



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:25 AM UTC

PDB ID : 6FNY / pdb_00006fny
Title : CRYSTAL STRUCTURE OF A CHOLINE SULFATASE FROM SINORHIZOBIIUM MELLILOTI
Authors : Valkov, E.; Van Loo, B.; Hollfelder, F.; Hyvonen, M.
Deposited on : 2018-02-05
Resolution : 2.79 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
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

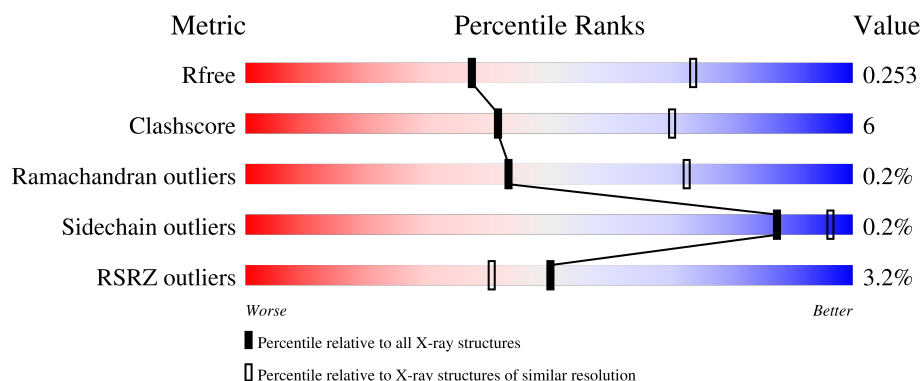
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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	516	2% 86% 14%
1	B	516	3% 84% 15%
1	C	516	4% 85% 14%
1	D	516	3% 83% 15%
1	E	516	3% 83% 16%

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Mol	Chain	Length	Quality of chain
1	F	516	
1	G	516	
1	H	516	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CA	D	601	-	-	-	X
2	CA	E	601	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 34715 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 Choline-sulfatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	515	Total	C	N	O	S	0	1	0
			4148	2619	723	785	21			
1	B	515	Total	C	N	O	S	0	1	0
			4148	2619	723	785	21			
1	C	513	Total	C	N	O	S	0	1	0
			4136	2613	721	781	21			
1	D	510	Total	C	N	O	S	0	1	0
			4115	2599	718	777	21			
1	E	510	Total	C	N	O	S	0	1	0
			4115	2599	718	777	21			
1	F	509	Total	C	N	O	S	0	1	0
			4108	2595	717	775	21			
1	G	509	Total	C	N	O	S	0	1	0
			4108	2595	717	775	21			
1	H	510	Total	C	N	O	S	0	1	0
			4116	2601	718	776	21			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP O69787
A	-1	ASP	-	expression tag	UNP O69787
A	0	PRO	-	expression tag	UNP O69787
A	1	VAL	-	expression tag	UNP O69787
B	-2	GLY	-	expression tag	UNP O69787
B	-1	ASP	-	expression tag	UNP O69787
B	0	PRO	-	expression tag	UNP O69787
B	1	VAL	-	expression tag	UNP O69787
C	-2	GLY	-	expression tag	UNP O69787
C	-1	ASP	-	expression tag	UNP O69787
C	0	PRO	-	expression tag	UNP O69787
C	1	VAL	-	expression tag	UNP O69787
D	-2	GLY	-	expression tag	UNP O69787

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	ASP	-	expression tag	UNP O69787
D	0	PRO	-	expression tag	UNP O69787
D	1	VAL	-	expression tag	UNP O69787
E	-2	GLY	-	expression tag	UNP O69787
E	-1	ASP	-	expression tag	UNP O69787
E	0	PRO	-	expression tag	UNP O69787
E	1	VAL	-	expression tag	UNP O69787
F	-2	GLY	-	expression tag	UNP O69787
F	-1	ASP	-	expression tag	UNP O69787
F	0	PRO	-	expression tag	UNP O69787
F	1	VAL	-	expression tag	UNP O69787
G	-2	GLY	-	expression tag	UNP O69787
G	-1	ASP	-	expression tag	UNP O69787
G	0	PRO	-	expression tag	UNP O69787
G	1	VAL	-	expression tag	UNP O69787
H	-2	GLY	-	expression tag	UNP O69787
H	-1	ASP	-	expression tag	UNP O69787
H	0	PRO	-	expression tag	UNP O69787
H	1	VAL	-	expression tag	UNP O69787

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

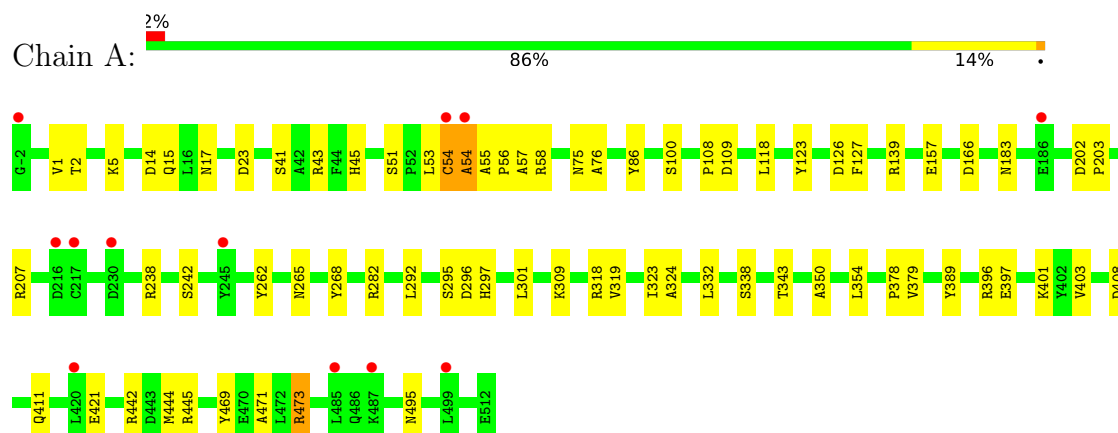
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	172	Total 172	O 172	0	0
3	B	296	Total 296	O 296	0	0
3	C	184	Total 184	O 184	0	0
3	D	218	Total 218	O 218	0	0
3	E	259	Total 259	O 259	0	0
3	F	136	Total 136	O 136	0	0
3	G	169	Total 169	O 169	0	0
3	H	279	Total 279	O 279	0	0

