



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:18 AM UTC

PDB ID : 8S9J / pdb_00008s9j
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 : 4-5-2 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

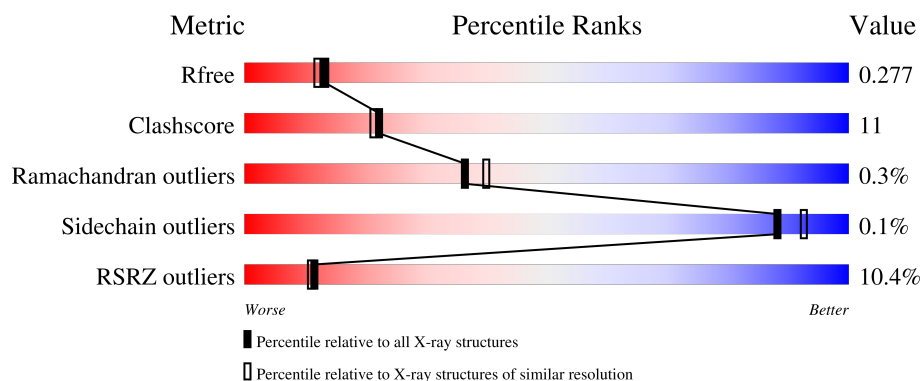
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (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	2% 87% 13%
1	B	453	3% 77% 23%
1	C	453	5% 82% 18%
1	D	453	4% 81% 19%
1	E	453	15% 76% 23% .

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

2 Entry composition

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

There are 21 discrepancies between the modelled and reference sequences:

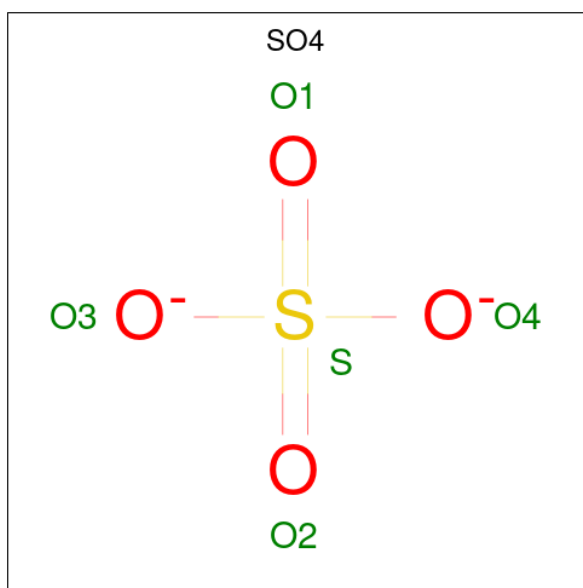
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A0A0D6GYZ4
A	-1	PRO	-	expression tag	UNP A0A0D6GYZ4
A	0	GLY	-	expression tag	UNP A0A0D6GYZ4
B	-2	GLY	-	expression tag	UNP A0A0D6GYZ4
B	-1	PRO	-	expression tag	UNP A0A0D6GYZ4
B	0	GLY	-	expression tag	UNP A0A0D6GYZ4
C	-2	GLY	-	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 (CCD ID: 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		

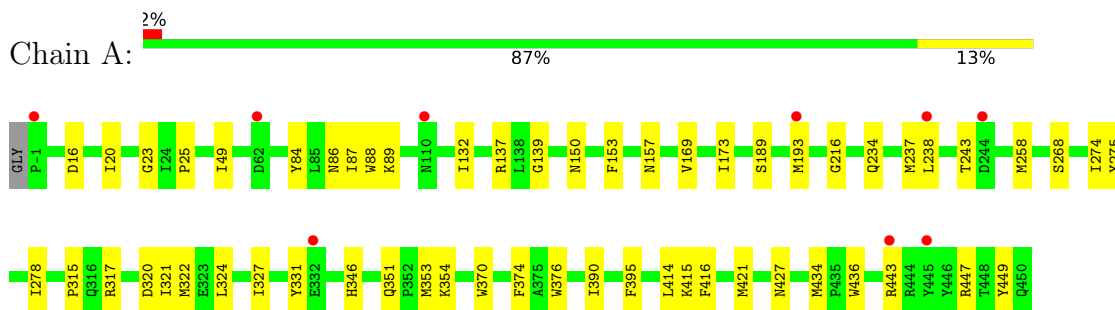
- Molecule 3 is water.

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

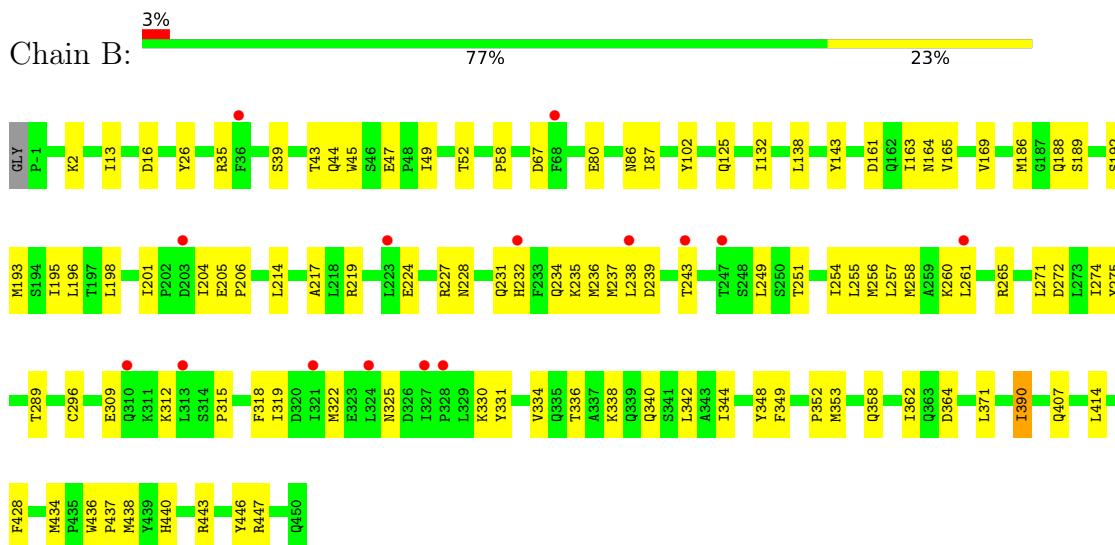
3 Residue-property plots [i](#)

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.

