



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 1, 2024 – 02:13 PM EDT

PDB ID : 8S9J
Title : FphA, Staphylococcus aureus fluorophosphonate-binding serine hydrolases A, apo form
Authors : Fellner, M.
Deposited on : 2023-03-28
Resolution : 2.25 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.1

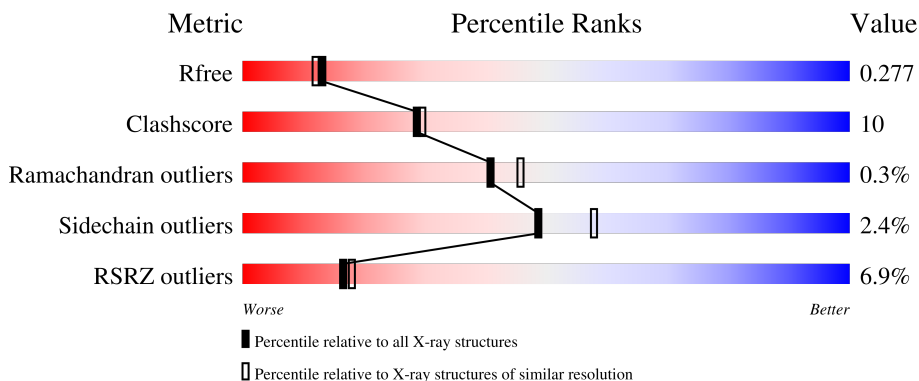
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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.



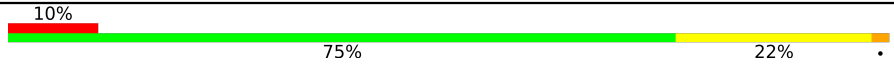

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	453	
1	B	453	
1	C	453	
1	D	453	
1	E	453	

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Mol	Chain	Length	Quality of chain
1	F	453	
1	G	453	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 26026 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 Fluorophosphonate-binding serine hydrolase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	452	3705	2372	619	696	18	0	3	0
1	B	452	3668	2350	613	687	18	0	1	0
1	C	452	3686	2363	619	686	18	0	3	0
1	D	451	3664	2350	612	684	18	0	2	0
1	E	452	3581	2296	599	670	16	0	1	0
1	F	452	3577	2290	602	668	17	0	1	0
1	G	452	3605	2315	603	671	16	0	1	0

There are 21 discrepancies between the modelled and reference sequences:

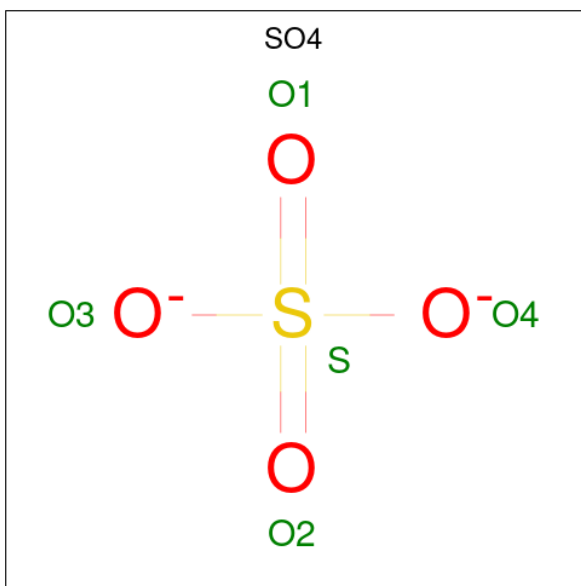
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A0A0D6GYZ4
A	-1	PRO	-	expression tag	UNP A0A0D6GYZ4
A	0	GLY	-	expression tag	UNP A0A0D6GYZ4
B	-2	GLY	-	expression tag	UNP A0A0D6GYZ4
B	-1	PRO	-	expression tag	UNP A0A0D6GYZ4
B	0	GLY	-	expression tag	UNP A0A0D6GYZ4
C	-2	GLY	-	expression tag	UNP A0A0D6GYZ4
C	-1	PRO	-	expression tag	UNP A0A0D6GYZ4
C	0	GLY	-	expression tag	UNP A0A0D6GYZ4
D	-2	GLY	-	expression tag	UNP A0A0D6GYZ4
D	-1	PRO	-	expression tag	UNP A0A0D6GYZ4
D	0	GLY	-	expression tag	UNP A0A0D6GYZ4
E	-2	GLY	-	expression tag	UNP A0A0D6GYZ4
E	-1	PRO	-	expression tag	UNP A0A0D6GYZ4
E	0	GLY	-	expression tag	UNP A0A0D6GYZ4

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	GLY	-	expression tag	UNP A0A0D6GYZ4
F	-1	PRO	-	expression tag	UNP A0A0D6GYZ4
F	0	GLY	-	expression tag	UNP A0A0D6GYZ4
G	-2	GLY	-	expression tag	UNP A0A0D6GYZ4
G	-1	PRO	-	expression tag	UNP A0A0D6GYZ4
G	0	GLY	-	expression tag	UNP A0A0D6GYZ4

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		

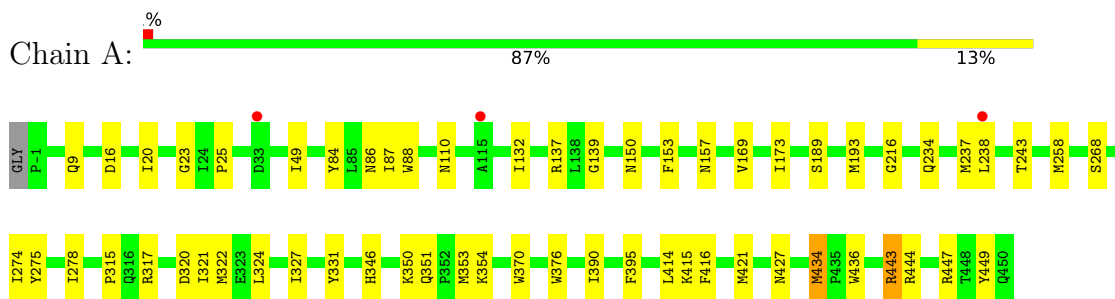
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	131	Total 131	O 131	0	0
3	B	47	Total 47	O 47	0	0
3	C	63	Total 63	O 63	0	0
3	D	65	Total 65	O 65	0	0
3	E	41	Total 41	O 41	0	0
3	F	30	Total 30	O 30	0	0
3	G	23	Total 23	O 23	0	0

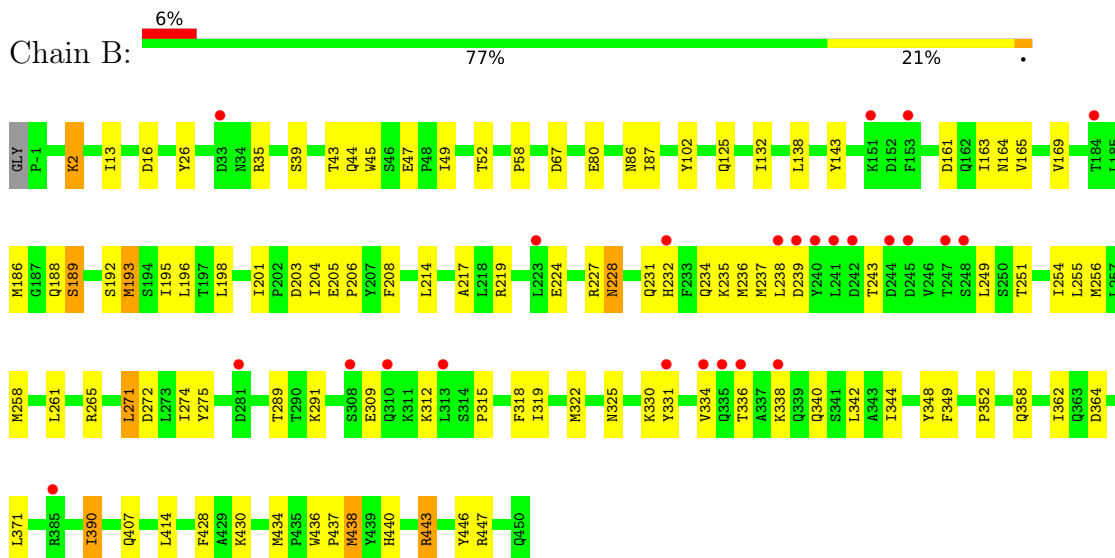
3 Residue-property plots [i](#)

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

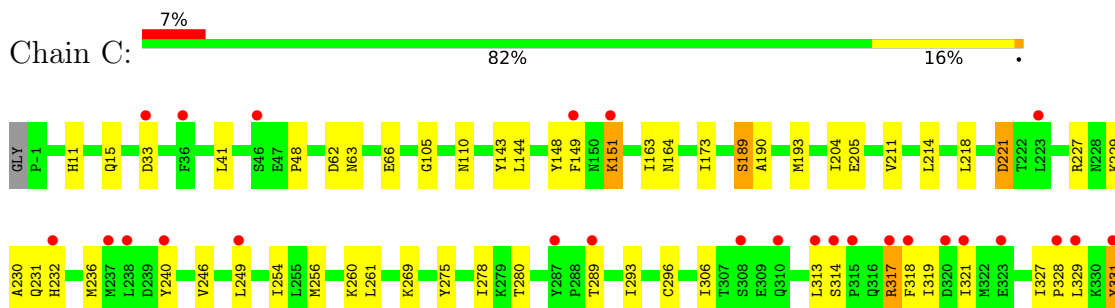
- Molecule 1: Fluorophosphonate-binding serine hydrolase A