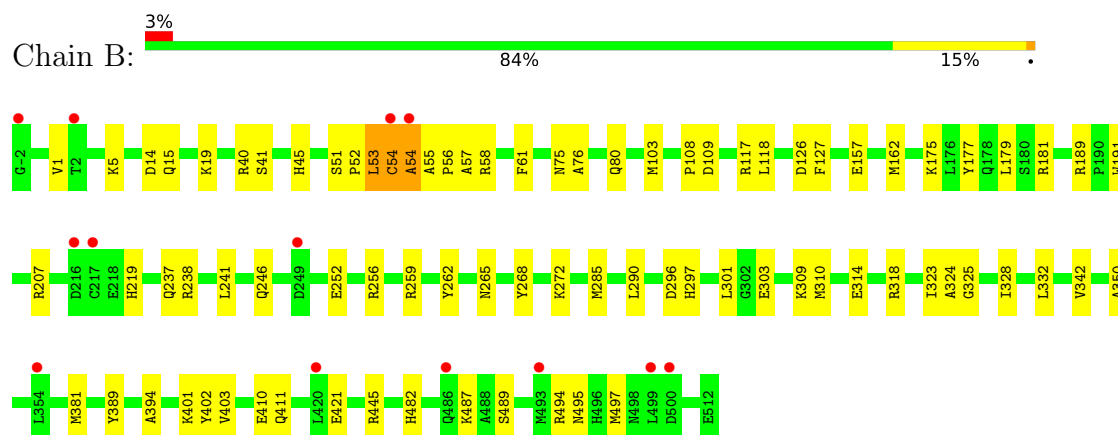
3 Residue-property plots

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

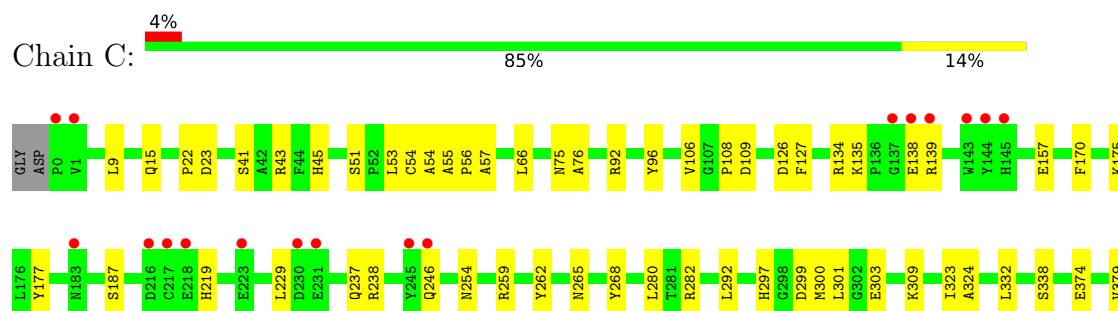
• Molecule 1: Choline-sulfatase



• Molecule 1: Choline-sulfatase

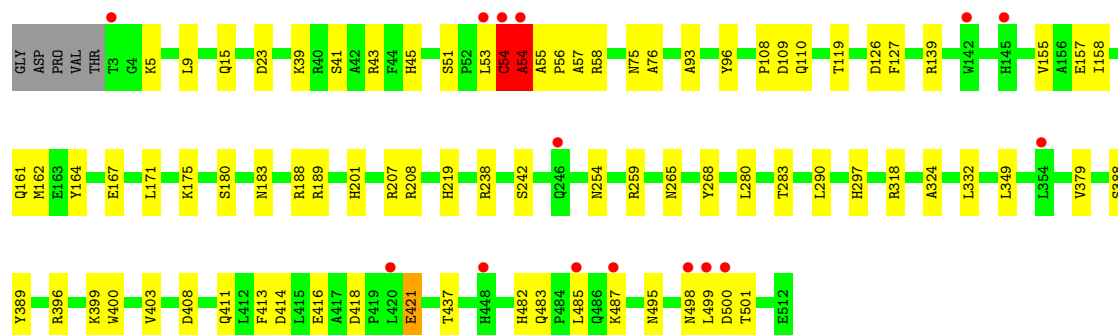
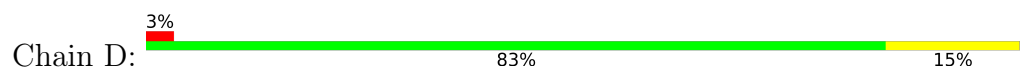


• Molecule 1: Choline-sulfatase

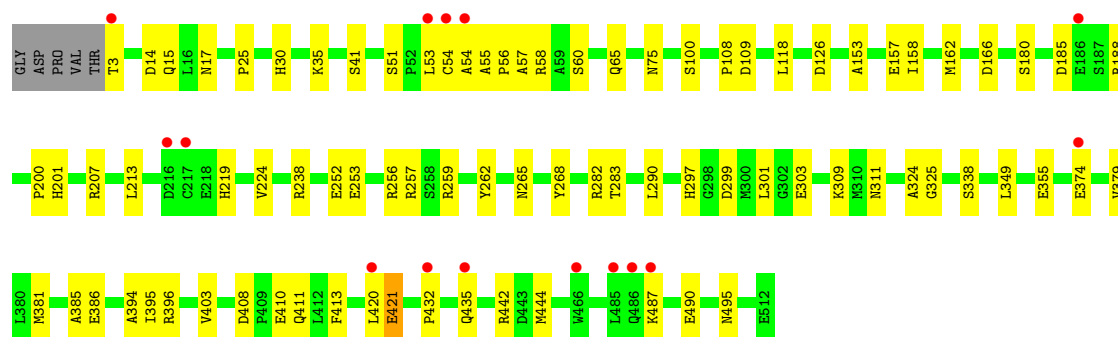
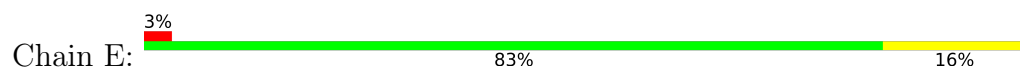




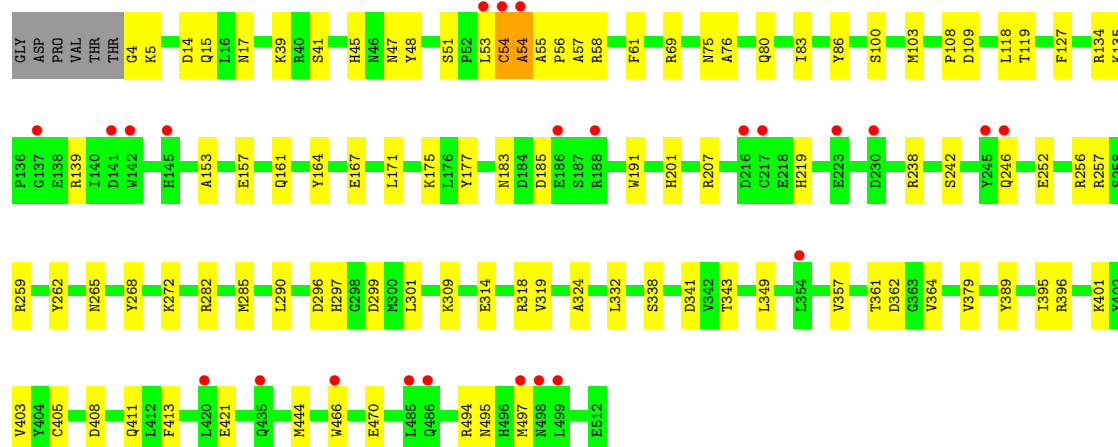
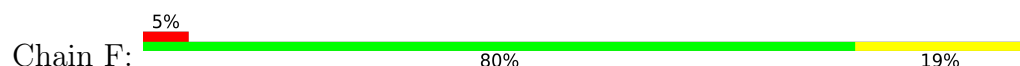
● Molecule 1: Choline-sulfatase