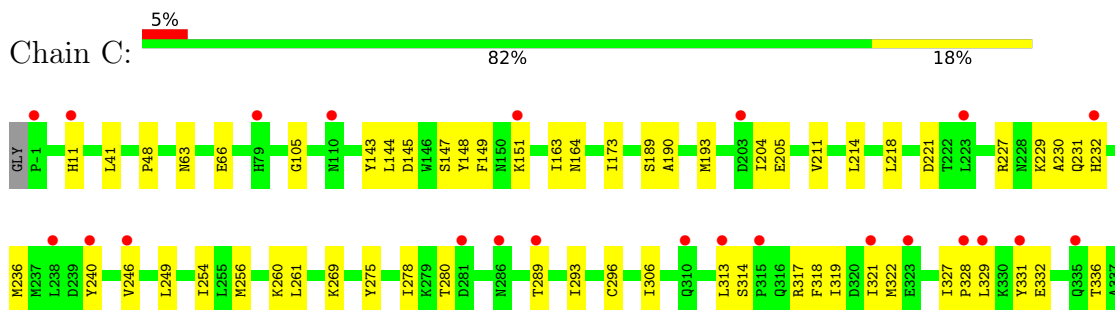
- Molecule 1: Fluorophosphonate-binding serine hydrolase A



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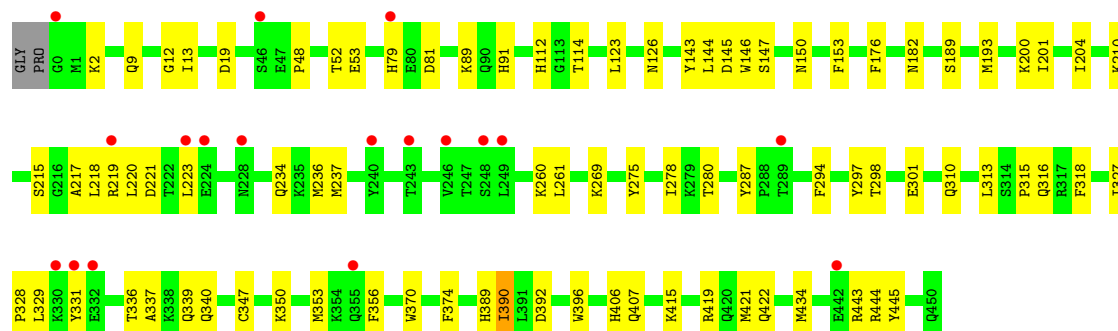
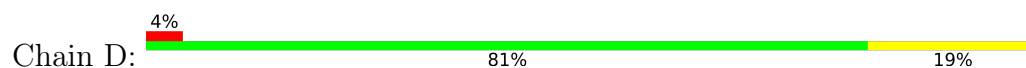


- Molecule 1: Fluorophosphonate-binding serine hydrolase A

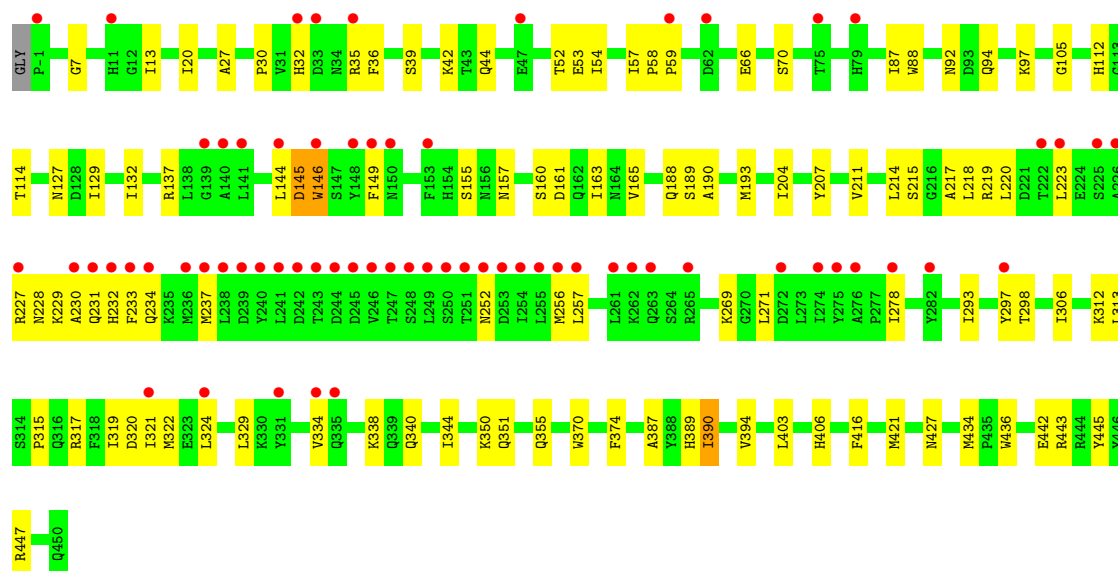
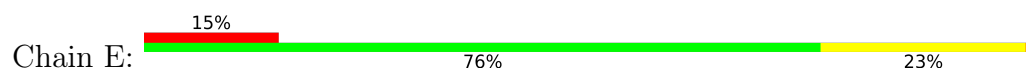