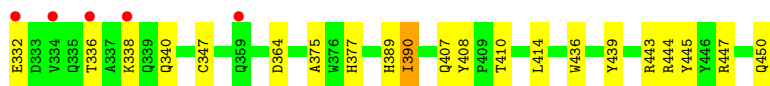


- Molecule 1: Fluorophosphonate-binding serine hydrolase A

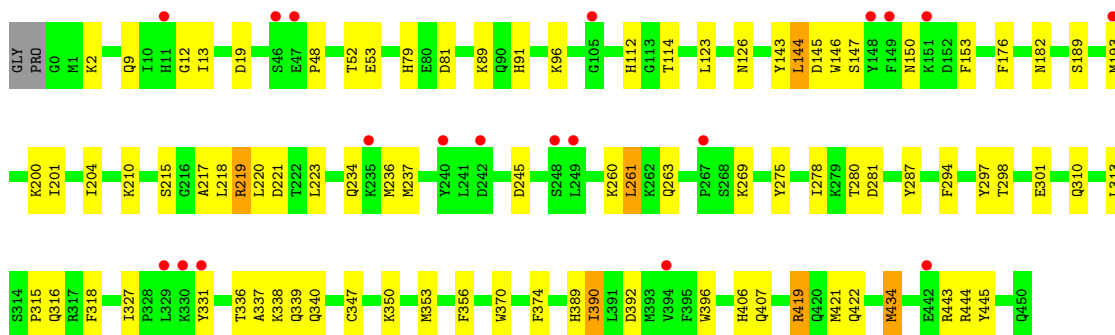
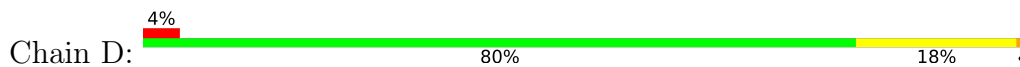


- Molecule 1: Fluorophosphonate-binding serine hydrolase A

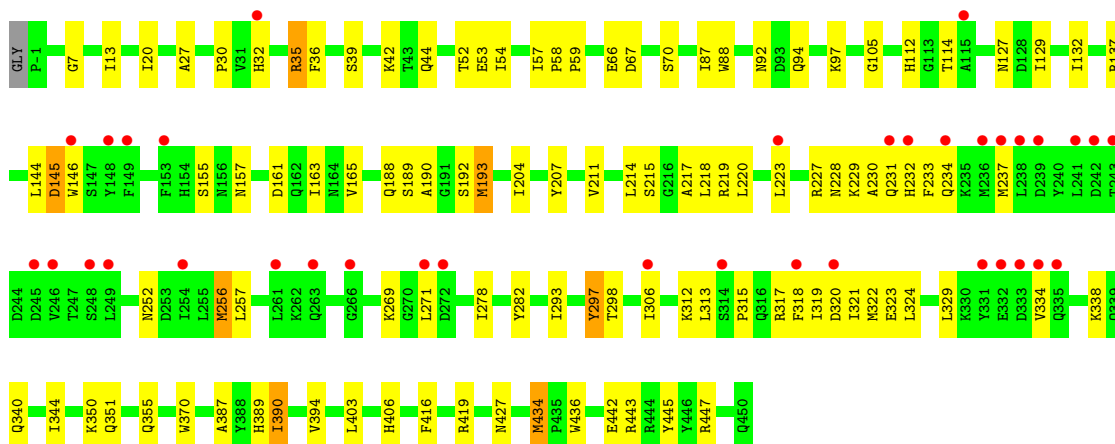
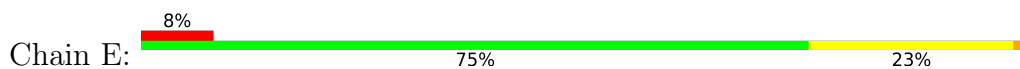




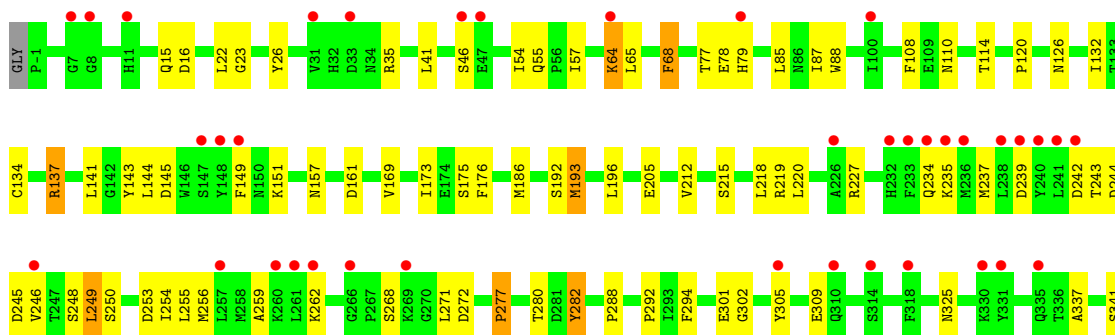
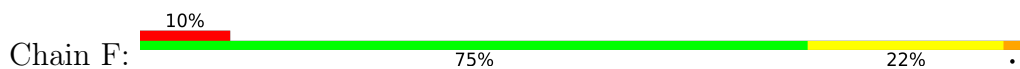
- Molecule 1: Fluorophosphonate-binding serine hydrolase A

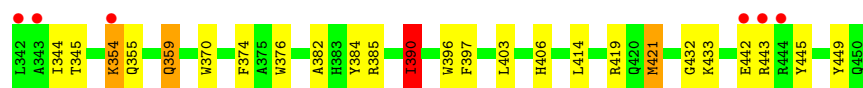


- Molecule 1: Fluorophosphonate-binding serine hydrolase A

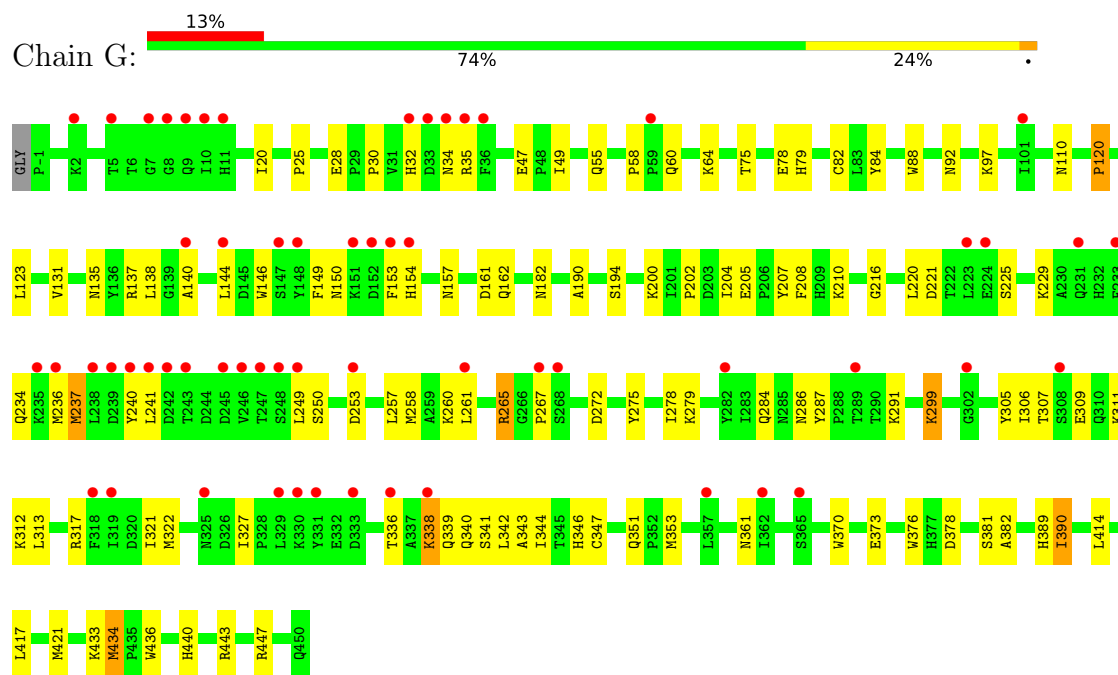


- Molecule 1: Fluorophosphonate-binding serine hydrolase A





● Molecule 1: Fluorophosphonate-binding serine hydrolase A



4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	313.04Å 313.04Å 185.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.50 – 2.25 49.50 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.5 (49.50-2.25) 98.5 (49.50-2.25)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.25Å)	Xtrriage
Refinement program	PHENIX 1.20.1-4487	Depositor
R, R_{free}	0.241 , 0.277 0.240 , 0.277	Depositor DCC
R_{free} test set	10754 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	41.9	Xtrriage
Anisotropy	0.192	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	26026	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.70% 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: SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.47	0/3807	0.63	1/5166 (0.0%)
1	B	0.43	0/3769	0.61	1/5117 (0.0%)
1	C	0.41	0/3790	0.60	0/5147
1	D	0.43	0/3766	0.60	0/5115
1	E	0.43	0/3678	0.64	2/5004 (0.0%)
1	F	0.43	1/3674 (0.0%)	0.66	4/4995 (0.1%)
1	G	0.42	1/3707 (0.0%)	0.60	0/5044
All	All	0.43	2/26191 (0.0%)	0.62	8/35588 (0.0%)

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	F	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	277	PRO	N-CD	9.55	1.61	1.47
1	G	202	PRO	N-CD	6.23	1.56	1.47

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	390	ILE	N-CA-C	8.28	133.35	111.00
1	F	390	ILE	CB-CA-C	-7.97	95.67	111.60
1	F	277	PRO	CA-N-CD	-6.86	101.90	111.50
1	F	41	LEU	CA-CB-CG	5.99	129.07	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	145	ASP	CB-CG-OD2	5.20	122.98	118.30
1	E	145	ASP	N-CA-C	-5.19	97.00	111.00
1	B	271	LEU	CA-CB-CG	5.15	127.15	115.30
1	A	350	LYS	CD-CE-NZ	5.06	123.34	111.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	137	ARG	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	3705	0	3583	38	0
1	B	3668	0	3547	68	0
1	C	3686	0	3549	60	0
1	D	3664	0	3527	66	0
1	E	3581	0	3402	81	0
1	F	3577	0	3373	88	0
1	G	3605	0	3417	93	0
2	A	30	0	0	1	0
2	B	20	0	0	0	0
2	C	25	0	0	2	0
2	D	20	0	0	1	0
2	E	20	0	0	2	0
2	F	15	0	0	1	0
2	G	10	0	0	0	0
3	A	131	0	0	3	0
3	B	47	0	0	0	0
3	C	63	0	0	0	0
3	D	65	0	0	2	0
3	E	41	0	0	1	0
3	F	30	0	0	0	0
3	G	23	0	0	0	0
All	All	26026	0	24398	487	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 10.