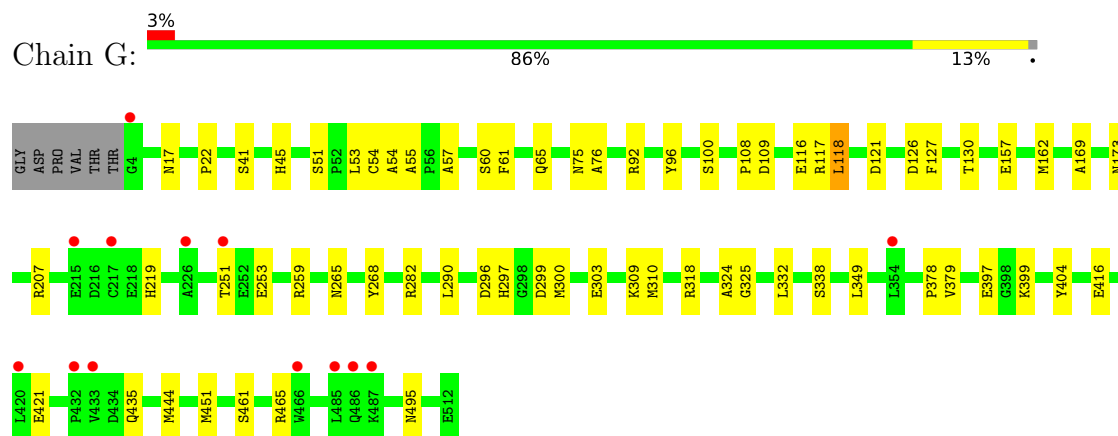
● Molecule 1: Choline-sulfatase



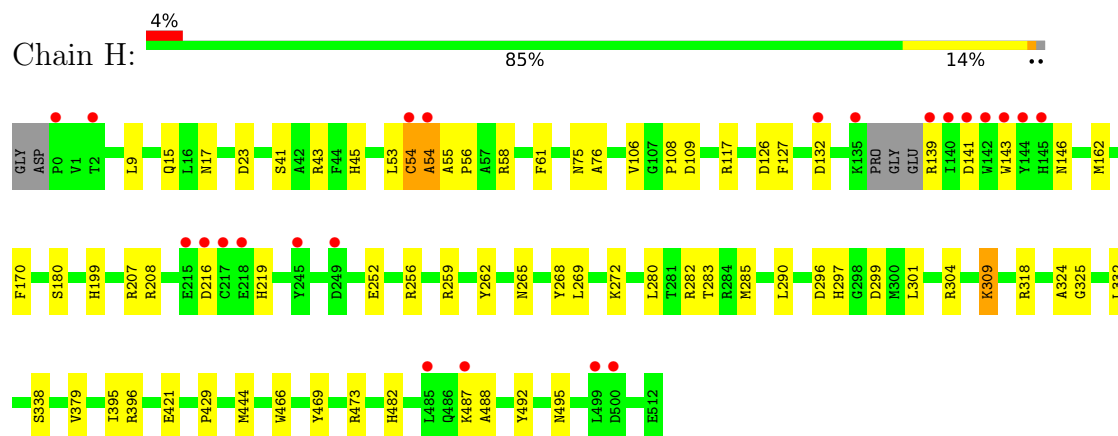
● Molecule 1: Choline-sulfatase



● Molecule 1: Choline-sulfatase



● Molecule 1: Choline-sulfatase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	119.56Å 163.25Å 177.62Å 90.00° 94.40° 90.00°	Depositor
Resolution (Å)	88.55 – 2.79 88.55 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.3 (88.55-2.79) 99.3 (88.55-2.79)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.77Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.205 , 0.252 0.208 , 0.253	Depositor DCC
R_{free} test set	8431 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	26.8	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	34715	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.16% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, DDZ

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	0.13	0/4256	0.33	0/5794
1	B	0.13	0/4256	0.33	0/5794
1	C	0.11	0/4244	0.30	0/5777
1	D	0.13	0/4222	0.34	0/5746
1	E	0.15	0/4222	0.33	0/5746
1	F	0.12	0/4215	0.32	0/5736
1	G	0.11	0/4215	0.31	0/5736
1	H	0.12	0/4222	0.32	0/5745
All	All	0.13	0/33852	0.32	0/46074

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	4148	0	3952	51	0
1	B	4148	0	3951	56	0
1	C	4136	0	3947	52	0
1	D	4115	0	3920	53	0
1	E	4115	0	3921	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	4108	0	3912	69	0
1	G	4108	0	3911	44	0
1	H	4116	0	3928	57	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	172	0	0	3	0
3	B	296	0	0	8	0
3	C	184	0	0	4	0
3	D	218	0	0	1	0
3	E	259	0	0	4	0
3	F	136	0	0	3	0
3	G	169	0	0	2	0
3	H	279	0	0	5	0
All	All	34715	0	31442	406	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 6.