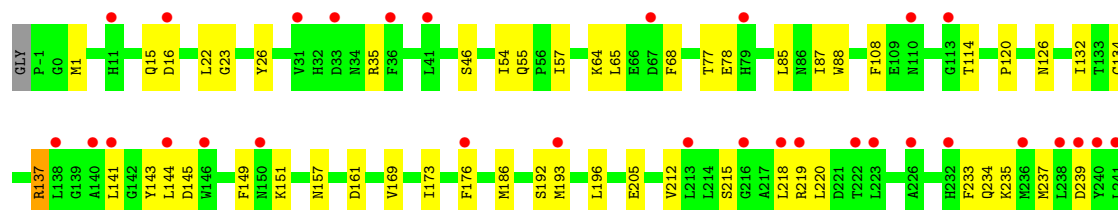
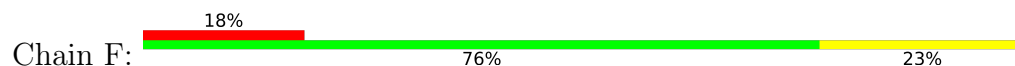
• Molecule 1: Fluorophosphonate-binding serine hydrolase A

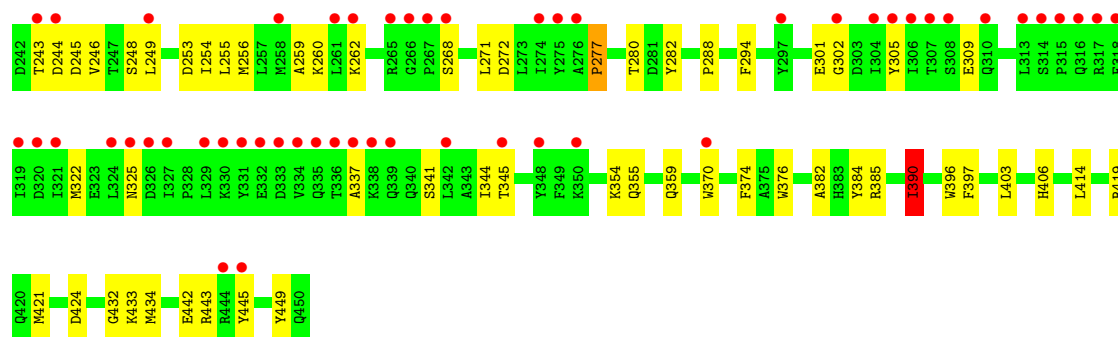


• Molecule 1: Fluorophosphonate-binding serine hydrolase A

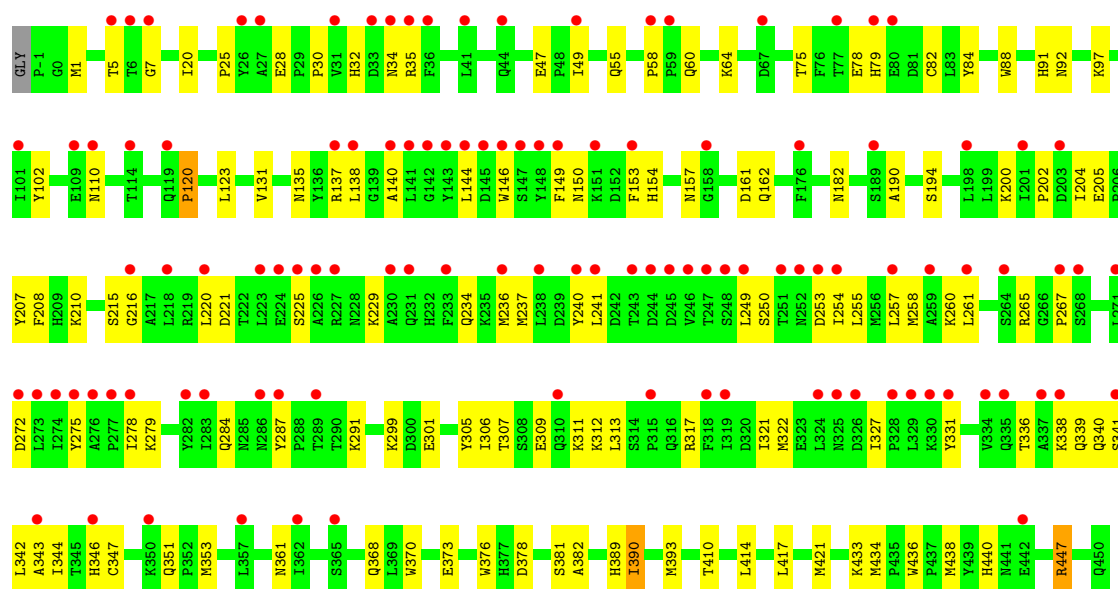


• Molecule 1: Fluorophosphonate-binding serine hydrolase A





● 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) 98.6 (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)	Xtriage
Refinement program	PHENIX 1.20.1-4487	Depositor
R, R_{free}	0.241 , 0.277 0.241 , 0.277	Depositor DCC
R_{free} test set	10754 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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

5.1 Standard geometry

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	0.41	0/3807	0.60	0/5166
1	B	0.36	0/3769	0.55	0/5117
1	C	0.36	0/3790	0.55	0/5147
1	D	0.37	0/3766	0.54	0/5115
1	E	0.37	0/3678	0.59	2/5004 (0.0%)
1	F	0.38	1/3674 (0.0%)	0.61	3/4995 (0.1%)
1	G	0.35	1/3707 (0.0%)	0.55	0/5044
All	All	0.37	2/26191 (0.0%)	0.57	5/35588 (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	9.62	1.61	1.47
1	G	202	PRO	N-CD	6.30	1.56	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	390	ILE	N-CA-C	11.54	133.35	109.34
1	F	390	ILE	CB-CA-C	-9.53	95.67	111.29
1	F	277	PRO	CA-N-CD	-7.22	101.90	112.00
1	E	146	TRP	N-CA-C	-7.15	104.71	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	145	ASP	N-CA-C	-6.48	97.00	110.80

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 [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	3705	0	3583	44	0
1	B	3668	0	3547	72	0
1	C	3686	0	3549	65	0
1	D	3664	0	3527	68	0
1	E	3581	0	3402	85	0
1	F	3577	0	3373	94	0
1	G	3605	0	3417	109	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	4	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	529	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 11.

