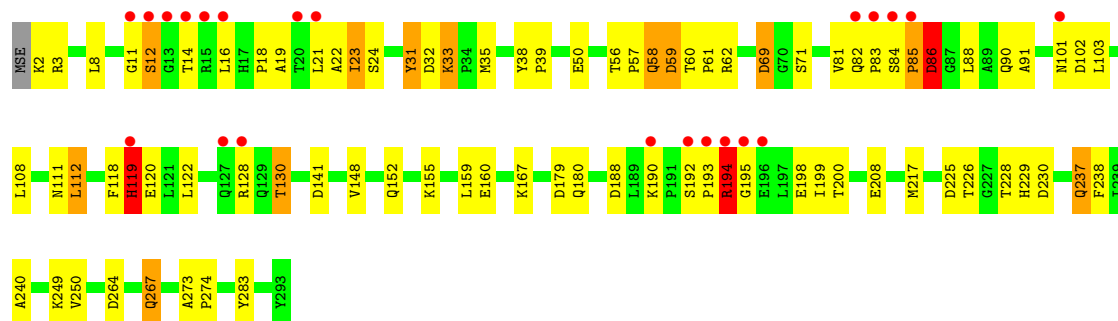




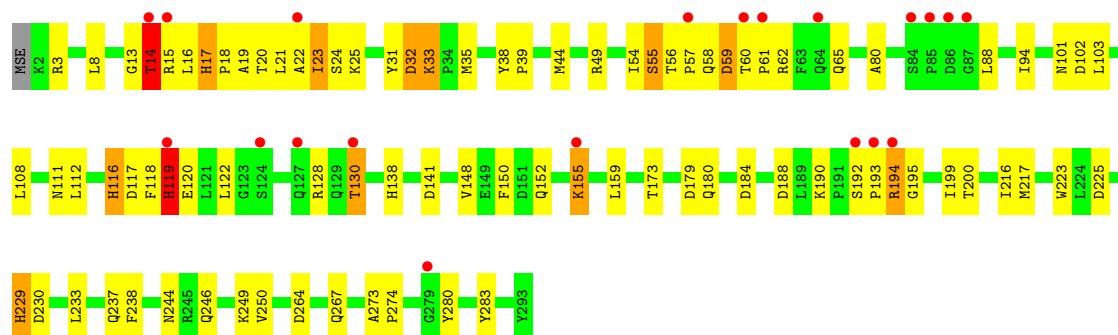
● Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE



● Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

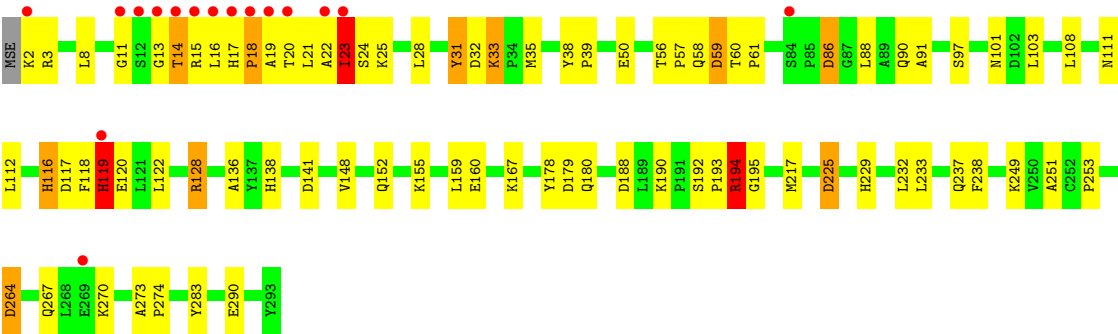


● Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

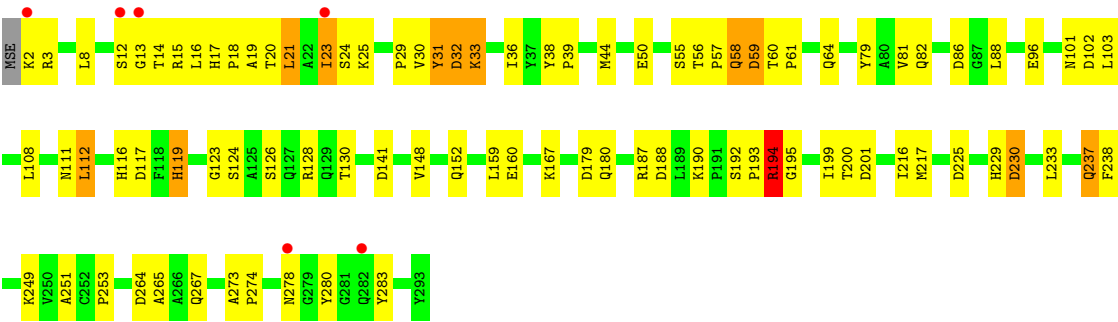


● Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE





● Molecule 1: GLUCOSE-1-PHOSPHATE THYMDYLYLTRANSFERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	71.58Å 73.90Å 133.75Å 89.81° 80.31° 80.18°	Depositor
Resolution (Å)	72.55 – 2.80 72.55 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.1 (72.55-2.80) 94.6 (72.55-2.80)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.70 (at 2.79Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.199 , 0.226 0.215 , 0.240	Depositor DCC
R_{free} test set	3103 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	34.4	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	18473	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% of the height of the origin peak. No significant pseudotranslation is detected.*

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: SO4, G1P

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.20	10/2332 (0.4%)	1.16	13/3159 (0.4%)
1	B	1.28	19/2332 (0.8%)	1.15	11/3159 (0.3%)
1	C	1.27	15/2332 (0.6%)	1.23	13/3159 (0.4%)
1	D	1.39	17/2332 (0.7%)	1.29	17/3159 (0.5%)
1	E	1.56	17/2332 (0.7%)	1.31	21/3159 (0.7%)
1	F	1.50	24/2332 (1.0%)	1.19	19/3159 (0.6%)
1	G	1.29	14/2332 (0.6%)	1.13	10/3159 (0.3%)
1	H	1.36	16/2332 (0.7%)	1.26	18/3159 (0.6%)
All	All	1.36	132/18656 (0.7%)	1.22	122/25272 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	3
1	G	0	2
1	H	0	1
All	All	0	10

All (132) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	194	ARG	CZ-NH1	-26.66	0.98	1.33
1	D	194	ARG	CZ-NH1	-26.41	0.98	1.33
1	E	267	GLN	CB-CG	-22.59	0.91	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	155	LYS	CB-CG	-19.42	1.00	1.52
1	H	237	GLN	CB-CG	-17.86	1.04	1.52
1	F	155	LYS	CD-CE	-17.75	1.06	1.51
1	H	23	ILE	CG1-CD1	-17.22	0.31	1.50
1	D	194	ARG	CB-CG	-15.66	1.10	1.52
1	E	194	ARG	CB-CG	-15.32	1.11	1.52
1	F	237	GLN	CB-CG	-14.81	1.12	1.52
1	C	141	ASP	CB-CG	-14.22	1.21	1.51
1	E	267	GLN	CG-CD	-14.04	1.18	1.51
1	E	190	LYS	CB-CG	-13.83	1.15	1.52
1	E	190	LYS	CD-CE	-13.49	1.17	1.51
1	D	119	HIS	CB-CG	-13.03	1.26	1.50
1	B	194	ARG	CZ-NH1	-13.00	1.16	1.33
1	F	194	ARG	CZ-NH1	-12.75	1.16	1.33
1	A	194	ARG	CZ-NH1	-12.39	1.17	1.33
1	F	130	THR	CB-CG2	-12.08	1.12	1.52
1	G	152	GLN	CD-OE1	-11.94	0.97	1.24
1	B	152	GLN	CD-OE1	-11.53	0.98	1.24
1	D	130	THR	CB-CG2	-11.40	1.14	1.52
1	E	119	HIS	CB-CG	-11.35	1.29	1.50
1	H	237	GLN	CG-CD	-11.28	1.25	1.51
1	G	97	SER	CB-OG	-10.97	1.27	1.42
1	F	155	LYS	CG-CD	-10.93	1.15	1.52
1	H	23	ILE	CB-CG2	-10.89	1.19	1.52
1	E	194	ARG	NE-CZ	-10.56	1.19	1.33
1	D	194	ARG	CZ-NH2	-10.53	1.19	1.33
1	E	194	ARG	CZ-NH2	-10.40	1.19	1.33
1	D	194	ARG	NE-CZ	-10.20	1.19	1.33
1	H	194	ARG	CZ-NH1	-10.18	1.19	1.33
1	G	194	ARG	CZ-NH1	-10.17	1.19	1.33
1	F	244	ASN	CG-ND2	-10.00	1.07	1.32
1	C	194	ARG	CZ-NH1	-9.99	1.20	1.33
1	F	55	SER	CB-OG	-9.78	1.29	1.42
1	F	237	GLN	CG-CD	-9.57	1.29	1.51
1	B	152	GLN	CG-CD	-9.34	1.29	1.51
1	F	244	ASN	CG-OD1	-9.31	1.03	1.24
1	F	155	LYS	CE-NZ	-8.99	1.26	1.49
1	G	152	GLN	CG-CD	-8.92	1.30	1.51
1	B	194	ARG	CB-CG	-8.89	1.28	1.52
1	A	194	ARG	CB-CG	-8.49	1.29	1.52
1	C	26	GLN	CD-OE1	-8.18	1.05	1.24
1	H	23	ILE	CB-CG1	-8.16	1.31	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	217	MSE	SE-CE	-7.97	1.48	1.95
1	H	194	ARG	CB-CG	-7.82	1.31	1.52
1	G	194	ARG	CB-CG	-7.74	1.31	1.52
1	C	217	MSE	SE-CE	-7.72	1.50	1.95
1	H	119	HIS	CB-CG	-7.66	1.36	1.50
1	H	119	HIS	CG-CD2	-7.56	1.22	1.35
1	B	26	GLN	CD-OE1	-7.43	1.07	1.24
1	C	26	GLN	CD-NE2	-7.42	1.14	1.32
1	H	119	HIS	CA-CB	-7.30	1.37	1.53
1	C	65	GLN	CD-NE2	-7.22	1.14	1.32
1	C	194	ARG	CB-CG	-7.14	1.33	1.52
1	B	119	HIS	CB-CG	-7.08	1.37	1.50
1	E	190	LYS	CG-CD	-7.05	1.28	1.52
1	A	217	MSE	SE-CE	-7.04	1.53	1.95
1	F	194	ARG	CB-CG	-6.97	1.33	1.52
1	B	23	ILE	CB-CG2	-6.94	1.31	1.52
1	G	194	ARG	CZ-NH2	-6.91	1.24	1.33
1	A	119	HIS	CB-CG	-6.91	1.37	1.50
1	B	237	GLN	CB-CG	-6.85	1.34	1.52
1	H	194	ARG	CZ-NH2	-6.79	1.24	1.33
1	G	119	HIS	CB-CG	-6.76	1.37	1.50
1	C	119	HIS	CB-CG	-6.72	1.38	1.50
1	E	217	MSE	SE-CE	-6.70	1.55	1.95
1	B	217	MSE	SE-CE	-6.68	1.56	1.95
1	F	119	HIS	CB-CG	-6.62	1.38	1.50
1	C	65	GLN	CD-OE1	-6.59	1.09	1.24
1	H	217	MSE	SE-CE	-6.51	1.57	1.95
1	C	141	ASP	CG-OD1	-6.49	1.10	1.25
1	D	44	MSE	SE-CE	-6.46	1.57	1.95
1	D	237	GLN	CB-CG	-6.36	1.35	1.52
1	G	237	GLN	CB-CG	-6.36	1.35	1.52
1	C	194	ARG	CZ-NH2	-6.34	1.24	1.33
1	F	217	MSE	SE-CE	-6.33	1.58	1.95
1	F	237	GLN	CD-OE1	-6.29	1.10	1.24
1	F	35	MSE	SE-CE	-6.24	1.58	1.95
1	F	23	ILE	CA-CB	-6.24	1.40	1.54
1	D	23	ILE	CB-CG2	-6.22	1.33	1.52
1	G	178	TYR	CD1-CE1	-6.21	1.30	1.39
1	E	237	GLN	CB-CG	-6.13	1.36	1.52
1	D	119	HIS	CA-CB	-6.13	1.40	1.53
1	E	267	GLN	CD-OE1	-6.10	1.10	1.24
1	C	23	ILE	CA-CB	-6.04	1.41	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	23	ILE	CA-CB	-5.94	1.41	1.54
1	F	194	ARG	CZ-NH2	-5.89	1.25	1.33
1	B	194	ARG	CZ-NH2	-5.88	1.25	1.33
1	H	30	VAL	CA-CB	-5.87	1.42	1.54
1	G	23	ILE	CB-CG2	-5.86	1.34	1.52
1	G	217	MSE	SE-CE	-5.77	1.61	1.95
1	B	26	GLN	CD-NE2	-5.76	1.18	1.32
1	B	136	ALA	CA-CB	-5.71	1.40	1.52
1	E	194	ARG	CD-NE	-5.68	1.36	1.46
1	H	190	LYS	CB-CG	-5.68	1.37	1.52
1	E	194	ARG	CG-CD	-5.67	1.37	1.51
1	D	194	ARG	CG-CD	-5.65	1.37	1.51
1	A	23	ILE	CB-CG2	-5.64	1.35	1.52
1	E	152	GLN	CG-CD	-5.59	1.38	1.51
1	E	119	HIS	CA-CB	-5.55	1.41	1.53
1	G	155	LYS	CD-CE	-5.51	1.37	1.51
1	A	155	LYS	CD-CE	-5.50	1.37	1.51
1	D	119	HIS	CG-CD2	-5.47	1.26	1.35
1	B	155	LYS	CD-CE	-5.46	1.37	1.51
1	D	194	ARG	CD-NE	-5.45	1.37	1.46
1	B	44	MSE	SE-CE	-5.44	1.63	1.95
1	C	2	LYS	CD-CE	-5.32	1.38	1.51
1	D	190	LYS	CB-CG	-5.31	1.38	1.52
1	D	155	LYS	CD-CE	-5.30	1.38	1.51
1	F	44	MSE	SE-CE	-5.29	1.64	1.95
1	F	152	GLN	CG-CD	-5.28	1.38	1.51
1	B	155	LYS	CB-CG	-5.28	1.38	1.52
1	H	130	THR	CB-CG2	-5.26	1.34	1.52
1	A	130	THR	CB-CG2	-5.25	1.35	1.52
1	A	190	LYS	CB-CG	-5.25	1.38	1.52
1	F	65	GLN	CD-NE2	-5.24	1.19	1.32
1	F	23	ILE	CB-CG2	-5.21	1.36	1.52
1	F	190	LYS	CB-CG	-5.18	1.38	1.52
1	A	119	HIS	CA-CB	-5.17	1.42	1.53
1	F	65	GLN	CD-OE1	-5.16	1.12	1.24
1	C	152	GLN	CG-CD	-5.13	1.39	1.51
1	G	136	ALA	CA-CB	-5.10	1.41	1.52
1	B	190	LYS	CB-CG	-5.10	1.38	1.52
1	A	194	ARG	CZ-NH2	-5.10	1.26	1.33
1	B	119	HIS	CA-CB	-5.09	1.42	1.53
1	C	35	MSE	SE-CE	-5.09	1.65	1.95
1	B	229	HIS	CG-CD2	-5.06	1.27	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	190	LYS	CB-CG	-5.05	1.39	1.52
1	H	44	MSE	SE-CE	-5.04	1.65	1.95
1	D	152	GLN	CG-CD	-5.03	1.39	1.51