All (487) 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:G:216:GLY:H	1:G:353:MET:HE3	1.17	1.08
1:F:137:ARG:HH21	1:F:157:ASN:HB3	1.39	0.86
1:F:120:PRO:HB3	1:F:397:PHE:CE2	2.14	0.82
1:F:141:LEU:H	1:F:141:LEU:HD12	1.45	0.82
1:D:297:TYR:CE1	1:D:350:LYS:HD2	2.19	0.78
1:G:208:PHE:O	1:G:291:LYS:NZ	2.17	0.78
1:C:249:LEU:HD23	1:C:254:ILE:HG13	1.66	0.78
1:G:216:GLY:N	1:G:353:MET:HE3	1.97	0.77
1:F:243:THR:HG22	1:F:245:ASP:H	1.50	0.77
1:G:200:LYS:HE2	1:G:287:TYR:CE1	2.19	0.77
1:F:57:ILE:HD11	1:F:78:GLU:HG2	1.68	0.75
1:D:236:MET:HE1	1:D:260:LYS:HB2	1.69	0.74
1:E:145:ASP:OD2	1:E:223:LEU:HD11	1.88	0.73
1:B:440:HIS:HB2	1:B:443:ARG:HH21	1.50	0.73
1:E:252:ASN:O	1:E:256:MET:SD	2.47	0.73
1:E:315:PRO:O	1:E:319:ILE:HD13	1.88	0.73
1:D:310:GLN:N	1:D:310:GLN:OE1	2.22	0.73
1:C:269:LYS:HD3	1:C:313:LEU:HD21	1.70	0.72
1:D:336:THR:HG23	1:D:339:GLN:H	1.53	0.72
1:D:123:LEU:HD13	1:D:422:GLN:HG2	1.73	0.71
1:F:259:ALA:HA	1:F:262:LYS:HD2	1.72	0.71
1:A:354:LYS:NZ	2:A:506:SO4:O3	2.21	0.71
1:C:377:HIS:NE2	2:C:505:SO4:O4	2.21	0.71
1:G:340:GLN:O	1:G:344:ILE:HD12	1.89	0.70
1:C:332:GLU:OE1	1:C:332:GLU:N	2.18	0.70
1:F:120:PRO:HB3	1:F:397:PHE:CD2	2.27	0.70
1:C:443:ARG:HH11	1:C:443:ARG:HG2	1.56	0.70
1:B:13:ILE:HD11	1:B:52:THR:HA	1.72	0.70
1:F:443:ARG:HB3	1:F:445:TYR:CE1	2.26	0.70
1:E:322:MET:HG3	1:E:329:LEU:CD1	2.22	0.70
1:G:234:GLN:HA	1:G:237:MET:HG3	1.73	0.70
1:F:370:TRP:CH2	1:F:433:LYS:HA	2.27	0.69
1:F:302:GLY:H	1:F:345:THR:HG22	1.57	0.69
1:E:137:ARG:HH21	1:E:157:ASN:CB	2.06	0.69
1:F:87:ILE:HG12	1:F:132:ILE:HG12	1.73	0.68
1:F:309:GLU:HG3	1:F:337:ALA:HB2	1.74	0.68
1:E:442:GLU:HG2	1:E:443:ARG:H	1.56	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:TYR:HB2	1:C:275:TYR:HB3	1.76	0.68
1:G:190:ALA:O	1:G:194:SER:OG	2.12	0.68
1:B:188:GLN:HE22	1:B:390:ILE:HG12	1.59	0.67
1:A:278:ILE:CD1	3:A:649:HOH:O	2.42	0.67
1:E:442:GLU:HG2	1:E:443:ARG:N	2.10	0.67
1:F:143:TYR:CE2	1:F:277:PRO:HD3	2.31	0.66
1:C:221:ASP:OD2	1:C:229:LYS:NZ	2.27	0.66
1:E:351:GLN:O	1:E:355:GLN:HG2	1.94	0.66
1:G:32:HIS:H	1:G:35:ARG:HH21	1.41	0.66
1:E:297:TYR:CD2	1:E:350:LYS:HG2	2.31	0.66
1:F:302:GLY:HA2	1:F:305:TYR:HD2	1.60	0.66
1:G:341:SER:HA	1:G:344:ILE:HD13	1.76	0.66
1:C:246:VAL:HA	1:C:249:LEU:HD13	1.78	0.65
1:E:229:LYS:O	1:E:233:PHE:HB2	1.97	0.65
1:C:163:ILE:HG23	1:C:204:ILE:HG21	1.77	0.65
1:C:227:ARG:HG3	1:C:227:ARG:HH11	1.60	0.65
1:A:139:GLY:HA2	1:A:275:TYR:CD2	2.31	0.65
1:F:219:ARG:NH1	1:F:325:ASN:O	2.29	0.65
1:E:338:LYS:NZ	3:E:603:HOH:O	2.30	0.65
1:F:126:ASN:HB3	1:F:419:ARG:NH1	2.13	0.64
1:D:297:TYR:CZ	1:D:350:LYS:HD2	2.33	0.64
1:E:20:ILE:HG12	1:E:88:TRP:CD1	2.33	0.64
1:A:234:GLN:HA	1:A:237:MET:HE3	1.80	0.63
1:A:278:ILE:HD12	3:A:649:HOH:O	1.97	0.63
1:B:201:ILE:HB	1:B:204:ILE:HD11	1.79	0.63
1:E:237:MET:HG3	1:E:257:LEU:HD11	1.79	0.63
1:B:254:ILE:O	1:B:258:MET:HG3	1.98	0.63
1:A:139:GLY:HA2	1:A:275:TYR:HD2	1.63	0.63
1:D:114:THR:HG21	3:D:649:HOH:O	1.97	0.63
1:E:322:MET:HG3	1:E:329:LEU:HD11	1.81	0.63
1:F:215:SER:OG	1:F:301:GLU:OE2	2.17	0.63
1:D:114:THR:CG2	3:D:649:HOH:O	2.47	0.62
1:G:47:GLU:OE1	1:G:47:GLU:HA	1.98	0.62
1:F:137:ARG:HH21	1:F:157:ASN:CB	2.10	0.62
1:C:319:ILE:HD11	1:C:331:TYR:HA	1.81	0.62
1:B:35:ARG:NH2	1:B:80:GLU:OE2	2.30	0.62
1:D:234:GLN:HA	1:D:237:MET:HG3	1.81	0.62
1:E:317:ARG:O	1:E:321:ILE:HG13	2.00	0.62
1:B:315:PRO:HB2	1:B:331:TYR:CE1	2.35	0.62
1:F:385:ARG:HG3	1:F:385:ARG:HH11	1.64	0.61
1:A:268:SER:HB2	1:A:321:ILE:HD12	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:212:VAL:HG13	1:F:294:PHE:HD2	1.65	0.61
1:B:255:LEU:HD23	1:B:258:MET:HE3	1.83	0.61
1:E:227:ARG:O	1:E:231:GLN:N	2.28	0.61
1:A:258:MET:HE2	3:A:717:HOH:O	2.01	0.61
1:F:246:VAL:HA	1:F:249:LEU:CD1	2.31	0.60
1:G:240:TYR:CE2	1:G:260:LYS:HE3	2.36	0.60
1:F:249:LEU:HB3	1:F:253:ASP:HB2	1.83	0.60
1:A:421:MET:HE3	1:A:449:TYR:CG	2.37	0.60
1:B:2:LYS:H	1:B:2:LYS:HD3	1.66	0.60
1:D:182:ASN:OD1	1:D:210:LYS:NZ	2.34	0.60
1:A:415:LYS:NZ	1:C:410:THR:O	2.34	0.60
1:G:249:LEU:CD2	1:G:253:ASP:HB3	2.32	0.60
1:G:261:LEU:O	1:G:261:LEU:HD12	2.02	0.59
1:G:110:ASN:HA	1:G:138:LEU:HD13	1.84	0.59
1:D:193[A]:MET:HG2	1:D:217:ALA:O	2.02	0.59
1:F:243:THR:HG21	1:F:248:SER:OG	2.03	0.59
1:C:249:LEU:HD23	1:C:254:ILE:CG1	2.31	0.59
1:A:274:ILE:HG22	1:A:275:TYR:CE1	2.38	0.59
1:G:417:LEU:O	1:G:421:MET:HG3	2.02	0.59
1:G:261:LEU:O	1:G:265:ARG:HG3	2.03	0.59
1:E:54:ILE:HG23	1:E:114:THR:HG21	1.84	0.58
1:B:192:SER:O	1:B:196:LEU:HD13	2.04	0.58
1:C:11[B]:HIS:CE1	1:C:48:PRO:HB2	2.38	0.58
1:C:306:ILE:HG13	1:C:340:GLN:HB3	1.85	0.58
1:D:89:LYS:HE3	1:D:176:PHE:O	2.03	0.58
1:F:370:TRP:CZ3	1:F:433:LYS:HA	2.38	0.58
1:E:443:ARG:HD3	1:E:445:TYR:CE2	2.38	0.58
1:E:271:LEU:HD23	1:E:322:MET:HE1	1.86	0.58
1:B:219:ARG:NH2	1:B:348:TYR:O	2.36	0.58
1:F:442:GLU:HA	1:F:442:GLU:OE1	2.03	0.58
1:B:163:ILE:HG23	1:B:204:ILE:CG2	2.34	0.58
1:G:317:ARG:CZ	1:G:321:ILE:HD11	2.34	0.58
1:C:318:PHE:CD1	1:C:340:GLN:HG2	2.39	0.57
1:E:370:TRP:CD1	1:E:434:MET:HB2	2.39	0.57
1:G:299:LYS:HG3	1:G:373:GLU:OE2	2.04	0.57
1:C:11[B]:HIS:CE1	1:C:48:PRO:CB	2.87	0.57
1:C:204:ILE:C	1:C:204:ILE:HD12	2.24	0.57
1:G:361:ASN:ND2	1:G:440:HIS:HA	2.19	0.57
1:A:25:PRO:HD2	1:A:49:ILE:HD13	1.87	0.57
1:B:237:MET:SD	1:B:249:LEU:HD11	2.44	0.57
1:B:47:GLU:OE1	1:B:47:GLU:HA	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:440:HIS:HB2	1:B:443:ARG:NH2	2.20	0.57
1:C:193[A]:MET:HG3	1:C:218:LEU:HD12	1.86	0.57
1:E:256:MET:SD	1:E:256:MET:N	2.78	0.56
1:B:318:PHE:CD1	1:B:334:VAL:HG11	2.40	0.56
1:B:195:ILE:HA	1:B:198:LEU:HD12	1.86	0.56
1:F:141:LEU:H	1:F:141:LEU:CD1	2.10	0.56
1:B:16:ASP:O	1:B:125:GLN:NE2	2.38	0.56
1:D:297:TYR:HB3	1:D:353:MET:CE	2.36	0.56
1:B:371:LEU:HD23	1:B:446:TYR:HB3	1.88	0.56
1:D:297:TYR:CE1	1:D:350:LYS:CD	2.89	0.56
1:E:105:GLY:HA2	1:E:190:ALA:HB3	1.88	0.56
1:E:322:MET:HG3	1:E:329:LEU:HD12	1.88	0.55
1:C:144:LEU:HD11	1:C:230:ALA:HA	1.89	0.55
1:D:370:TRP:CD1	1:D:434:MET:HB2	2.41	0.55
1:F:173:ILE:HD12	1:F:176:PHE:HD2	1.72	0.55
1:F:192:SER:O	1:F:196:LEU:HD12	2.06	0.55
1:A:189:SER:O	1:A:193[A]:MET:HG3	2.06	0.55
1:E:218:LEU:HD11	1:E:220:LEU:HG	1.89	0.55
1:E:297:TYR:CE2	1:E:350:LYS:HG2	2.42	0.55
1:G:25:PRO:HD2	1:G:49:ILE:HD12	1.89	0.54
1:E:271:LEU:HD23	1:E:322:MET:CE	2.37	0.54
1:F:271:LEU:HD11	1:F:344:ILE:HD11	1.89	0.54
1:G:92:ASN:OD1	1:G:97:LYS:NZ	2.40	0.54
1:A:370:TRP:CD1	1:A:434:MET:HB2	2.42	0.54
1:E:137:ARG:HH21	1:E:157:ASN:HB3	1.71	0.54
1:F:35:ARG:NH2	1:F:254:ILE:HD11	2.23	0.54
1:E:436:TRP:CD2	1:E:447:ARG:HB2	2.43	0.54
1:G:344:ILE:HD12	1:G:344:ILE:H	1.72	0.54
1:C:328:PRO:O	1:C:329:LEU:HD23	2.07	0.54
1:D:294:PHE:CD2	1:D:434:MET:HE2	2.42	0.54
1:F:143:TYR:CD2	1:F:277:PRO:HD3	2.43	0.54
1:G:309:GLU:OE1	1:G:312:LYS:HD3	2.07	0.54
1:C:336:THR:HG22	1:C:338:LYS:N	2.23	0.53
1:A:20:ILE:HG12	1:A:88:TRP:CD1	2.44	0.53
1:A:436:TRP:CD2	1:A:447:ARG:HB2	2.44	0.53
1:E:30:PRO:HB3	1:E:137:ARG:HH11	1.73	0.53
1:C:211:VAL:HG22	1:C:293:ILE:HG12	1.91	0.53
1:G:336:THR:OG1	1:G:339:GLN:HG3	2.09	0.53
1:B:189:SER:O	1:B:193[B]:MET:HG3	2.08	0.53
1:B:87:ILE:HG12	1:B:132:ILE:HG12	1.90	0.53
1:D:13:ILE:CD1	1:D:52:THR:HG22	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:317:ARG:HG3	1:E:321:ILE:HD11	1.91	0.53
1:B:436:TRP:CD2	1:B:447:ARG:HB2	2.43	0.53
1:F:271:LEU:HD11	1:F:344:ILE:CD1	2.39	0.53
1:C:443:ARG:HD2	1:C:445:TYR:CE2	2.44	0.53