All (529) 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: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: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:D:294:PHE:CG	1:D:434:MET:HE2	2.20	0.76
1:F:57:ILE:HD11	1:F:78:GLU:HG2	1.68	0.75
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:B:236:MET:HE3	1:B:257:LEU:HD22	1.70	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:B:256:MET:HE2	1:B:260:LYS:HG3	1.73	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:216:GLY:H	1:G:353:MET:HE3	1.57	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:G:102:TYR:CZ	1:G:393:MET:HE2	2.28	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
1:A:234:GLN:HA	1:A:237:MET:HE3	1.75	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:E:271:LEU:HD23	1:E:322:MET:HE1	1.76	0.67
1:E:193:MET:HE2	1:E:219:ARG:H	1.58	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:G:216:GLY:H	1:G:353:MET:CE	2.08	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:B:254:ILE:HG22	1:B:258:MET:HE2	1.77	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:1:MET:HA	1:F:1:MET:HE2	1.79	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: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:E:374:PHE:CD1	1:E:421:MET:HE1	2.34	0.62
1:F:137:ARG:HH21	1:F:157:ASN:CB	2.10	0.62
1:C:368:GLN:HA	1:C:438:MET:HE3	1.82	0.62
1:C:319:ILE:HD11	1:C:331:TYR:HA	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:ARG:NH2	1:B:80:GLU:OE2	2.30	0.62
1:C:204:ILE:C	1:C:204:ILE:HD12	2.24	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
1:A:421:MET:HE3	1:A:449:TYR:HB3	1.82	0.61
1:F:212:VAL:HG13	1:F:294:PHE:HD2	1.65	0.61
1:E:227:ARG:O	1:E:231:GLN:N	2.28	0.61
1:A:374:PHE:CD1	1:A:421:MET:HE1	2.36	0.61
1:D:236:MET:HE1	1:D:260:LYS:HB2	1.82	0.60
1:B:255:LEU:HA	1:B:258:MET:HE3	1.83	0.60
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: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:A:258:MET:HE2	3:A:717:HOH:O	2.02	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:G:254:ILE:HG22	1:G:258:MET:HE2	1.85	0.58
1:B:219:ARG:NH2	1:B:348:TYR:O	2.36	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:G:216:GLY:O	1:G:353:MET:HE3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:318:PHE:CD1	1:C:340:GLN:HG2	2.39	0.57
1:C:332:GLU:H	1:C:332:GLU:CD	2.09	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:G:361:ASN:ND2	1:G:440:HIS:HA	2.19	0.57
1:B:296:CYS:O	1:B:353:MET:HE1	2.04	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
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:294:PHE:CD2	1:D:434:MET:HE2	2.40	0.56
1:F:442:GLU:HA	1:F:442:GLU:OE1	2.03	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:F:256:MET:HE2	1:F:260:LYS:HG2	1.87	0.55
1:F:322:MET:HE2	1:F:322:MET:HA	1.87	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:B:255:LEU:HD23	1:B:258:MET:HE3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:234:GLN:HA	1:F:237:MET:HE3	1.90	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: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:F:374:PHE:CD1	1:F:421:MET:HE1	2.42	0.53
1:C:211:VAL:HG22	1:C:293:ILE:HG12	1.91	0.53
1:D:310:GLN:H	1:D:310:GLN:CD	2.16	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:A:374:PHE:HD1	1:A:421:MET:HE1	1.74	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
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: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:E:149:PHE:HE2	1:E:237:MET:HE1	1.74	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:E:149:PHE:CE2	1:E:237:MET:HE1	2.45	0.51
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:G:389:HIS:C	1:G:390:ILE:HG13	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:GLU:O	1:B:228:ASN:HB2	2.10	0.51
1:B:234:GLN:HA	1:B:237:MET:HE2	1.92	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:O	1:F:390:ILE:HG22	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: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:368:GLN:HA	1:G:438:MET:HE2	1.93	0.50
1:F:374:PHE:CE1	1:F:421:MET:HE1	2.46	0.50
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: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:322:MET:HE2	1:G:322:MET:HA	1.94	0.50
1:G:338:LYS:HD3	1:G:342:LEU:HD12	1.93	0.50
1:G:1:MET:HE1	1:G:91:HIS:HE1	1.75	0.50
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:D:297:TYR:HB3	1:D:353:MET:HE1	1.94	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:F:68:PHE:C	1:F:68:PHE:CD1	2.90	0.49
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:E:137:ARG:HH21	1:E:157:ASN:CG	2.19	0.49
1:G:305:TYR:C	1:G:306:ILE:HD13	2.37	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:407:GLN:HE22	1:F:16:ASP:CG	2.21	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:E:157:ASN:O	1:E:160:SER:OG	2.27	0.49
1:E:193:MET:CE	1:E:219:ARG:H	2.23	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:C:145:ASP:OD1	1:C:147:SER:OG	2.30	0.48
1:D:12:GLY:C	1:D:13:ILE:HD12	2.38	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:F:421:MET:HE3	1:F:449:TYR:HB3	1.95	0.48
1:A:317:ARG:O	1:A:321:ILE:HG12	2.13	0.48
1:D:415:LYS:NZ	1:G:410:THR:O	2.30	0.48
1:E:52:THR:C	1:E:53:GLU:HG2	2.38	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: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: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
1:D:236:MET:HE1	1:D:260:LYS:CB	2.44	0.48
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:89:LYS:NZ	3:A:611:HOH:O	2.46	0.47
1:B:438:MET:HB2	1:B:438:MET:HE2	1.68	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:140:ALA:C	1:G:146:TRP:HZ2	2.23	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:A:421:MET:HE3	1:A:449:TYR:CB	2.45	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:F:193:MET:HE2	1:F:193:MET:HB2	1.79	0.47
1:B:271:LEU:HD13	1:B:322:MET:HE2	1.97	0.46
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:D:236:MET:CE	1:D:260:LYS:HB2	2.45	0.46
1:F:354:LYS:HD2	1:F:354:LYS:C	2.41	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:233:PHE:CD1	1:F:237:MET:HE2	2.51	0.46
1:F:301:GLU:HB2	1:F:345:THR:HG22	1.97	0.46
1:G:1:MET:HE1	1:G:91:HIS:CE1	2.50	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:A:216:GLY:H	1:A:353:MET:HE3	1.82	0.44
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:E:389:HIS:O	1:E:390:ILE:HB	2.16	0.44
1:F:424:ASP:OD2	1:F:449:TYR:OH	2.29	0.44
1:G:88:TRP:CZ3	1:G:120:PRO:HD3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:249:LEU:HD23	1:G:253:ASP:HB3	1.99	0.44
1:A:274:ILE:C	1:A:275:TYR:CD1	2.95	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: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:349:PHE:O	1:B:352:PRO:HD2	2.18	0.44
1:G:236:MET:C	1:G:257:LEU:HD21	2.43	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:B:338:LYS:HZ2	1:B:342:LEU:HD21	1.83	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:A:374:PHE:CE1	1:A:421:MET:HE1	2.53	0.43
1:D:126:ASN:OD1	1:D:419:ARG:NH2	2.52	0.43
1:G:215:SER:OG	1:G:301:GLU:OE2	2.28	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:C:327:ILE:HG21	1:C:347:CYS:HB3	2.01	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150:ASN:HB3	1:D:153:PHE:CD2	2.54	0.42
1:E:36:PHE:C	1:E:157:ASN:HD21	2.27	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:OD1	1:F:244:ASP:N	2.53	0.42
1:F:294:PHE:CG	1:F:434:MET:HE2	2.55	0.42
1:C:322:MET:HE3	1:C:322:MET:HB3	1.68	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:G:205:GLU:C	1:G:205:GLU:OE1	2.63	0.42
1:B:45:TRP:CE2	1:B:49:ILE:HD12	2.55	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:5:THR:C	1:G:7:GLY:H	2.28	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:G:102:TYR:CE1	1:G:393:MET:HE2	2.54	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:331:TYR:CD1	1:G:331:TYR:C	2.98	0.42
1:D:328:PRO:C	1:D:329:LEU:HD12	2.45	0.41
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: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:204:ILE:C	1:C:204:ILE:CD1	2.92	0.41
1:C:256:MET:O	1:C:260:LYS:HG2	2.20	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:G:255:LEU:HA	1:G:258:MET:HE3	2.02	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:C:349:PHE:C	1:C:352:PRO:HD2	2.46	0.41
1:D:298:THR:O	1:D:301:GLU:HG2	2.21	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:B:338:LYS:HZ3	1:B:338:LYS:HG3	1.71	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:19:ASP:CG	1:D:91:HIS:HD1	2.25	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:261:LEU:HA	1:D:261:LEU:HD23	1.80	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:D:336:THR:OG1	1:D:337:ALA:N	2.53	0.40
1:G:215:SER:N	1:G:353:MET:HE1	2.35	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: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

