



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 03:10 PM UTC

PDB ID : 4BUJ / pdb_00004buj
Title : Crystal structure of the S. cerevisiae Ski2-3-8 complex
Authors : Halbach, F.; Reichelt, P.; Rode, M.; Conti, E.
Deposited on : 2013-06-20
Resolution : 3.70 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

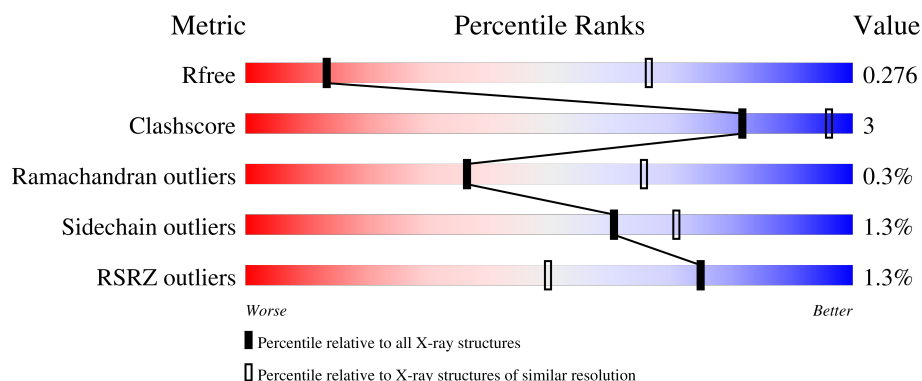
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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	1044	
1	E	1044	
2	B	1436	
2	F	1436	
3	C	397	

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Mol	Chain	Length	Quality of chain
3	D	397	2% 88% 8%
3	G	397	% 88% 9%
3	H	397	3% 85% 12%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 43019 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 ANTIVIRAL HELICASE SKI2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	903	Total	C	N	O	S	0	0	0
			6621	4236	1132	1223	30			
1	E	881	Total	C	N	O	S	0	0	0
			6016	3836	1046	1106	28			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P35207
A	-2	PRO	-	expression tag	UNP P35207
A	-1	ASP	-	expression tag	UNP P35207
A	0	SER	-	expression tag	UNP P35207
A	835	GLY	-	linker	UNP P35207
A	836	SER	-	linker	UNP P35207
A	837	ARG	-	linker	UNP P35207
A	1085	GLY	-	linker	UNP P35207
E	-3	GLY	-	expression tag	UNP P35207
E	-2	PRO	-	expression tag	UNP P35207
E	-1	ASP	-	expression tag	UNP P35207
E	0	SER	-	expression tag	UNP P35207
E	835	GLY	-	linker	UNP P35207
E	836	SER	-	linker	UNP P35207
E	837	ARG	-	linker	UNP P35207
E	1085	GLY	-	linker	UNP P35207

- Molecule 2 is a protein called SUPERKILLER PROTEIN 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1367	Total	C	N	O	S	0	0	0
			9800	6281	1660	1822	37			
2	F	1351	Total	C	N	O	S	0	0	0
			9328	5966	1597	1733	32			

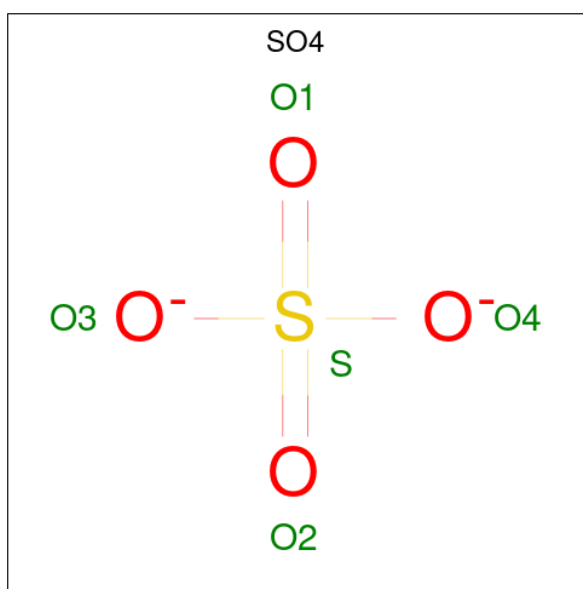
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P17883
B	-2	PRO	-	expression tag	UNP P17883
B	-1	ASP	-	expression tag	UNP P17883
B	0	SER	-	expression tag	UNP P17883
F	-3	GLY	-	expression tag	UNP P17883
F	-2	PRO	-	expression tag	UNP P17883
F	-1	ASP	-	expression tag	UNP P17883
F	0	SER	-	expression tag	UNP P17883

- Molecule 3 is a protein called ANTIVIRAL PROTEIN SKI8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	392	Total	C	N	O	S	0	0	0
			2931	1860	499	558	14			
3	D	381	Total	C	N	O	S	0	0	0
			2790	1778	478	521	13			
3	G	387	Total	C	N	O	S	0	0	0
			2904	1846	497	547	14			
3	H	351	Total	C	N	O	S	0	0	0
			2529	1615	427	474	13			

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

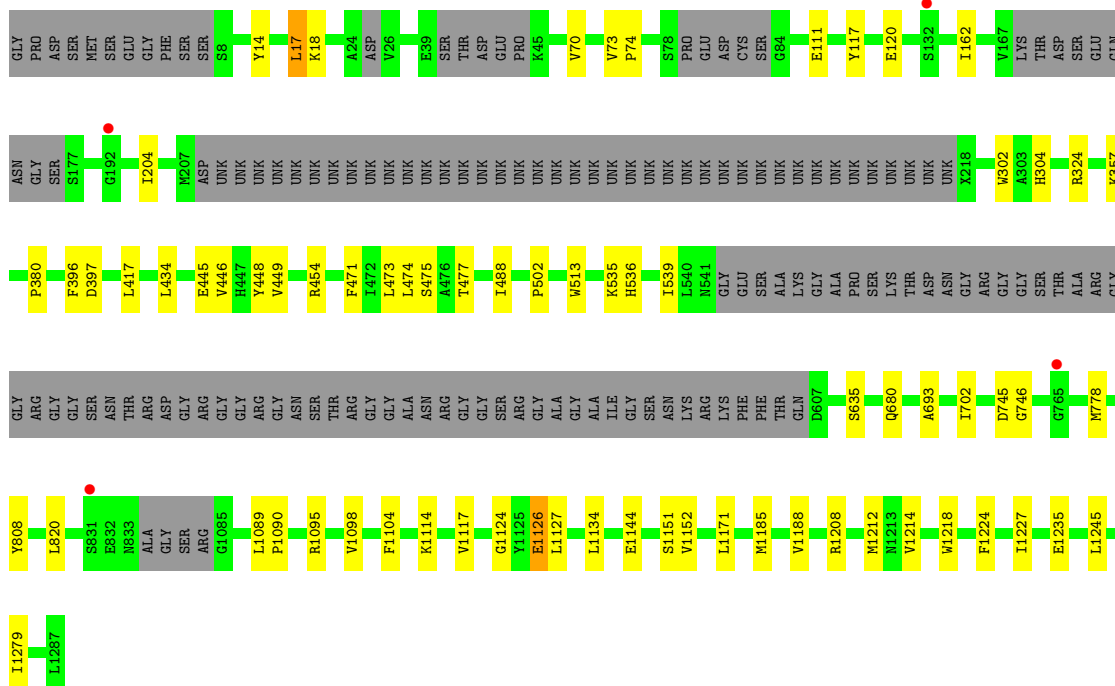
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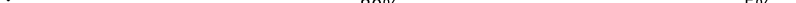
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total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