All (406) 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:224:VAL:HG23	1:E:420:LEU:HD22	1.45	0.99
1:D:403:VAL:HG22	1:D:411:GLN:HB2	1.56	0.85
1:E:15:GLN:HG3	1:E:297:HIS:CE1	2.13	0.82
1:B:487:LYS:HE3	1:B:489:SER:H	1.45	0.81
1:E:224:VAL:CG2	1:E:420:LEU:HD22	2.12	0.80
1:D:498:ASN:HB2	1:D:501:THR:HB	1.67	0.77
1:B:285:MET:SD	3:B:802:HOH:O	2.45	0.74
1:G:251:THR:HG22	1:G:253:GLU:H	1.51	0.74
1:B:157:GLU:O	1:B:207:ARG:NH1	2.20	0.74
1:B:445:ARG:NH1	3:B:701:HOH:O	2.21	0.73
1:D:157:GLU:HG2	1:H:282:ARG:HB3	1.71	0.71
1:C:23:ASP:OD1	1:C:43:ARG:NH1	2.24	0.70
1:H:283:THR:HG22	1:H:285:MET:HG3	1.73	0.69
1:B:15:GLN:HG3	1:B:297:HIS:HE1	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:487:LYS:HE2	1:E:490:GLU:HG3	1.74	0.69
1:D:108:PRO:HG2	1:E:108:PRO:HG2	1.73	0.69
1:A:157:GLU:O	1:A:207:ARG:NH1	2.24	0.69
1:B:109:ASP:HB2	1:H:108:PRO:HG3	1.75	0.69
1:H:283:THR:HG21	1:H:285:MET:HE2	1.73	0.69
1:F:494:ARG:H	1:F:497:MET:HE3	1.59	0.68
1:B:15:GLN:HG3	1:B:297:HIS:CE1	2.30	0.67
1:A:15:GLN:HG2	1:A:297:HIS:HE1	1.60	0.67
1:B:41:SER:HB3	1:B:324:ALA:HB2	1.74	0.67
1:E:157:GLU:O	1:E:207:ARG:NH1	2.27	0.67
1:F:108:PRO:HG2	1:G:108:PRO:HG2	1.77	0.66
1:G:219:HIS:O	1:G:259:ARG:NH1	2.29	0.65
1:D:155:VAL:HG11	1:D:208:ARG:HG2	1.77	0.65
1:D:157:GLU:O	1:D:207:ARG:NH1	2.30	0.65
1:B:108:PRO:HG3	1:H:109:ASP:HB2	1.78	0.65
1:D:108:PRO:HG3	1:E:109:ASP:HB2	1.77	0.65
1:D:41:SER:HB3	1:D:324:ALA:HB2	1.79	0.65
1:A:126:ASP:OD1	1:G:495:ASN:ND2	2.26	0.64
1:C:41:SER:HB3	1:C:324:ALA:HB2	1.80	0.64
1:A:15:GLN:HG2	1:A:297:HIS:CE1	2.32	0.64
1:E:41:SER:HB3	1:E:324:ALA:HB2	1.80	0.64
1:C:374:GLU:CD	1:C:374:GLU:H	2.04	0.64
1:C:219:HIS:O	1:C:259:ARG:NH1	2.30	0.64
1:D:109:ASP:HB2	1:E:108:PRO:HG3	1.80	0.64
1:A:108:PRO:HG2	1:C:108:PRO:HG2	1.78	0.63
1:H:23:ASP:OD1	1:H:43:ARG:NE	2.31	0.63
1:F:219:HIS:O	1:F:259:ARG:NH1	2.32	0.63
1:G:53:LEU:HD12	1:G:309:LYS:HE2	1.80	0.63
1:E:53:LEU:HB3	1:E:56:PRO:HD2	1.80	0.62
1:F:466:TRP:O	1:F:470:GLU:HG3	1.98	0.62
1:B:108:PRO:HG2	1:H:108:PRO:HG2	1.81	0.62
1:F:108:PRO:HG3	1:G:109:ASP:HB2	1.81	0.62
1:E:15:GLN:HG3	1:E:297:HIS:HE1	1.61	0.62
1:F:153:ALA:O	1:F:257:ARG:NH2	2.32	0.62
1:H:54[A]:CYS:SG	3:H:841:HOH:O	2.51	0.62
1:A:45:HIS:HB2	1:A:332:LEU:HD11	1.81	0.62
1:C:157:GLU:HG3	1:F:282:ARG:HB3	1.80	0.62
1:H:297:HIS:CE1	1:H:309:LYS:HD2	2.34	0.61
1:E:238:ARG:NH2	1:E:408:ASP:OD2	2.34	0.61
1:G:41:SER:HB3	1:G:324:ALA:HB2	1.81	0.61
1:A:55:ALA:HB3	1:A:75:ASN:HA	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:ARG:HB3	1:G:157:GLU:HG3	1.83	0.61
1:D:45:HIS:O	1:D:318:ARG:NH2	2.33	0.60
1:A:297:HIS:CE1	1:A:309:LYS:HD2	2.37	0.60
1:F:41:SER:HB3	1:F:324:ALA:HB2	1.84	0.60
1:C:487:LYS:HE3	1:C:490:GLU:HG3	1.84	0.60
1:A:379:VAL:HB	1:A:396:ARG:HB3	1.82	0.60
1:E:219:HIS:O	1:E:259:ARG:NH1	2.35	0.60
1:H:55:ALA:HB3	1:H:75:ASN:HA	1.84	0.60
1:D:399:LYS:HB2	1:D:416:GLU:HG3	1.84	0.59
1:G:399:LYS:HB2	1:G:416:GLU:HG3	1.84	0.59
1:D:483:GLN:NE2	1:H:488:ALA:H	2.00	0.59
1:B:256:ARG:NH1	3:B:705:HOH:O	2.34	0.59
1:E:435:GLN:OE1	1:E:435:GLN:N	2.25	0.59
1:E:55:ALA:HB3	1:E:75:ASN:HA	1.84	0.58
1:E:432:PRO:HA	1:E:435:GLN:NE2	2.17	0.58
1:H:132:ASP:OD2	3:H:701:HOH:O	2.17	0.58
1:A:1:VAL:HG11	1:H:429:PRO:HG2	1.84	0.58
1:A:41:SER:HB3	1:A:324:ALA:HB2	1.86	0.58
1:F:48:TYR:OH	1:F:314:GLU:OE1	2.21	0.58
1:C:177:TYR:OH	1:C:282:ARG:NH2	2.32	0.58
1:C:379:VAL:HB	1:C:396:ARG:HB3	1.84	0.58
1:E:185:ASP:HB3	1:E:188:ARG:HB3	1.85	0.58
1:B:45:HIS:O	1:B:318:ARG:NH2	2.37	0.58
1:E:53:LEU:O	1:E:297:HIS:HD2	1.86	0.57
1:F:69:ARG:NH1	1:F:362:ASP:OD1	2.36	0.57
1:B:219:HIS:O	1:B:259:ARG:NH1	2.37	0.57
1:D:53:LEU:HB3	1:D:56:PRO:HD2	1.85	0.57
1:A:108:PRO:HG3	1:C:109:ASP:HB2	1.85	0.57
1:H:45:HIS:HB2	1:H:332:LEU:HD11	1.87	0.57
1:E:153:ALA:O	1:E:257:ARG:NH1	2.37	0.57
1:E:374:GLU:OE2	3:E:701:HOH:O	2.17	0.57
1:F:109:ASP:HB2	1:G:108:PRO:HG3	1.85	0.57
1:E:303:GLU:OE2	1:E:420:LEU:HD23	2.05	0.57
1:H:487:LYS:H	1:H:487:LYS:HD2	1.71	0.56
1:C:55:ALA:HB3	1:C:75:ASN:HA	1.88	0.56
1:B:15:GLN:OE1	1:B:309:LYS:NZ	2.27	0.56
1:E:180:SER:HB2	1:E:283:THR:HG23	1.88	0.56
1:G:55:ALA:HB3	1:G:75:ASN:HA	1.88	0.56
1:E:290:LEU:HD23	1:E:325:GLY:HA3	1.87	0.56
1:H:45:HIS:O	1:H:318:ARG:NH2	2.39	0.56
1:B:55:ALA:HB3	1:B:75:ASN:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ARG:HD3	1:A:389:TYR:CE2	2.41	0.56
1:B:445:ARG:NH2	3:B:722:HOH:O	2.37	0.56
1:C:126:ASP:OD1	1:F:495:ASN:ND2	2.35	0.56
1:D:55:ALA:HB3	1:D:75:ASN:HA	1.89	0.55
1:H:54[A]:CYS:O	1:H:58:ARG:HG3	2.06	0.55
1:D:15:GLN:HG3	1:D:297:HIS:CE1	2.42	0.55
1:F:39:LYS:HD2	1:F:39:LYS:N	2.21	0.55
1:F:55:ALA:HB3	1:F:75:ASN:HA	1.87	0.55
1:F:297:HIS:CE1	1:F:309:LYS:HD3	2.40	0.55
1:A:109:ASP:HB2	1:C:108:PRO:HG3	1.87	0.55
1:A:157:GLU:HG3	1:G:282:ARG:HB3	1.88	0.55
1:C:238:ARG:NH2	1:C:408:ASP:OD2	2.39	0.55
1:H:180:SER:HB2	1:H:283:THR:HG23	1.88	0.55
1:H:41:SER:HB3	1:H:324:ALA:HB2	1.88	0.55
1:A:100:SER:HB2	1:A:118:LEU:HD22	1.89	0.55
1:F:53:LEU:HB3	1:F:56:PRO:HD2	1.89	0.55
1:E:3:THR:N	3:E:717:HOH:O	2.39	0.55
1:H:15:GLN:HG3	1:H:297:HIS:CE1	2.42	0.55
1:A:495:ASN:ND2	1:G:126:ASP:OD1	2.36	0.55
1:C:45:HIS:HB2	1:C:332:LEU:HD11	1.89	0.55
1:E:297:HIS:CE1	1:E:309:LYS:HD2	2.42	0.54
1:A:45:HIS:O	1:A:318:ARG:NH2	2.40	0.54
1:H:139:ARG:NH1	1:H:141:ASP:OD1	2.40	0.54
1:F:139:ARG:NH1	1:F:242:SER:O	2.40	0.54
1:E:432:PRO:HA	1:E:435:GLN:HE22	1.73	0.54
1:B:381:MET:HB2	1:B:394:ALA:HB3	1.90	0.54
1:F:45:HIS:O	1:F:318:ARG:NH2	2.39	0.54
1:D:379:VAL:HB	1:D:396:ARG:HB3	1.88	0.53
1:B:53:LEU:HB3	1:B:56:PRO:HD2	1.89	0.53
1:D:119:THR:HG22	1:D:171:LEU:HD12	1.90	0.53
1:F:45:HIS:HB2	1:F:332:LEU:HD11	1.89	0.53
1:A:86:TYR:HB3	1:A:343:THR:HG23	1.89	0.53
1:H:395:ILE:HD13	1:H:444:MET:HE2	1.91	0.53
1:E:51:SER:O	1:E:57:ALA:HB2	2.09	0.53
1:D:5:LYS:NZ	1:D:93:ALA:O	2.41	0.53
1:E:290:LEU:HD13	1:E:349:LEU:HD13	1.91	0.53
1:F:265:ASN:HA	1:F:268:TYR:HB3	1.91	0.53
1:A:2:THR:HA	1:A:5:LYS:HD2	1.91	0.52
1:D:39:LYS:N	1:D:39:LYS:HD2	2.24	0.52
1:G:100:SER:HB2	1:G:118:LEU:HD22	1.90	0.52
1:B:314:GLU:OE1	1:B:401:LYS:NZ	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:58:ARG:HG2	1:E:58:ARG:HH11	1.74	0.52