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	453/453 (100%)	429 (95%)	23 (5%)	1 (0%)	43	50
1	B	451/453 (100%)	424 (94%)	26 (6%)	1 (0%)	43	50
1	C	453/453 (100%)	427 (94%)	25 (6%)	1 (0%)	43	50
1	D	451/453 (100%)	423 (94%)	27 (6%)	1 (0%)	43	50
1	E	451/453 (100%)	418 (93%)	31 (7%)	2 (0%)	30	31
1	F	451/453 (100%)	418 (93%)	32 (7%)	1 (0%)	43	50
1	G	451/453 (100%)	419 (93%)	30 (7%)	2 (0%)	30	31
All	All	3161/3171 (100%)	2958 (94%)	194 (6%)	9 (0%)	36	40

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

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%)	407 (100%)	0	100	100
1	B	401/404 (99%)	400 (100%)	1 (0%)	87	92
1	C	401/404 (99%)	401 (100%)	0	100	100
1	D	398/404 (98%)	398 (100%)	0	100	100
1	E	378/404 (94%)	378 (100%)	0	100	100
1	F	374/404 (93%)	374 (100%)	0	100	100
1	G	381/404 (94%)	380 (100%)	1 (0%)	86	90
All	All	2740/2828 (97%)	2738 (100%)	2 (0%)	88	92

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	86	ASN
1	G	447	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	A	335	GLN
1	A	383	HIS
1	A	422	GLN
1	B	188	GLN
1	B	232	HIS
1	B	316	GLN
1	B	346	HIS
1	B	401	GLN
1	B	407	GLN
1	C	44	GLN
1	C	110	ASN
1	C	122	HIS
1	C	181	ASN
1	C	232	HIS
1	C	383	HIS
1	D	94	GLN
1	D	284	GLN
1	D	316	GLN
1	D	406	HIS
1	E	406	HIS