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	194	ARG	NE-CZ-NH2	29.21	134.91	120.30
1	E	194	ARG	NE-CZ-NH2	29.21	134.90	120.30
1	H	23	ILE	CG1-CB-CG2	-26.59	52.90	111.40
1	C	141	ASP	CB-CG-OD1	-22.25	98.28	118.30
1	C	141	ASP	CB-CG-OD2	19.32	135.69	118.30
1	A	194	ARG	NE-CZ-NH2	15.67	128.14	120.30
1	B	194	ARG	NE-CZ-NH2	15.42	128.01	120.30
1	F	194	ARG	NE-CZ-NH2	14.28	127.44	120.30
1	E	194	ARG	CG-CD-NE	13.36	139.85	111.80
1	D	194	ARG	CG-CD-NE	12.96	139.02	111.80
1	G	194	ARG	NE-CZ-NH2	10.91	125.76	120.30
1	E	194	ARG	NE-CZ-NH1	-10.82	114.89	120.30
1	C	194	ARG	NE-CZ-NH2	10.50	125.55	120.30
1	F	130	THR	OG1-CB-CG2	-10.20	86.55	110.00
1	H	194	ARG	NE-CZ-NH2	10.18	125.39	120.30
1	H	23	ILE	CA-CB-CG1	10.06	130.12	111.00
1	D	194	ARG	NH1-CZ-NH2	-10.02	108.38	119.40
1	E	194	ARG	NH1-CZ-NH2	-9.74	108.68	119.40
1	D	194	ARG	NE-CZ-NH1	-9.74	115.43	120.30
1	F	155	LYS	CD-CE-NZ	9.10	132.62	111.70
1	D	119	HIS	CB-CA-C	-8.56	93.28	110.40
1	D	130	THR	OG1-CB-CG2	-8.31	90.89	110.00
1	D	119	HIS	N-CA-CB	7.95	124.91	110.60
1	G	128	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	B	141	ASP	CB-CG-OD2	7.52	125.07	118.30
1	F	141	ASP	CB-CG-OD2	7.42	124.98	118.30
1	H	102	ASP	CB-CG-OD2	7.41	124.97	118.30
1	F	155	LYS	CA-CB-CG	7.31	129.48	113.40
1	D	141	ASP	CB-CG-OD2	7.30	124.87	118.30
1	G	141	ASP	CB-CG-OD2	7.25	124.83	118.30
1	E	119	HIS	N-CA-CB	7.18	123.53	110.60
1	G	188	ASP	CB-CG-OD2	7.17	124.76	118.30
1	A	86	ASP	CB-CG-OD2	6.97	124.58	118.30
1	F	32	ASP	CB-CG-OD2	6.88	124.49	118.30
1	F	59	ASP	CB-CG-OD2	6.73	124.36	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	119	HIS	N-CA-CB	-6.71	98.52	110.60
1	A	23	ILE	CB-CA-C	-6.71	98.18	111.60
1	B	188	ASP	CB-CG-OD2	6.67	124.30	118.30
1	B	32	ASP	CB-CG-OD2	6.67	124.30	118.30
1	E	141	ASP	CB-CG-OD2	6.55	124.20	118.30
1	H	32	ASP	CB-CG-OD2	6.53	124.18	118.30
1	D	194	ARG	CB-CG-CD	6.51	128.53	111.60
1	F	23	ILE	CB-CA-C	-6.45	98.71	111.60
1	A	194	ARG	NE-CZ-NH1	-6.41	117.10	120.30
1	A	141	ASP	CB-CG-OD2	6.39	124.05	118.30
1	C	11	GLY	N-CA-C	6.29	128.82	113.10
1	D	23	ILE	CB-CA-C	-6.27	99.05	111.60
1	A	128	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	H	216	ILE	CB-CA-C	-6.25	99.10	111.60
1	H	86	ASP	CB-CG-OD2	6.21	123.89	118.30
1	E	194	ARG	CB-CG-CD	6.11	127.48	111.60
1	E	119	HIS	CB-CA-C	-6.09	98.23	110.40
1	F	184	ASP	CB-CG-OD2	6.08	123.78	118.30
1	H	59	ASP	CB-CG-OD2	6.08	123.77	118.30
1	E	264	ASP	CB-CG-OD2	6.02	123.72	118.30
1	B	119	HIS	N-CA-CB	-5.99	99.82	110.60
1	H	119	HIS	CB-CG-CD2	-5.99	112.24	130.80
1	H	23	ILE	N-CA-CB	-5.99	97.03	110.80
1	B	102	ASP	CB-CG-OD2	5.98	123.68	118.30
1	F	17	HIS	CB-CA-C	-5.98	98.45	110.40
1	H	141	ASP	CB-CG-OD2	5.98	123.68	118.30
1	B	152	GLN	CB-CG-CD	5.97	127.13	111.60
1	B	110	ASP	CB-CG-OD2	5.95	123.65	118.30
1	C	216	ILE	CB-CA-C	-5.93	99.75	111.60
1	C	59	ASP	CB-CG-OD2	5.92	123.63	118.30
1	E	23	ILE	CB-CA-C	-5.90	99.81	111.60
1	F	155	LYS	CB-CA-C	-5.89	98.63	110.40
1	C	201	ASP	CB-CG-OD2	5.88	123.59	118.30
1	E	102	ASP	CB-CG-OD2	5.86	123.57	118.30
1	A	188	ASP	CB-CG-OD2	5.79	123.52	118.30
1	H	230	ASP	CB-CG-OD1	5.79	123.51	118.30
1	A	201	ASP	CB-CG-OD2	5.73	123.46	118.30
1	H	112	LEU	CB-CG-CD1	-5.68	101.34	111.00
1	G	59	ASP	CB-CG-OD2	5.67	123.41	118.30
1	E	59	ASP	CB-CG-OD2	5.67	123.40	118.30
1	H	201	ASP	CB-CG-OD2	5.67	123.40	118.30
1	F	194	ARG	NH1-CZ-NH2	-5.62	113.22	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	102	ASP	CB-CG-OD2	5.62	123.35	118.30
1	C	86	ASP	CB-CG-OD2	5.60	123.34	118.30
1	H	188	ASP	CB-CG-OD2	5.58	123.33	118.30
1	F	188	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	179	ASP	CB-CG-OD2	5.57	123.31	118.30
1	D	59	ASP	CB-CG-OD2	5.56	123.30	118.30
1	B	216	ILE	CB-CA-C	-5.55	100.49	111.60
1	D	102	ASP	CB-CG-OD2	5.53	123.27	118.30
1	A	32	ASP	CB-CG-OD2	5.53	123.27	118.30
1	F	237	GLN	CB-CG-CD	5.51	125.92	111.60
1	B	264	ASP	CB-CG-OD2	5.50	123.25	118.30
1	E	112	LEU	CB-CG-CD1	-5.50	101.66	111.00
1	D	32	ASP	CB-CG-OD2	5.46	123.22	118.30
1	B	23	ILE	CB-CA-C	-5.44	100.72	111.60
1	H	21	LEU	CA-CB-CG	-5.41	102.85	115.30
1	F	216	ILE	CB-CA-C	-5.41	100.79	111.60
1	F	230	ASP	CB-CG-OD1	5.38	123.14	118.30
1	E	11	GLY	N-CA-C	5.33	126.41	113.10
1	D	216	ILE	CB-CA-C	-5.31	100.98	111.60
1	A	230	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	59	ASP	CB-CG-OD2	5.29	123.06	118.30
1	G	194	ARG	NH1-CZ-NH2	-5.29	113.58	119.40
1	F	233	LEU	CB-CG-CD2	-5.28	102.02	111.00
1	E	188	ASP	CB-CG-OD2	5.27	123.04	118.30
1	G	152	GLN	CB-CG-CD	5.26	125.29	111.60
1	C	188	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	102	ASP	CB-CG-OD2	5.25	123.02	118.30
1	E	190	LYS	CB-CG-CD	-5.25	97.96	111.60
1	C	230	ASP	CB-CG-OD1	5.21	122.99	118.30
1	C	151	ASP	CB-CG-OD2	5.19	122.97	118.30
1	C	112	LEU	CB-CG-CD1	-5.19	102.19	111.00
1	D	188	ASP	CB-CG-OD2	5.18	122.96	118.30
1	D	194	ARG	CD-NE-CZ	5.16	130.82	123.60
1	E	267	GLN	N-CA-CB	-5.15	101.34	110.60
1	G	119	HIS	CB-CA-C	5.13	120.66	110.40
1	F	49	ARG	NE-CZ-NH1	-5.10	117.75	120.30
1	E	69	ASP	CB-CG-OD1	5.09	122.89	118.30
1	D	184	ASP	CB-CG-OD2	5.08	122.87	118.30
1	E	194	ARG	CD-NE-CZ	5.08	130.71	123.60
1	C	102	ASP	CB-CG-OD2	5.06	122.86	118.30
1	H	233	LEU	CB-CG-CD2	-5.04	102.43	111.00
1	G	86	ASP	CB-CG-OD2	5.03	122.82	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	230	ASP	CB-CG-OD2	5.02	122.82	118.30
1	G	264	ASP	CB-CG-OD2	5.02	122.81	118.30
1	E	86	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	119	HIS	Sidechain
1	C	119	HIS	Sidechain
1	D	119	HIS	Sidechain
1	E	119	HIS	Sidechain
1	F	116	HIS	Sidechain
1	F	119	HIS	Sidechain
1	F	229	HIS	Sidechain
1	G	116	HIS	Sidechain
1	G	119	HIS	Sidechain
1	H	119	HIS	Sidechain