1:D:162:MET:SD	1:D:207:ARG:HG3	2.49	0.52
1:F:177:TYR:OH	1:F:282:ARG:NH2	2.38	0.52
1:F:259:ARG:NH2	3:F:713:HOH:O	2.42	0.52
1:G:338:SER:HB2	1:G:379:VAL:HG13	1.92	0.52
1:A:17:ASN:ND2	3:A:709:HOH:O	2.38	0.52
1:A:23:ASP:OD1	1:A:43:ARG:NE	2.34	0.52
1:E:265:ASN:HA	1:E:268:TYR:HB3	1.92	0.52
1:E:487:LYS:CE	1:E:490:GLU:HG3	2.39	0.52
1:F:4:GLY:N	3:F:715:HOH:O	2.43	0.52
1:C:265:ASN:HA	1:C:268:TYR:HB3	1.91	0.52
1:B:494:ARG:HB2	1:B:497:MET:HE3	1.92	0.52
1:B:157:GLU:HA	1:B:207:ARG:HG2	1.93	0.51
1:C:187:SER:O	1:C:187:SER:OG	2.27	0.51
1:B:189:ARG:NH2	3:B:712:HOH:O	2.30	0.51
1:D:238:ARG:NH2	1:D:408:ASP:OD2	2.44	0.51
1:G:162:MET:SD	1:G:207:ARG:HG3	2.50	0.51
1:D:45:HIS:HB2	1:D:332:LEU:HD11	1.92	0.51
1:H:219:HIS:O	1:H:259:ARG:NH1	2.44	0.51
1:E:338:SER:HB2	1:E:379:VAL:HG13	1.92	0.51
1:A:295:SER:HB3	1:A:319:VAL:HB	1.93	0.50
1:B:495:ASN:ND2	1:E:126:ASP:OD1	2.44	0.50
1:C:338:SER:HB2	1:C:379:VAL:HG13	1.92	0.50
1:F:17:ASN:ND2	1:F:299:ASP:O	2.45	0.50
1:C:246:GLN:H	1:C:246:GLN:CD	2.17	0.50
1:B:403:VAL:HB	1:B:411:GLN:HB2	1.93	0.50
1:B:290:LEU:HD23	1:B:325:GLY:HA3	1.94	0.50
1:C:134:ARG:NH2	3:C:707:HOH:O	2.39	0.50
1:C:238:ARG:HH11	1:C:388:SER:HA	1.77	0.50
1:D:76:ALA:HB1	1:D:127:PHE:HA	1.93	0.50
1:E:421:GLU:OE2	3:E:702:HOH:O	2.19	0.50
1:H:379:VAL:HB	1:H:396:ARG:HB3	1.94	0.50
1:C:229:LEU:O	1:C:237:GLN:NE2	2.45	0.50
1:G:290:LEU:HD23	1:G:325:GLY:HA3	1.93	0.50
1:G:96:TYR:OH	1:G:116:GLU:OE1	2.27	0.50
1:H:17:ASN:ND2	1:H:299:ASP:O	2.45	0.50
1:C:139:ARG:NH2	3:C:717:HOH:O	2.44	0.50
1:A:442:ARG:HG2	1:A:445:ARG:HH11	1.77	0.49
1:E:395:ILE:HD13	1:E:444:MET:HE2	1.92	0.49
1:F:80:GLN:HB2	1:F:83:ILE:HG13	1.94	0.49
1:C:135:LYS:HB2	1:C:138:GLU:OE2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:413:PHE:CD1	1:D:421:GLU:HB3	2.48	0.49
1:G:17:ASN:ND2	1:G:299:ASP:O	2.46	0.49
1:A:76:ALA:HB1	1:A:127:PHE:HA	1.95	0.49
1:B:238:ARG:HD3	1:B:389:TYR:CE2	2.47	0.49
1:E:381:MET:HB2	1:E:394:ALA:HB3	1.94	0.49
1:F:238:ARG:HD3	1:F:389:TYR:CE2	2.48	0.49
1:D:180:SER:HB2	1:D:283:THR:HG23	1.93	0.49
1:D:265:ASN:HA	1:D:268:TYR:HB3	1.93	0.49
1:B:118:LEU:HD11	1:B:175:LYS:HD2	1.95	0.48
1:C:254:ASN:ND2	3:C:706:HOH:O	2.36	0.48
1:D:238:ARG:HD3	1:D:389:TYR:CE2	2.48	0.48
1:H:304:ARG:NH2	3:H:730:HOH:O	2.46	0.48
1:A:58:ARG:HH11	1:A:58:ARG:HG2	1.77	0.48
1:D:219:HIS:O	1:D:259:ARG:NH1	2.46	0.48
1:C:15:GLN:NE2	1:C:299:ASP:OD2	2.47	0.48
1:F:58:ARG:HD3	1:F:103:MET:HA	1.95	0.48
1:F:470:GLU:HB2	1:G:92:ARG:HD2	1.96	0.48
1:G:251:THR:HG22	1:G:253:GLU:N	2.25	0.48
1:H:9:LEU:HD22	1:H:280:LEU:HD11	1.96	0.48
1:D:126:ASP:OD1	1:H:495:ASN:ND2	2.44	0.48
1:B:297:HIS:CE1	1:B:309:LYS:HD2	2.48	0.48
1:E:379:VAL:HB	1:E:396:ARG:HB3	1.95	0.48
1:A:338:SER:HB2	1:A:379:VAL:HG13	1.95	0.48
1:E:297:HIS:HE1	1:E:309:LYS:HD2	1.78	0.48
1:F:53:LEU:HA	1:F:309:LYS:HD2	1.95	0.48
1:H:15:GLN:HG3	1:H:297:HIS:HE1	1.75	0.48
1:H:76:ALA:HB1	1:H:127:PHE:HA	1.94	0.48
1:A:444:MET:HE2	1:A:444:MET:HB3	1.75	0.48
1:B:76:ALA:HB1	1:B:127:PHE:HA	1.96	0.47
1:E:385:ALA:HB1	1:E:386:GLU:OE2	2.14	0.47
1:F:119:THR:HG22	1:F:171:LEU:HD12	1.94	0.47
1:H:15:GLN:HG2	1:H:299:ASP:HB2	1.95	0.47
1:B:162:MET:SD	1:B:207:ARG:HG3	2.54	0.47
1:B:246:GLN:NE2	3:B:724:HOH:O	2.39	0.47
1:B:265:ASN:HA	1:B:268:TYR:HB3	1.95	0.47
1:F:405:CYS:HB3	1:F:408:ASP:HB2	1.96	0.47
1:H:296:ASP:OD1	1:H:297:HIS:N	2.48	0.47
1:H:338:SER:HB2	1:H:379:VAL:HG13	1.95	0.47
1:A:238:ARG:NH2	1:A:408:ASP:OD2	2.46	0.47
1:C:282:ARG:HB3	1:F:157:GLU:HG3	1.95	0.47
1:D:9:LEU:HD22	1:D:280:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:414:ASP:O	1:D:418:ASP:N	2.47	0.47
1:D:157:GLU:HA	1:D:207:ARG:HG2	1.97	0.47
1:F:338:SER:HB2	1:F:379:VAL:HG13	1.97	0.47
1:H:162:MET:SD	1:H:207:ARG:HG3	2.54	0.47
1:D:254:ASN:ND2	3:D:715:HOH:O	2.36	0.47
1:D:499:LEU:HD13	1:H:143:TRP:HA	1.97	0.47
1:A:183:ASN:O	1:A:183:ASN:ND2	2.48	0.47
1:A:354:LEU:HD12	1:A:354:LEU:H	1.80	0.47
1:B:157:GLU:HG3	1:E:282:ARG:HB3	1.96	0.47
1:C:76:ALA:HB1	1:C:127:PHE:HA	1.97	0.47
1:C:297:HIS:CE1	1:C:309:LYS:HD2	2.49	0.47
1:D:54[A]:CYS:O	1:D:58:ARG:HG3	2.13	0.47
1:H:469:TYR:OH	1:H:473:ARG:HD2	2.14	0.47
1:D:96:TYR:OH	1:D:175:LYS:HE3	2.14	0.47
1:A:5:LYS:HE3	1:A:350:ALA:O	2.14	0.46
1:A:108:PRO:HB2	1:C:108:PRO:HB2	1.97	0.46
1:E:413:PHE:CG	1:E:421:GLU:HG2	2.51	0.46
1:G:265:ASN:HA	1:G:268:TYR:HB3	1.96	0.46
1:B:252:GLU:O	1:B:256:ARG:HG3	2.15	0.46
1:E:262:TYR:CE1	1:E:301:LEU:HD11	2.50	0.46
1:F:157:GLU:HA	1:F:207:ARG:HG2	1.97	0.46
1:H:208:ARG:NH2	3:H:725:HOH:O	2.44	0.46
1:B:19:LYS:NZ	1:B:303:GLU:OE1	2.49	0.46
1:B:5:LYS:HD3	1:B:350:ALA:O	2.16	0.46
1:H:487:LYS:H	1:H:487:LYS:CD	2.28	0.46
1:D:23:ASP:OD1	1:D:43:ARG:NE	2.37	0.46
1:F:51:SER:O	1:F:57:ALA:HB2	2.16	0.46
1:G:76:ALA:HB1	1:G:127:PHE:HA	1.98	0.46
1:H:207:ARG:NH1	3:H:738:HOH:O	2.49	0.46
1:B:117:ARG:HB3	1:B:482:HIS:NE2	2.30	0.46
1:E:60:SER:OG	1:E:65:GLN:O	2.30	0.46
1:C:66:LEU:HD22	1:C:382:GLU:HG3	1.97	0.46
1:C:238:ARG:HD3	1:C:389:TYR:CE2	2.50	0.46
1:D:167:GLU:HA	1:H:170:PHE:CZ	2.51	0.46
1:D:238:ARG:HH11	1:D:388:SER:HA	1.80	0.46
1:F:86:TYR:HB3	1:F:343:THR:HG23	1.98	0.46
1:F:444:MET:HE2	1:F:444:MET:HB3	1.78	0.46
1:G:60:SER:OG	1:G:65:GLN:O	2.31	0.46
1:E:15:GLN:OE1	1:E:201:HIS:CD2	2.69	0.45
1:F:15:GLN:HG3	1:F:297:HIS:CE1	2.50	0.45
1:C:444:MET:HE2	1:C:444:MET:HB3	1.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:SER:O	1:A:57:ALA:HB2	2.16	0.45
1:C:22:PRO:O	1:C:45:HIS:ND1	2.39	0.45
1:C:492:TYR:CZ	1:F:164:TYR:HD1	2.35	0.45
1:G:45:HIS:O	1:G:318:ARG:NH2	2.49	0.45
1:F:15:GLN:HG2	1:F:299:ASP:HB2	1.98	0.45
1:B:40:ARG:NH1	3:B:737:HOH:O	2.49	0.45
1:E:403:VAL:HB	1:E:411:GLN:HB2	1.99	0.45
1:C:96:TYR:OH	1:C:175:LYS:HE2	2.17	0.45
1:A:469:TYR:OH	1:A:473:ARG:NH1	2.43	0.45
1:C:262:TYR:CE1	1:C:301:LEU:HD11	2.52	0.45
1:E:410:GLU:OE1	1:E:442:ARG:NH2	2.46	0.45
1:B:181:ARG:HH21	1:E:158:ILE:HG13	1.81	0.44
1:C:374:GLU:OE2	1:C:374:GLU:N	2.42	0.44
1:D:15:GLN:HG3	1:D:297:HIS:HE1	1.82	0.44
1:F:341:ASP:HB3	1:F:364:VAL:O	2.17	0.44
1:G:378:PRO:HB3	1:G:397:GLU:HG3	1.98	0.44
1:H:132:ASP:HA	1:H:466:TRP:HZ2	1.82	0.44
1:C:76:ALA:HA	1:C:106:VAL:HG21	1.99	0.44