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Mol	Chain	Res	Type
1	F	44	GLN
1	F	55	GLN
1	F	122	HIS
1	F	389	HIS
1	G	91	HIS
1	G	94	GLN
1	G	110	ASN
1	G	122	HIS
1	G	286	ASN
1	G	355	GLN
1	G	383	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 oligosaccharides 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	D	502	-	4,4,4	0.27	0	6,6,6	0.24	0
2	SO4	F	502	-	4,4,4	0.28	0	6,6,6	0.15	0
2	SO4	F	501	-	4,4,4	0.30	0	6,6,6	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	C	505	-	4,4,4	0.26	0	6,6,6	0.23	0
2	SO4	D	501	-	4,4,4	0.28	0	6,6,6	0.23	0
2	SO4	E	504	-	4,4,4	0.29	0	6,6,6	0.28	0
2	SO4	B	502	-	4,4,4	0.28	0	6,6,6	0.27	0
2	SO4	C	502	-	4,4,4	0.25	0	6,6,6	0.21	0
2	SO4	E	502	-	4,4,4	0.25	0	6,6,6	0.13	0
2	SO4	C	504	-	4,4,4	0.20	0	6,6,6	0.36	0
2	SO4	A	506	-	4,4,4	0.29	0	6,6,6	0.43	0
2	SO4	D	504	-	4,4,4	0.30	0	6,6,6	0.34	0
2	SO4	A	502	-	4,4,4	0.29	0	6,6,6	0.23	0
2	SO4	B	504	-	4,4,4	0.31	0	6,6,6	0.36	0
2	SO4	G	502	-	4,4,4	0.24	0	6,6,6	0.14	0
2	SO4	E	503	-	4,4,4	0.24	0	6,6,6	0.18	0
2	SO4	A	503	-	4,4,4	0.29	0	6,6,6	0.22	0
2	SO4	B	501	-	4,4,4	0.30	0	6,6,6	0.28	0
2	SO4	E	501	-	4,4,4	0.26	0	6,6,6	0.11	0
2	SO4	A	504	-	4,4,4	0.23	0	6,6,6	0.06	0
2	SO4	C	501	-	4,4,4	0.30	0	6,6,6	0.16	0
2	SO4	F	503	-	4,4,4	0.26	0	6,6,6	0.19	0
2	SO4	A	505	-	4,4,4	0.23	0	6,6,6	0.32	0
2	SO4	A	501	-	4,4,4	0.31	0	6,6,6	0.29	0
2	SO4	C	503	-	4,4,4	0.23	0	6,6,6	0.18	0
2	SO4	D	503	-	4,4,4	0.26	0	6,6,6	0.20	0
2	SO4	G	501	-	4,4,4	0.23	0	6,6,6	0.43	0
2	SO4	B	503	-	4,4,4	0.29	0	6,6,6	0.20	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	F	501	SO4	1	0
2	C	505	SO4	1	0
2	E	502	SO4	1	0
2	C	504	SO4	1	0
2	A	506	SO4	1	0
2	D	504	SO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	501	SO4	1	0

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	452/453 (99%)	0.18	9 (1%) 65 65	23, 51, 67, 72	3 (0%)
1	B	452/453 (99%)	0.73	15 (3%) 49 49	31, 65, 85, 102	1 (0%)
1	C	452/453 (99%)	0.51	24 (5%) 32 30	26, 58, 84, 104	3 (0%)
1	D	451/453 (99%)	0.45	18 (3%) 42 42	26, 59, 82, 95	2 (0%)
1	E	452/453 (99%)	1.00	67 (14%) 5 5	26, 66, 99, 120	1 (0%)
1	F	452/453 (99%)	1.32	83 (18%) 3 3	33, 73, 109, 133	1 (0%)
1	G	452/453 (99%)	1.47	112 (24%) 2 1	34, 77, 102, 116	1 (0%)
All	All	3163/3171 (99%)	0.81	328 (10%) 11 11	23, 65, 97, 133	12 (0%)

All (328) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	331	TYR	6.7
1	G	246	VAL	6.5
1	G	268	SER	5.6
1	F	333	ASP	5.5
1	E	242	ASP	5.5
1	E	243	THR	5.2
1	E	236	MET	5.0
1	G	245	ASP	4.9
1	C	79[A]	HIS	4.9
1	G	278	ILE	4.9
1	F	308	SER	4.6
1	E	274	ILE	4.6
1	E	248	SER	4.5
1	G	331	TYR	4.5
1	E	238	LEU	4.5
1	E	232	HIS	4.4
1	G	335	GLN	4.3

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Mol	Chain	Res	Type	RSRZ
1	F	320	ASP	4.3
1	G	141	LEU	4.2
1	G	329	LEU	4.2
1	G	33	ASP	4.1
1	F	335	GLN	4.1
1	G	223	LEU	4.1
1	F	330	LYS	4.1
1	E	261	LEU	4.1
1	G	149	PHE	4.1
1	A	193[A]	MET	4.1
1	G	251	THR	4.0
1	E	149	PHE	4.0
1	F	314	SER	3.9
1	E	246	VAL	3.9
1	F	326	ASP	3.8
1	D	79[A]	HIS	3.8
1	G	244	ASP	3.8
1	F	319	ILE	3.8
1	F	315	PRO	3.8
1	E	275	TYR	3.7
1	E	331	TYR	3.7
1	G	143	TYR	3.7
1	G	227	ARG	3.7
1	C	240	TYR	3.7
1	E	244	ASP	3.7
1	E	33	ASP	3.7
1	F	313	LEU	3.7
1	E	148	TYR	3.7
1	F	318	PHE	3.6
1	G	27	ALA	3.6
1	F	305	TYR	3.6
1	E	249	LEU	3.6
1	D	331	TYR	3.6
1	G	224	GLU	3.6
1	E	227	ARG	3.6
1	G	362	ILE	3.5
1	C	289	THR	3.5
1	D	248	SER	3.5
1	F	329	LEU	3.5
1	F	336	THR	3.5
1	G	226	ALA	3.4
1	E	146	TRP	3.4