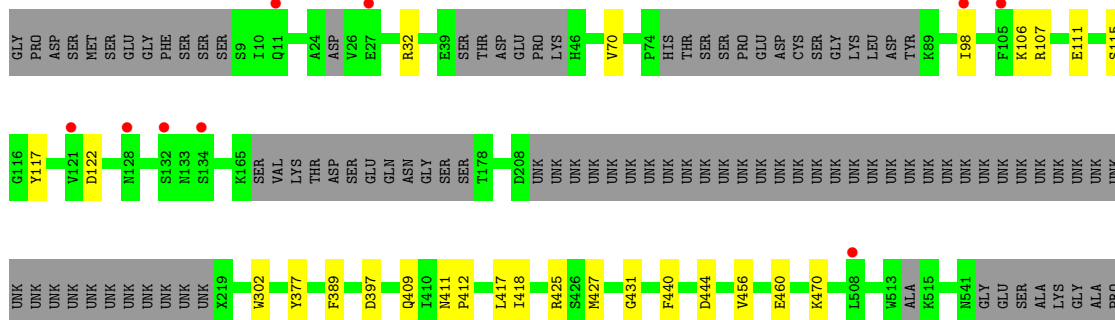
● Molecule 1: ANTIVIRAL HELICASE SKI2

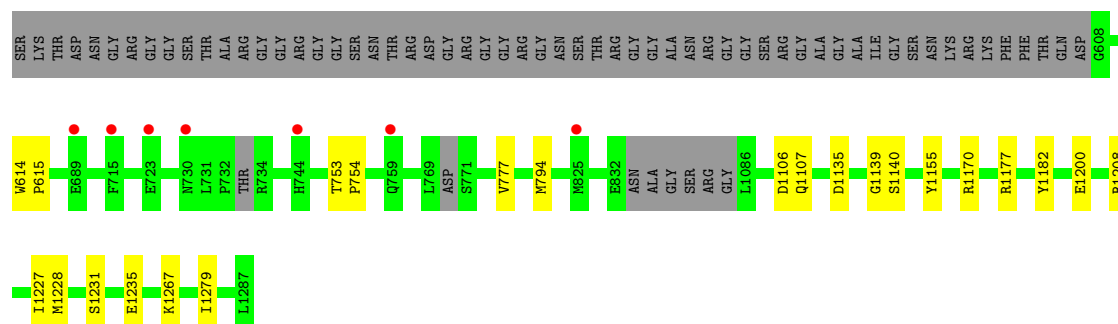
Responsibility	Percentage
Current government	80%
Previous government	7%
No government	14%



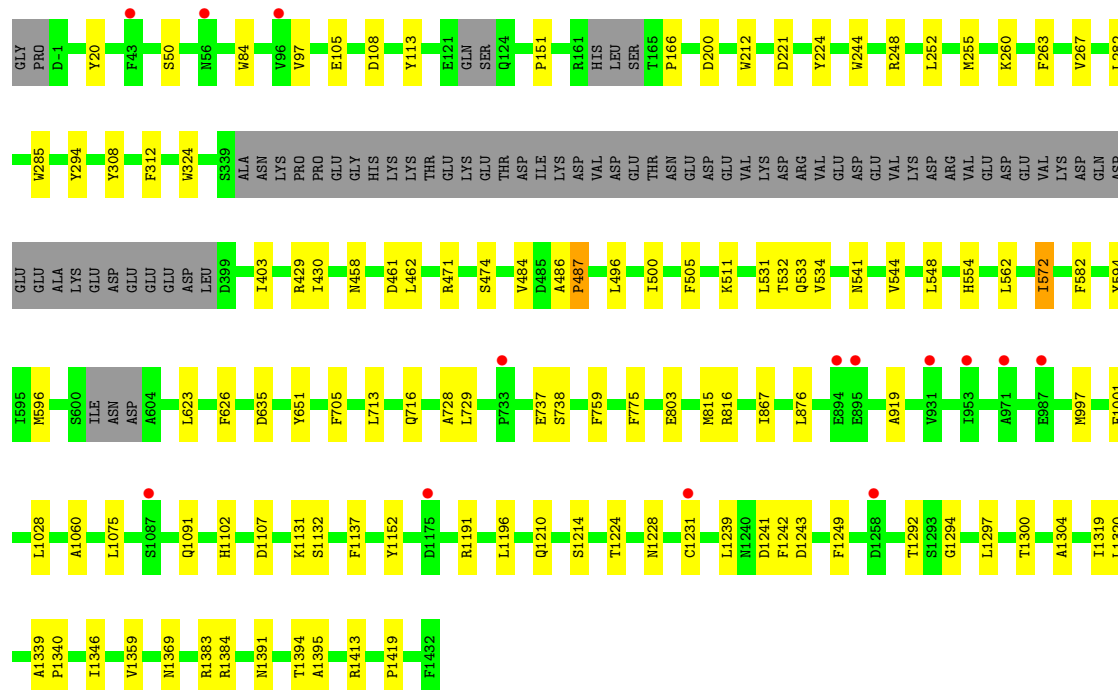
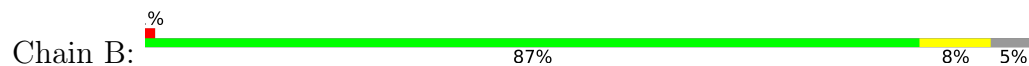
- Molecule 1: ANTIVIRAL HELICASE SKI2