1:F:290:LEU:HD22	1:F:349:LEU:HD13	1.99	0.44
1:G:309:LYS:HG3	1:G:310:MET:SD	2.57	0.44
1:H:76:ALA:HA	1:H:106:VAL:HG21	1.98	0.44
1:E:253:GLU:O	1:E:257:ARG:HG3	2.18	0.44
1:H:265:ASN:HA	1:H:268:TYR:HB3	1.98	0.44
1:H:216:ASP:OD1	1:H:216:ASP:N	2.49	0.44
1:B:268:TYR:OH	1:B:272:LYS:HE2	2.16	0.44
1:G:259:ARG:NH2	3:G:722:HOH:O	2.50	0.44
1:B:51:SER:O	1:B:57:ALA:HB2	2.18	0.44
1:A:43:ARG:NH2	3:A:724:HOH:O	2.51	0.44
1:A:75:ASN:ND2	3:A:708:HOH:O	2.37	0.44
1:F:191:TRP:HE1	1:F:285:MET:HE2	1.82	0.44
1:E:15:GLN:OE1	1:E:309:LYS:NZ	2.40	0.44
1:H:139:ARG:HH22	1:H:146:ASN:HB3	1.82	0.44
1:D:485:LEU:CD1	1:D:487:LYS:HG3	2.47	0.43
1:F:395:ILE:HD13	1:F:444:MET:HE2	2.00	0.43
1:G:404:TYR:HE2	1:G:451:MET:HG3	1.83	0.43
1:A:262:TYR:CE2	1:A:301:LEU:HD11	2.53	0.43
1:E:162:MET:HG2	1:E:207:ARG:NH2	2.33	0.43
1:G:117:ARG:NH2	1:G:121:ASP:OD2	2.48	0.43
1:A:53:LEU:HB3	1:A:56:PRO:HD2	1.99	0.43
1:B:487:LYS:HA	1:B:487:LYS:HD2	1.73	0.43
1:C:9:LEU:HD22	1:C:280:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:LEU:HD13	1:B:191:TRP:CG	2.53	0.43
1:D:158:ILE:HD12	1:D:158:ILE:HA	1.87	0.43
1:F:296:ASP:OD1	1:F:296:ASP:N	2.51	0.43
1:A:265:ASN:HA	1:A:268:TYR:HB3	1.99	0.43
1:E:166:ASP:OD2	1:E:207:ARG:NH2	2.51	0.43
1:F:76:ALA:HB1	1:F:127:PHE:HA	2.00	0.43
1:F:252:GLU:O	1:F:256:ARG:HG3	2.18	0.43
1:F:379:VAL:HB	1:F:396:ARG:HB3	2.00	0.43
1:E:311:ASN:ND2	3:E:739:HOH:O	2.51	0.43
1:F:262:TYR:CE1	1:F:301:LEU:HD11	2.54	0.43
1:H:268:TYR:CZ	1:H:272:LYS:HE2	2.53	0.43
1:C:300:MET:HE3	1:C:303:GLU:HB3	1.99	0.43
1:F:403:VAL:HB	1:F:411:GLN:HB2	1.99	0.43
1:G:169:ALA:O	1:G:173:ASN:ND2	2.47	0.43
1:H:444:MET:HE2	1:H:444:MET:HB3	1.82	0.43
1:C:53:LEU:HB3	1:C:56:PRO:HD2	2.00	0.43
1:B:177:TYR:HB3	1:E:158:ILE:HG12	2.00	0.43
1:C:414:ASP:O	1:C:418:ASP:N	2.52	0.43
1:A:166:ASP:OD2	1:A:207:ARG:NH2	2.49	0.43
1:B:52:PRO:HB2	1:B:310:MET:H	1.82	0.43
1:C:51:SER:O	1:C:57:ALA:HB2	2.19	0.43
1:E:53:LEU:O	1:E:297:HIS:CD2	2.71	0.43
1:G:300:MET:HE3	1:G:303:GLU:HB3	2.00	0.43
1:G:461:SER:O	1:G:465:ARG:HG3	2.19	0.43
1:C:170:PHE:CZ	1:F:167:GLU:HA	2.54	0.42
1:D:139:ARG:NH1	1:D:242:SER:O	2.51	0.42
1:E:14:ASP:O	1:E:200:PRO:HD2	2.19	0.42
1:F:14:ASP:OD2	1:F:296:ASP:OD2	2.36	0.42
1:F:396:ARG:HD3	1:F:401:LYS:HD3	2.01	0.42
1:G:444:MET:HE2	1:G:444:MET:HB3	1.81	0.42
1:C:15:GLN:HG2	1:C:299:ASP:HB2	2.01	0.42
1:F:357:VAL:O	1:F:361:THR:HG22	2.19	0.42
1:H:139:ARG:NH2	1:H:146:ASN:HB3	2.35	0.42
1:B:1:VAL:HG11	1:C:429:PRO:HG2	2.01	0.42
1:D:161:GLN:OE1	1:D:201:HIS:HB3	2.18	0.42
1:E:17:ASN:ND2	1:E:299:ASP:O	2.52	0.42
1:A:403:VAL:HB	1:A:411:GLN:HB2	2.01	0.42
1:C:466:TRP:O	1:C:470:GLU:HB2	2.19	0.42
1:F:268:TYR:CZ	1:F:272:LYS:HE2	2.55	0.42
1:G:57:ALA:O	1:G:61:PHE:N	2.46	0.42
1:A:378:PRO:HB3	1:A:397:GLU:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:SER:O	1:D:183:ASN:HB2	2.20	0.42
1:E:30:HIS:HD2	1:E:213:LEU:HB3	1.85	0.42
1:E:355:GLU:H	1:E:355:GLU:HG3	1.67	0.42
1:G:130:THR:HG23	1:G:465:ARG:HH21	1.84	0.42
1:H:262:TYR:CE2	1:H:301:LEU:HD11	2.54	0.42
1:F:118:LEU:HD21	1:F:175:LYS:HD2	2.02	0.42
1:E:25:PRO:HG2	1:E:35:LYS:HG3	2.02	0.42
1:F:268:TYR:OH	1:F:272:LYS:HE2	2.20	0.42
1:F:413:PHE:CD1	1:F:421:GLU:HB3	2.55	0.42
1:A:139:ARG:NH1	1:A:242:SER:O	2.53	0.42
1:B:402:TYR:OH	1:B:410:GLU:OE2	2.33	0.42
1:H:117:ARG:HB3	1:H:482:HIS:NE2	2.34	0.42
1:B:80:GLN:HG3	3:B:772:HOH:O	2.20	0.42
1:D:51:SER:O	1:D:57:ALA:HB2	2.20	0.42
1:F:47:ASN:HD22	1:F:319:VAL:HG23	1.85	0.42
1:H:58:ARG:HA	1:H:61:PHE:HB3	2.01	0.42
1:B:14:ASP:OD1	1:B:296:ASP:OD2	2.37	0.41
1:F:5:LYS:NZ	3:F:719:HOH:O	2.49	0.41
1:G:297:HIS:CE1	1:G:309:LYS:HD3	2.55	0.41
1:G:404:TYR:CE2	1:G:451:MET:HG3	2.55	0.41
1:A:14:ASP:HA	1:A:296:ASP:OD1	2.19	0.41
1:B:45:HIS:HB2	1:B:332:LEU:HD11	2.01	0.41
1:B:61:PHE:CE1	1:B:342:VAL:HG11	2.55	0.41
1:C:445:ARG:NH1	3:C:701:HOH:O	2.34	0.41
1:E:252:GLU:O	1:E:256:ARG:HG3	2.20	0.41
1:G:296:ASP:OD1	1:G:296:ASP:N	2.52	0.41
1:D:110:GLN:CB	1:D:482:HIS:HB2	2.51	0.41
1:D:164:TYR:HD1	1:H:492:TYR:CZ	2.38	0.41
1:D:290:LEU:HD13	1:D:349:LEU:HD13	2.01	0.41
1:F:15:GLN:HG3	1:F:297:HIS:HE1	1.85	0.41
1:H:252:GLU:O	1:H:256:ARG:HG3	2.21	0.41
1:C:292:LEU:HG	1:C:323:ILE:HG12	2.01	0.41
1:F:470:GLU:OE2	1:G:92:ARG:NH1	2.53	0.41
1:G:51:SER:O	1:G:57:ALA:HB2	2.19	0.41
1:H:199:HIS:HB2	1:H:269:LEU:HD21	2.02	0.41
1:F:57:ALA:O	1:F:61:PHE:N	2.45	0.41
1:F:100:SER:HB2	1:F:118:LEU:HD22	2.02	0.41
1:F:183:ASN:C	1:F:185:ASP:H	2.28	0.41
1:A:123:TYR:HD1	1:A:123:TYR:HA	1.75	0.41
1:G:290:LEU:HD13	1:G:349:LEU:HD13	2.01	0.41
1:G:435:GLN:HB3	3:G:795:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:ARG:HD3	1:A:401:LYS:HD3	2.02	0.41
1:B:58:ARG:HD3	1:B:103:MET:HA	2.01	0.41
1:D:400:TRP:CD2	1:D:437:THR:HG21	2.55	0.41
1:G:45:HIS:HB2	1:G:332:LEU:HD11	2.02	0.41
1:D:188:ARG:HG2	1:D:189:ARG:N	2.35	0.41
1:F:134:ARG:C	1:F:135:LYS:HE2	2.46	0.41
1:B:262:TYR:CE1	1:B:301:LEU:HD11	2.55	0.40
1:D:495:ASN:ND2	1:H:126:ASP:OD1	2.50	0.40
1:C:238:ARG:NH1	1:C:388:SER:HA	2.36	0.40
1:A:202:ASP:HA	1:A:203:PRO:C	2.47	0.40
1:D:499:LEU:HD23	1:D:500:ASP:H	1.86	0.40
1:E:158:ILE:HD12	1:E:158:ILE:HA	1.94	0.40
1:H:290:LEU:HD23	1:H:325:GLY:HA3	2.03	0.40
1:B:237:GLN:O	1:B:241:LEU:HG	2.21	0.40
1:F:48:TYR:HB2	1:F:379:VAL:HG11	2.03	0.40
1:A:292:LEU:HG	1:A:323:ILE:HG12	2.03	0.40
1:A:471:ALA:HB2	1:C:92:ARG:HB2	2.03	0.40
1:B:126:ASP:OD1	1:E:495:ASN:ND2	2.45	0.40
1:B:323:ILE:O	1:B:328:ILE:HG21	2.21	0.40
1:E:100:SER:HB2	1:E:118:LEU:HD22	2.03	0.40
1:F:161:GLN:OE1	1:F:201:HIS:HB3	2.21	0.40
1:F:246:GLN:H	1:F:246:GLN:HG2	1.72	0.40
1:H:53:LEU:HB3	1:H:56:PRO:HD2	2.04	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	512/516 (99%)	490 (96%)	21 (4%)	1 (0%)	43 72
1	B	512/516 (99%)	494 (96%)	17 (3%)	1 (0%)	43 72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	510/516 (99%)	481 (94%)	29 (6%)	0	100	100
1	D	507/516 (98%)	484 (96%)	22 (4%)	1 (0%)	43	72
1	E	507/516 (98%)	485 (96%)	21 (4%)	1 (0%)	43	72
1	F	506/516 (98%)	481 (95%)	25 (5%)	0	100	100
1	G	506/516 (98%)	491 (97%)	13 (3%)	2 (0%)	30	60
1	H	505/516 (98%)	485 (96%)	19 (4%)	1 (0%)	43	72
All	All	4065/4128 (98%)	3891 (96%)	167 (4%)	7 (0%)	43	72