1:A:322:MET:HB3	1:A:327:ILE:HB	1.90	0.52
1:B:163:ILE:HG12	1:B:204:ILE:HD13	1.91	0.52
1:D:53:GLU:OE2	1:G:75:THR:HG23	2.09	0.52
1:A:87:ILE:HG12	1:A:132:ILE:HG12	1.92	0.52
1:F:144:LEU:HD12	1:F:145:ASP:H	1.75	0.52
1:G:376:TRP:CE2	1:G:414:LEU:HD21	2.44	0.52
1:G:88:TRP:CD2	1:G:120:PRO:HD2	2.45	0.52
1:E:193:MET:CE	1:E:219:ARG:H	2.23	0.52
1:F:341:SER:O	1:F:345:THR:HG23	2.09	0.52
1:B:80:GLU:OE2	1:B:251:THR:HG22	2.10	0.52
1:E:87:ILE:HG12	1:E:132:ILE:HG12	1.92	0.52
1:B:232:HIS:CE1	1:B:261:LEU:HD13	2.44	0.52
1:E:297:TYR:CD1	1:E:297:TYR:N	2.77	0.52
1:F:302:GLY:HA2	1:F:305:TYR:CD2	2.43	0.51
1:G:58:PRO:HG2	1:G:138:LEU:HD12	1.91	0.51
1:F:57:ILE:CD1	1:F:78:GLU:HG2	2.38	0.51
1:B:163:ILE:HG12	1:B:204:ILE:HG21	1.93	0.51
1:B:224:GLU:O	1:B:228:ASN:HB2	2.10	0.51
1:D:389:HIS:CD2	1:D:390:ILE:HG13	2.46	0.51
1:C:336:THR:HG22	1:C:338:LYS:H	1.73	0.51
1:F:390:ILE:HG22	1:F:390:ILE:O	2.09	0.51
1:D:9:GLN:HB3	1:D:48:PRO:HB3	1.91	0.51
1:F:64:LYS:HG3	1:F:65:LEU:HD22	1.93	0.51
1:B:255:LEU:HA	1:B:258:MET:HE2	1.93	0.51
1:B:336:THR:HG22	1:B:338:LYS:N	2.25	0.51
1:D:406:HIS:O	1:D:407:GLN:HG2	2.11	0.51
1:D:278:ILE:N	1:D:278:ILE:HD12	2.26	0.51
1:G:265:ARG:NH1	1:G:272:ASP:OD2	2.45	0.50
1:G:327:ILE:HG21	1:G:347:CYS:HB3	1.93	0.50
1:B:235:LYS:HE2	1:B:239:ASP:OD2	2.11	0.50
1:B:265:ARG:NH1	1:B:272:ASP:OD1	2.44	0.50
1:F:205:GLU:OE2	1:F:288:PRO:HB3	2.11	0.50
1:G:140:ALA:O	1:G:146:TRP:HZ2	1.94	0.50
1:E:193:MET:HE3	1:E:219:ARG:H	1.77	0.50
1:C:204:ILE:HD12	1:C:205:GLU:N	2.26	0.50
1:G:137:ARG:CZ	1:G:157:ASN:HB3	2.41	0.50
1:G:338:LYS:HD3	1:G:342:LEU:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:443:ARG:HD2	1:C:445:TYR:HE2	1.76	0.50
1:C:444:ARG:HD2	2:C:504:SO4:O2	2.12	0.50
1:G:182:ASN:OD1	1:G:210:LYS:NZ	2.44	0.50
1:G:220:LEU:HD13	1:G:279:LYS:HG2	1.94	0.50
1:G:137:ARG:NH2	1:G:161:ASP:OD1	2.42	0.49
1:A:238:LEU:HD23	1:A:243:THR:O	2.13	0.49
1:B:39:SER:OG	1:B:164:ASN:ND2	2.42	0.49
1:E:30:PRO:HB3	1:E:137:ARG:NH1	2.27	0.49
1:D:297:TYR:HB3	1:D:353:MET:HE1	1.94	0.49
1:F:235:LYS:NZ	1:F:239:ASP:OD2	2.39	0.49
1:F:246:VAL:HA	1:F:249:LEU:HD11	1.93	0.49
1:F:396:TRP:CE3	1:F:421:MET:HB3	2.47	0.49
1:G:312:LYS:HB2	1:G:340:GLN:OE1	2.13	0.49
1:A:376:TRP:CZ2	1:A:414:LEU:HD21	2.47	0.49
1:E:394:VAL:HG11	1:E:403:LEU:HD21	1.94	0.49
1:G:221:ASP:HB3	1:G:278:ILE:HD12	1.95	0.49
1:B:340:GLN:O	1:B:344:ILE:HD12	2.13	0.49
1:C:318:PHE:HB2	1:C:340:GLN:HE21	1.77	0.49
1:D:79[A]:HIS:ND1	1:D:81:ASP:HB3	2.28	0.49
1:C:149:PHE:CG	1:C:246:VAL:HG21	2.48	0.49
1:C:318:PHE:CE1	1:C:340:GLN:HG2	2.48	0.49
1:B:165:VAL:O	1:B:169:VAL:HG23	2.13	0.48
1:D:336:THR:CG2	1:D:339:GLN:HB2	2.43	0.48
1:E:112:HIS:ND1	1:E:114:THR:OG1	2.40	0.48
1:B:58:PRO:HB2	1:B:138:LEU:HD12	1.96	0.48
1:B:188:GLN:NE2	1:B:390:ILE:HG12	2.28	0.48
1:F:151:LYS:HE2	1:F:151:LYS:H	1.79	0.48
1:B:334:VAL:HG12	1:B:334:VAL:O	2.14	0.48
1:D:221:ASP:HB3	1:D:278:ILE:HG13	1.96	0.48
1:F:212:VAL:HG13	1:F:294:PHE:CD2	2.46	0.48
1:A:216:GLY:H	1:A:353:MET:HE1	1.78	0.48
1:A:317:ARG:O	1:A:321:ILE:HG12	2.13	0.48
1:E:297:TYR:HE2	1:E:350:LYS:CE	2.27	0.48
1:G:361:ASN:HD21	1:G:440:HIS:HA	1.77	0.48
1:B:236:MET:HE2	1:B:236:MET:HB2	1.52	0.48
1:A:346:HIS:CE1	1:A:351:GLN:HG3	2.49	0.48
1:D:200:LYS:HE3	1:D:287:TYR:CE1	2.49	0.48
1:G:267:PRO:HB2	1:G:313:LEU:HD21	1.95	0.48
1:B:234:GLN:HA	1:B:237:MET:HE2	1.96	0.48
1:B:315:PRO:O	1:B:319:ILE:HD13	2.14	0.48
1:C:289:THR:HG21	1:C:364:ASP:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:268:SER:HB2	1:F:272:ASP:H	1.78	0.48
1:G:370:TRP:CD1	1:G:434:MET:HB2	2.49	0.48
1:F:302:GLY:H	1:F:345:THR:CG2	2.24	0.47
1:F:421:MET:HE3	1:F:449:TYR:CG	2.49	0.47
1:G:225:SER:OG	1:G:229:LYS:HE3	2.14	0.47
1:G:340:GLN:O	1:G:343:ALA:N	2.47	0.47
1:C:314:SER:HB3	1:C:317:ARG:HB3	1.96	0.47
1:F:250:SER:OG	1:F:253:ASP:OD1	2.26	0.47
1:B:227:ARG:O	1:B:231:GLN:HG3	2.14	0.47
1:C:214:LEU:HD23	1:C:296:CYS:HB3	1.96	0.47
1:D:19:ASP:OD1	1:D:91:HIS:ND1	2.39	0.47
1:D:396:TRP:CZ3	1:D:421:MET:HB3	2.49	0.47
1:F:376:TRP:CZ2	1:F:414:LEU:HD11	2.49	0.47
1:F:382:ALA:HA	1:F:385:ARG:NH2	2.30	0.47
1:G:60:GLN:OE1	1:G:110:ASN:HB2	2.15	0.47
1:G:249:LEU:HD22	1:G:253:ASP:HB3	1.95	0.47
1:G:307:THR:OG1	1:G:311:LYS:HD2	2.14	0.47
1:E:57:ILE:HD12	1:E:58:PRO:O	2.15	0.47
1:F:370:TRP:CZ3	1:F:432:GLY:O	2.68	0.47
1:G:150:ASN:HB3	1:G:153:PHE:CD2	2.49	0.47
1:C:436:TRP:CD2	1:C:447:ARG:HB2	2.50	0.47
1:D:193[B]:MET:HG3	1:D:218:LEU:HA	1.97	0.47
1:F:54:ILE:HG23	1:F:114:THR:HG21	1.96	0.47
1:F:376:TRP:CE2	1:F:414:LEU:HD11	2.49	0.47
1:B:436:TRP:HB2	1:B:437:PRO:HD2	1.96	0.47
1:C:240:TYR:CE2	1:C:260:LYS:HE2	2.50	0.47
1:G:389:HIS:C	1:G:390:ILE:HG13	2.35	0.47
1:F:249:LEU:HD12	1:F:249:LEU:H	1.80	0.47
1:A:16:ASP:OD1	1:C:407:GLN:NE2	2.37	0.47
1:G:28:GLU:OE1	1:G:28:GLU:HA	2.15	0.46
1:G:200:LYS:HD3	1:G:284:GLN:O	2.15	0.46
1:G:237:MET:O	1:G:241:LEU:HB2	2.16	0.46
1:E:297:TYR:HE2	1:E:350:LYS:CD	2.28	0.46
1:D:143:TYR:HB2	1:D:275:TYR:HB3	1.98	0.46
1:G:221:ASP:HB3	1:G:278:ILE:CD1	2.46	0.46
1:A:169:VAL:HG13	1:A:173:ILE:HB	1.96	0.46
1:B:265:ARG:HD2	1:B:274:ILE:HG12	1.98	0.46
1:F:301:GLU:HB2	1:F:345:THR:HG22	1.97	0.46
1:B:208:PHE:O	1:B:291:LYS:NZ	2.35	0.46
1:F:173:ILE:HD12	1:F:176:PHE:CD2	2.51	0.46
1:F:23:GLY:HA3	1:F:55:GLN:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:30:PRO:HA	1:G:34:ASN:HB2	1.97	0.46
1:G:370:TRP:CH2	1:G:433:LYS:HG2	2.51	0.46
1:B:309:GLU:O	1:B:312:LYS:HD3	2.15	0.46
1:E:42:LYS:NZ	2:E:501:SO4:O1	2.49	0.46
1:E:269:LYS:HG2	1:E:313:LEU:HD21	1.98	0.46
1:G:20:ILE:HG12	1:G:88:TRP:CD1	2.50	0.46
1:G:250:SER:H	1:G:253:ASP:HB2	1.81	0.46
1:G:322:MET:HB3	1:G:327:ILE:HB	1.98	0.46
1:C:443:ARG:HG2	1:C:443:ARG:NH1	2.23	0.46
1:F:186:MET:HG3	1:F:212:VAL:HB	1.98	0.46
1:G:88:TRP:CE3	1:G:120:PRO:CD	2.99	0.46
1:F:193:MET:HE2	1:F:193:MET:HB2	1.81	0.45
1:G:317:ARG:HA	1:G:317:ARG:HD2	1.74	0.45
1:E:163:ILE:HG23	1:E:204:ILE:HD13	1.98	0.45
1:F:370:TRP:HZ3	1:F:432:GLY:O	1.99	0.45
1:G:436:TRP:CE3	1:G:447:ARG:HD3	2.51	0.45
1:E:230:ALA:O	1:E:234:GLN:N	2.46	0.45
1:G:25:PRO:CD	1:G:49:ILE:HD12	2.46	0.45
1:G:146:TRP:HD1	1:G:154:HIS:O	1.99	0.45
1:C:105:GLY:HA2	1:C:190:ALA:HB3	1.97	0.45
1:C:317:ARG:NH1	1:C:321:ILE:HD11	2.31	0.45
1:E:228:ASN:O	1:E:232:HIS:N	2.28	0.45
1:G:140:ALA:O	1:G:146:TRP:CZ2	2.69	0.45
1:C:41:LEU:HB2	1:C:164:ASN:OD1	2.17	0.45
1:D:219:ARG:CG	1:D:219:ARG:HH11	2.29	0.45
1:E:389:HIS:O	1:E:390:ILE:HB	2.16	0.45
1:F:68:PHE:C	1:F:68:PHE:CD1	2.90	0.45
1:G:88:TRP:CE3	1:G:120:PRO:HD2	2.51	0.45
1:B:289:THR:HG21	1:B:364:ASP:HB2	1.99	0.45
1:G:258:MET:HG2	1:G:275:TYR:OH	2.15	0.45
1:G:381:SER:OG	1:G:382:ALA:N	2.50	0.45
1:E:137:ARG:HH21	1:E:157:ASN:CG	2.19	0.45
1:F:169:VAL:HG13	1:F:173:ILE:HB	1.99	0.45
1:F:280:THR:OG1	1:F:282:TYR:CD1	2.65	0.45
1:F:385:ARG:HH11	1:F:385:ARG:CG	2.29	0.45
1:B:43:THR:HG22	1:B:44:GLN:HG2	1.99	0.45
1:B:414:LEU:HD23	1:B:414:LEU:HA	1.81	0.45
1:E:193:MET:HG3	1:E:217:ALA:O	2.17	0.45
1:F:88:TRP:CD2	1:F:120:PRO:HD2	2.51	0.45
1:G:144:LEU:HD23	1:G:146:TRP:CZ3	2.51	0.45
1:G:305:TYR:C	1:G:306:ILE:HD13	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:444:ARG:NH1	2:D:504:SO4:O4	2.50	0.44
1:E:319:ILE:HD11	1:E:334:VAL:HG21	1.99	0.44
1:F:384:TYR:CE1	1:F:403:LEU:HD22	2.52	0.44
1:E:298:THR:HB	1:E:387:ALA:O	2.16	0.44
1:G:88:TRP:CZ3	1:G:120:PRO:HD3	2.52	0.44
1:G:249:LEU:HD23	1:G:253:ASP:HB3	1.99	0.44