Chain E:  2% 80% 5% 16%

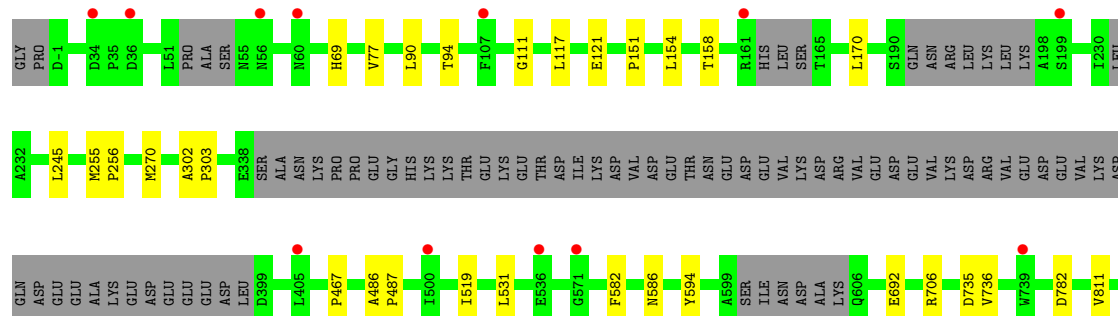
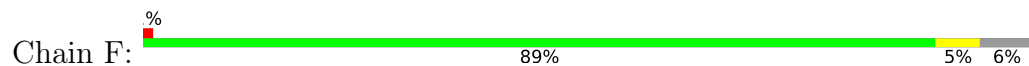


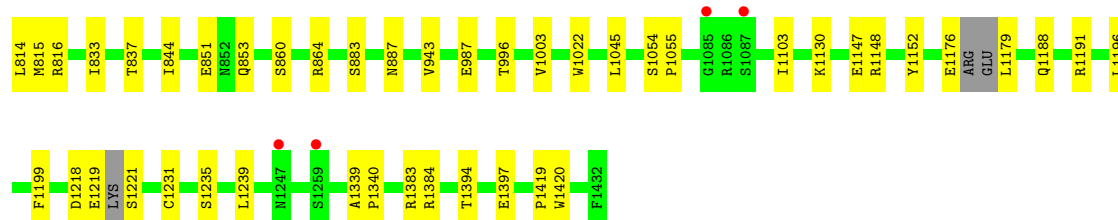


• Molecule 2: SUPERKILLER PROTEIN 3

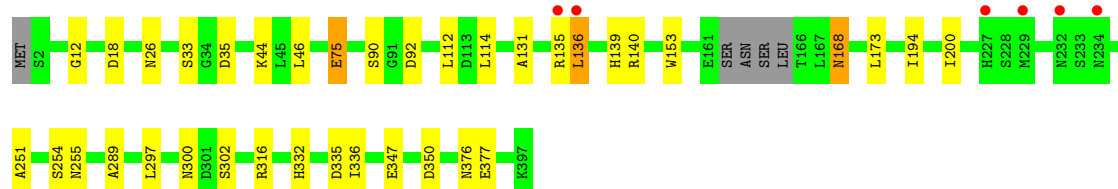
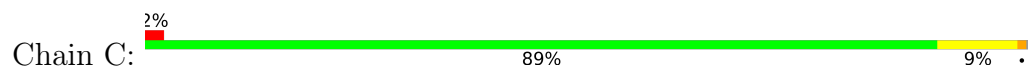


• Molecule 2: SUPERKILLER PROTEIN 3

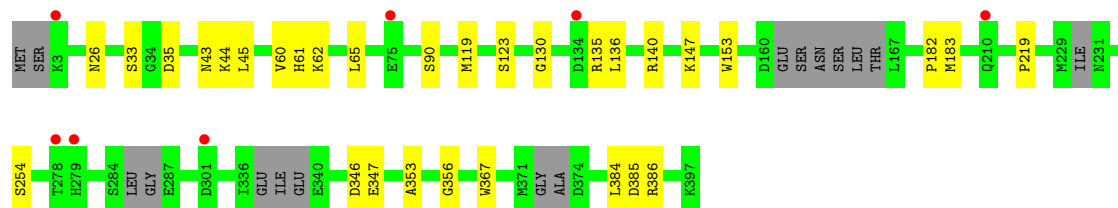
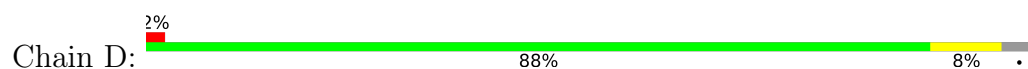




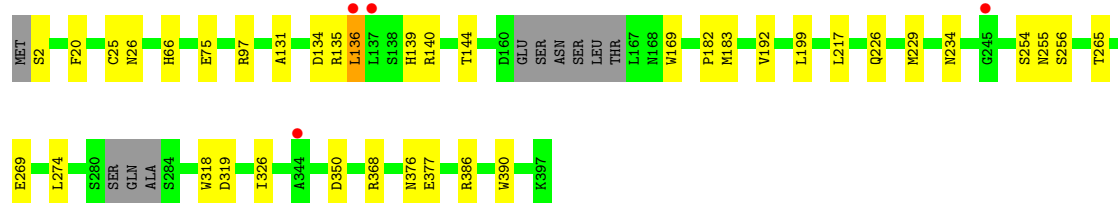
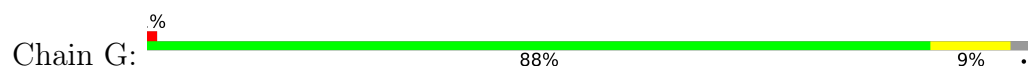
● Molecule 3: ANTIVIRAL PROTEIN SKI8



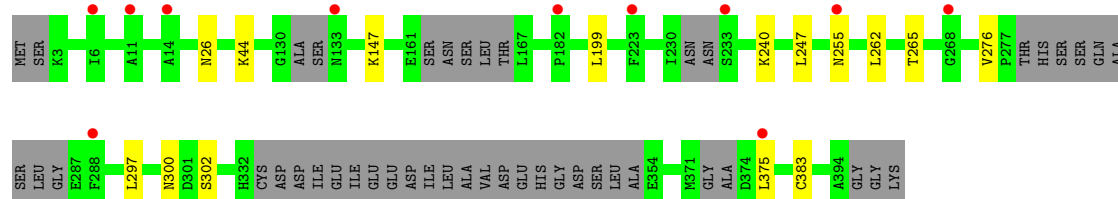
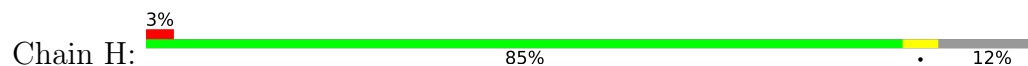
● Molecule 3: ANTIVIRAL PROTEIN SKI8