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	2285	0	2272	63	0
1	B	2285	0	2272	60	0
1	C	2285	0	2272	71	1
1	D	2285	0	2272	84	0
1	E	2285	0	2272	81	0
1	F	2285	0	2272	68	0
1	G	2285	0	2272	86	1
1	H	2285	0	2272	67	0
2	A	16	0	11	1	0
2	B	16	0	11	1	0
2	C	16	0	11	1	0
2	D	16	0	11	1	0
2	E	16	0	11	1	0
2	F	16	0	11	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	16	0	11	1	0
2	H	16	0	11	1	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	10	0	0	1	0
3	E	10	0	0	0	0
3	F	15	0	0	1	0
3	G	10	0	0	0	0
3	H	5	0	0	0	0
All	All	18473	0	18264	536	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (536) 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:E:267:GLN:CB	1:E:267:GLN:CD	1.82	1.45
1:E:267:GLN:CG	1:E:267:GLN:CA	2.06	1.32
1:C:141:ASP:OD1	1:C:141:ASP:N	1.71	1.12
1:E:267:GLN:CB	1:E:267:GLN:HG3	1.51	1.02
1:E:267:GLN:CG	1:E:267:GLN:HB2	1.52	1.02
1:E:267:GLN:CG	1:E:267:GLN:HB3	1.52	1.02
1:A:22:ALA:C	1:A:23:ILE:HG13	1.80	1.00
1:E:267:GLN:CB	1:E:267:GLN:HG2	1.51	0.99
1:D:119:HIS:H	1:D:119:HIS:HD2	1.10	0.98
1:F:60:THR:HB	1:F:61:PRO:HD3	1.47	0.94
1:E:267:GLN:CB	1:E:267:GLN:OE1	2.14	0.94
1:E:23:ILE:HD13	1:F:23:ILE:HD13	1.51	0.93
1:C:18:PRO:O	1:C:21:LEU:HB2	1.70	0.92
1:D:16:LEU:HB3	1:D:20:THR:HG23	1.51	0.92
1:C:22:ALA:C	1:C:23:ILE:HG13	1.89	0.91
1:E:267:GLN:CB	1:E:267:GLN:CG	0.91	0.91
1:D:18:PRO:HB2	1:D:21:LEU:HD12	1.55	0.89
1:A:273:ALA:HB3	1:A:274:PRO:HD3	1.53	0.89
1:B:22:ALA:C	1:B:23:ILE:HG13	1.94	0.88
1:F:273:ALA:HB3	1:F:274:PRO:HD3	1.54	0.87
1:H:273:ALA:HB3	1:H:274:PRO:HD3	1.55	0.87
1:B:22:ALA:O	1:B:23:ILE:HG13	1.75	0.87
1:F:22:ALA:C	1:F:23:ILE:HG13	1.94	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:119:HIS:H	1:D:119:HIS:CD2	1.92	0.86
1:E:23:ILE:CD1	1:F:23:ILE:HD13	2.05	0.86
1:A:16:LEU:HD13	1:A:25:LYS:HG3	1.58	0.85
1:D:273:ALA:HB3	1:D:274:PRO:HD3	1.58	0.85
1:G:16:LEU:HD12	1:G:25:LYS:HD3	1.59	0.84
1:B:273:ALA:HB3	1:B:274:PRO:HD3	1.60	0.83
1:C:273:ALA:HB3	1:C:274:PRO:HD3	1.58	0.83
1:G:273:ALA:HB3	1:G:274:PRO:HD3	1.59	0.83
1:A:22:ALA:O	1:A:23:ILE:HG13	1.78	0.82
1:B:58:GLN:OE1	1:B:58:GLN:N	2.13	0.81
1:D:130:THR:HG23	3:D:608:SO4:O4	1.81	0.80
1:D:22:ALA:C	1:D:23:ILE:HG13	2.01	0.80
1:F:60:THR:HB	1:F:61:PRO:CD	2.13	0.79
1:E:273:ALA:HB3	1:E:274:PRO:HD3	1.65	0.79
1:B:180:GLN:NE2	1:E:208:GLU:OE1	2.17	0.78
1:C:23:ILE:HD13	1:D:23:ILE:CD1	2.15	0.77
1:B:103:LEU:HD21	1:E:208:GLU:HG2	1.66	0.77
1:C:193:PRO:C	1:C:195:GLY:H	1.87	0.77
1:D:193:PRO:O	1:D:195:GLY:N	2.19	0.76
1:G:16:LEU:CD1	1:G:25:LYS:HG3	2.16	0.75
1:G:16:LEU:HD12	1:G:25:LYS:CD	2.17	0.74
1:G:22:ALA:C	1:G:23:ILE:HG13	2.08	0.74
1:H:101:ASN:O	1:H:180:GLN:NE2	2.20	0.74
1:E:193:PRO:O	1:E:195:GLY:N	2.20	0.74
1:D:22:ALA:O	1:D:23:ILE:HG13	1.88	0.74
1:E:22:ALA:C	1:E:23:ILE:HG13	2.07	0.73
1:G:16:LEU:CD1	1:G:25:LYS:CD	2.66	0.73
1:D:60:THR:HB	1:D:61:PRO:HD3	1.71	0.73
1:E:88:LEU:HD13	1:E:108:LEU:HD21	1.69	0.73
1:B:60:THR:HB	1:B:61:PRO:HD3	1.70	0.73
1:E:193:PRO:C	1:E:195:GLY:H	1.90	0.73
1:A:193:PRO:C	1:A:195:GLY:H	1.92	0.72
1:F:13:GLY:HA3	1:F:20:THR:OG1	1.89	0.72
1:D:88:LEU:HD13	1:D:108:LEU:HD21	1.71	0.72
1:H:60:THR:HB	1:H:61:PRO:HD3	1.71	0.72
1:G:119:HIS:C	1:G:119:HIS:CD2	2.60	0.72
1:A:101:ASN:O	1:A:180:GLN:NE2	2.22	0.72
1:D:119:HIS:CD2	1:D:119:HIS:N	2.49	0.72
1:D:264:ASP:OD1	1:D:267:GLN:HG3	1.90	0.72
1:C:17:HIS:CD2	1:C:20:THR:OG1	2.43	0.71
1:H:193:PRO:C	1:H:195:GLY:H	1.93	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:PRO:C	1:D:195:GLY:H	1.94	0.71
1:E:18:PRO:HB3	1:E:21:LEU:HD12	1.73	0.71
1:C:88:LEU:HD13	1:C:108:LEU:HD21	1.73	0.71
1:G:60:THR:HB	1:G:61:PRO:HD3	1.72	0.70
1:D:18:PRO:HA	1:D:21:LEU:HG	1.74	0.69
1:B:23:ILE:HG22	1:B:24:SER:N	2.06	0.69
1:C:193:PRO:O	1:C:195:GLY:N	2.25	0.69
1:E:119:HIS:H	1:E:119:HIS:CD2	2.09	0.69
1:B:16:LEU:HA	1:B:229:HIS:NE2	2.08	0.69
1:B:101:ASN:O	1:B:180:GLN:NE2	2.25	0.69
1:H:88:LEU:HD13	1:H:108:LEU:HD21	1.74	0.69
1:E:267:GLN:HB2	1:E:267:GLN:OE1	1.82	0.69
1:E:23:ILE:HD11	1:F:23:ILE:HG21	1.74	0.68
1:G:16:LEU:HB3	1:G:20:THR:CG2	2.23	0.68
1:B:264:ASP:OD1	1:B:267:GLN:HG3	1.93	0.68
1:C:249:LYS:HG3	1:C:283:TYR:CE2	2.29	0.68
1:F:249:LYS:HG3	1:F:283:TYR:CE2	2.28	0.68
1:H:23:ILE:O	1:H:23:ILE:HG22	1.92	0.68
1:E:18:PRO:HD3	1:F:280:TYR:CD1	2.30	0.67
1:E:60:THR:HB	1:E:61:PRO:HD3	1.76	0.67
1:D:16:LEU:HB3	1:D:20:THR:CG2	2.23	0.66
1:B:88:LEU:HD11	2:B:501:G1P:H1	1.78	0.66
1:G:19:ALA:HB1	1:H:29:PRO:HB3	1.77	0.66
1:E:193:PRO:C	1:E:195:GLY:N	2.49	0.66
1:F:88:LEU:HD13	1:F:108:LEU:HD21	1.76	0.66
1:F:22:ALA:C	1:F:23:ILE:CG1	2.64	0.66
1:F:264:ASP:OD1	1:F:267:GLN:HG3	1.94	0.66
1:A:60:THR:HB	1:A:61:PRO:HD3	1.76	0.66
1:D:33:LYS:NZ	1:D:250:VAL:O	2.24	0.65
1:H:32:ASP:OD1	1:H:33:LYS:HE3	1.95	0.65
1:A:32:ASP:O	1:B:18:PRO:HD2	1.96	0.65
1:C:23:ILE:HD13	1:D:23:ILE:HG12	1.79	0.65
1:D:32:ASP:OD1	1:D:33:LYS:HE3	1.97	0.65
1:F:101:ASN:O	1:F:180:GLN:NE2	2.29	0.65
1:G:88:LEU:HD13	1:G:108:LEU:HD21	1.79	0.65
1:C:17:HIS:HD2	1:C:20:THR:OG1	1.78	0.65
1:A:160:GLU:OE2	1:A:167:LYS:NZ	2.30	0.64
1:C:23:ILE:CD1	1:D:23:ILE:HG12	2.26	0.64
1:G:17:HIS:HB2	1:H:278:ASN:ND2	2.11	0.64
1:C:60:THR:HB	1:C:61:PRO:HD3	1.78	0.64
1:G:264:ASP:OD1	1:G:267:GLN:HG3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:PRO:O	1:A:195:GLY:N	2.31	0.64
1:H:15:ARG:HG3	1:H:15:ARG:HH11	1.63	0.64
1:F:138:HIS:NE2	1:G:290:GLU:OE2	2.26	0.64
1:G:16:LEU:CD1	1:G:25:LYS:CG	2.76	0.64
1:D:17:HIS:NE2	1:D:21:LEU:HD23	2.12	0.64
1:H:193:PRO:C	1:H:195:GLY:N	2.51	0.64
1:D:249:LYS:HG3	1:D:283:TYR:CE2	2.32	0.63
1:D:193:PRO:C	1:D:195:GLY:N	2.51	0.63
1:E:86:ASP:N	1:E:86:ASP:OD1	2.29	0.63
1:E:119:HIS:H	1:E:119:HIS:HD2	1.43	0.63
1:F:14:THR:HG22	1:F:15:ARG:N	2.13	0.63
1:B:16:LEU:HD13	1:B:25:LYS:HG3	1.79	0.63
1:G:16:LEU:HB3	1:G:20:THR:HG21	1.81	0.63
1:A:16:LEU:HD12	1:A:25:LYS:CD	2.29	0.62
1:D:24:SER:HB2	1:D:59:ASP:OD2	1.99	0.62
1:B:88:LEU:HD13	1:B:108:LEU:HD21	1.80	0.62
1:H:103:LEU:HD23	1:H:179:ASP:HA	1.81	0.62
1:E:88:LEU:HD11	2:E:504:G1P:H1	1.81	0.62
1:G:16:LEU:CB	1:G:20:THR:HG21	2.29	0.62
1:A:88:LEU:HD13	1:A:108:LEU:HD21	1.82	0.62
1:A:193:PRO:C	1:A:195:GLY:N	2.52	0.62
1:F:88:LEU:HD11	2:F:505:G1P:H1	1.80	0.62
1:E:23:ILE:HD13	1:F:23:ILE:CD1	2.28	0.62
1:E:249:LYS:HG3	1:E:283:TYR:CE2	2.35	0.62
1:A:32:ASP:OD1	1:A:33:LYS:HE3	1.99	0.62
1:H:193:PRO:O	1:H:195:GLY:N	2.32	0.62
1:G:32:ASP:OD1	1:G:33:LYS:HE3	1.99	0.61
1:D:2:LYS:NZ	1:D:50:GLU:OE1	2.24	0.61
1:C:193:PRO:C	1:C:195:GLY:N	2.54	0.61
1:D:18:PRO:CB	1:D:21:LEU:HD12	2.29	0.61
1:A:16:LEU:CD1	1:A:25:LYS:HG3	2.30	0.61
1:H:16:LEU:HA	1:H:229:HIS:CE1	2.35	0.61
1:E:16:LEU:O	1:E:19:ALA:HB3	2.01	0.60
1:A:16:LEU:CD1	1:A:25:LYS:CD	2.79	0.60
1:F:32:ASP:OD1	1:F:33:LYS:HE3	2.02	0.60
1:C:119:HIS:C	1:C:119:HIS:CD2	2.74	0.60
1:B:193:PRO:O	1:B:195:GLY:N	2.35	0.60
1:D:101:ASN:O	1:D:180:GLN:NE2	2.34	0.60
1:A:16:LEU:HB3	1:A:20:THR:HG23	1.83	0.59
1:F:13:GLY:HA3	1:F:20:THR:CB	2.32	0.59
1:A:58:GLN:N	1:A:58:GLN:OE1	2.30	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:160:GLU:OE2	1:H:167:LYS:NZ	2.35	0.59
1:B:3:ARG:NH2	1:B:128:ARG:O	2.36	0.59
1:B:193:PRO:C	1:B:195:GLY:N	2.55	0.59
1:E:16:LEU:HD22	1:E:229:HIS:CE1	2.38	0.59
1:E:22:ALA:O	1:E:23:ILE:HG13	2.03	0.58
1:A:88:LEU:HD11	2:A:500:G1P:H1	1.86	0.58
1:B:116:HIS:O	1:B:117:ASP:HB2	2.03	0.58
1:G:17:HIS:CD2	1:G:21:LEU:HD23	2.37	0.58
1:D:16:LEU:O	1:D:17:HIS:C	2.38	0.58
1:E:237:GLN:HG2	1:H:237:GLN:HE22	1.68	0.58
1:A:103:LEU:HD23	1:A:179:ASP:HA	1.86	0.58
1:B:16:LEU:CD1	1:B:25:LYS:HG3	2.33	0.58
1:H:58:GLN:N	1:H:58:GLN:OE1	2.35	0.58
1:A:119:HIS:C	1:A:119:HIS:CD2	2.76	0.57
1:H:88:LEU:HD11	2:H:507:G1P:H1	1.85	0.57
1:F:273:ALA:HB3	1:F:274:PRO:CD	2.32	0.57
1:D:18:PRO:CB	1:D:21:LEU:CD1	2.83	0.57
1:H:12:SER:OG	1:H:13:GLY:N	2.37	0.57
1:B:290:GLU:OE2	1:D:138:HIS:NE2	2.34	0.57
1:G:3:ARG:NH2	1:G:128:ARG:O	2.38	0.57
1:H:249:LYS:HG3	1:H:283:TYR:CE2	2.39	0.57
1:E:119:HIS:CD2	1:E:119:HIS:N	2.66	0.57
1:H:60:THR:HB	1:H:61:PRO:CD	2.34	0.57
1:H:3:ARG:NH2	1:H:128:ARG:O	2.38	0.56
1:B:18:PRO:HB3	1:B:21:LEU:HD12	1.86	0.56
1:C:23:ILE:HD13	1:D:23:ILE:CG1	2.34	0.56
1:C:88:LEU:HD11	2:C:502:G1P:H1	1.86	0.56
1:D:103:LEU:HD23	1:D:179:ASP:HA	1.88	0.56
1:G:160:GLU:OE2	1:G:167:LYS:NZ	2.38	0.56
1:A:12:SER:OG	1:A:13:GLY:N	2.39	0.56
1:D:8:LEU:HD23	1:D:88:LEU:HD22	1.87	0.56
1:E:16:LEU:HD21	1:E:228:THR:HA	1.87	0.56
1:F:116:HIS:O	1:F:117:ASP:HB2	2.06	0.56
1:G:16:LEU:O	1:G:20:THR:OG1	2.21	0.56
1:G:16:LEU:HD13	1:G:25:LYS:HG3	1.87	0.56
1:A:3:ARG:NH2	1:A:128:ARG:O	2.38	0.56
1:C:119:HIS:HD2	1:C:120:GLU:OE1	1.89	0.56
1:C:18:PRO:HD3	1:D:280:TYR:CD1	2.41	0.56
1:G:58:GLN:OE1	1:G:58:GLN:N	2.32	0.56
1:B:32:ASP:OD1	1:B:33:LYS:HE3	2.06	0.56
1:F:24:SER:HB2	1:F:59:ASP:OD2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:LEU:HD23	1:B:179:ASP:HA	1.89	0.55
1:D:18:PRO:O	1:D:21:LEU:HB2	2.06	0.55
1:G:18:PRO:HD2	1:H:32:ASP:O	2.06	0.55
1:G:103:LEU:HD23	1:G:179:ASP:HA	1.89	0.55
1:G:16:LEU:HD11	1:G:25:LYS:HD2	1.89	0.55
1:C:24:SER:HB2	1:C:59:ASP:OD2	2.06	0.55
1:G:88:LEU:HD11	2:G:506:G1P:H1	1.87	0.55
1:D:56:THR:HB	1:D:57:PRO:HD2	1.89	0.55
1:A:2:LYS:NZ	1:A:50:GLU:OE1	2.34	0.54
1:C:24:SER:HB2	1:C:59:ASP:CG	2.27	0.54
1:C:56:THR:HB	1:C:57:PRO:HD2	1.89	0.54
1:F:14:THR:CG2	1:F:15:ARG:N	2.71	0.54
1:G:116:HIS:O	1:G:117:ASP:HB2	2.06	0.54
1:D:3:ARG:NH2	1:D:128:ARG:O	2.41	0.54
1:H:24:SER:HB2	1:H:59:ASP:OD2	2.08	0.54
1:C:112:LEU:C	1:C:112:LEU:HD23	2.27	0.54
1:B:249:LYS:HG3	1:B:283:TYR:CE2	2.43	0.54
1:G:18:PRO:HD3	1:H:280:TYR:CD1	2.43	0.54
1:A:16:LEU:CD1	1:A:25:LYS:HD2	2.38	0.54
1:B:16:LEU:CD1	1:B:25:LYS:CD	2.85	0.54
1:D:58:GLN:OE1	1:D:58:GLN:N	2.39	0.54
1:G:8:LEU:HD23	1:G:88:LEU:HD22	1.90	0.54
1:G:16:LEU:C	1:G:20:THR:HG1	2.11	0.54
1:C:15:ARG:O	1:C:17:HIS:N	2.41	0.54
1:C:116:HIS:O	1:C:117:ASP:HB2	2.07	0.54
1:F:249:LYS:HG3	1:F:283:TYR:CD2	2.43	0.54
1:G:16:LEU:HD11	1:G:25:LYS:CD	2.38	0.54
1:B:56:THR:HB	1:B:57:PRO:HD2	1.90	0.54
1:D:60:THR:HB	1:D:61:PRO:CD	2.37	0.54
1:C:23:ILE:HD11	1:D:23:ILE:HG21	1.90	0.53
1:E:56:THR:HB	1:E:57:PRO:HD2	1.91	0.53
1:E:112:LEU:C	1:E:112:LEU:HD23	2.29	0.53
1:D:23:ILE:HG22	1:D:24:SER:N	2.24	0.53
1:A:8:LEU:HD23	1:A:88:LEU:HD22	1.90	0.53
1:D:24:SER:HB2	1:D:59:ASP:CG	2.29	0.53
1:D:88:LEU:HD11	2:D:503:G1P:H1	1.90	0.53
1:A:56:THR:HB	1:A:57:PRO:HD2	1.90	0.53
1:A:249:LYS:HG3	1:A:283:TYR:CE2	2.43	0.53
1:F:60:THR:N	1:F:61:PRO:HD2	2.24	0.53
1:C:32:ASP:OD1	1:C:33:LYS:HE3	2.08	0.52
1:C:23:ILE:HD13	1:D:23:ILE:HD13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:LEU:C	1:D:112:LEU:HD23	2.29	0.52
1:F:16:LEU:O	1:F:19:ALA:HB3	2.09	0.52
1:G:119:HIS:HD2	1:G:120:GLU:N	2.08	0.52
1:C:8:LEU:HD23	1:C:88:LEU:HD22	1.92	0.52
1:C:16:LEU:HB3	1:C:20:THR:HG23	1.90	0.52
1:F:60:THR:CB	1:F:61:PRO:CD	2.81	0.52
1:H:56:THR:HB	1:H:57:PRO:HD2	1.91	0.52
1:A:16:LEU:HD12	1:A:25:LYS:HD3	1.92	0.52
1:E:32:ASP:OD1	1:E:33:LYS:HE3	2.09	0.52
1:H:24:SER:HB2	1:H:59:ASP:CG	2.30	0.52
1:E:58:GLN:OE1	1:E:58:GLN:N	2.40	0.52
1:B:60:THR:HB	1:B:61:PRO:CD	2.39	0.52
1:B:193:PRO:C	1:B:195:GLY:H	2.13	0.52
1:D:249:LYS:HG3	1:D:283:TYR:CD2	2.44	0.52
1:E:60:THR:HB	1:E:61:PRO:CD	2.39	0.52
1:G:28:LEU:HD22	1:H:29:PRO:HD3	1.90	0.52
1:G:233:LEU:HD21	1:H:237:GLN:HA	1.92	0.52
1:H:116:HIS:O	1:H:117:ASP:HB2	2.08	0.52
1:G:101:ASN:O	1:G:180:GLN:NE2	2.42	0.52
1:A:24:SER:HB2	1:A:59:ASP:OD2	2.07	0.52
1:G:16:LEU:C	1:G:20:THR:OG1	2.49	0.52
1:E:103:LEU:HD23	1:E:179:ASP:HA	1.91	0.52
1:F:3:ARG:NH2	1:F:128:ARG:O	2.42	0.52
1:G:60:THR:HB	1:G:61:PRO:CD	2.39	0.52
1:B:119:HIS:C	1:B:119:HIS:CD2	2.83	0.51
1:H:251:ALA:O	1:H:253:PRO:HD3	2.10	0.51
1:C:273:ALA:HB3	1:C:274:PRO:CD	2.37	0.51
1:F:56:THR:HB	1:F:57:PRO:HD2	1.93	0.51
1:D:16:LEU:CB	1:D:20:THR:CG2	2.87	0.51
1:G:14:THR:C	1:G:16:LEU:H	2.12	0.51
1:H:273:ALA:N	1:H:274:PRO:CD	2.73	0.51
1:B:24:SER:HB2	1:B:59:ASP:CG	2.31	0.51
1:G:56:THR:HB	1:G:57:PRO:HD2	1.91	0.51