1:C:163:ILE:CG2	1:C:204:ILE:HG21	2.44	0.44
1:D:327:ILE:HG21	1:D:347:CYS:HB3	1.99	0.44
1:B:407:GLN:HE22	1:F:16:ASP:CG	2.21	0.44
1:E:35:ARG:HD3	1:E:36:PHE:N	2.33	0.44
1:A:275:TYR:CD1	1:A:275:TYR:N	2.86	0.44
1:D:145:ASP:OD1	1:D:147:SER:OG	2.33	0.44
1:A:427:ASN:HB3	1:E:416:PHE:CD2	2.53	0.44
1:B:338:LYS:HZ2	1:B:342:LEU:HD21	1.83	0.44
1:E:52:THR:C	1:E:53:GLU:HG2	2.38	0.44
1:B:349:PHE:O	1:B:352:PRO:HD2	2.18	0.44
1:D:12:GLY:C	1:D:13:ILE:HD12	2.38	0.44
1:B:67:ASP:HB2	1:F:15:GLN:HG3	2.00	0.44
1:D:144:LEU:O	1:D:146:TRP:N	2.51	0.44
1:E:189:SER:HA	1:E:215:SER:O	2.18	0.44
1:C:443:ARG:HG2	1:C:443:ARG:H	1.48	0.43
1:D:19:ASP:OD2	1:D:89:LYS:NZ	2.51	0.43
1:D:278:ILE:O	1:D:280:THR:HG23	2.18	0.43
1:E:92:ASN:HB2	2:E:502:SO4:O2	2.18	0.43
1:E:144:LEU:HD23	1:E:146:TRP:CH2	2.53	0.43
1:C:236:MET:HE1	1:C:261:LEU:N	2.32	0.43
1:G:64:LYS:HB3	1:G:64:LYS:HE2	1.72	0.43
1:D:126:ASN:OD1	1:D:419:ARG:NH2	2.52	0.43
1:D:236:MET:HE1	1:D:260:LYS:CB	2.45	0.43
1:A:443:ARG:H	1:A:443:ARG:HD3	1.83	0.43
1:E:237:MET:SD	1:E:237:MET:N	2.91	0.43
1:F:85:LEU:HA	1:F:134:CYS:HA	2.00	0.43
1:F:218:LEU:HD11	1:F:220:LEU:HG	1.98	0.43
1:F:234:GLN:HA	1:F:237:MET:HE3	2.00	0.43
1:C:327:ILE:HG21	1:C:347:CYS:HB3	2.01	0.43
1:D:294:PHE:CG	1:D:434:MET:HE2	2.53	0.43
1:C:278:ILE:O	1:C:280:THR:HG23	2.19	0.43
1:F:220:LEU:HA	1:F:220:LEU:HD23	1.75	0.43
1:G:82:CYS:O	1:G:135:ASN:HB2	2.18	0.43
1:G:123:LEU:HD23	1:G:131:VAL:HG21	1.99	0.43
1:G:204:ILE:HD12	1:G:207:TYR:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:TYR:OH	1:B:161:ASP:HB3	2.18	0.43
1:C:408:TYR:HE2	1:C:414:LEU:HD11	1.83	0.43
1:B:428:PHE:HB2	1:B:434:MET:SD	2.59	0.43
1:D:112:HIS:ND1	1:D:114:THR:OG1	2.44	0.43
1:G:378:ASP:O	1:G:381:SER:HB3	2.19	0.43
1:F:246:VAL:O	1:F:249:LEU:HD12	2.19	0.43
1:B:188:GLN:HA	1:B:214:LEU:O	2.19	0.42
1:D:150:ASN:HB3	1:D:153:PHE:CD2	2.54	0.42
1:E:7:GLY:HA2	1:E:44:GLN:NE2	2.34	0.42
1:G:265:ARG:O	1:G:317:ARG:NH2	2.52	0.42
1:G:346:HIS:O	1:G:351:GLN:HB2	2.19	0.42
1:B:234:GLN:O	1:B:238:LEU:CD2	2.68	0.42
1:C:227:ARG:HG3	1:C:227:ARG:NH1	2.31	0.42
1:E:313:LEU:N	1:E:313:LEU:HD23	2.35	0.42
1:F:244:ASP:N	1:F:244:ASP:OD1	2.53	0.42
1:C:439:TYR:OH	1:C:444:ARG:HD3	2.19	0.42
1:D:201:ILE:HB	1:D:204:ILE:HG22	2.00	0.42
1:E:70:SER:O	1:E:406:HIS:HE1	2.03	0.42
1:B:45:TRP:CE2	1:B:49:ILE:HD12	2.55	0.42
1:D:236:MET:CE	1:D:260:LYS:HB2	2.45	0.42
1:D:269:LYS:HG2	1:D:313:LEU:HD11	2.01	0.42
1:E:127:ASN:O	1:E:129:ILE:N	2.49	0.42
1:G:20:ILE:HG12	1:G:88:TRP:HD1	1.85	0.42
1:G:149:PHE:HE2	1:G:234:GLN:HG3	1.84	0.42
1:G:317:ARG:NH2	1:G:321:ILE:HD11	2.35	0.42
1:A:137:ARG:CZ	1:A:157:ASN:HB3	2.50	0.42
1:A:320:ASP:O	1:A:324:LEU:HG	2.20	0.42
1:C:151:LYS:HD3	1:C:151:LYS:N	2.34	0.42
1:D:220:LEU:HD23	1:D:220:LEU:HA	1.90	0.42
1:D:316:GLN:HG2	1:D:331:TYR:HE2	1.85	0.42
1:D:223:LEU:HD12	1:D:223:LEU:O	2.20	0.42
1:D:336:THR:HG23	1:D:339:GLN:HB2	2.02	0.42
1:F:22:LEU:N	1:F:22:LEU:HD22	2.34	0.42
1:C:63:ASN:OD1	1:C:66:GLU:HB2	2.20	0.42
1:C:189:SER:O	1:C:193[B]:MET:HG3	2.19	0.42
1:D:298:THR:HG22	1:D:374:PHE:HB3	2.00	0.42
1:G:110:ASN:CA	1:G:138:LEU:HD13	2.49	0.42
1:G:140:ALA:C	1:G:146:TRP:HZ2	2.23	0.42
1:C:375:ALA:HB3	1:C:450:GLN:HG3	2.01	0.42
1:D:287:TYR:CD2	1:D:356:PHE:HE1	2.38	0.42
1:E:188:GLN:HA	1:E:214:LEU:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:211:VAL:CG2	1:E:293:ILE:HG12	2.50	0.42
1:F:46:SER:N	2:F:501:SO4:O4	2.47	0.42
1:F:149:PHE:HE1	1:F:234:GLN:HB2	1.84	0.42
1:A:416:PHE:CD2	1:E:427:ASN:HB3	2.55	0.42
1:B:325:ASN:HD22	1:B:348:TYR:HE2	1.65	0.42
1:E:13:ILE:HD13	1:E:13:ILE:HA	1.84	0.42
1:F:57:ILE:HG13	1:F:77:THR:O	2.18	0.42
1:G:236:MET:CB	1:G:257:LEU:HD21	2.50	0.41
1:E:257:LEU:HD23	1:E:257:LEU:HA	1.90	0.41
1:F:68:PHE:O	1:F:406:HIS:CE1	2.72	0.41
1:F:108:PHE:CE2	1:F:277:PRO:HD2	2.55	0.41
1:F:354:LYS:HD2	1:F:354:LYS:C	2.41	0.41
1:G:88:TRP:CZ3	1:G:120:PRO:CD	3.03	0.41
1:A:23:GLY:HA2	1:A:84:TYR:HB3	2.01	0.41
1:G:78:GLU:O	1:G:79:HIS:ND1	2.45	0.41
1:B:232:HIS:CE1	1:B:236:MET:SD	3.13	0.41
1:C:256:MET:O	1:C:260:LYS:HG2	2.20	0.41
1:D:310:GLN:H	1:D:310:GLN:CD	2.16	0.41
1:D:318:PHE:CD1	1:D:340:GLN:HG2	2.55	0.41
1:E:20:ILE:CG1	1:E:88:TRP:CD1	3.03	0.41
1:E:204:ILE:HD12	1:E:207:TYR:CD1	2.55	0.41
1:F:355:GLN:O	1:F:359:GLN:HG2	2.21	0.41
1:G:240:TYR:CZ	1:G:260:LYS:HG2	2.55	0.41
1:A:315:PRO:HB2	1:A:331:TYR:CE1	2.56	0.41
1:C:173:ILE:HD12	1:C:173:ILE:HA	1.89	0.41
1:C:389:HIS:CD2	1:C:390:ILE:HG13	2.55	0.41
1:D:2:LYS:HD3	1:D:9:GLN:OE1	2.21	0.41
1:E:27:ALA:HB1	1:E:39:SER:HB2	2.02	0.41
1:A:395:PHE:HB3	1:A:421:MET:SD	2.60	0.41
1:B:102:TYR:HA	1:B:186:MET:O	2.20	0.41
1:B:271:LEU:HD13	1:B:322:MET:CE	2.50	0.41
1:E:297:TYR:N	1:E:297:TYR:HD1	2.19	0.41
1:F:137:ARG:HG3	1:F:161:ASP:OD2	2.19	0.41
1:F:255:LEU:HD23	1:F:255:LEU:HA	1.89	0.41
1:D:298:THR:O	1:D:301:GLU:HG2	2.21	0.41
1:F:374:PHE:HD1	1:F:421:MET:HE2	1.86	0.41
1:G:260:LYS:HA	1:G:260:LYS:HD3	1.81	0.41
1:A:173:ILE:HD12	1:A:173:ILE:HA	1.81	0.41
1:C:148:TYR:CE2	1:C:231:GLN:HG3	2.56	0.41
1:C:232:HIS:CD2	1:C:261:LEU:HD13	2.56	0.41
1:D:261:LEU:HA	1:D:261:LEU:HD23	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:336:THR:OG1	1:D:337:ALA:N	2.53	0.41
1:E:94:GLN:HB2	1:E:97:LYS:HE2	2.02	0.41
1:E:155:SER:HB2	1:E:278:ILE:HD13	2.02	0.41
1:E:306:ILE:HG23	1:E:312:LYS:HA	2.02	0.41
1:E:320:ASP:O	1:E:324:LEU:HD23	2.20	0.41
1:F:26:TYR:OH	1:F:161:ASP:HB3	2.20	0.41
1:F:173:ILE:HD12	1:F:173:ILE:HA	1.83	0.41
1:G:376:TRP:CZ2	1:G:414:LEU:HD21	2.54	0.41
1:A:150:ASN:HB3	1:A:153:PHE:CD2	2.56	0.41
1:B:205:GLU:HB3	1:B:206:PRO:HD3	2.02	0.41
1:B:358:GLN:O	1:B:362:ILE:HG13	2.20	0.41
1:D:443:ARG:HG3	1:D:445:TYR:CD2	2.56	0.41
1:G:240:TYR:CD1	1:G:240:TYR:N	2.89	0.41
1:A:86:ASN:HB2	1:A:88:TRP:CZ3	2.56	0.40
1:B:143:TYR:HB2	1:B:275:TYR:HB3	2.03	0.40
1:D:350:LYS:HE3	1:D:350:LYS:HB3	1.92	0.40
1:D:374:PHE:CG	1:D:392:ASP:HB3	2.56	0.40
1:E:58:PRO:HA	1:E:59:PRO:HD3	1.94	0.40
1:E:161:ASP:O	1:E:165:VAL:HG23	2.21	0.40
1:E:318:PHE:CZ	1:E:322:MET:HE3	2.56	0.40
1:B:238:LEU:HD13	1:B:243:THR:O	2.21	0.40
1:C:317:ARG:CZ	1:C:321:ILE:HD11	2.50	0.40
1:D:219:ARG:HH11	1:D:219:ARG:HG2	1.86	0.40
1:E:278:ILE:H	1:E:278:ILE:HD12	1.87	0.40
1:E:340:GLN:O	1:E:344:ILE:HD12	2.22	0.40
1:G:370:TRP:CG	1:G:434:MET:HB2	2.56	0.40
1:A:370:TRP:CG	1:A:434:MET:HB2	2.56	0.40
1:B:330:LYS:O	1:B:334:VAL:HG23	2.21	0.40
1:D:189:SER:HA	1:D:215:SER:O	2.22	0.40
1:D:315:PRO:HB2	1:D:331:TYR:CZ	2.56	0.40
1:G:55:GLN:HG3	1:G:84:TYR:CD2	2.56	0.40
1:G:162:GLN:OE1	1:G:194:SER:HB3	2.22	0.40
1:G:414:LEU:HD23	1:G:414:LEU:HA	1.84	0.40
1:B:193[B]:MET:HG2	1:B:217:ALA:O	2.21	0.40
1:B:438:MET:HE2	1:B:438:MET:HB2	1.96	0.40
1:C:33:ASP:N	1:C:33:ASP:OD1	2.55	0.40
1:D:112:HIS:CE1	1:D:114:THR:HG1	2.37	0.40
1:E:66:GLU:O	1:E:70:SER:HB2	2.21	0.40
1:E:146:TRP:CE3	1:E:146:TRP:HA	2.56	0.40
1:F:376:TRP:NE1	1:F:414:LEU:HD11	2.36	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	453/453 (100%)	429 (95%)	23 (5%)	1 (0%)	47	55
1	B	451/453 (100%)	424 (94%)	26 (6%)	1 (0%)	47	55
1	C	453/453 (100%)	427 (94%)	25 (6%)	1 (0%)	47	55
1	D	451/453 (100%)	423 (94%)	27 (6%)	1 (0%)	47	55
1	E	451/453 (100%)	418 (93%)	31 (7%)	2 (0%)	34	37
1	F	451/453 (100%)	418 (93%)	32 (7%)	1 (0%)	47	55
1	G	451/453 (100%)	419 (93%)	30 (7%)	2 (0%)	34	37
All	All	3161/3171 (100%)	2958 (94%)	194 (6%)	9 (0%)	41	46