● Molecule 3: ANTIVIRAL PROTEIN SKI8



● Molecule 3: ANTIVIRAL PROTEIN SKI8



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	183.38Å 200.41Å 340.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	96.12 – 3.70 96.12 – 3.70	Depositor EDS
% Data completeness (in resolution range)	98.8 (96.12-3.70) 98.6 (96.12-3.70)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 3.67Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.231 , 0.265 0.243 , 0.276	Depositor DCC
R_{free} test set	6669 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	139.9	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 180.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	43019	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% 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	0.37	0/6488	0.74	3/8829 (0.0%)
1	E	0.33	0/5886	0.73	1/8055 (0.0%)
2	B	0.36	0/10000	0.75	2/13675 (0.0%)
2	F	0.36	2/9511 (0.0%)	0.75	2/13043 (0.0%)
3	C	0.36	0/2999	0.68	0/4079
3	D	0.33	0/2855	0.69	1/3885 (0.0%)
3	G	0.34	0/2972	0.69	2/4039 (0.0%)
3	H	0.30	0/2588	0.62	0/3536
All	All	0.35	2/43299 (0.0%)	0.73	11/59141 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	69	HIS	CG-ND1	-5.55	1.32	1.38
2	F	69	HIS	CG-CD2	5.31	1.41	1.35

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	226	GLN	N-CA-C	6.03	118.30	110.53
3	G	254	SER	N-CA-C	-5.99	100.24	109.52
1	A	73	VAL	CB-CA-C	-5.72	105.62	110.94
1	E	70	VAL	N-CA-C	5.56	116.22	110.82
2	F	77	VAL	CA-C-N	5.47	125.56	119.32
2	F	77	VAL	C-N-CA	5.47	125.56	119.32
2	B	200	ASP	N-CA-C	-5.45	101.72	109.62
1	A	693	ALA	N-CA-C	5.40	115.67	108.38
3	D	254	SER	N-CA-C	-5.25	102.69	110.46
1	A	396	PHE	N-CA-C	5.19	118.16	110.48
2	B	97	VAL	CB-CA-C	-5.02	108.93	113.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6621	0	5996	40	0
1	E	6016	0	4947	24	0
2	B	9800	0	8525	60	0
2	F	9328	0	7703	39	0
3	C	2931	0	2691	22	0
3	D	2790	0	2487	13	0
3	G	2904	0	2658	17	0
3	H	2529	0	2218	6	0
4	A	20	0	0	2	0
4	B	5	0	0	0	0
4	C	20	0	0	0	0
4	D	10	0	0	0	0
4	E	15	0	0	0	0
4	G	20	0	0	0	0
4	H	10	0	0	0	0
All	All	43019	0	37225	203	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 3.