1:C:118:PHE:CE2	1:C:122:LEU:HD11	2.45	0.51
1:F:13:GLY:O	1:F:16:LEU:N	2.44	0.51
1:G:14:THR:C	1:G:16:LEU:N	2.63	0.51
1:E:18:PRO:O	1:E:21:LEU:HB2	2.10	0.51
1:E:8:LEU:HD23	1:E:88:LEU:HD22	1.93	0.51
1:F:8:LEU:HD23	1:F:88:LEU:HD22	1.93	0.51
1:B:58:GLN:H	1:B:58:GLN:CD	2.11	0.50
1:E:56:THR:HB	1:E:57:PRO:CD	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:120:GLU:N	1:E:120:GLU:OE1	2.43	0.50
1:A:116:HIS:O	1:A:117:ASP:HB2	2.10	0.50
1:E:90:GLN:O	1:E:91:ALA:C	2.48	0.50
1:F:118:PHE:CE2	1:F:122:LEU:HD11	2.46	0.50
1:D:56:THR:HB	1:D:57:PRO:CD	2.42	0.50
1:F:14:THR:HA	1:F:17:HIS:ND1	2.26	0.50
1:F:103:LEU:HD23	1:F:179:ASP:HA	1.94	0.50
1:B:56:THR:HB	1:B:57:PRO:CD	2.42	0.50
1:C:58:GLN:OE1	1:C:58:GLN:N	2.40	0.50
1:G:23:ILE:HG12	1:H:23:ILE:HD11	1.94	0.50
1:G:24:SER:HB2	1:G:59:ASP:CG	2.32	0.50
1:G:193:PRO:C	1:G:195:GLY:N	2.63	0.50
1:B:16:LEU:HD11	1:B:25:LYS:HD2	1.93	0.50
1:G:56:THR:HB	1:G:57:PRO:CD	2.42	0.50
1:G:119:HIS:CD2	1:G:120:GLU:N	2.80	0.50
1:A:290:GLU:OE2	1:C:138:HIS:NE2	2.35	0.50
1:C:249:LYS:HG3	1:C:283:TYR:CD2	2.46	0.49
1:E:237:GLN:HG2	1:H:237:GLN:NE2	2.26	0.49
1:G:28:LEU:HD22	1:H:29:PRO:CD	2.42	0.49
1:A:238:PHE:CE1	1:C:238:PHE:CE1	3.01	0.49
1:F:38:TYR:N	1:F:39:PRO:HD2	2.27	0.49
1:A:273:ALA:HB3	1:A:274:PRO:CD	2.35	0.49
1:D:273:ALA:HB3	1:D:274:PRO:CD	2.38	0.49
1:E:3:ARG:NH2	1:E:128:ARG:O	2.45	0.49
1:E:199:ILE:CG2	1:E:200:THR:N	2.75	0.49
1:A:264:ASP:OD1	1:A:267:GLN:HG3	2.13	0.49
1:G:193:PRO:C	1:G:195:GLY:H	2.15	0.49
1:D:16:LEU:N	1:D:16:LEU:HD23	2.27	0.49
1:F:238:PHE:CE1	1:G:238:PHE:CE1	3.00	0.49
1:D:38:TYR:N	1:D:39:PRO:HD2	2.28	0.49
1:H:18:PRO:O	1:H:19:ALA:C	2.50	0.49
1:C:58:GLN:H	1:C:58:GLN:CD	2.16	0.49
1:D:35:MSE:SE	1:D:226:THR:OG1	2.80	0.49
1:B:180:GLN:OE1	1:E:208:GLU:CB	2.61	0.49
1:H:249:LYS:HG3	1:H:283:TYR:CD2	2.47	0.48
1:F:119:HIS:HD2	1:F:120:GLU:OE1	1.97	0.48
1:B:8:LEU:HD23	1:B:88:LEU:HD22	1.95	0.48
1:G:58:GLN:H	1:G:58:GLN:CD	2.14	0.48
1:H:2:LYS:NZ	1:H:50:GLU:OE1	2.34	0.48
1:E:249:LYS:HG3	1:E:283:TYR:CD2	2.48	0.48
1:G:19:ALA:O	1:G:22:ALA:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:23:ILE:HG22	1:G:24:SER:N	2.28	0.48
1:A:58:GLN:H	1:A:58:GLN:CD	2.14	0.48
1:A:112:LEU:C	1:A:112:LEU:HD23	2.33	0.48
1:B:273:ALA:N	1:B:274:PRO:CD	2.76	0.48
1:C:194:ARG:O	1:C:194:ARG:HG2	2.14	0.48
1:C:273:ALA:N	1:C:274:PRO:CD	2.76	0.48
1:C:96:GLU:OE1	1:C:187:ARG:NH1	2.47	0.48
1:G:17:HIS:NE2	1:G:21:LEU:HD23	2.29	0.48
1:G:229:HIS:HB3	1:H:31:TYR:CE1	2.49	0.48
1:B:225:ASP:C	1:B:225:ASP:OD1	2.51	0.48
1:H:148:VAL:HB	1:H:159:LEU:HD23	1.96	0.48
1:A:56:THR:HB	1:A:57:PRO:CD	2.43	0.48
1:B:23:ILE:HG22	1:B:24:SER:H	1.75	0.48
1:H:56:THR:HB	1:H:57:PRO:CD	2.44	0.48
1:G:16:LEU:HB3	1:G:20:THR:HG23	1.96	0.47
1:C:3:ARG:NH2	1:C:128:ARG:O	2.47	0.47
1:E:69:ASP:OD1	1:E:71:SER:OG	2.28	0.47
1:G:112:LEU:HD23	1:G:112:LEU:C	2.34	0.47
1:A:24:SER:HB2	1:A:59:ASP:CG	2.35	0.47
1:A:60:THR:HB	1:A:61:PRO:CD	2.42	0.47
1:C:264:ASP:OD1	1:C:267:GLN:HG3	2.15	0.47
1:E:88:LEU:HD13	1:E:108:LEU:CD2	2.41	0.47
1:F:14:THR:O	1:F:17:HIS:HB2	2.14	0.47
1:G:15:ARG:HG3	1:G:15:ARG:HH11	1.79	0.47
1:F:179:ASP:OD1	1:F:179:ASP:C	2.52	0.47
1:C:60:THR:HB	1:C:61:PRO:CD	2.43	0.47
1:D:16:LEU:O	1:D:17:HIS:O	2.32	0.47
1:H:123:GLY:O	1:H:124:SER:C	2.52	0.47
1:C:119:HIS:CD2	1:C:120:GLU:N	2.83	0.47
1:D:21:LEU:HD23	1:D:21:LEU:HA	1.66	0.47
1:G:17:HIS:CB	1:H:278:ASN:ND2	2.77	0.47
1:C:148:VAL:HB	1:C:159:LEU:HD23	1.96	0.47
1:D:18:PRO:CA	1:D:21:LEU:HG	2.43	0.47
1:E:238:PHE:CE1	1:H:238:PHE:CE1	3.03	0.47
1:E:118:PHE:CE2	1:E:122:LEU:HD11	2.50	0.47
1:C:56:THR:HB	1:C:57:PRO:CD	2.45	0.47
1:D:273:ALA:N	1:D:274:PRO:CD	2.78	0.47
1:E:267:GLN:CG	1:E:267:GLN:HA	2.31	0.47
1:A:199:ILE:CG2	1:A:200:THR:N	2.78	0.46
1:D:119:HIS:HD2	1:D:119:HIS:N	1.84	0.46
1:D:148:VAL:HB	1:D:159:LEU:HD23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:130:THR:HG23	3:F:610:SO4:O1	2.15	0.46
1:C:249:LYS:HG3	1:C:283:TYR:CZ	2.51	0.46
1:E:2:LYS:NZ	1:E:50:GLU:OE1	2.31	0.46
1:F:14:THR:HA	1:F:17:HIS:CE1	2.51	0.46
1:A:264:ASP:OD1	1:A:264:ASP:C	2.53	0.46
1:C:21:LEU:HD23	1:C:21:LEU:HA	1.61	0.46
1:H:36:ILE:HG12	1:H:36:ILE:O	2.16	0.46
1:H:192:SER:OG	1:H:194:ARG:HB3	2.15	0.46
1:D:36:ILE:HG12	1:D:36:ILE:O	2.16	0.46
1:B:112:LEU:HD23	1:B:112:LEU:C	2.36	0.46
1:B:180:GLN:OE1	1:E:208:GLU:HB3	2.16	0.45
1:E:24:SER:HB2	1:E:59:ASP:CG	2.37	0.45
1:H:199:ILE:CG2	1:H:200:THR:N	2.79	0.45
1:B:238:PHE:CE1	1:D:238:PHE:CE1	3.04	0.45
1:E:148:VAL:HB	1:E:159:LEU:HD23	1.98	0.45
1:F:94:ILE:O	1:F:94:ILE:CG2	2.62	0.45
1:F:193:PRO:C	1:F:195:GLY:N	2.70	0.45
1:A:148:VAL:HB	1:A:159:LEU:HD23	1.97	0.45
1:H:38:TYR:N	1:H:39:PRO:HD2	2.31	0.45
1:H:16:LEU:HD13	1:H:25:LYS:HG3	1.98	0.45
1:H:96:GLU:OE1	1:H:187:ARG:NH1	2.49	0.45
1:B:249:LYS:HG3	1:B:283:TYR:CD2	2.51	0.45
1:C:103:LEU:HD23	1:C:179:ASP:HA	1.97	0.45
1:G:90:GLN:O	1:G:91:ALA:C	2.55	0.45
1:G:192:SER:OG	1:G:194:ARG:HB3	2.17	0.45
1:A:64:GLN:HG3	1:A:79:TYR:CE1	2.52	0.45
1:A:123:GLY:O	1:A:124:SER:C	2.52	0.45
1:D:179:ASP:C	1:D:179:ASP:OD1	2.55	0.45
1:G:17:HIS:CD2	1:G:21:LEU:CD2	2.99	0.45
1:G:193:PRO:O	1:G:195:GLY:N	2.50	0.45
1:H:8:LEU:HD23	1:H:88:LEU:HD22	1.99	0.45
1:F:59:ASP:OD1	1:F:62:ARG:NH1	2.49	0.45
1:G:179:ASP:C	1:G:179:ASP:OD1	2.55	0.45
1:H:273:ALA:HB3	1:H:274:PRO:CD	2.35	0.45
1:C:199:ILE:HD12	1:C:199:ILE:HA	1.85	0.44
1:D:199:ILE:CG2	1:D:200:THR:N	2.80	0.44
1:F:193:PRO:C	1:F:195:GLY:H	2.19	0.44
1:H:112:LEU:C	1:H:112:LEU:HD23	2.37	0.44
1:A:16:LEU:CD1	1:A:25:LYS:CG	2.94	0.44
1:E:59:ASP:OD1	1:E:62:ARG:NH1	2.47	0.44
1:G:38:TYR:N	1:G:39:PRO:HD2	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:LEU:N	1:D:16:LEU:CD2	2.80	0.44
1:F:18:PRO:O	1:F:19:ALA:C	2.56	0.44
1:H:264:ASP:OD1	1:H:267:GLN:HG3	2.17	0.44
1:F:24:SER:HB2	1:F:59:ASP:CG	2.38	0.44
1:F:112:LEU:C	1:F:112:LEU:HD23	2.38	0.44
1:E:58:GLN:H	1:E:58:GLN:CD	2.19	0.44
1:A:192:SER:HB2	1:A:193:PRO:CD	2.48	0.44
1:C:15:ARG:C	1:C:17:HIS:H	2.20	0.44
1:C:18:PRO:O	1:C:21:LEU:CB	2.55	0.44
1:C:35:MSE:SE	1:C:226:THR:OG1	2.86	0.44
1:F:33:LYS:NZ	1:F:250:VAL:O	2.30	0.44
1:D:14:THR:O	1:D:15:ARG:C	2.56	0.44
1:D:58:GLN:H	1:D:58:GLN:CD	2.21	0.44
1:E:160:GLU:OE2	1:E:167:LYS:NZ	2.51	0.44
1:B:160:GLU:OE2	1:B:167:LYS:NZ	2.51	0.44
1:C:23:ILE:HG12	1:D:23:ILE:HG12	2.00	0.44
1:D:120:GLU:OE1	1:D:120:GLU:N	2.51	0.44
1:H:17:HIS:HD2	1:H:20:THR:OG1	2.01	0.44
1:H:264:ASP:O	1:H:265:ALA:C	2.56	0.43
1:C:88:LEU:HD13	1:C:108:LEU:CD2	2.46	0.43
1:G:57:PRO:HD2	1:G:58:GLN:OE1	2.18	0.43
1:G:148:VAL:HB	1:G:159:LEU:HD23	2.00	0.43
1:E:81:VAL:CG1	1:E:82:GLN:N	2.80	0.43
1:E:130:THR:O	1:E:130:THR:HG23	2.18	0.43
1:G:15:ARG:HG3	1:G:15:ARG:NH1	2.32	0.43
1:A:249:LYS:HG3	1:A:283:TYR:CD2	2.54	0.43
1:E:84:SER:HA	1:E:85:PRO:HD3	1.84	0.43
1:A:55:SER:OG	1:A:56:THR:N	2.52	0.43
1:B:99:ILE:HG22	1:B:100:GLY:O	2.18	0.43
1:B:140:LEU:O	1:B:140:LEU:HG	2.18	0.43
1:B:264:ASP:OD1	1:B:264:ASP:C	2.57	0.43
1:G:25:LYS:O	1:G:35:MSE:HE3	2.19	0.43
1:B:138:HIS:NE2	1:D:290:GLU:OE2	2.49	0.43
1:C:225:ASP:OD1	1:C:225:ASP:C	2.57	0.43
1:D:88:LEU:HD13	1:D:108:LEU:CD2	2.44	0.43
1:E:31:TYR:CD1	1:E:240:ALA:HB2	2.54	0.43
1:E:192:SER:OG	1:E:194:ARG:HB2	2.19	0.43
1:H:55:SER:OG	1:H:56:THR:N	2.51	0.43
1:A:14:THR:HG22	1:A:17:HIS:CE1	2.54	0.43
1:B:61:PRO:O	1:B:65:GLN:N	2.43	0.43
1:D:17:HIS:CD2	1:D:21:LEU:HD23	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:SER:OG	1:D:194:ARG:HB2	2.19	0.43
1:A:273:ALA:N	1:A:274:PRO:CD	2.81	0.43
1:E:35:MSE:SE	1:E:226:THR:OG1	2.87	0.43
1:E:199:ILE:HD12	1:E:199:ILE:HA	1.90	0.43
1:F:56:THR:HB	1:F:57:PRO:CD	2.49	0.43
1:F:173:THR:HG22	1:F:223:TRP:CE3	2.54	0.43
1:F:192:SER:OG	1:F:194:ARG:HB3	2.19	0.43
1:G:273:ALA:HB3	1:G:274:PRO:CD	2.39	0.43
1:A:225:ASP:OD1	1:A:225:ASP:C	2.57	0.43
1:F:16:LEU:HD23	1:F:229:HIS:ND1	2.34	0.43
1:F:23:ILE:HD13	1:F:23:ILE:HG21	1.74	0.43
1:H:16:LEU:O	1:H:229:HIS:HE1	2.01	0.43
1:G:2:LYS:NZ	1:G:50:GLU:OE1	2.45	0.42
1:G:249:LYS:HG3	1:G:283:TYR:CE2	2.54	0.42
1:B:16:LEU:CD1	1:B:25:LYS:CG	2.97	0.42
1:G:273:ALA:N	1:G:274:PRO:CD	2.81	0.42
1:A:38:TYR:HB2	1:A:39:PRO:CD	2.49	0.42
1:G:23:ILE:HG22	1:G:24:SER:H	1.83	0.42
1:A:59:ASP:OD1	1:A:62:ARG:NH1	2.53	0.42
1:B:24:SER:HB2	1:B:59:ASP:OD2	2.19	0.42
1:B:93:LEU:O	1:B:94:ILE:C	2.56	0.42
1:E:101:ASN:O	1:E:180:GLN:NE2	2.50	0.42
1:F:249:LYS:HG3	1:F:283:TYR:CZ	2.54	0.42
1:H:58:GLN:H	1:H:58:GLN:CD	2.20	0.42
1:A:138:HIS:NE2	1:C:290:GLU:OE2	2.43	0.42
1:G:13:GLY:O	1:G:16:LEU:HB2	2.19	0.42
1:D:152:GLN:H	1:D:152:GLN:HG2	1.49	0.42
1:E:23:ILE:HG22	1:E:24:SER:N	2.35	0.42
1:E:273:ALA:N	1:E:274:PRO:CD	2.82	0.42
1:F:148:VAL:HB	1:F:159:LEU:HD23	2.02	0.42
1:F:192:SER:HB2	1:F:193:PRO:HD2	2.02	0.42
1:G:16:LEU:HB2	1:G:20:THR:HG21	2.00	0.42
1:C:101:ASN:O	1:C:180:GLN:NE2	2.53	0.42
1:C:119:HIS:HD2	1:C:120:GLU:CD	2.23	0.42
1:E:267:GLN:CD	1:E:267:GLN:CA	2.57	0.42
1:C:23:ILE:HG21	1:D:23:ILE:HD11	2.02	0.42
1:C:60:THR:N	1:C:61:PRO:HD2	2.35	0.42
1:E:194:ARG:NH1	1:E:198:GLU:OE2	2.53	0.42
1:F:13:GLY:CA	1:F:20:THR:OG1	2.65	0.42
1:G:24:SER:HB2	1:G:59:ASP:OD2	2.19	0.42
1:A:38:TYR:N	1:A:39:PRO:HD2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:PHE:CE2	1:D:122:LEU:HD11	2.55	0.41
1:D:194:ARG:NH1	1:D:198:GLU:OE2	2.53	0.41
1:E:18:PRO:HB3	1:E:21:LEU:CD1	2.47	0.41
1:F:199:ILE:CG2	1:F:200:THR:N	2.83	0.41
1:G:225:ASP:C	1:G:225:ASP:OD1	2.58	0.41
1:E:38:TYR:N	1:E:39:PRO:HD2	2.35	0.41
1:F:16:LEU:CD1	1:F:25:LYS:HG3	2.50	0.41
1:H:192:SER:HB2	1:H:193:PRO:CD	2.50	0.41
1:B:16:LEU:HD11	1:B:25:LYS:CD	2.50	0.41
1:E:33:LYS:NZ	1:E:250:VAL:O	2.33	0.41
1:A:86:ASP:OD1	1:A:86:ASP:N	2.53	0.41
1:D:84:SER:HA	1:D:85:PRO:HD3	1.83	0.41
1:E:81:VAL:HG12	1:E:83:PRO:HD3	2.02	0.41
1:G:86:ASP:N	1:G:86:ASP:OD1	2.51	0.41
1:A:16:LEU:HA	1:A:229:HIS:CE1	2.55	0.41
1:C:93:LEU:O	1:C:94:ILE:C	2.55	0.41
1:D:116:HIS:O	1:D:117:ASP:HB2	2.19	0.41
1:F:18:PRO:HB3	1:F:21:LEU:CD1	2.49	0.41
1:F:117:ASP:C	1:F:119:HIS:N	2.73	0.41
1:F:246:GLN:O	1:G:138:HIS:ND1	2.54	0.41
1:H:199:ILE:HD12	1:H:199:ILE:HA	1.84	0.41
1:C:84:SER:HA	1:C:85:PRO:HD3	1.87	0.41
1:G:38:TYR:HB2	1:G:39:PRO:CD	2.51	0.41
1:H:16:LEU:O	1:H:19:ALA:HB3	2.21	0.41
1:B:148:VAL:HB	1:B:159:LEU:HD23	2.03	0.41
1:B:273:ALA:HB3	1:B:274:PRO:CD	2.40	0.41
1:C:23:ILE:CG1	1:D:23:ILE:HG12	2.51	0.41
1:F:54:ILE:HA	1:F:80:ALA:O	2.21	0.41
1:F:150:PHE:HA	1:F:155:LYS:O	2.20	0.41
1:F:192:SER:HB2	1:F:193:PRO:CD	2.50	0.41
1:F:122:LEU:HD23	1:F:122:LEU:HA	1.89	0.41
1:G:251:ALA:O	1:G:253:PRO:HD3	2.20	0.41
1:B:122:LEU:HD23	1:B:122:LEU:HA	1.90	0.41
1:C:141:ASP:HB3	1:C:143:GLU:OE2	2.21	0.41
1:C:199:ILE:CG2	1:C:200:THR:N	2.84	0.41
1:D:18:PRO:HB2	1:D:21:LEU:CD1	2.32	0.41
1:D:49:ARG:HD2	1:D:262:TRP:CE2	2.56	0.41
1:D:129:GLN:C	1:D:130:THR:HG22	2.40	0.41
1:E:24:SER:HB2	1:E:59:ASP:OD2	2.21	0.41
1:G:192:SER:HB2	1:G:193:PRO:CD	2.50	0.41
1:G:232:LEU:O	1:G:232:LEU:HD12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:152:GLN:H	1:H:152:GLN:HG2	1.52	0.41
1:H:237:GLN:HE21	1:H:237:GLN:HB3	1.57	0.41
1:C:242:LEU:HD23	1:C:242:LEU:HA	1.94	0.41
1:H:81:VAL:CG1	1:H:82:GLN:N	2.84	0.41
1:A:23:ILE:HG12	1:B:23:ILE:HG12	2.03	0.40
1:A:93:LEU:O	1:A:94:ILE:C	2.57	0.40
1:A:287:LEU:HD23	1:A:287:LEU:HA	1.87	0.40
1:B:179:ASP:C	1:B:179:ASP:OD1	2.58	0.40
1:D:251:ALA:O	1:D:253:PRO:HD3	2.20	0.40
1:E:21:LEU:HD23	1:E:21:LEU:HA	1.88	0.40
1:G:118:PHE:CE2	1:G:122:LEU:HD11	2.56	0.40
1:H:64:GLN:HG3	1:H:79:TYR:CE1	2.55	0.40
1:B:16:LEU:HD12	1:B:25:LYS:HD3	2.03	0.40
1:A:111:ASN:N	1:A:111:ASN:HD22	2.19	0.40
1:A:173:THR:HG22	1:A:223:TRP:CE3	2.57	0.40
1:B:33:LYS:NZ	1:B:250:VAL:O	2.30	0.40
1:C:86:ASP:OD1	1:C:86:ASP:N	2.54	0.40
1:D:232:LEU:HD12	1:D:232:LEU:O	2.21	0.40
1:C:38:TYR:N	1:C:39:PRO:HD2	2.36	0.40
1:G:31:TYR:OH	1:H:230:ASP:OD1	2.32	0.40
1:C:179:ASP:OD1	1:C:179:ASP:C	2.59	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:GLU:OE1	1:G:180:GLN:NE2[1_556]	2.09	0.11