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	390	ILE
1	C	390	ILE
1	D	390	ILE
1	E	390	ILE
1	G	390	ILE
1	A	390	ILE
1	F	390	ILE
1	E	32	HIS
1	G	120	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	407/404 (101%)	402 (99%)	5 (1%)	71	80
1	B	401/404 (99%)	390 (97%)	11 (3%)	44	54
1	C	401/404 (99%)	393 (98%)	8 (2%)	55	64
1	D	398/404 (98%)	388 (98%)	10 (2%)	47	56
1	E	378/404 (94%)	368 (97%)	10 (3%)	46	55
1	F	374/404 (93%)	359 (96%)	15 (4%)	31	37
1	G	381/404 (94%)	373 (98%)	8 (2%)	53	62
All	All	2740/2828 (97%)	2673 (98%)	67 (2%)	49	58

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	110	ASN
1	A	434	MET
1	A	443	ARG
1	A	444	ARG
1	B	2	LYS
1	B	86	ASN
1	B	189	SER
1	B	193[A]	MET
1	B	193[B]	MET
1	B	203	ASP
1	B	228	ASN
1	B	256	MET
1	B	430	LYS
1	B	438	MET
1	B	443	ARG
1	C	15	GLN
1	C	62	ASP
1	C	110	ASN
1	C	151	LYS
1	C	189	SER
1	C	221	ASP
1	C	317	ARG
1	C	331	TYR
1	D	96	LYS
1	D	144	LEU
1	D	219	ARG
1	D	245	ASP
1	D	261	LEU