All (203) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:680:GLN:NE2	1:A:1235:GLU:OE1	2.17	0.77
3:D:356:GLY:O	3:D:384:LEU:N	2.22	0.72
2:B:1224:THR:O	2:B:1228:ASN:ND2	2.25	0.70
1:A:18:LYS:NZ	3:C:92:ASP:OD1	2.26	0.67
2:B:1383:ARG:NH1	3:C:350:ASP:OD2	2.30	0.64
1:A:14:TYR:OH	2:B:1419:PRO:O	2.14	0.63
1:A:380:PRO:O	1:A:454:ARG:NH2	2.31	0.63
3:C:131:ALA:O	3:C:135:ARG:NH1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1104:PHE:HE2	1:A:1127:LEU:HG	1.65	0.61
3:C:168:ASN:N	3:C:168:ASN:OD1	2.33	0.61
2:F:735:ASP:OD1	2:F:736:VAL:N	2.33	0.61
1:A:324:ARG:NH1	1:A:397:ASP:OD1	2.32	0.61
3:H:300:ASN:ND2	3:H:302:SER:OG	2.34	0.60
2:F:1383:ARG:NH1	3:G:350:ASP:OD2	2.35	0.59
3:D:60:VAL:HG11	3:D:65:LEU:HD11	1.84	0.59
3:D:33:SER:OG	3:D:35:ASP:OD1	2.20	0.59
1:E:106:LYS:O	1:E:115:SER:N	2.37	0.58
1:A:471:PHE:HB3	1:A:473:LEU:CD1	2.34	0.57
2:B:252:LEU:HD11	2:B:267:VAL:HG11	1.86	0.57
1:E:1139:GLY:O	1:E:1267:LYS:NZ	2.38	0.57
1:A:446:VAL:O	1:A:449:VAL:N	2.37	0.56
3:C:300:ASN:ND2	3:C:302:SER:OG	2.39	0.56
2:F:883:SER:O	2:F:887:ASN:ND2	2.37	0.56
2:B:294:TYR:O	2:B:429:ARG:NH2	2.38	0.56
2:F:117:LEU:O	2:F:121:GLU:N	2.38	0.55
2:F:1103:ILE:O	2:F:1148:ARG:NH2	2.38	0.55
2:B:1369:ASN:OD1	2:B:1391:ASN:ND2	2.37	0.55
2:F:814:LEU:HB3	2:F:837:THR:HG22	1.88	0.55
3:D:130:GLY:N	3:D:140:ARG:O	2.40	0.55
3:H:26:ASN:O	3:H:44:LYS:NZ	2.40	0.55
3:H:240:LYS:NZ	3:H:297:LEU:O	2.40	0.55
1:A:635:SER:OG	4:A:2002:SO4:O4	2.26	0.54
1:E:122:ASP:OD1	1:E:122:ASP:N	2.40	0.54
1:E:1140:SER:O	1:E:1170:ARG:NH1	2.40	0.54
2:B:815:MET:HG3	2:B:816:ARG:N	2.23	0.54
2:B:531:LEU:HA	2:B:534:VAL:HG12	1.92	0.52
1:A:1224:PHE:HA	1:A:1227:ILE:CG2	2.40	0.52
1:A:111:GLU:HG2	2:B:737:GLU:HB2	1.93	0.51
1:A:117:TYR:OH	2:B:803:GLU:OE1	2.29	0.51
2:B:324:TRP:CB	2:B:430:ILE:HD11	2.41	0.51
1:A:1224:PHE:HA	1:A:1227:ILE:HG22	1.93	0.51
1:A:357:LYS:HZ2	1:A:475:SER:C	2.17	0.51
1:E:1155:TYR:O	1:E:1208:ARG:NH1	2.44	0.51
1:A:357:LYS:N	4:A:2001:SO4:O1	2.44	0.51
2:B:471:ARG:NH2	2:B:500:ILE:O	2.44	0.50
1:E:1135:ASP:OD2	1:E:1177:ARG:NH2	2.44	0.50
2:F:486:ALA:HB3	2:F:487:PRO:HD3	1.92	0.50
3:C:26:ASN:O	3:C:44:LYS:NZ	2.45	0.50
3:C:75:GLU:OE1	3:C:139:HIS:NE2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:635:ASP:OD1	2:B:651:TYR:OH	2.27	0.49
2:F:1218:ASP:O	2:F:1221:SER:N	2.45	0.49
2:F:1219:GLU:O	2:F:1221:SER:N	2.46	0.49
1:E:409:GLN:O	3:G:2:SER:N	2.45	0.49
1:A:702:ILE:HG21	1:A:1279:ILE:HD11	1.95	0.49
1:A:808:TYR:CG	1:A:1127:LEU:HD11	2.48	0.49
2:B:324:TRP:CG	2:B:430:ILE:HD11	2.48	0.49
2:F:1384:ARG:O	3:H:147:LYS:NZ	2.43	0.49
3:G:131:ALA:O	3:G:135:ARG:NH1	2.45	0.49
1:A:1126:GLU:HG2	1:A:1127:LEU:HD12	1.96	0.48
2:B:221:ASP:OD1	2:B:244:TRP:NE1	2.39	0.48
1:A:513:TRP:HB3	1:A:778:MET:HE2	1.96	0.48
2:B:84:TRP:HB3	2:B:113:TYR:CD2	2.48	0.48
3:C:114:LEU:HD23	3:C:173:LEU:HG	1.94	0.48
1:A:304:HIS:N	1:A:304:HIS:CD2	2.82	0.48
2:B:759:PHE:CE2	2:B:775:PHE:HB3	2.49	0.48
3:D:346:ASP:OD1	3:D:347:GLU:N	2.44	0.47
2:F:1419:PRO:HD2	2:F:1420:TRP:CE3	2.50	0.47
2:B:1384:ARG:O	3:D:147:LYS:NZ	2.46	0.47
1:A:1171:LEU:HB3	1:A:1212:MET:CE	2.45	0.47
1:E:1227:ILE:O	1:E:1231:SER:N	2.43	0.47
2:F:90:LEU:O	2:F:94:THR:N	2.43	0.47
2:F:1339:ALA:HB3	2:F:1340:PRO:HD3	1.97	0.47
2:B:623:LEU:CB	2:B:626:PHE:HB2	2.45	0.47
2:F:245:LEU:HD13	2:F:270:MET:HE3	1.96	0.47
2:B:1339:ALA:HB3	2:B:1340:PRO:HD3	1.97	0.47
2:B:1102:HIS:ND1	2:B:1107:ASP:OD2	2.47	0.47
2:B:532:THR:HA	2:B:548:LEU:HD11	1.96	0.46
2:F:302:ALA:HB3	2:F:303:PRO:HD3	1.96	0.46
2:F:111:GLY:HA3	2:F:154:LEU:HD11	1.97	0.46
3:C:112:LEU:HB3	3:C:114:LEU:CD1	2.45	0.46
2:F:1152:TYR:HB3	2:F:1196:LEU:HD12	1.98	0.46
2:B:282:LEU:HD21	2:B:312:PHE:CG	2.51	0.46
2:B:876:LEU:HD22	2:B:919:ALA:HB2	1.98	0.46
1:E:389:PHE:HA	1:E:418:ILE:HD12	1.98	0.46
1:E:425:ARG:NE	1:E:460:GLU:OE1	2.47	0.46
1:E:427:MET:O	1:E:431:GLY:N	2.48	0.46
3:G:25:CYS:SG	3:G:26:ASN:N	2.89	0.46
2:B:729:LEU:HD11	2:B:738:SER:HB3	1.98	0.46
2:F:1130:LYS:NZ	3:G:269:GLU:OE1	2.49	0.46
1:A:1152:VAL:O	1:A:1208:ARG:NH1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1384:ARG:NH1	3:D:123:SER:OG	2.48	0.46
2:B:1132:SER:O	2:B:1132:SER:OG	2.31	0.46
2:F:853:GLN:HE22	2:F:943:VAL:HG21	1.80	0.45
1:E:377:TYR:OH	1:E:444:ASP:OD2	2.35	0.45
2:F:1022:TRP:HB2	2:F:1045:LEU:HD21	1.97	0.45
2:B:486:ALA:HB3	2:B:487:PRO:HD3	1.98	0.45
2:B:1152:TYR:HB3	2:B:1196:LEU:HD12	1.98	0.45
2:B:1304:ALA:HA	2:B:1319:ILE:HG12	1.98	0.45
2:F:811:VAL:CG2	2:F:844:ILE:HD11	2.46	0.45
3:G:136:LEU:HB3	3:G:140:ARG:HH12	1.81	0.45
1:A:446:VAL:O	1:A:448:TYR:N	2.50	0.45
2:F:996:THR:HG21	2:F:1003:VAL:HB	1.99	0.45
1:E:111:GLU:CB	2:F:706:ARG:CZ	2.95	0.45
1:A:17:LEU:CD2	3:C:90:SER:HA	2.46	0.45
2:B:84:TRP:HB3	2:B:113:TYR:HD2	1.82	0.45
3:C:136:LEU:HB3	3:C:140:ARG:HH12	1.81	0.45
1:A:1151:SER:HA	1:A:1245:LEU:HD21	1.98	0.45