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	290/293 (99%)	281 (97%)	7 (2%)	2 (1%)	19	48
1	B	290/293 (99%)	278 (96%)	10 (3%)	2 (1%)	19	48
1	C	290/293 (99%)	276 (95%)	8 (3%)	6 (2%)	5	20
1	D	290/293 (99%)	280 (97%)	8 (3%)	2 (1%)	19	48
1	E	290/293 (99%)	273 (94%)	12 (4%)	5 (2%)	7	26
1	F	290/293 (99%)	279 (96%)	9 (3%)	2 (1%)	19	48
1	G	290/293 (99%)	281 (97%)	6 (2%)	3 (1%)	13	39
1	H	290/293 (99%)	279 (96%)	8 (3%)	3 (1%)	13	39
All	All	2320/2344 (99%)	2227 (96%)	68 (3%)	25 (1%)	12	37

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	16	LEU
1	C	194	ARG
1	E	12	SER
1	B	194	ARG
1	D	194	ARG
1	E	194	ARG
1	G	11	GLY
1	A	194	ARG
1	B	31	TYR
1	E	31	TYR
1	G	194	ARG
1	H	194	ARG
1	A	31	TYR
1	C	15	ARG
1	C	31	TYR
1	F	14	THR
1	G	31	TYR
1	H	31	TYR
1	C	12	SER
1	F	31	TYR
1	H	21	LEU
1	C	14	THR
1	D	31	TYR
1	E	14	THR
1	E	85	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	239/236 (101%)	230 (96%)	9 (4%)	28	62
1	B	239/236 (101%)	228 (95%)	11 (5%)	23	55
1	C	239/236 (101%)	230 (96%)	9 (4%)	28	62
1	D	239/236 (101%)	230 (96%)	9 (4%)	28	62
1	E	239/236 (101%)	230 (96%)	9 (4%)	28	62
1	F	239/236 (101%)	232 (97%)	7 (3%)	37	71
1	G	239/236 (101%)	231 (97%)	8 (3%)	33	67
1	H	239/236 (101%)	233 (98%)	6 (2%)	42	75
All	All	1912/1888 (101%)	1844 (96%)	68 (4%)	30	64

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	THR
1	A	33	LYS
1	A	58	GLN
1	A	111	ASN
1	A	119	HIS
1	A	126	SER
1	A	152	GLN
1	A	225	ASP
1	A	270	LYS
1	B	14	THR
1	B	15	ARG
1	B	20	THR
1	B	23	ILE
1	B	33	LYS
1	B	58	GLN
1	B	85	PRO
1	B	111	ASN
1	B	119	HIS
1	B	133	SER

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Mol	Chain	Res	Type
1	B	225	ASP
1	C	14	THR
1	C	26	GLN
1	C	33	LYS
1	C	111	ASN
1	C	119	HIS
1	C	130	THR
1	C	141	ASP
1	C	155	LYS
1	C	225	ASP
1	D	16	LEU
1	D	33	LYS
1	D	58	GLN
1	D	111	ASN
1	D	119	HIS
1	D	130	THR
1	D	155	LYS
1	D	225	ASP
1	D	252	CYS
1	E	12	SER
1	E	33	LYS
1	E	58	GLN
1	E	86	ASP
1	E	111	ASN
1	E	119	HIS
1	E	130	THR
1	E	155	LYS
1	E	225	ASP
1	F	14	THR
1	F	33	LYS
1	F	55	SER
1	F	58	GLN
1	F	111	ASN
1	F	119	HIS
1	F	225	ASP
1	G	14	THR
1	G	18	PRO
1	G	23	ILE
1	G	33	LYS
1	G	111	ASN
1	G	119	HIS
1	G	225	ASP

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Mol	Chain	Res	Type
1	G	270	LYS
1	H	14	THR
1	H	33	LYS
1	H	58	GLN
1	H	111	ASN
1	H	126	SER
1	H	225	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	HIS
1	A	229	HIS
1	B	119	HIS
1	C	17	HIS
1	C	26	GLN
1	C	65	GLN
1	C	119	HIS
1	D	119	HIS
1	E	119	HIS
1	F	17	HIS
1	F	65	GLN
1	F	119	HIS
1	G	65	GLN
1	G	119	HIS
1	H	17	HIS
1	H	229	HIS
1	H	237	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

21 ligands 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
2	G1P	H	507	-	15,16,16	1.96	4 (26%)	24,24,24	3.83	5 (20%)
3	SO4	C	602	-	4,4,4	0.36	0	6,6,6	0.26	0
3	SO4	E	604	-	4,4,4	0.25	0	6,6,6	1.30	1 (16%)
2	G1P	F	505	-	15,16,16	2.10	3 (20%)	24,24,24	4.54	8 (33%)
3	SO4	F	611	-	4,4,4	0.32	0	6,6,6	0.76	0
2	G1P	D	503	-	15,16,16	2.03	3 (20%)	24,24,24	4.18	8 (33%)
3	SO4	F	605	-	4,4,4	0.27	0	6,6,6	1.04	0
2	G1P	C	502	-	15,16,16	2.11	3 (20%)	24,24,24	3.50	8 (33%)
3	SO4	G	606	-	4,4,4	0.26	0	6,6,6	1.00	0
3	SO4	D	603	-	4,4,4	0.29	0	6,6,6	1.01	0
2	G1P	A	500	-	15,16,16	2.09	4 (26%)	24,24,24	3.95	8 (33%)
3	SO4	B	601	-	4,4,4	0.26	0	6,6,6	0.77	0
3	SO4	G	612	-	4,4,4	0.33	0	6,6,6	0.45	0
2	G1P	B	501	-	15,16,16	2.00	3 (20%)	24,24,24	4.64	6 (25%)
2	G1P	G	506	-	15,16,16	2.07	3 (20%)	24,24,24	3.67	5 (20%)
3	SO4	A	600	-	4,4,4	0.14	0	6,6,6	1.02	0
3	SO4	D	608	-	4,4,4	0.46	0	6,6,6	0.46	0
3	SO4	F	610	-	4,4,4	0.33	0	6,6,6	0.96	1 (16%)
2	G1P	E	504	-	15,16,16	2.08	3 (20%)	24,24,24	4.48	11 (45%)
3	SO4	H	607	-	4,4,4	0.23	0	6,6,6	0.60	0
3	SO4	E	609	-	4,4,4	0.56	0	6,6,6	0.21	0

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
2	G1P	G	506	-	-	0/7/27/27	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	G1P	E	504	-	-	0/7/27/27	0/1/1/1
2	G1P	C	502	-	-	0/7/27/27	0/1/1/1
2	G1P	F	505	-	-	0/7/27/27	0/1/1/1
2	G1P	B	501	-	-	0/7/27/27	0/1/1/1
2	G1P	H	507	-	-	0/7/27/27	0/1/1/1
2	G1P	D	503	-	-	0/7/27/27	0/1/1/1
2	G1P	A	500	-	-	0/7/27/27	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	504	G1P	P-O3P	4.87	1.72	1.54
2	C	502	G1P	P-O3P	4.65	1.72	1.54
2	C	502	G1P	P-O2P	4.63	1.72	1.54
2	D	503	G1P	P-O2P	4.60	1.71	1.54
2	F	505	G1P	P-O3P	4.58	1.71	1.54
2	A	500	G1P	P-O1P	4.57	1.64	1.50
2	F	505	G1P	P-O2P	4.43	1.71	1.54
2	G	506	G1P	P-O2P	4.37	1.71	1.54
2	C	502	G1P	P-O1P	4.36	1.64	1.50
2	E	504	G1P	P-O2P	4.34	1.70	1.54
2	B	501	G1P	P-O2P	4.34	1.70	1.54
2	G	506	G1P	P-O1P	4.33	1.64	1.50
2	B	501	G1P	P-O1P	4.27	1.63	1.50
2	F	505	G1P	P-O1P	4.25	1.63	1.50
2	G	506	G1P	P-O3P	4.23	1.70	1.54
2	H	507	G1P	P-O1P	4.19	1.63	1.50
2	D	503	G1P	P-O3P	4.19	1.70	1.54
2	B	501	G1P	P-O3P	4.17	1.70	1.54
2	A	500	G1P	P-O3P	4.14	1.70	1.54
2	H	507	G1P	P-O3P	4.07	1.69	1.54
2	D	503	G1P	P-O1P	4.01	1.62	1.50
2	A	500	G1P	P-O2P	3.96	1.69	1.54
2	E	504	G1P	P-O1P	3.79	1.62	1.50
2	H	507	G1P	P-O2P	3.65	1.68	1.54
2	H	507	G1P	P-O1	2.22	1.63	1.59
2	A	500	G1P	P-O1	2.00	1.63	1.59

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	G1P	O5-C1-O1	-20.37	84.74	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	505	G1P	O5-C1-O1	-19.05	86.47	111.36
2	E	504	G1P	O5-C1-O1	-18.54	87.13	111.36
2	D	503	G1P	O5-C1-O1	-17.22	88.86	111.36
2	A	500	G1P	O5-C1-O1	-16.53	89.76	111.36
2	H	507	G1P	O5-C1-O1	-16.52	89.77	111.36
2	G	506	G1P	O5-C1-O1	-15.70	90.85	111.36
2	C	502	G1P	O5-C1-O1	-13.73	93.42	111.36
2	D	503	G1P	O5-C1-C2	5.48	121.64	110.37
2	F	505	G1P	O5-C1-C2	5.45	121.57	110.37
2	A	500	G1P	O5-C1-C2	5.42	121.50	110.37
2	B	501	G1P	O5-C1-C2	4.88	120.41	110.37
2	E	504	G1P	O2-C2-C3	-4.87	98.90	110.38
2	E	504	G1P	O5-C1-C2	4.87	120.37	110.37
2	F	505	G1P	O3-C3-C2	-4.83	99.00	110.38
2	G	506	G1P	O5-C1-C2	4.76	120.15	110.37
2	H	507	G1P	O5-C1-C2	4.74	120.11	110.37
2	B	501	G1P	C1-O5-C5	4.74	122.98	113.72
2	A	500	G1P	P-O1-C1	-4.71	110.92	123.54
2	D	503	G1P	P-O1-C1	-4.66	111.04	123.54
2	G	506	G1P	P-O1-C1	-4.44	111.62	123.54
2	C	502	G1P	O2-C2-C3	-4.36	100.09	110.38
2	F	505	G1P	O2-C2-C3	-4.33	100.16	110.38
2	C	502	G1P	O5-C5-C4	4.27	117.40	109.70
2	E	504	G1P	C1-O5-C5	4.25	122.03	113.72
2	H	507	G1P	P-O1-C1	-4.25	112.13	123.54
2	H	507	G1P	C1-O5-C5	4.21	121.94	113.72
2	B	501	G1P	P-O1-C1	-4.19	112.30	123.54
2	C	502	G1P	P-O1-C1	-3.97	112.88	123.54
2	C	502	G1P	O5-C1-C2	3.87	118.32	110.37
2	B	501	G1P	O1-C1-C2	-3.84	101.35	108.38
2	E	504	G1P	O3-C3-C2	-3.70	101.64	110.38
2	D	503	G1P	C4-C3-C2	-3.68	104.37	110.83
2	F	505	G1P	O5-C5-C4	3.62	116.23	109.70
2	F	505	G1P	O1-C1-C2	-3.57	101.85	108.38
2	G	506	G1P	C1-O5-C5	3.56	120.67	113.72
2	D	503	G1P	O2-C2-C3	-3.49	102.16	110.38
2	D	503	G1P	O5-C5-C4	3.48	115.96	109.70
2	E	504	G1P	P-O1-C1	-3.38	114.47	123.54
2	F	505	G1P	C1-O5-C5	3.11	119.79	113.72
2	D	503	G1P	O3-C3-C2	-3.09	103.09	110.38
2	A	500	G1P	C1-O5-C5	3.04	119.65	113.72
2	E	504	G1P	O2-C2-C1	2.74	116.61	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	504	G1P	C4-C3-C2	-2.68	106.13	110.83
2	C	502	G1P	C4-C3-C2	-2.65	106.18	110.83
2	C	502	G1P	C1-O5-C5	2.58	118.76	113.72
2	G	506	G1P	C4-C3-C2	-2.53	106.40	110.83
2	A	500	G1P	C4-C3-C2	-2.51	106.42	110.83
2	C	502	G1P	O1-C1-C2	-2.49	103.82	108.38
2	E	504	G1P	O4-C4-C3	2.46	116.19	110.38
2	E	504	G1P	O1-C1-C2	-2.46	103.87	108.38
2	F	505	G1P	O3-C3-C4	2.29	115.78	110.38
2	D	503	G1P	O2-C2-C1	2.29	115.53	110.08
2	A	500	G1P	O4-C4-C5	-2.25	103.79	109.32
2	H	507	G1P	O2P-P-O1P	-2.20	102.26	110.83
2	B	501	G1P	O5-C5-C4	2.18	113.62	109.70
2	A	500	G1P	O2P-P-O1P	-2.16	102.43	110.83
2	A	500	G1P	O3-C3-C2	-2.14	105.33	110.38
3	E	604	SO4	O3-S-O1	2.11	120.61	109.56
2	E	504	G1P	O4-C4-C5	-2.05	104.27	109.32
3	F	610	SO4	O4-S-O2	2.03	120.17	109.56

There are no chirality outliers.

There are no torsion outliers.

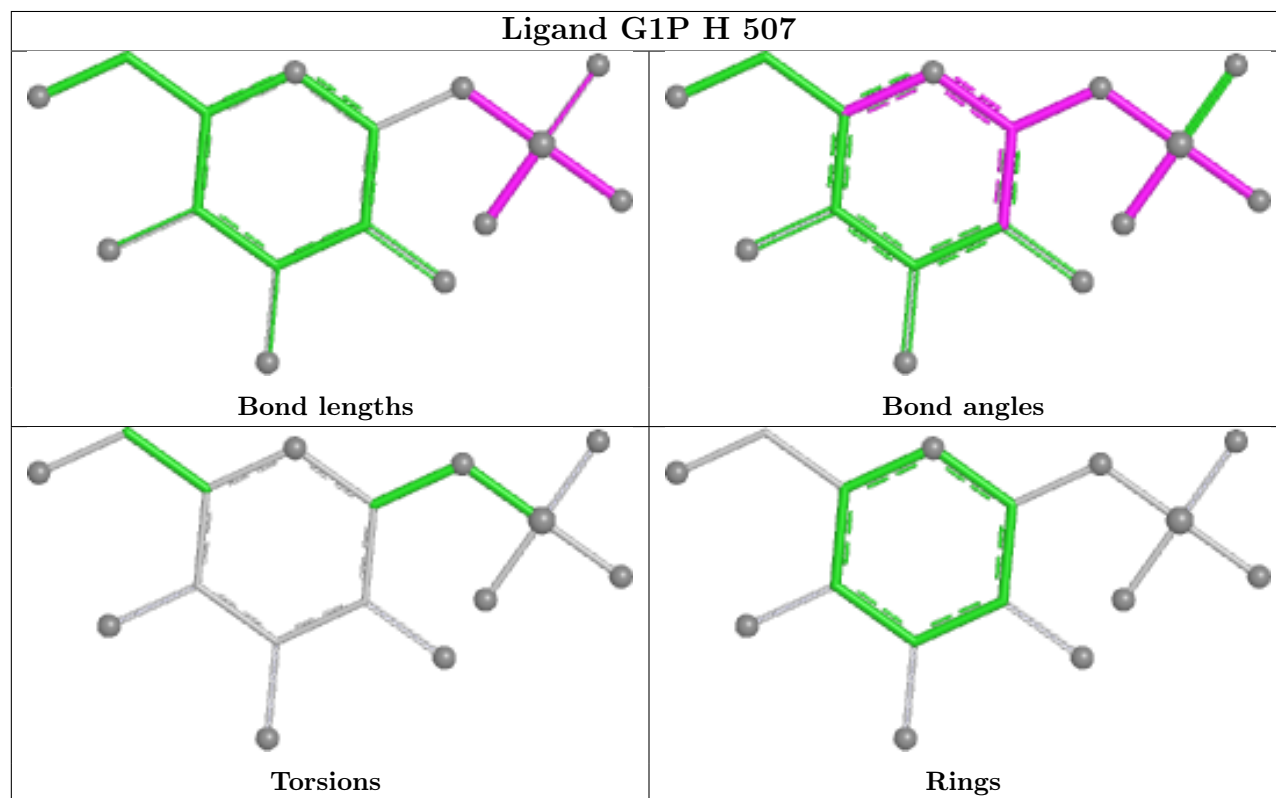
There are no ring outliers.