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Mol	Chain	Res	Type
1	D	263	GLN
1	D	281	ASP
1	D	338	LYS
1	D	419	ARG
1	D	434	MET
1	E	35	ARG
1	E	67	ASP
1	E	192	SER
1	E	193	MET
1	E	256	MET
1	E	282	TYR
1	E	297	TYR
1	E	323	GLU
1	E	419	ARG
1	E	434	MET
1	F	64	LYS
1	F	68	PHE
1	F	79	HIS
1	F	110	ASN
1	F	175	SER
1	F	193	MET
1	F	227	ARG
1	F	242	ASP
1	F	249	LEU
1	F	256	MET
1	F	282	TYR
1	F	292	PRO
1	F	354	LYS
1	F	359	GLN
1	F	421	MET
1	G	205	GLU
1	G	237	MET
1	G	265	ARG
1	G	286	ASN
1	G	299	LYS
1	G	338	LYS
1	G	434	MET
1	G	443	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	232	HIS
1	B	346	HIS
1	F	389	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

28 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	SO4	A	501	-	4,4,4	0.20	0	6,6,6	0.38	0
2	SO4	A	503	-	4,4,4	0.18	0	6,6,6	0.24	0
2	SO4	E	501	-	4,4,4	0.16	0	6,6,6	0.12	0
2	SO4	D	501	-	4,4,4	0.17	0	6,6,6	0.23	0
2	SO4	E	502	-	4,4,4	0.15	0	6,6,6	0.13	0
2	SO4	A	502	-	4,4,4	0.18	0	6,6,6	0.24	0
2	SO4	D	503	-	4,4,4	0.14	0	6,6,6	0.16	0
2	SO4	C	503	-	4,4,4	0.13	0	6,6,6	0.15	0
2	SO4	E	504	-	4,4,4	0.18	0	6,6,6	0.32	0
2	SO4	B	501	-	4,4,4	0.19	0	6,6,6	0.24	0
2	SO4	E	503	-	4,4,4	0.13	0	6,6,6	0.18	0
2	SO4	B	503	-	4,4,4	0.18	0	6,6,6	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	C	502	-	4,4,4	0.14	0	6,6,6	0.23	0
2	SO4	G	502	-	4,4,4	0.13	0	6,6,6	0.12	0
2	SO4	A	505	-	4,4,4	0.12	0	6,6,6	0.35	0
2	SO4	B	504	-	4,4,4	0.20	0	6,6,6	0.31	0
2	SO4	C	504	-	4,4,4	0.12	0	6,6,6	0.37	0
2	SO4	A	504	-	4,4,4	0.11	0	6,6,6	0.09	0
2	SO4	F	503	-	4,4,4	0.14	0	6,6,6	0.19	0
2	SO4	C	505	-	4,4,4	0.15	0	6,6,6	0.22	0
2	SO4	D	502	-	4,4,4	0.15	0	6,6,6	0.24	0
2	SO4	B	502	-	4,4,4	0.17	0	6,6,6	0.24	0
2	SO4	F	501	-	4,4,4	0.19	0	6,6,6	0.10	0
2	SO4	D	504	-	4,4,4	0.19	0	6,6,6	0.29	0
2	SO4	G	501	-	4,4,4	0.12	0	6,6,6	0.41	0
2	SO4	A	506	-	4,4,4	0.18	0	6,6,6	0.42	0
2	SO4	C	501	-	4,4,4	0.18	0	6,6,6	0.23	0
2	SO4	F	502	-	4,4,4	0.16	0	6,6,6	0.13	0

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.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	501	SO4	1	0
2	E	502	SO4	1	0
2	C	504	SO4	1	0
2	C	505	SO4	1	0
2	F	501	SO4	1	0
2	D	504	SO4	1	0
2	A	506	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	452/453 (99%)	0.06	3 (0%) 87 88	42, 51, 67, 72	0
1	B	452/453 (99%)	0.44	25 (5%) 25 27	52, 65, 85, 102	0
1	C	452/453 (99%)	0.38	31 (6%) 16 18	46, 59, 84, 104	0
1	D	451/453 (99%)	0.40	19 (4%) 36 38	43, 59, 82, 95	0
1	E	452/453 (99%)	0.57	36 (7%) 12 13	48, 66, 99, 120	0
1	F	452/453 (99%)	0.85	44 (9%) 7 8	61, 73, 109, 133	0
1	G	452/453 (99%)	0.88	59 (13%) 3 3	54, 77, 102, 116	0
All	All	3163/3171 (99%)	0.51	217 (6%) 16 18	42, 65, 97, 133	0