2:B:1241:ASP:O	2:B:1243:ASP:N	2.50	0.45
2:B:1297:LEU:O	2:B:1300:THR:N	2.50	0.45
1:A:70:VAL:HG11	2:B:1191:ARG:HD3	1.98	0.44
2:F:1176:GLU:O	2:F:1179:LEU:N	2.51	0.44
3:G:182:PRO:HD2	3:G:183:MET:HE3	1.98	0.44
2:F:833:ILE:O	2:F:837:THR:HG23	2.18	0.44
2:B:1060:ALA:HB2	2:B:1075:LEU:HB3	1.99	0.44
1:E:1182:TYR:OH	1:E:1200:GLU:O	2.34	0.44
1:E:409:GLN:HG2	1:E:412:PRO:HG3	1.99	0.44
2:F:782:ASP:OD1	2:F:816:ARG:NH1	2.50	0.44
2:F:1394:THR:HB	2:F:1397:GLU:HG3	2.00	0.44
1:E:1106:ASP:OD1	1:E:1107:GLN:N	2.51	0.44
2:B:997:MET:HE3	2:B:1028:LEU:HA	2.00	0.44
3:C:112:LEU:HB3	3:C:114:LEU:HD11	1.99	0.44
2:F:519:ILE:HD11	2:F:531:LEU:HD11	1.98	0.44
1:A:417:LEU:HD11	1:A:434:LEU:HD11	1.99	0.44
2:B:461:ASP:OD1	2:B:462:LEU:N	2.49	0.44
2:F:1188:GLN:OE1	2:F:1191:ARG:NH2	2.51	0.44
3:G:75:GLU:OE1	3:G:139:HIS:NE2	2.51	0.44
3:C:376:ASN:OD1	3:C:377:GLU:N	2.42	0.43
3:D:26:ASN:HA	3:D:367:TRP:CG	2.53	0.43
3:C:289:ALA:O	3:C:316:ARG:NH1	2.51	0.43
1:E:397:ASP:OD1	1:E:397:ASP:N	2.50	0.43
2:B:1191:ARG:HG2	2:B:1231:CYS:SG	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:511:LYS:NZ	2:B:533:GLN:OE1	2.51	0.43
2:F:1147:GLU:OE1	2:F:1188:GLN:NE2	2.50	0.43
1:A:204:ILE:HD11	2:B:1001:PHE:CE1	2.53	0.43
2:F:1199:PHE:O	2:F:1235:SER:OG	2.36	0.43
1:E:1228:MET:SD	1:E:1235:GLU:HG2	2.59	0.43
1:A:74:PRO:HB2	2:B:1137:PHE:CE2	2.54	0.43
2:B:244:TRP:NE1	2:B:248:ARG:HD3	2.34	0.43
2:B:541:ASN:HB3	2:B:544:VAL:HG12	2.01	0.43
3:C:254:SER:O	3:C:255:ASN:C	2.62	0.43
3:G:20:PHE:HB2	3:G:66:HIS:HA	2.00	0.43
3:G:199:LEU:HD22	3:G:265:THR:HG21	2.00	0.43
2:F:1054:SER:N	2:F:1055:PRO:HD2	2.34	0.42
3:G:256:SER:O	3:G:256:SER:OG	2.34	0.42
3:H:247:LEU:HD11	3:H:262:LEU:HB3	2.01	0.42
2:B:1394:THR:OG1	2:B:1395:ALA:N	2.52	0.42
1:E:753:THR:HB	1:E:754:PRO:HD2	2.00	0.42
2:B:252:LEU:HD21	2:B:263:PHE:HD1	1.85	0.42
2:B:1210:GLN:O	2:B:1214:SER:N	2.50	0.42
3:C:332:HIS:N	3:C:335:ASP:OD2	2.47	0.42
3:D:384:LEU:C	3:D:386:ARG:H	2.28	0.42
1:E:411:ASN:N	1:E:412:PRO:HD3	2.35	0.42
3:G:97:ARG:HD2	3:G:169:TRP:CZ2	2.55	0.42
3:G:319:ASP:HB2	3:G:326:ILE:HD11	2.00	0.42
2:B:285:TRP:HB3	2:B:308:TYR:CE1	2.55	0.42
2:B:263:PHE:CD1	2:B:263:PHE:C	2.97	0.42
2:B:1320:LEU:HD12	2:B:1346:ILE:HB	2.02	0.42
3:C:33:SER:OG	3:C:35:ASP:OD1	2.37	0.42
1:A:162:ILE:HG21	1:A:820:LEU:HD12	2.00	0.42
2:B:474:SER:HB2	2:B:496:LEU:HD11	2.02	0.42
1:A:445:GLU:N	1:A:474:LEU:O	2.53	0.41
1:A:1089:LEU:HB3	1:A:1090:PRO:HD3	2.02	0.41
2:B:1413:ARG:NE	3:C:18:ASP:OD2	2.52	0.41
3:D:182:PRO:HD2	3:D:183:MET:HE2	2.01	0.41
2:F:582:PHE:O	2:F:586:ASN:ND2	2.52	0.41
2:B:705:PHE:HB2	2:B:728:ALA:HB2	2.02	0.41
3:G:368:ARG:HH12	3:G:390:TRP:CG	2.38	0.41
3:G:376:ASN:OD1	3:G:377:GLU:N	2.52	0.41
1:A:1104:PHE:CD1	1:A:1114:LYS:HB3	2.55	0.41
2:B:20:TYR:CE2	2:B:50:SER:CB	3.04	0.41
3:C:251:ALA:HB2	3:C:297:LEU:HD13	2.02	0.41
1:E:614:TRP:HB2	1:E:615:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1214:VAL:HG13	1:A:1227:ILE:HG13	2.03	0.41
3:D:61:HIS:CE1	3:D:90:SER:HB2	2.55	0.41
2:B:151:PRO:HG3	2:B:166:PRO:HB2	2.03	0.41
3:C:153:TRP:HB3	3:C:173:LEU:HD22	2.03	0.41
3:C:12:GLY:HA3	3:C:336:ILE:HD13	2.03	0.41
1:E:98:ILE:HD11	2:F:987:GLU:HG3	2.03	0.41
3:H:199:LEU:CD2	3:H:265:THR:HG21	2.51	0.41
1:A:1185:MET:HA	1:A:1188:VAL:HG12	2.02	0.41
2:B:729:LEU:HD11	2:B:738:SER:CB	2.50	0.41
3:C:194:ILE:HG22	3:C:200:ILE:HG12	2.03	0.41
1:E:107:ARG:HA	1:E:115:SER:H	1.86	0.41
2:F:255:MET:HB2	2:F:256:PRO:HD2	2.03	0.41
3:G:144:THR:HG23	3:G:192:VAL:HG21	2.03	0.41
1:A:1218:TRP:HB2	1:A:1227:ILE:HD12	2.02	0.41
2:B:212:TRP:CZ3	2:B:255:MET:HB3	2.56	0.41
2:B:255:MET:SD	2:B:260:LYS:HA	2.61	0.41
2:F:860:SER:O	2:F:864:ARG:HG2	2.21	0.41
2:F:1191:ARG:HG2	2:F:1231:CYS:SG	2.61	0.41
3:G:274:LEU:HB3	3:G:318:TRP:CE3	2.56	0.41
1:A:473:LEU:HD21	1:A:488:ILE:CD1	2.51	0.40
1:A:535:LYS:O	1:A:539:ILE:HG13	2.21	0.40
2:B:554:HIS:HA	2:B:596:MET:HE1	2.03	0.40
2:F:151:PRO:HD3	2:F:170:LEU:HD11	2.02	0.40
2:F:154:LEU:O	2:F:158:THR:N	2.54	0.40
1:A:1095:ARG:HA	1:A:1098:VAL:HG12	2.03	0.40
2:B:105:GLU:HA	2:B:108:ASP:HB2	2.03	0.40
1:E:440:PHE:CE1	1:E:470:LYS:HD2	2.57	0.40
1:A:745:ASP:OD1	1:A:746:GLY:N	2.54	0.40
2:B:572:ILE:HD13	2:B:582:PHE:CD2	2.56	0.40
3:D:43:ASN:O	3:D:45:LEU:N	2.55	0.40
3:D:119:MET:HE2	3:D:153:TRP:HZ2	1.87	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	835/1044 (80%)	797 (95%)	36 (4%)	2 (0%)	43	72
1	E	810/1044 (78%)	785 (97%)	24 (3%)	1 (0%)	48	78
2	B	1357/1436 (94%)	1298 (96%)	52 (4%)	7 (0%)	24	56
2	F	1333/1436 (93%)	1284 (96%)	48 (4%)	1 (0%)	48	78
3	C	388/397 (98%)	364 (94%)	23 (6%)	1 (0%)	36	65
3	D	369/397 (93%)	347 (94%)	17 (5%)	5 (1%)	9	37
3	G	381/397 (96%)	358 (94%)	22 (6%)	1 (0%)	36	65
3	H	337/397 (85%)	313 (93%)	23 (7%)	1 (0%)	36	65
All	All	5810/6548 (89%)	5546 (96%)	245 (4%)	19 (0%)	36	65