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Mol	Chain	Res	Type	RSRZ
1	G	249	LEU	3.4
1	G	140	ALA	3.4
1	G	261	LEU	3.4
1	G	148	TYR	3.4
1	G	318	PHE	3.4
1	E	75	THR	3.4
1	G	264	SER	3.4
1	F	316	GLN	3.3
1	C	329	LEU	3.3
1	F	317	ARG	3.3
1	F	307	THR	3.3
1	E	247	THR	3.2
1	F	275	TYR	3.2
1	G	138	LEU	3.2
1	G	233	PHE	3.2
1	G	273	LEU	3.2
1	G	247	THR	3.2
1	B	36	PHE	3.2
1	E	272	ASP	3.2
1	G	145	ASP	3.2
1	C	-1	PRO	3.2
1	E	223	LEU	3.2
1	E	241	LEU	3.2
1	G	238	LEU	3.2
1	G	257	LEU	3.2
1	F	274	ILE	3.2
1	E	239	ASP	3.1
1	G	310	GLN	3.1
1	F	241	LEU	3.1
1	C	11[A]	HIS	3.1
1	E	263	GLN	3.1
1	C	238	LEU	3.1
1	E	153	PHE	3.1
1	E	141	LEU	3.1
1	F	324	LEU	3.1
1	G	151	LYS	3.0
1	F	342	LEU	3.0
1	G	146	TRP	3.0
1	F	266	GLY	3.0
1	B	238	LEU	3.0
1	E	250	SER	3.0
1	G	216	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	223	LEU	2.9
1	G	240	TYR	2.9
1	C	323	GLU	2.9
1	A	-1	PRO	2.9
1	F	262	LYS	2.9
1	F	350	LYS	2.9
1	D	249	LEU	2.9
1	E	335	GLN	2.9
1	F	310	GLN	2.9
1	F	306	ILE	2.9
1	G	203	ASP	2.9
1	E	251	THR	2.9
1	A	62	ASP	2.9
1	E	245	ASP	2.9
1	F	267	PRO	2.8
1	G	275	TYR	2.8
1	F	144	LEU	2.8
1	E	278	ILE	2.8
1	F	244	ASP	2.8
1	G	272	ASP	2.8
1	G	286	ASN	2.8
1	E	144	LEU	2.8
1	F	334	VAL	2.8
1	G	236	MET	2.8
1	G	259	ALA	2.8
1	E	35	ARG	2.8
1	G	79	HIS	2.8
1	G	282	TYR	2.8
1	G	277	PRO	2.7
1	G	315	PRO	2.7
1	C	331	TYR	2.7
1	D	246	VAL	2.7
1	D	289	THR	2.7
1	E	150	ASN	2.7
1	E	253	ASP	2.7
1	F	110	ASN	2.7
1	E	282	TYR	2.7
1	G	289	THR	2.7
1	B	327	ILE	2.7
1	E	139	GLY	2.7
1	F	321	ILE	2.7
1	E	324	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	223	LEU	2.7
1	G	36	PHE	2.7
1	G	114	THR	2.7
1	G	330	LYS	2.7
1	F	113	GLY	2.7
1	E	237	MET	2.7
1	G	231	GLN	2.6
1	G	328	PRO	2.6
1	C	310	GLN	2.6
1	F	332	GLU	2.6
1	G	7	GLY	2.6
1	E	256	MET	2.6
1	F	11	HIS	2.6
1	B	261	LEU	2.6
1	F	141	LEU	2.6
1	A	443	ARG	2.6
1	C	286	ASN	2.6
1	B	328	PRO	2.6
1	C	445	TYR	2.6
1	E	240	TYR	2.6
1	F	236	MET	2.6
1	G	319	ILE	2.6
1	F	232	HIS	2.6
1	F	337	ALA	2.6
1	G	77	THR	2.6
1	B	313	LEU	2.5
1	C	223	LEU	2.5
1	D	224	GLU	2.5
1	D	219	ARG	2.5
1	E	140	ALA	2.5
1	F	36	PHE	2.5
1	A	445	TYR	2.5
1	F	445	TYR	2.5
1	F	218	LEU	2.5
1	G	324	LEU	2.5
1	A	244	ASP	2.5
1	F	150	ASN	2.5
1	E	262	LYS	2.5
1	E	222	THR	2.5
1	G	243	THR	2.5
1	C	321	ILE	2.5
1	F	348	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	257	LEU	2.5
1	G	271	LEU	2.5
1	F	338	LYS	2.5
1	G	252	ASN	2.5
1	C	335	GLN	2.5
1	F	339	GLN	2.5
1	G	153	PHE	2.5
1	G	254	ILE	2.5
1	F	240	TYR	2.5
1	B	310	GLN	2.5
1	G	59	PRO	2.5
1	G	274	ILE	2.4
1	G	144	LEU	2.4
1	G	198	LEU	2.4
1	G	287	TYR	2.4
1	E	231	GLN	2.4
1	F	268	SER	2.4
1	F	327	ILE	2.4
1	G	176	PHE	2.4
1	G	283	ILE	2.4
1	A	238	LEU	2.4
1	G	26	TYR	2.4
1	F	79	HIS	2.4
1	F	216	GLY	2.4
1	G	276	ALA	2.4
1	B	243	THR	2.4
1	G	248	SER	2.4
1	E	254	ILE	2.4
1	E	255	LEU	2.4
1	G	241	LEU	2.4
1	G	346	HIS	2.4
1	E	265	ARG	2.4
1	C	281	ASP	2.4
1	G	325	ASN	2.4
1	E	-1	PRO	2.4
1	G	147	SER	2.4
1	G	341	SER	2.4
1	F	238	LEU	2.4
1	G	357	LEU	2.4
1	C	232	HIS	2.4
1	D	240	TYR	2.3
1	G	267	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	225	SER	2.3