All (217) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	331	TYR	10.1
1	E	238	LEU	7.6
1	C	329	LEU	6.8
1	F	241	LEU	5.5
1	C	334	VAL	5.5
1	E	149	PHE	5.4
1	F	318	PHE	5.3
1	F	236	MET	5.1
1	G	329	LEU	5.0
1	G	148	TYR	5.0
1	E	242	ASP	5.0
1	B	310	GLN	5.0
1	E	153	PHE	4.9
1	G	7	GLY	4.9
1	C	240	TYR	4.6
1	C	331	TYR	4.5
1	F	261	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	E	148	TYR	4.4
1	F	240	TYR	4.3
1	G	268	SER	4.3
1	C	313	LEU	4.3
1	G	238	LEU	4.3
1	G	233	PHE	4.3
1	G	147	SER	4.2
1	D	329	LEU	4.2
1	G	246	VAL	4.1
1	E	261	LEU	4.1
1	D	46	SER	4.1
1	D	240	TYR	4.0
1	B	232	HIS	4.0
1	F	47	GLU	3.9
1	F	266	GLY	3.9
1	G	33	ASP	3.9
1	E	236	MET	3.9
1	G	241	LEU	3.8
1	G	331	TYR	3.8
1	D	330	LYS	3.7
1	B	240	TYR	3.7
1	C	323	GLU	3.7
1	G	319	ILE	3.7
1	F	149	PHE	3.7
1	G	32	HIS	3.7
1	B	238	LEU	3.6
1	B	248	SER	3.6
1	E	335	GLN	3.6
1	F	46	SER	3.6
1	G	318	PHE	3.6
1	F	330	LYS	3.6
1	F	232	HIS	3.6
1	C	223	LEU	3.5
1	G	236	MET	3.5
1	C	315	PRO	3.5
1	E	245	ASP	3.5
1	G	231	GLN	3.4
1	F	305	TYR	3.4
1	E	246	VAL	3.4
1	F	31	VAL	3.3
1	E	249	LEU	3.3
1	E	272	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	242	ASP	3.3
1	E	334	VAL	3.3
1	G	267	PRO	3.3
1	G	248	SER	3.3
1	E	318	PHE	3.2
1	G	253	ASP	3.2
1	G	308	SER	3.2
1	B	334	VAL	3.2
1	C	328	PRO	3.2
1	F	11	HIS	3.2
1	G	245	ASP	3.2
1	E	333	ASP	3.1
1	G	336	THR	3.1
1	C	238	LEU	3.1
1	D	442	GLU	3.0
1	E	237	MET	3.0
1	G	243	THR	3.0
1	G	330	LYS	3.0
1	D	242	ASP	3.0
1	G	333	ASP	3.0
1	F	7	GLY	3.0
1	D	331	TYR	3.0
1	F	79	HIS	3.0
1	E	271	LEU	3.0
1	D	249	LEU	2.9
1	F	257	LEU	2.9
1	B	153	PHE	2.9
1	G	338	LYS	2.9
1	D	148	TYR	2.9
1	F	342	LEU	2.9
1	E	248	SER	2.8
1	G	365	SER	2.8
1	D	149	PHE	2.8
1	G	2	LYS	2.8
1	G	153	PHE	2.8
1	C	338	LYS	2.8
1	F	354	LYS	2.8
1	G	9	GLN	2.8
1	G	36	PHE	2.7
1	C	308	SER	2.7
1	F	314	SER	2.7
1	B	241	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	444	ARG	2.7
1	C	321	ILE	2.7
1	D	235	LYS	2.7
1	C	289	THR	2.7
1	D	193[A]	MET	2.7
1	F	33	ASP	2.7
1	C	332	GLU	2.7
1	C	287	TYR	2.7
1	E	231	GLN	2.6
1	E	232	HIS	2.6
1	G	223	LEU	2.6
1	E	32	HIS	2.6
1	F	310	GLN	2.6
1	G	10	ILE	2.6
1	E	243	THR	2.5
1	E	306	ILE	2.5
1	B	245	ASP	2.5
1	C	151	LYS	2.5
1	C	318	PHE	2.5
1	F	443	ARG	2.5
1	G	240	TYR	2.5
1	G	140	ALA	2.5
1	E	239	ASP	2.5
1	G	282	TYR	2.5
1	C	232	HIS	2.5
1	G	249	LEU	2.5
1	F	100	ILE	2.5
1	G	362	ILE	2.5
1	F	260	LYS	2.5
1	F	8	GLY	2.5
1	E	146	TRP	2.4
1	G	59	PRO	2.4
1	G	289	THR	2.4
1	G	11	HIS	2.4
1	E	234	GLN	2.4
1	F	238	LEU	2.4
1	D	11	HIS	2.4
1	E	320	ASP	2.4
1	F	262	LYS	2.4
1	C	237	MET	2.4
1	E	332	GLU	2.4
1	G	8	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	302	GLY	2.4
1	E	314	SER	2.4
1	E	241	LEU	2.4
1	G	261	LEU	2.4
1	G	357	LEU	2.4
1	G	35	ARG	2.4
1	C	149	PHE	2.4
1	E	254	ILE	2.4
1	D	394	VAL	2.4
1	F	233	PHE	2.4
1	F	246	VAL	2.4
1	B	33	ASP	2.3
1	D	105	GLY	2.3
1	E	266	GLY	2.3
1	C	310	GLN	2.3
1	C	336	THR	2.3
1	G	34	ASN	2.3
1	F	239	ASP	2.3
1	B	335	GLN	2.3
1	F	147	SER	2.3
1	B	151	LYS	2.3
1	G	239	ASP	2.3
1	G	325	ASN	2.3
1	D	267	PRO	2.3
1	F	226	ALA	2.3
1	C	317	ARG	2.2
1	B	331	TYR	2.2
1	B	239	ASP	2.2
1	G	154	HIS	2.2
1	C	314	SER	2.2
1	B	308	SER	2.2
1	G	247	THR	2.2
1	G	235	LYS	2.2
1	B	313	LEU	2.2
1	C	46	SER	2.2
1	D	248	SER	2.2
1	F	335	GLN	2.2
1	B	336	THR	2.2
1	A	238	LEU	2.2
1	D	47	GLU	2.2
1	C	320	ASP	2.2
1	E	331	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	36	PHE	2.1
1	F	64	LYS	2.1
1	G	152	ASP	2.1
1	F	442	GLU	2.1
1	B	242	ASP	2.1
1	B	244	ASP	2.1
1	C	249	LEU	2.1
1	F	234	GLN	2.1
1	G	242	ASP	2.1
1	G	224	GLU	2.1
1	D	151	LYS	2.1
1	F	343	ALA	2.1
1	G	5	THR	2.1
1	F	148	TYR	2.1
1	F	235	LYS	2.1
1	E	223	LEU	2.1
1	A	33	ASP	2.1
1	C	33	ASP	2.1
1	B	184	THR	2.1
1	B	247	THR	2.1
1	B	338	LYS	2.0
1	G	151	LYS	2.0
1	B	223	LEU	2.0
1	G	101	ILE	2.0
1	G	144	LEU	2.0
1	A	115	ALA	2.0
1	E	263	GLN	2.0
1	B	281	ASP	2.0
1	B	385	ARG	2.0
1	C	359	GLN	2.0
1	E	115	ALA	2.0
1	F	269	LYS	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(Å ²)	Q<0.9
2	SO4	E	501	5/5	0.73	0.20	77,78,86,87	5
2	SO4	B	504	5/5	0.77	0.26	63,63,72,74	5
2	SO4	F	501	5/5	0.83	0.19	81,82,87,88	5
2	SO4	D	504	5/5	0.86	0.15	66,67,76,78	5
2	SO4	B	503	5/5	0.86	0.14	65,72,74,80	5
2	SO4	A	506	5/5	0.86	0.16	58,61,65,69	5
2	SO4	G	502	5/5	0.86	0.17	86,88,93,94	5
2	SO4	F	503	5/5	0.87	0.13	88,89,91,92	5
2	SO4	A	504	5/5	0.87	0.21	57,58,62,63	5
2	SO4	B	502	5/5	0.88	0.17	56,58,61,63	5
2	SO4	A	505	5/5	0.88	0.16	61,63,65,68	5
2	SO4	C	505	5/5	0.89	0.24	51,53,59,60	5
2	SO4	C	504	5/5	0.90	0.19	62,68,72,73	5
2	SO4	B	501	5/5	0.90	0.16	70,73,78,78	5
2	SO4	E	504	5/5	0.90	0.13	83,85,88,90	5
2	SO4	G	501	5/5	0.91	0.17	64,65,69,70	5
2	SO4	D	503	5/5	0.91	0.21	74,75,80,84	5
2	SO4	A	502	5/5	0.92	0.15	54,55,61,62	5
2	SO4	C	501	5/5	0.92	0.10	66,72,73,76	0
2	SO4	F	502	5/5	0.93	0.17	66,67,68,70	5
2	SO4	D	502	5/5	0.94	0.10	62,68,72,72	5
2	SO4	E	503	5/5	0.94	0.12	65,67,73,73	5
2	SO4	C	503	5/5	0.95	0.21	74,75,77,78	5
2	SO4	A	501	5/5	0.95	0.12	51,59,61,64	5
2	SO4	D	501	5/5	0.96	0.13	59,61,63,63	5
2	SO4	E	502	5/5	0.96	0.11	58,62,63,63	5
2	SO4	A	503	5/5	0.96	0.14	49,51,52,55	5
2	SO4	C	502	5/5	0.97	0.12	58,60,62,63	5

6.5 Other polymers [i](#)

There are no such residues in this entry.