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	484	VAL
2	B	1239	LEU
3	C	75	GLU
3	D	44	LYS
3	H	255	ASN
3	D	353	ALA
3	G	255	ASN
1	A	1124	GLY
3	D	135	ARG
2	F	467	PRO
2	B	1292	THR
3	D	385	ASP
2	B	403	ILE
2	B	1242	PHE
1	E	1279	ILE
3	D	219	PRO
2	B	487	PRO
2	B	1294	GLY
1	A	502	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	614/832 (74%)	605 (98%)	9 (2%)	57	68
1	E	466/832 (56%)	459 (98%)	7 (2%)	57	68
2	B	836/1282 (65%)	823 (98%)	13 (2%)	55	68
2	F	715/1282 (56%)	710 (99%)	5 (1%)	76	77
3	C	295/347 (85%)	291 (99%)	4 (1%)	59	70
3	D	266/347 (77%)	264 (99%)	2 (1%)	73	76
3	G	289/347 (83%)	283 (98%)	6 (2%)	47	64
3	H	240/347 (69%)	237 (99%)	3 (1%)	61	71
All	All	3721/5616 (66%)	3672 (99%)	49 (1%)	61	71

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	120	GLU
1	A	302	TRP
1	A	477	THR
1	A	536	HIS
1	A	1117	VAL
1	A	1126	GLU
1	A	1134	LEU
1	A	1144	GLU
2	B	224	TYR
2	B	458	ASN
2	B	505	PHE
2	B	562	LEU
2	B	572	ILE
2	B	594	TYR
2	B	713	LEU
2	B	716	GLN
2	B	867	ILE
2	B	1091	GLN
2	B	1131	LYS
2	B	1249	PHE
2	B	1359	VAL
3	C	46	LEU

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Mol	Chain	Res	Type
3	C	136	LEU
3	C	168	ASN
3	C	347	GLU
3	D	62	LYS
3	D	136	LEU
1	E	32	ARG
1	E	117	TYR
1	E	302	TRP
1	E	417	LEU
1	E	456	VAL
1	E	777	VAL
1	E	794	MET
2	F	594	TYR
2	F	692	GLU
2	F	815	MET
2	F	851	GLU
2	F	1239	LEU
3	G	134	ASP
3	G	136	LEU
3	G	217	LEU
3	G	229	MET
3	G	234	ASN
3	G	386	ARG
3	H	276	VAL
3	H	375	LEU
3	H	383	CYS

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

Mol	Chain	Res	Type
1	A	15	GLN
1	A	60	ASN
1	A	343	GLN
1	A	450	ASN
2	B	172	ASN
2	B	433	GLN
2	B	458	ASN
2	B	491	ASN
2	B	1066	GLN
3	C	10	ASN
3	C	43	ASN
3	C	66	HIS

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Mol	Chain	Res	Type
3	C	176	GLN
3	D	58	HIS
3	D	330	ASN
1	E	22	ASN
1	E	340	HIS
1	E	1265	HIS
1	E	1272	GLN
2	F	279	HIS
2	F	1101	ASN
2	F	1205	ASN
2	F	1261	HIS
2	F	1331	GLN
2	F	1361	GLN
3	G	176	GLN
3	G	210	GLN
3	H	122	HIS
3	H	252	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](#)