1	G	31	VAL	2.3
1	C	313	LEU	2.3
1	F	261	LEU	2.3
1	G	220	LEU	2.3
1	G	35	ARG	2.3
1	E	11	HIS	2.3
1	E	32	HIS	2.3
1	E	233	PHE	2.3
1	F	176	PHE	2.3
1	G	80	GLU	2.3
1	G	41	LEU	2.3
1	F	67	ASP	2.3
1	G	110	ASN	2.3
1	G	338	LYS	2.3
1	E	226	ALA	2.3
1	F	193	MET	2.3
1	B	247	THR	2.3
1	F	226	ALA	2.3
1	D	332	GLU	2.3
1	G	44	GLN	2.3
1	G	334	VAL	2.3
1	G	326	ASP	2.2
1	C	315	PRO	2.2
1	G	58	PRO	2.2
1	F	265	ARG	2.2
1	B	232	HIS	2.2
1	G	337	ALA	2.2
1	D	243	THR	2.2
1	E	47	GLU	2.2
1	G	365	SER	2.2
1	D	330	LYS	2.2
1	G	350	LYS	2.2
1	F	249	LEU	2.2
1	G	218	LEU	2.2
1	E	62	ASP	2.2
1	F	16	ASP	2.2
1	F	219	ARG	2.2
1	F	444	ARG	2.2
1	D	442	GLU	2.2
1	C	151	LYS	2.2
1	E	230	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	5	THR	2.2
1	G	6	THR	2.2
1	E	321	ILE	2.2
1	B	203	ASP	2.2
1	F	258	MET	2.2
1	G	442	GLU	2.2
1	D	355	GLN	2.2
1	F	370	TRP	2.2
1	F	41	LEU	2.2
1	F	138	LEU	2.2
1	F	31	VAL	2.2
1	D	0	GLY	2.2
1	G	119	GLN	2.2
1	F	140	ALA	2.2
1	F	243	THR	2.2
1	G	230	ALA	2.2
1	F	297	TYR	2.1
1	B	223	LEU	2.1
1	B	321	ILE	2.1
1	C	246	VAL	2.1
1	G	34	ASN	2.1
1	G	253	ASP	2.1
1	E	59	PRO	2.1
1	E	234	GLN	2.1
1	E	276	ALA	2.1
1	G	189	SER	2.1
1	G	137	ARG	2.1
1	E	297	TYR	2.1
1	E	252	ASN	2.1
1	F	325	ASN	2.1
1	G	109	GLU	2.1
1	A	110	ASN	2.1
1	C	203	ASP	2.1
1	F	239	ASP	2.1
1	G	49	ILE	2.1
1	G	67	ASP	2.1
1	E	334	VAL	2.1
1	F	146	TRP	2.1
1	F	302	GLY	2.1
1	G	158	GLY	2.1
1	D	46	SER	2.1
1	G	142	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	222	THR	2.0
1	A	332	GLU	2.0
1	F	276	ALA	2.0
1	C	110	ASN	2.0
1	D	228	ASN	2.0
1	F	33	ASP	2.0
1	F	213	LEU	2.0
1	F	304	ILE	2.0
1	G	101	ILE	2.0
1	G	201	ILE	2.0
1	C	328	PRO	2.0
1	B	68	PHE	2.0
1	E	225	SER	2.0
1	F	345	THR	2.0
1	G	343	ALA	2.0
1	E	79	HIS	2.0
1	B	324	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	E	501	5/5	0.57	0.17	77,78,86,87	5
2	SO4	G	502	5/5	0.63	0.17	86,88,93,94	5
2	SO4	F	503	5/5	0.69	0.16	88,89,91,92	5
2	SO4	F	501	5/5	0.72	0.14	81,82,87,88	5
2	SO4	E	504	5/5	0.74	0.13	83,85,88,90	5
2	SO4	B	504	5/5	0.75	0.17	63,63,72,74	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	B	501	5/5	0.76	0.12	70,73,78,78	5
2	SO4	A	505	5/5	0.79	0.15	61,63,65,68	5
2	SO4	A	506	5/5	0.80	0.15	58,61,65,69	5
2	SO4	A	504	5/5	0.80	0.13	57,58,62,63	5
2	SO4	B	503	5/5	0.81	0.15	65,72,74,80	5
2	SO4	G	501	5/5	0.83	0.15	64,65,69,70	5
2	SO4	D	503	5/5	0.83	0.12	74,75,80,84	5
2	SO4	C	504	5/5	0.84	0.16	62,68,72,73	5
2	SO4	C	503	5/5	0.86	0.10	74,75,77,78	5
2	SO4	D	504	5/5	0.86	0.11	66,67,76,78	5
2	SO4	A	502	5/5	0.87	0.12	54,55,61,62	5
2	SO4	B	502	5/5	0.87	0.15	56,58,61,63	5
2	SO4	A	501	5/5	0.88	0.12	51,59,61,64	5
2	SO4	C	501	5/5	0.88	0.10	66,72,73,76	0
2	SO4	C	505	5/5	0.88	0.12	51,53,59,60	5
2	SO4	D	502	5/5	0.88	0.12	62,68,72,72	5
2	SO4	F	502	5/5	0.89	0.15	66,67,68,70	5
2	SO4	E	503	5/5	0.89	0.09	65,67,73,73	5
2	SO4	C	502	5/5	0.90	0.12	58,60,62,63	5
2	SO4	D	501	5/5	0.91	0.11	59,61,63,63	5
2	SO4	E	502	5/5	0.92	0.10	58,62,63,63	5
2	SO4	A	503	5/5	0.93	0.10	49,51,52,55	5

6.5 Other polymers [i](#)

There are no such residues in this entry.