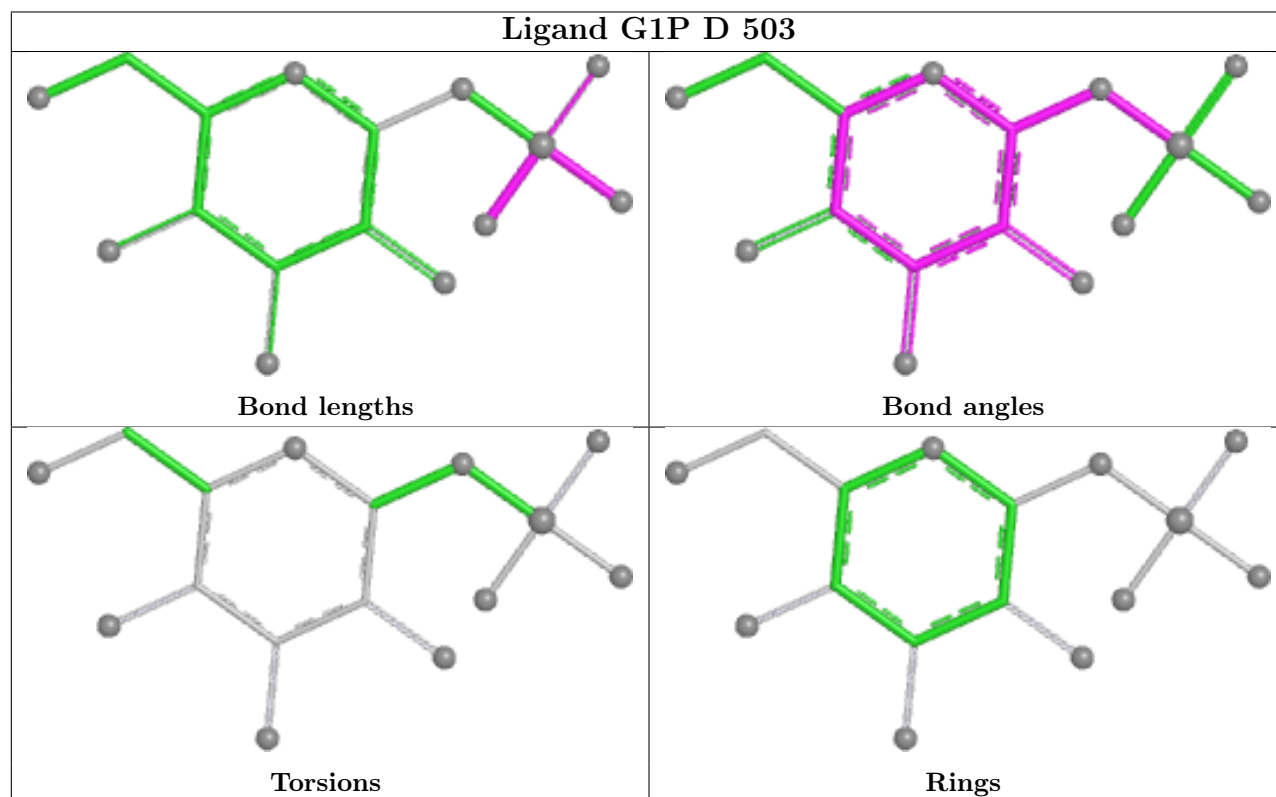
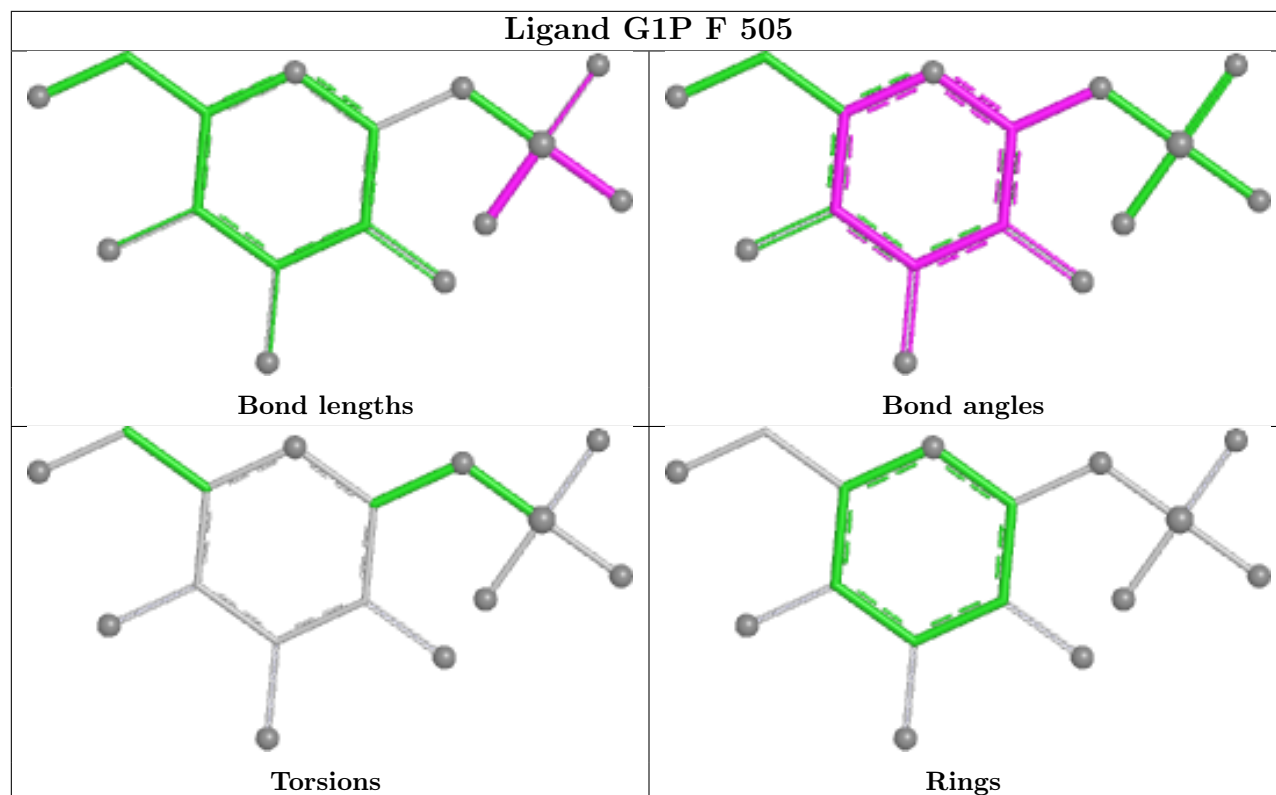
10 monomers are involved in 10 short contacts:

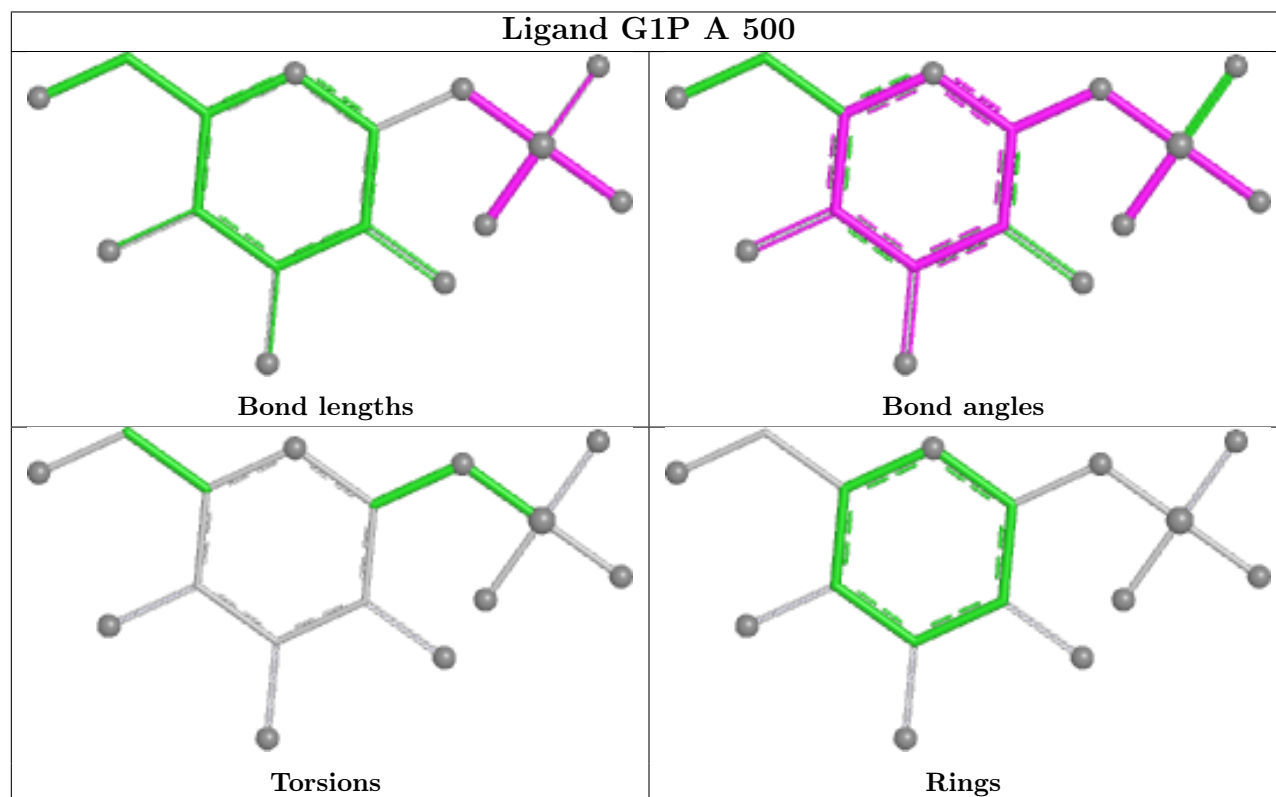
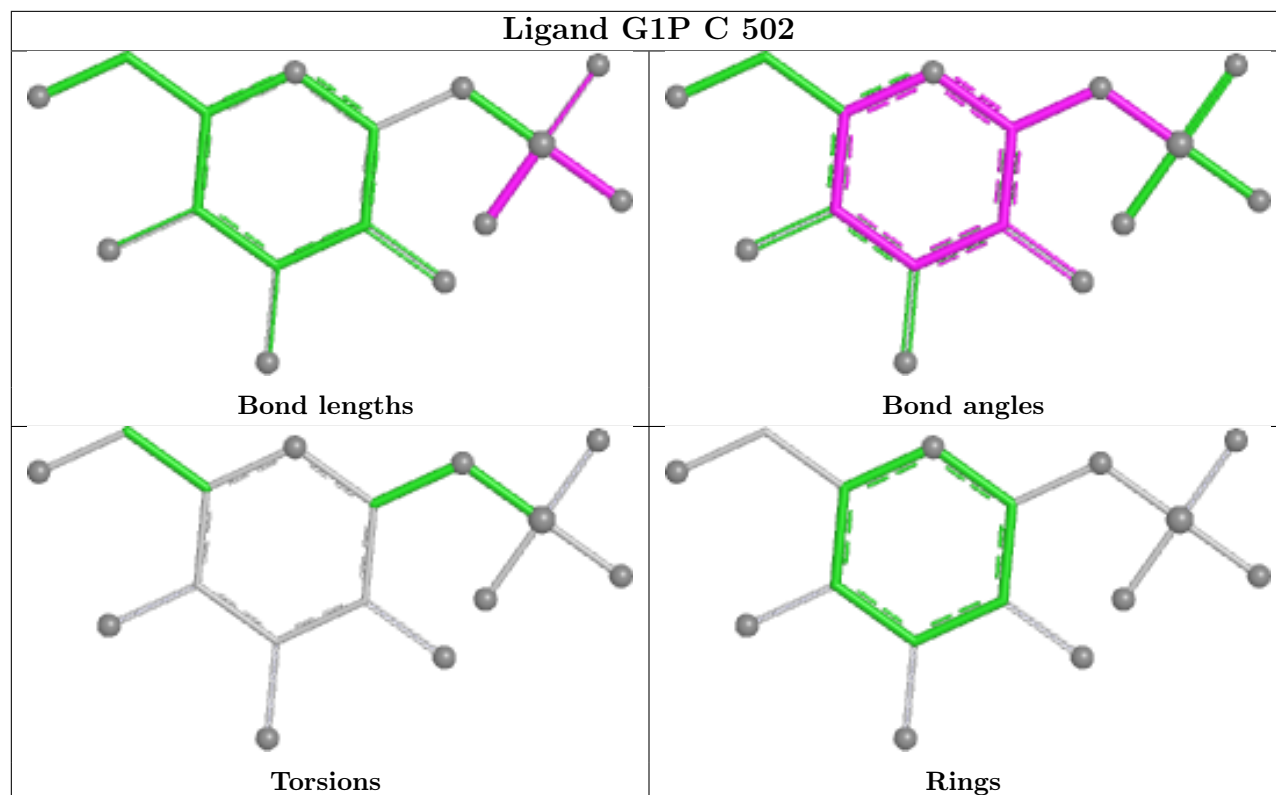
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	507	G1P	1	0
2	F	505	G1P	1	0
2	D	503	G1P	1	0
2	C	502	G1P	1	0
2	A	500	G1P	1	0
2	B	501	G1P	1	0
2	G	506	G1P	1	0
3	D	608	SO4	1	0
3	F	610	SO4	1	0
2	E	504	G1P	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

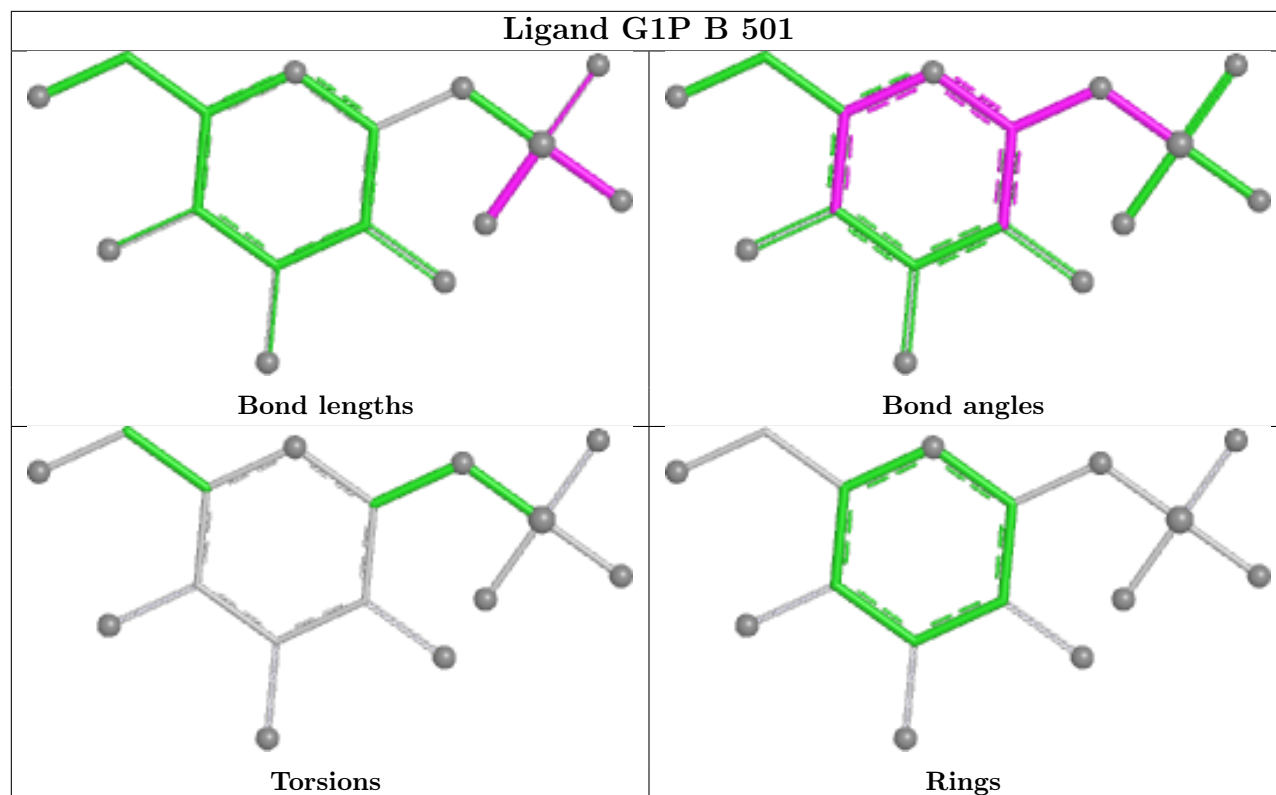
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