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	421	GLU
1	G	421	GLU
1	A	421	GLU
1	E	421	GLU
1	H	421	GLU
1	B	421	GLU
1	G	22	PRO

5.3.2 Protein sidechains [i](#)

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	438/438 (100%)	436 (100%)	2 (0%)	81	93
1	B	438/438 (100%)	436 (100%)	2 (0%)	81	93
1	C	437/438 (100%)	437 (100%)	0	100	100
1	D	434/438 (99%)	433 (100%)	1 (0%)	87	96
1	E	434/438 (99%)	434 (100%)	0	100	100
1	F	433/438 (99%)	432 (100%)	1 (0%)	87	96
1	G	433/438 (99%)	432 (100%)	1 (0%)	87	96
1	H	435/438 (99%)	434 (100%)	1 (0%)	87	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3482/3504 (99%)	3474 (100%)	8 (0%)	87 96

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54[A]	CYS
1	A	473	ARG
1	B	53	LEU
1	B	54[A]	CYS
1	D	54[A]	CYS
1	F	54[A]	CYS
1	G	118	LEU
1	H	309	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	46	ASN
1	A	47	ASN
1	A	232	GLN
1	A	237	GLN
1	A	411	GLN
1	A	496	HIS
1	B	33	ASN
1	B	174	GLN
1	B	232	GLN
1	C	33	ASN
1	C	80	GLN
1	C	174	GLN
1	C	482	HIS
1	D	483	GLN
1	E	7	ASN
1	E	30	HIS
1	E	80	GLN
1	E	237	GLN
1	E	247	ASN
1	E	411	GLN
1	F	46	ASN
1	F	47	ASN
1	F	219	HIS

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Mol	Chain	Res	Type
1	F	371	ASN
1	G	15	GLN
1	G	80	GLN
1	H	33	ASN
1	H	80	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	DDZ	H	54[B]	1,2	4,6,7	0.68	0	3,7,9	2.37	1 (33%)
1	DDZ	G	54[B]	1,2	4,6,7	0.67	0	3,7,9	1.95	1 (33%)
1	DDZ	F	54[B]	1,2	4,6,7	0.81	0	3,7,9	2.40	1 (33%)
1	DDZ	E	54[B]	1,2	4,6,7	0.91	0	3,7,9	2.28	1 (33%)
1	DDZ	A	54[B]	1,2	4,6,7	0.75	0	3,7,9	2.39	1 (33%)
1	DDZ	B	54[B]	1,2	4,6,7	0.88	0	3,7,9	2.24	1 (33%)
1	DDZ	C	54[B]	1,2	4,6,7	0.75	0	3,7,9	1.88	1 (33%)
1	DDZ	D	54[B]	1,2	4,6,7	0.79	0	3,7,9	2.54	1 (33%)