20 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
4	SO4	C	1002	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	G	1003	-	4,4,4	0.24	0	6,6,6	0.06	0
4	SO4	G	1002	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	G	1004	-	4,4,4	0.24	0	6,6,6	0.11	0
4	SO4	A	2002	-	4,4,4	0.26	0	6,6,6	0.05	0
4	SO4	B	2001	-	4,4,4	0.23	0	6,6,6	0.07	0
4	SO4	G	1001	-	4,4,4	0.23	0	6,6,6	0.10	0
4	SO4	E	2001	-	4,4,4	0.23	0	6,6,6	0.07	0
4	SO4	D	1001	-	4,4,4	0.23	0	6,6,6	0.06	0
4	SO4	H	1002	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	A	2003	-	4,4,4	0.22	0	6,6,6	0.13	0
4	SO4	C	1003	-	4,4,4	0.22	0	6,6,6	0.08	0
4	SO4	A	2001	-	4,4,4	0.23	0	6,6,6	0.06	0
4	SO4	E	2003	-	4,4,4	0.23	0	6,6,6	0.08	0
4	SO4	E	2002	-	4,4,4	0.25	0	6,6,6	0.09	0
4	SO4	C	1004	-	4,4,4	0.24	0	6,6,6	0.12	0
4	SO4	D	1002	-	4,4,4	0.24	0	6,6,6	0.11	0
4	SO4	C	1001	-	4,4,4	0.23	0	6,6,6	0.09	0
4	SO4	A	2004	-	4,4,4	0.23	0	6,6,6	0.08	0
4	SO4	H	1001	-	4,4,4	0.23	0	6,6,6	0.08	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2002	SO4	1	0
4	A	2001	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
1	E	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	281:UNK	C	301:GLU	N	44.66
1	E	281:UNK	C	301:GLU	N	41.85
1	E	255:UNK	C	270:UNK	N	19.58
1	A	256:UNK	C	269:UNK	N	16.09

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	851/1044 (81%)	-0.22	4 (0%) 87 69	49, 86, 153, 361	0
1	E	832/1044 (79%)	0.09	16 (1%) 66 42	79, 150, 224, 363	0
2	B	1367/1436 (95%)	-0.16	14 (1%) 79 55	51, 101, 164, 277	0
2	F	1351/1436 (94%)	-0.06	16 (1%) 76 51	61, 128, 199, 310	0
3	C	392/397 (98%)	-0.19	6 (1%) 72 46	40, 67, 140, 322	0
3	D	381/397 (95%)	-0.02	7 (1%) 67 42	56, 92, 169, 265	0
3	G	387/397 (97%)	-0.10	4 (1%) 79 55	45, 87, 151, 235	0
3	H	351/397 (88%)	0.18	11 (3%) 51 32	115, 180, 260, 351	0
All	All	5912/6548 (90%)	-0.08	78 (1%) 75 50	40, 112, 203, 363	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	1087	SER	4.7
3	H	233	SER	4.5
1	A	132	SER	4.2
3	H	182	PRO	3.9
1	E	508	LEU	3.5
2	B	56	ASN	3.3
1	E	27	GLU	3.3
3	D	278	THR	3.2
3	D	75	GLU	3.2
3	D	279	HIS	3.2
3	H	6	ILE	3.2
3	G	245	GLY	3.2
2	B	1087	SER	3.1
2	F	500	ILE	3.0
3	H	11	ALA	3.0
3	C	229	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	715	PHE	2.9
1	E	825	MET	2.9
2	F	161	ARG	2.8
1	E	98	ILE	2.8
3	H	255	ASN	2.8
2	B	987	GLU	2.6
2	B	43	PHE	2.6
1	E	759	GLN	2.6
2	F	571	GLY	2.6
2	F	34	ASP	2.5
3	C	232	ASN	2.5
3	D	301	ASP	2.5
3	G	136	LEU	2.5
1	E	730	ASN	2.5
2	F	56	ASN	2.5
2	B	1258	ASP	2.5
3	H	288	PHE	2.5
1	E	744	HIS	2.5
2	F	1247	ASN	2.5
3	C	234	ASN	2.4
2	B	1231	CYS	2.4
2	F	739	TRP	2.4
2	F	1085	GLY	2.4
2	B	931	VAL	2.4
2	F	36	ASP	2.4
1	A	831	SER	2.3
1	E	11	GLN	2.3
2	B	895	GLU	2.3
1	E	132	SER	2.3
1	E	689	GLU	2.3
2	B	894	GLU	2.3
2	F	60	ASN	2.3
3	H	133	ASN	2.3
1	E	105	PHE	2.3
1	E	121	VAL	2.2
3	H	14	ALA	2.2
3	C	136	LEU	2.2
3	H	268	GLY	2.2
3	H	375	LEU	2.2
3	D	134	ASP	2.2
2	B	971	ALA	2.2
2	B	733	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
3	G	344	ALA	2.2
2	F	199	SER	2.2
3	H	223	PHE	2.2
2	B	953	ILE	2.1
2	F	107	PHE	2.1
2	F	405	LEU	2.1
3	D	210	GLN	2.1
1	E	723	GLU	2.1
3	C	135	ARG	2.1
1	E	128	ASN	2.1
2	B	96	VAL	2.1
2	B	1175	ASP	2.1
3	C	227	HIS	2.1
1	A	192	GLY	2.1
1	A	765	GLY	2.1
3	D	3	LYS	2.1
2	F	1259	SER	2.0
2	F	536	GLU	2.0
3	G	137	LEU	2.0
1	E	134	SER	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	A	2004	5/5	0.44	0.15	205,205,205,205	0
4	SO4	E	2003	5/5	0.52	0.17	252,252,252,252	0
4	SO4	H	1001	5/5	0.65	0.14	256,256,256,256	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	B	2001	5/5	0.69	0.09	212,212,212,212	0
4	SO4	E	2002	5/5	0.70	0.07	208,208,208,208	0
4	SO4	A	2002	5/5	0.73	0.23	133,133,133,133	0
4	SO4	H	1002	5/5	0.74	0.07	267,267,267,267	0
4	SO4	C	1004	5/5	0.76	0.20	182,182,182,182	0
4	SO4	E	2001	5/5	0.80	0.14	238,238,238,238	0
4	SO4	G	1004	5/5	0.80	0.17	191,191,191,191	0
4	SO4	A	2003	5/5	0.85	0.14	97,97,97,97	0
4	SO4	C	1001	5/5	0.87	0.15	173,173,173,173	0
4	SO4	D	1001	5/5	0.89	0.15	174,174,174,174	0
4	SO4	G	1003	5/5	0.90	0.13	142,142,142,142	0
4	SO4	G	1001	5/5	0.90	0.16	178,178,178,178	0
4	SO4	A	2001	5/5	0.91	0.14	175,175,175,175	0
4	SO4	G	1002	5/5	0.91	0.24	151,151,151,151	0
4	SO4	C	1002	5/5	0.94	0.25	162,162,162,162	0
4	SO4	C	1003	5/5	0.95	0.11	122,122,122,122	0
4	SO4	D	1002	5/5	0.97	0.16	142,142,142,142	0

6.5 Other polymers [i](#)

There are no such residues in this entry.