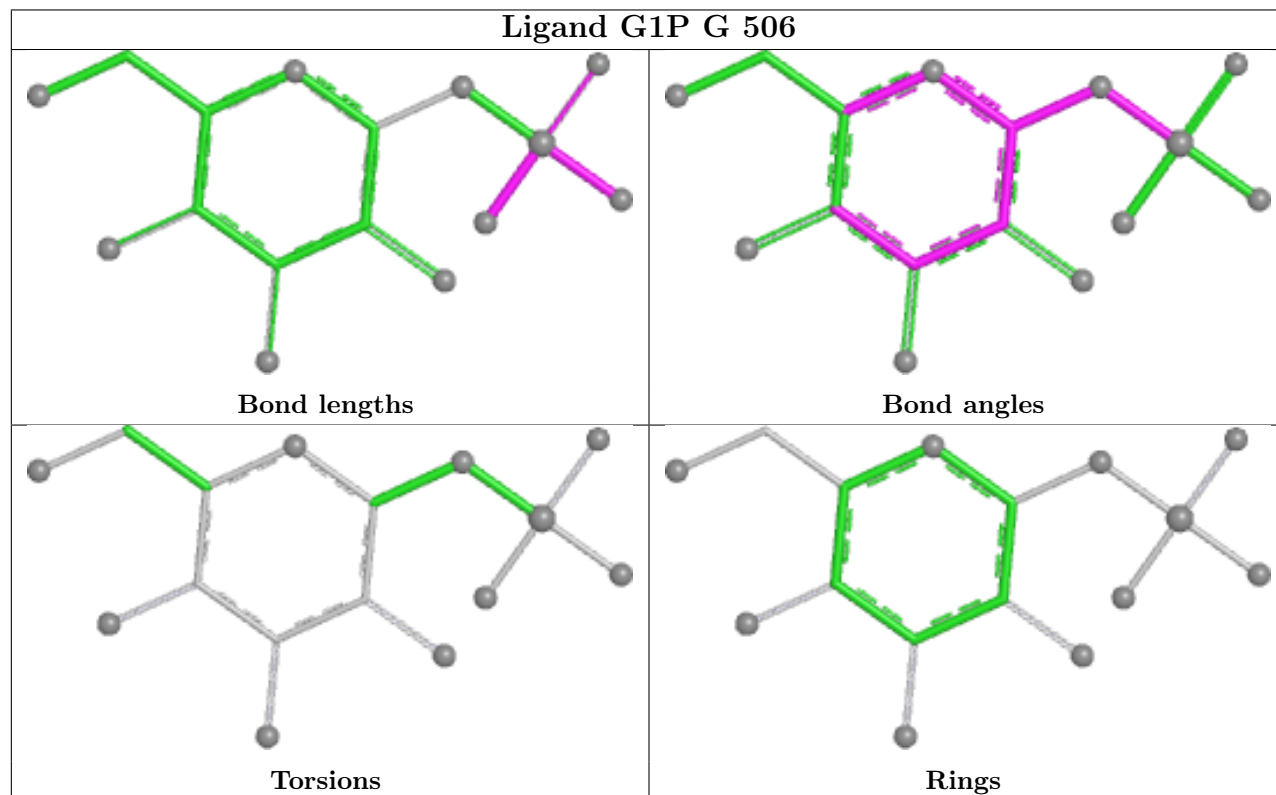


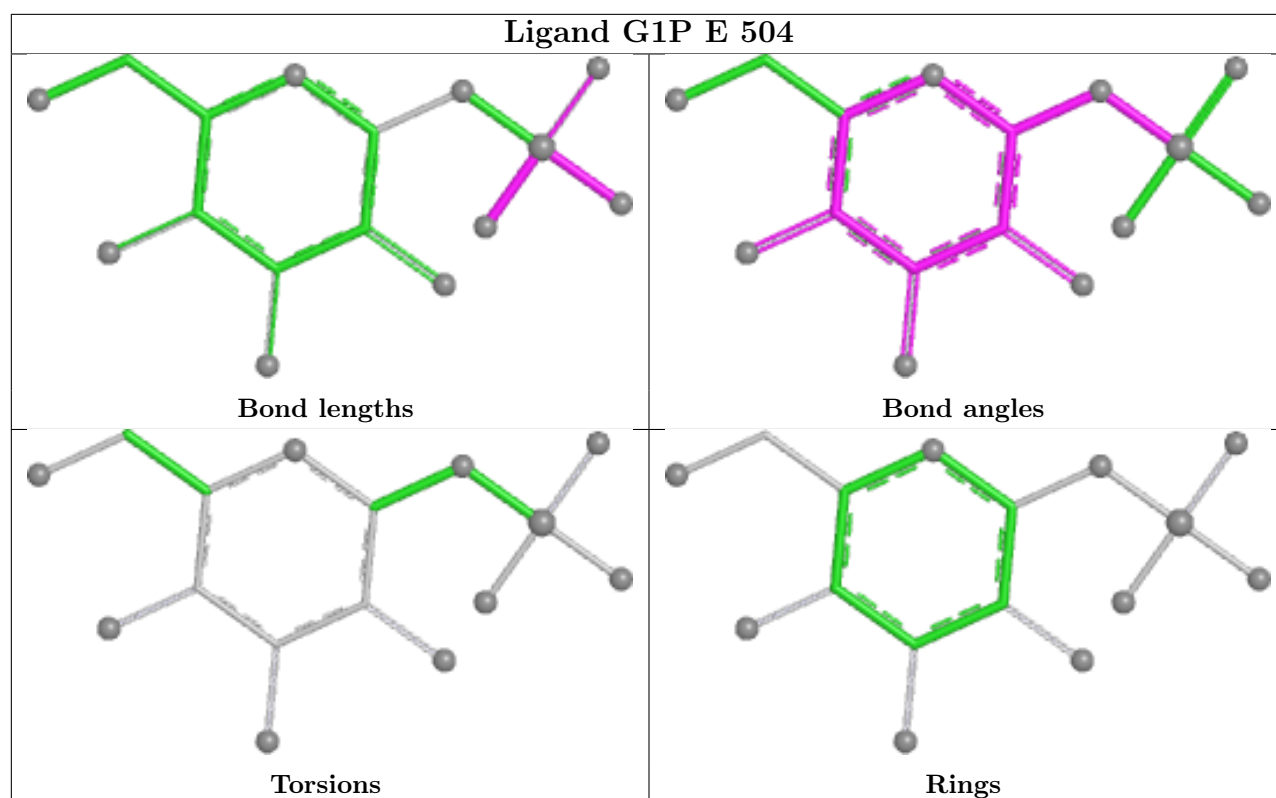


Ligand G1P B 501



Ligand G1P G 506





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	289/293 (98%)	-0.07	6 (2%) 63 55	11, 27, 53, 69	0
1	B	289/293 (98%)	-0.10	9 (3%) 51 43	11, 27, 51, 69	0
1	C	289/293 (98%)	-0.11	6 (2%) 63 55	11, 27, 52, 69	0
1	D	289/293 (98%)	-0.02	13 (4%) 39 31	11, 27, 54, 69	0
1	E	289/293 (98%)	0.11	22 (7%) 21 16	11, 27, 54, 69	0
1	F	289/293 (98%)	0.16	20 (6%) 24 18	11, 27, 50, 69	0
1	G	289/293 (98%)	0.11	16 (5%) 32 25	11, 27, 54, 69	0
1	H	289/293 (98%)	-0.13	6 (2%) 63 55	11, 27, 49, 69	0
All	All	2312/2344 (98%)	-0.01	98 (4%) 41 33	11, 27, 52, 69	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	194	ARG	6.3
1	E	193	PRO	5.2
1	A	13	GLY	5.1
1	F	84	SER	5.1
1	G	13	GLY	4.7
1	G	11	GLY	4.6
1	E	195	GLY	4.6
1	D	127	GLN	4.5
1	D	194	ARG	4.5
1	D	13	GLY	4.4
1	F	60	THR	4.0
1	C	127	GLN	4.0
1	G	15	ARG	4.0
1	E	12	SER	3.9
1	G	18	PRO	3.8
1	D	15	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	155	LYS	3.7
1	E	13	GLY	3.6
1	B	11	GLY	3.5
1	D	14	THR	3.4
1	E	190	LYS	3.3
1	H	23	ILE	3.3
1	C	13	GLY	3.3
1	A	22	ALA	3.3
1	G	23	ILE	3.3
1	B	12	SER	3.2
1	C	12	SER	3.2
1	D	16	LEU	3.2
1	F	194	ARG	3.1
1	G	12	SER	3.0
1	D	192	SER	3.0
1	G	16	LEU	2.9
1	G	14	THR	2.9
1	G	22	ALA	2.9
1	D	12	SER	2.9
1	G	119	HIS	2.9
1	E	82	GLN	2.8
1	E	15	ARG	2.8
1	D	23	ILE	2.8
1	A	12	SER	2.7
1	E	16	LEU	2.7
1	F	192	SER	2.7
1	H	12	SER	2.7
1	D	119	HIS	2.7
1	H	278	ASN	2.7
1	F	127	GLN	2.7
1	E	119	HIS	2.7
1	F	119	HIS	2.7
1	E	192	SER	2.6
1	B	13	GLY	2.6
1	E	14	THR	2.6
1	F	155	LYS	2.6
1	B	15	ARG	2.6
1	G	20	THR	2.6
1	F	86	ASP	2.6
1	F	64	GLN	2.6
1	B	119	HIS	2.6
1	F	14	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	84	SER	2.6
1	A	152	GLN	2.5
1	E	196	GLU	2.5
1	H	2	LYS	2.5
1	E	127	GLN	2.5
1	B	18	PRO	2.5
1	H	13	GLY	2.5
1	E	101	ASN	2.4
1	G	2	LYS	2.4
1	F	193	PRO	2.4
1	F	279	GLY	2.4
1	D	22	ALA	2.4
1	C	193	PRO	2.4
1	E	85	PRO	2.4
1	E	11	GLY	2.4
1	E	128	ARG	2.4
1	B	24	SER	2.4
1	E	20	THR	2.4
1	G	17	HIS	2.3
1	D	193	PRO	2.3
1	F	85	PRO	2.3
1	F	87	GLY	2.3
1	A	2	LYS	2.3
1	F	22	ALA	2.3
1	E	84	SER	2.3
1	E	21	LEU	2.3
1	D	17	HIS	2.2
1	F	124	SER	2.2
1	C	14	THR	2.2
1	E	83	PRO	2.2
1	F	57	PRO	2.2
1	F	15	ARG	2.2
1	F	130	THR	2.1
1	A	15	ARG	2.1
1	B	194	ARG	2.1
1	H	282	GLN	2.1
1	G	19	ALA	2.1
1	F	61	PRO	2.1
1	B	23	ILE	2.0
1	G	269	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

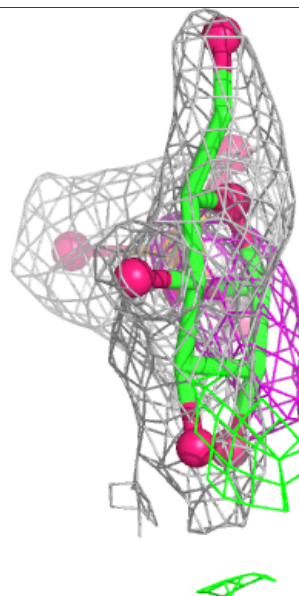
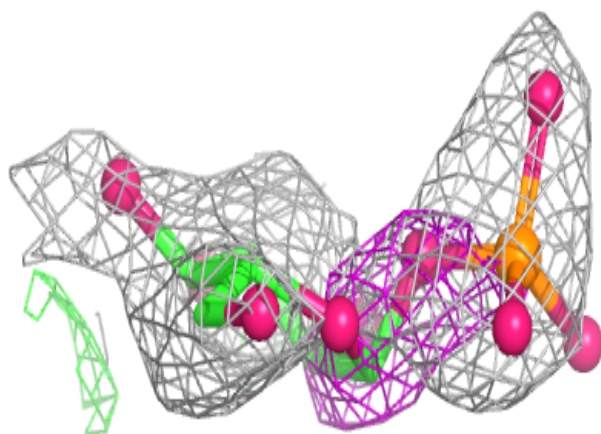
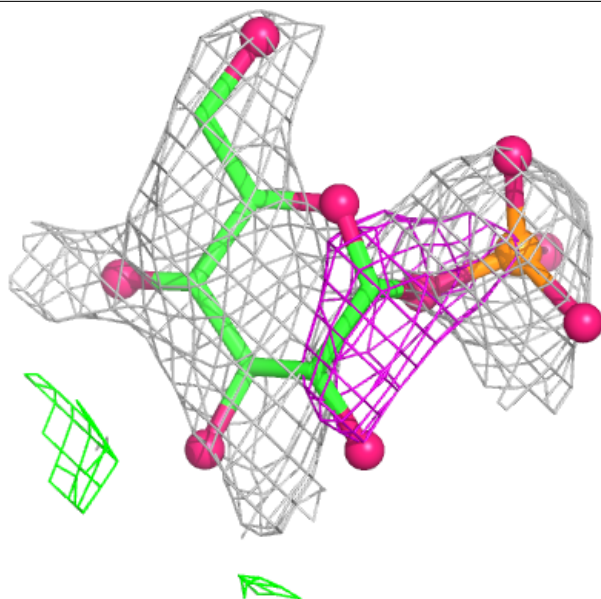
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	G1P	F	505	16/16	0.66	0.17	53,58,62,62	0
3	SO4	E	609	5/5	0.77	0.13	55,56,57,58	0
3	SO4	F	611	5/5	0.82	0.18	62,62,62,63	0
2	G1P	B	501	16/16	0.86	0.16	41,43,44,45	0
2	G1P	H	507	16/16	0.86	0.16	27,30,34,34	0
2	G1P	A	500	16/16	0.89	0.16	26,29,33,33	0
3	SO4	F	610	5/5	0.89	0.16	44,45,47,49	0
2	G1P	D	503	16/16	0.89	0.12	28,35,43,43	0
3	SO4	G	612	5/5	0.89	0.14	46,46,47,48	0
2	G1P	E	504	16/16	0.91	0.15	22,25,29,30	0
2	G1P	C	502	16/16	0.92	0.12	24,26,28,29	0
3	SO4	D	608	5/5	0.92	0.11	47,48,49,49	0
2	G1P	G	506	16/16	0.93	0.14	25,26,28,29	0
3	SO4	E	604	5/5	0.98	0.07	13,17,20,22	0
3	SO4	B	601	5/5	0.98	0.05	16,19,20,23	0
3	SO4	F	605	5/5	0.98	0.08	15,15,17,18	0
3	SO4	C	602	5/5	0.98	0.06	19,19,21,22	0
3	SO4	D	603	5/5	0.98	0.07	13,14,18,19	0
3	SO4	A	600	5/5	0.98	0.05	17,19,20,22	0
3	SO4	H	607	5/5	0.98	0.07	14,15,16,18	0
3	SO4	G	606	5/5	0.99	0.04	11,13,15,16	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.