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	DDZ	H	54[B]	1,2	-	0/2/6/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	DDZ	G	54[B]	1,2	-	0/2/6/8	-
1	DDZ	F	54[B]	1,2	-	2/2/6/8	-
1	DDZ	E	54[B]	1,2	-	0/2/6/8	-
1	DDZ	A	54[B]	1,2	-	2/2/6/8	-
1	DDZ	B	54[B]	1,2	-	2/2/6/8	-
1	DDZ	C	54[B]	1,2	-	1/2/6/8	-
1	DDZ	D	54[B]	1,2	-	2/2/6/8	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	54[B]	DDZ	OG2-CB-OG1	-4.34	103.77	111.26
1	F	54[B]	DDZ	OG2-CB-OG1	-4.11	104.17	111.26
1	A	54[B]	DDZ	OG2-CB-OG1	-4.09	104.20	111.26
1	H	54[B]	DDZ	OG2-CB-OG1	-3.99	104.38	111.26
1	E	54[B]	DDZ	OG2-CB-OG1	-3.90	104.53	111.26
1	B	54[B]	DDZ	OG2-CB-OG1	-3.71	104.86	111.26
1	G	54[B]	DDZ	OG2-CB-OG1	-3.31	105.56	111.26
1	C	54[B]	DDZ	OG2-CB-OG1	-3.20	105.74	111.26

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	54[B]	DDZ	N-CA-CB-OG1
1	A	54[B]	DDZ	N-CA-CB-OG2
1	B	54[B]	DDZ	N-CA-CB-OG1
1	B	54[B]	DDZ	N-CA-CB-OG2
1	D	54[B]	DDZ	N-CA-CB-OG1
1	F	54[B]	DDZ	N-CA-CB-OG2
1	C	54[B]	DDZ	N-CA-CB-OG1
1	D	54[B]	DDZ	N-CA-CB-OG2
1	F	54[B]	DDZ	N-CA-CB-OG1

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 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	514/516 (99%)	0.23	10 (1%) 66 57	17, 29, 54, 83	0
1	B	514/516 (99%)	-0.14	11 (2%) 63 54	8, 17, 40, 80	0
1	C	512/516 (99%)	0.23	20 (3%) 43 34	12, 28, 52, 84	0
1	D	509/516 (98%)	0.19	13 (2%) 57 47	9, 23, 49, 100	0
1	E	509/516 (98%)	-0.02	13 (2%) 57 47	7, 18, 43, 74	0
1	F	508/516 (98%)	0.49	22 (4%) 40 31	18, 34, 56, 88	0
1	G	508/516 (98%)	0.25	13 (2%) 57 47	14, 29, 53, 73	0
1	H	509/516 (98%)	-0.08	21 (4%) 41 33	6, 17, 45, 78	0
All	All	4083/4128 (98%)	0.14	123 (3%) 50 42	6, 25, 51, 100	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	499	LEU	5.8
1	C	0	PRO	5.1
1	E	432	PRO	5.1
1	E	3	THR	5.0
1	B	216	ASP	5.0
1	D	3	THR	4.7
1	C	245	TYR	4.5
1	F	486	GLN	4.3
1	A	485	LEU	4.3
1	E	420	LEU	4.1
1	B	217	CYS	4.0
1	E	485	LEU	3.8
1	G	485	LEU	3.7
1	H	216	ASP	3.6
1	F	466	TRP	3.6
1	H	143	TRP	3.5

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Mol	Chain	Res	Type	RSRZ
1	F	223	GLU	3.5
1	B	-2	GLY	3.5
1	G	487	LYS	3.5
1	E	186	GLU	3.5
1	B	499	LEU	3.4
1	F	354	LEU	3.4
1	C	145	HIS	3.4
1	E	216	ASP	3.3
1	F	245	TYR	3.3
1	B	420	LEU	3.3
1	H	0	PRO	3.3
1	H	144	TYR	3.3
1	H	485	LEU	3.3
1	F	216	ASP	3.3
1	E	435	GLN	3.2
1	A	-2	GLY	3.2
1	F	497	MET	3.2
1	D	485	LEU	3.2
1	C	1	VAL	3.1
1	G	432	PRO	3.1
1	G	486	GLN	3.1
1	H	215	GLU	3.0
1	D	354	LEU	3.0
1	C	230	ASP	3.0
1	D	448	HIS	3.0
1	H	245	TYR	3.0
1	C	485	LEU	2.9
1	H	499	LEU	2.9
1	F	142	TRP	2.9
1	D	500	ASP	2.9
1	A	186	GLU	2.9
1	G	420	LEU	2.9
1	E	374	GLU	2.9
1	H	145	HIS	2.9
1	D	498	ASN	2.9
1	F	420	LEU	2.9
1	E	486	GLN	2.9
1	F	145	HIS	2.9
1	B	249	ASP	2.8
1	H	500	ASP	2.8
1	C	137	GLY	2.8
1	D	420	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	2	THR	2.8
1	H	141	ASP	2.7
1	G	354	LEU	2.7
1	E	217	CYS	2.7
1	A	499	LEU	2.7
1	E	466	TRP	2.6
1	H	132	ASP	2.6
1	F	53	LEU	2.6
1	C	498	ASN	2.6
1	H	142	TRP	2.5
1	D	487	LYS	2.5
1	F	186	GLU	2.5
1	F	435	GLN	2.5
1	F	217	CYS	2.5
1	A	216	ASP	2.5
1	C	143	TRP	2.5
1	C	216	ASP	2.5
1	G	433	VAL	2.5
1	C	223	GLU	2.4
1	A	245	TYR	2.4
1	F	498	ASN	2.4
1	A	230	ASP	2.4
1	C	217	CYS	2.4
1	H	218	GLU	2.4
1	C	138	GLU	2.4
1	B	500	ASP	2.4
1	G	4	GLY	2.4
1	F	485	LEU	2.3
1	D	53	LEU	2.3
1	D	142	TRP	2.3
1	H	139	ARG	2.3
1	G	226	ALA	2.3
1	H	140	ILE	2.3
1	B	354	LEU	2.3
1	D	145	HIS	2.3
1	H	487	LYS	2.3
1	B	486	GLN	2.3
1	G	466	TRP	2.3
1	A	487	LYS	2.2
1	F	188	ARG	2.2
1	C	466	TRP	2.2
1	A	217	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	217	CYS	2.2
1	G	251	THR	2.1
1	B	493	MET	2.1
1	E	53	LEU	2.1
1	G	215	GLU	2.1
1	C	139	ARG	2.1
1	C	246	GLN	2.1
1	A	420	LEU	2.1
1	F	141	ASP	2.1
1	F	230	ASP	2.1
1	H	249	ASP	2.1
1	C	218	GLU	2.1
1	B	2	THR	2.1
1	G	217	CYS	2.1
1	E	487	LYS	2.1
1	D	246	GLN	2.1
1	F	499	LEU	2.1
1	F	137	GLY	2.1
1	C	144	TYR	2.1
1	C	231	GLU	2.0
1	H	135	LYS	2.0
1	C	183	ASN	2.0
1	F	246	GLN	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	DDZ	A	54[B]	7/8	-	-	25,32,34,36	7
1	DDZ	B	54[B]	7/8	-	-	21,25,32,36	7
1	DDZ	C	54[B]	7/8	-	-	28,31,34,52	7
1	DDZ	D	54[B]	7/8	-	-	25,27,34,38	7
1	DDZ	E	54[B]	7/8	-	-	25,30,44,54	7
1	DDZ	F	54[B]	7/8	-	-	32,35,37,45	7
1	DDZ	G	54[B]	7/8	-	-	31,33,33,35	7
1	DDZ	H	54[B]	7/8	-	-	38,43,62,62	7

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
2	CA	E	601	1/1	0.09	0.52	61,61,61,61	1
2	CA	D	601	1/1	0.32	0.40	48,48,48,48	1
2	CA	B	601	1/1	0.43	0.31	48,48,48,48	1
2	CA	F	601	1/1	0.55	0.21	42,42,42,42	1
2	CA	A	601	1/1	0.59	0.16	45,45,45,45	1
2	CA	H	601	1/1	0.76	0.22	50,50,50,50	1
2	CA	G	601	1/1	0.91	0.11	47,47,47,47	1
2	CA	C	601	1/1	0.95	0.07	21,21,21,21	1

6.5 Other polymers [i](#)

There are no such residues in this entry.