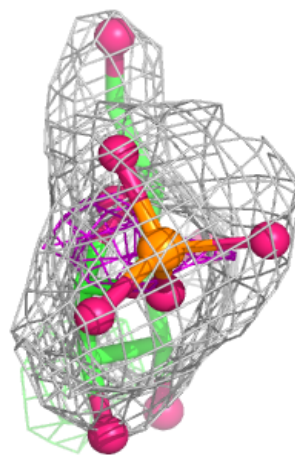
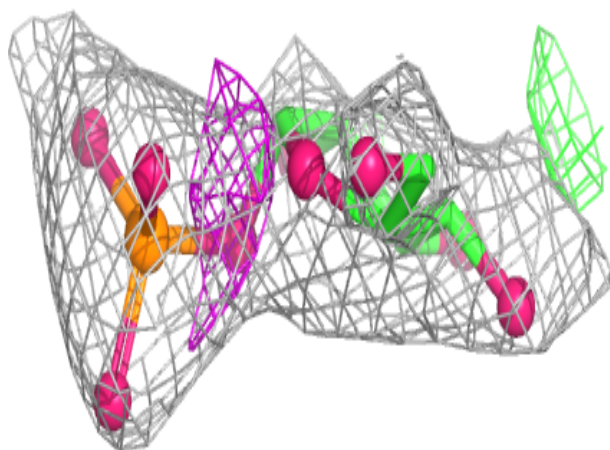
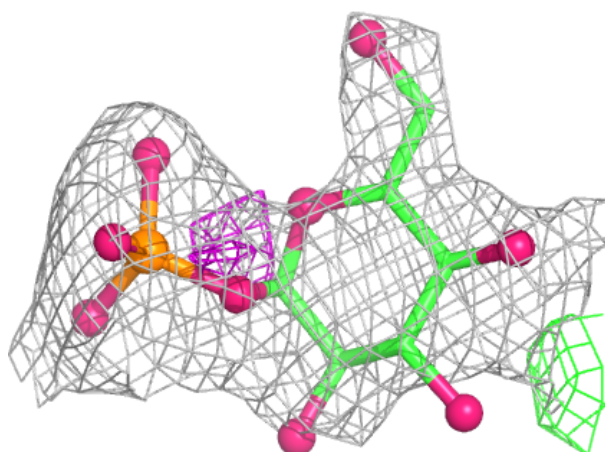
Electron density around G1P F 505:

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



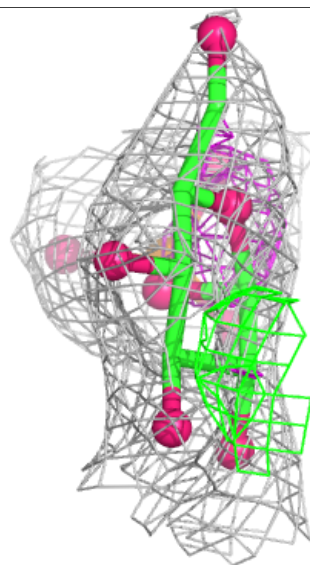
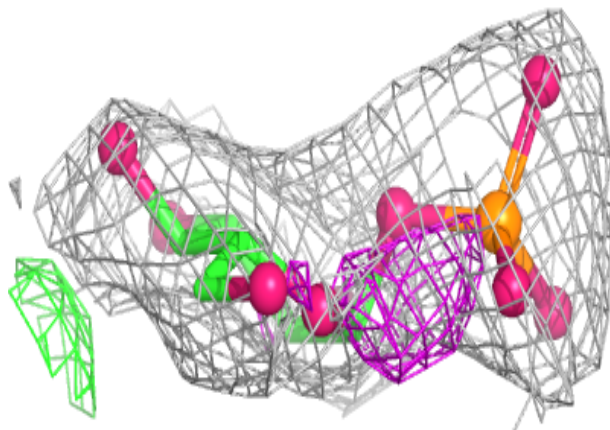
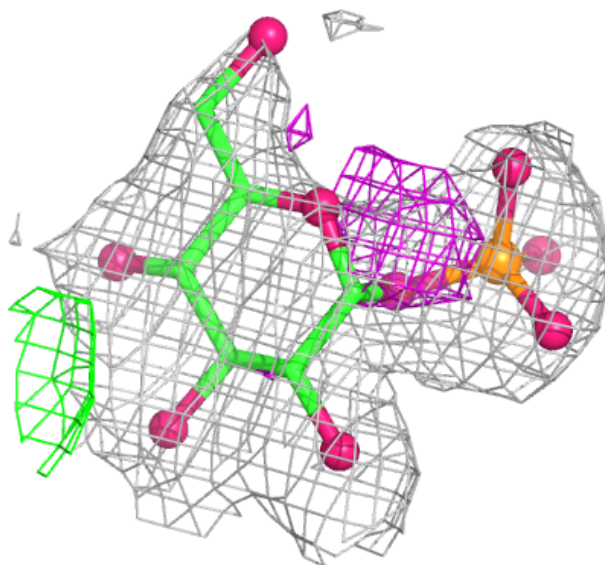
Electron density around G1P B 501:

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



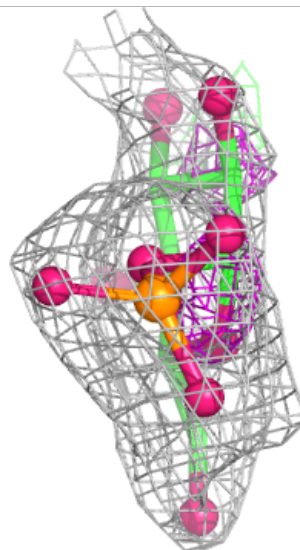
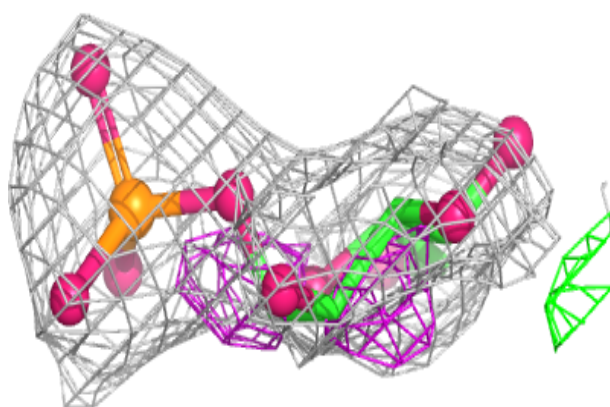
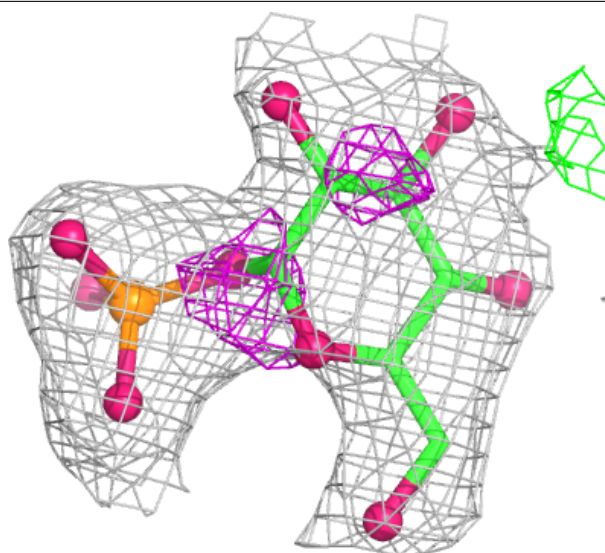
Electron density around G1P H 507:

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



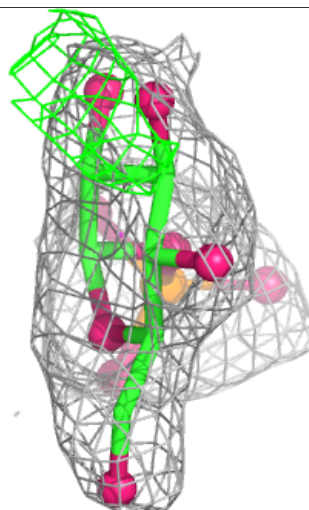
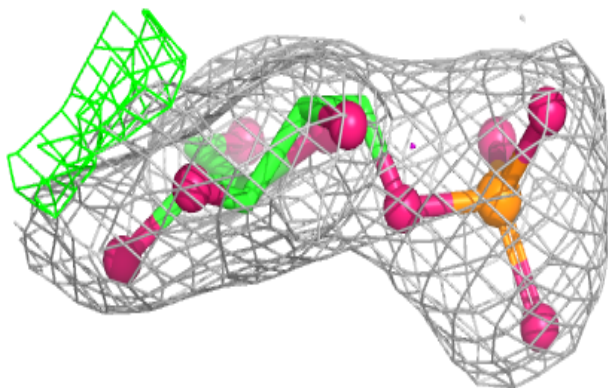
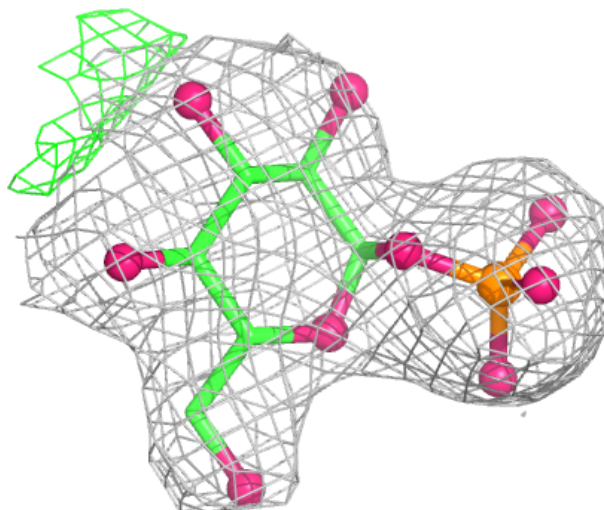
Electron density around G1P A 500:

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



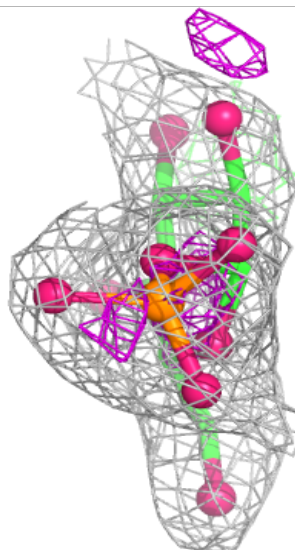
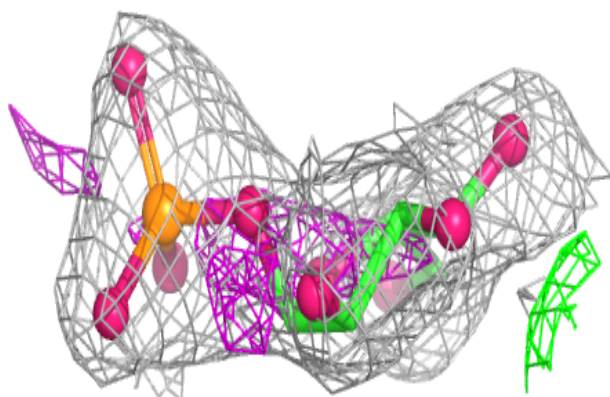
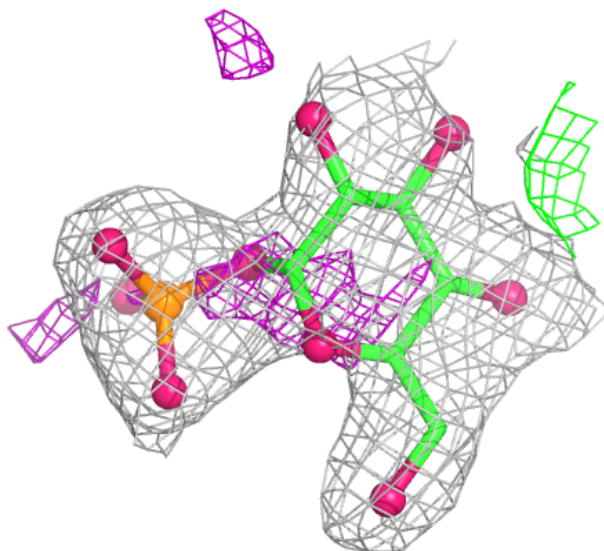
Electron density around G1P D 503:

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



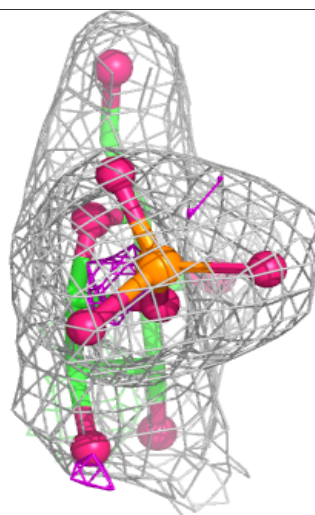
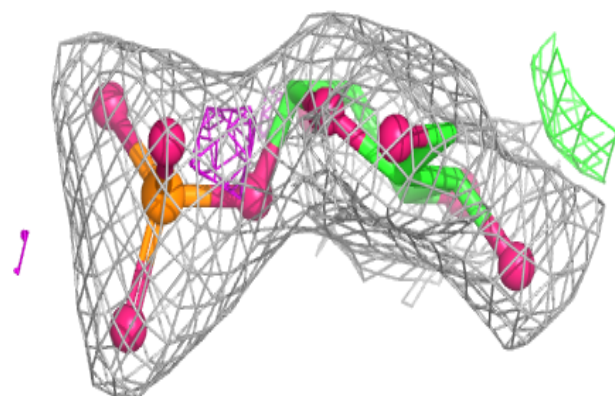
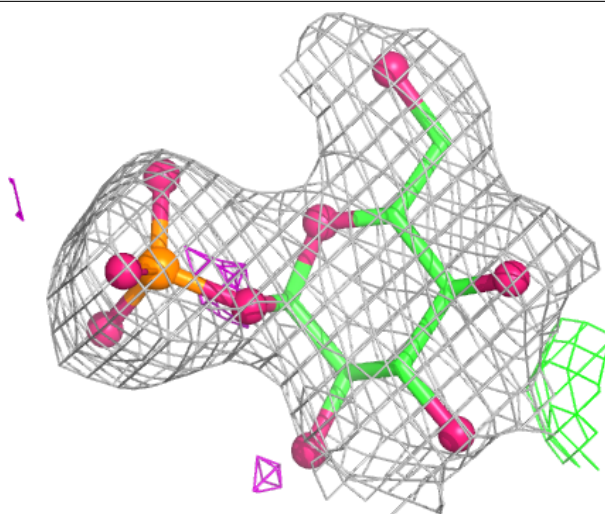
Electron density around G1P E 504:

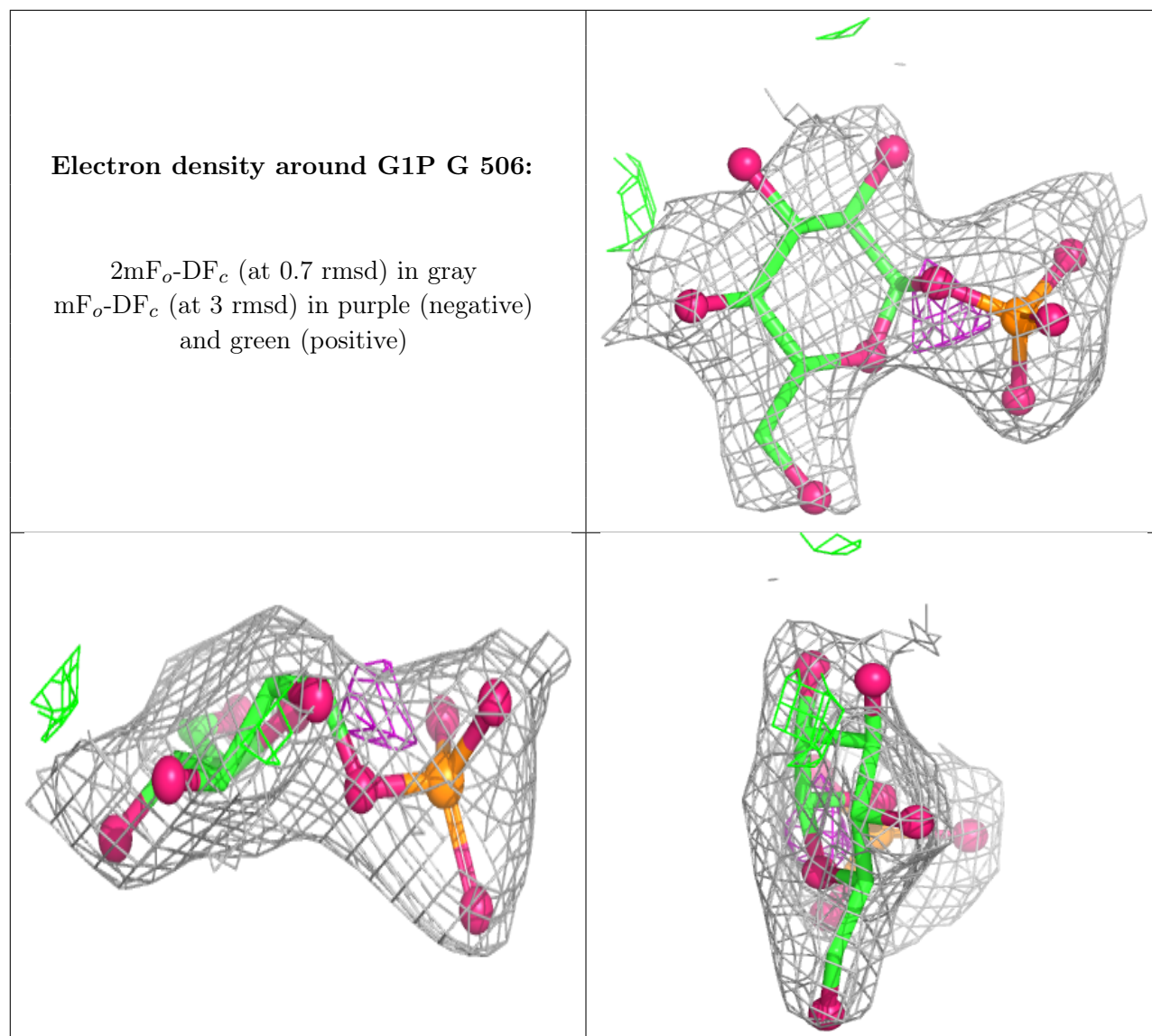
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around G1P C 502:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.