



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:16 PM GMT

PDB ID : 4BUJ  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

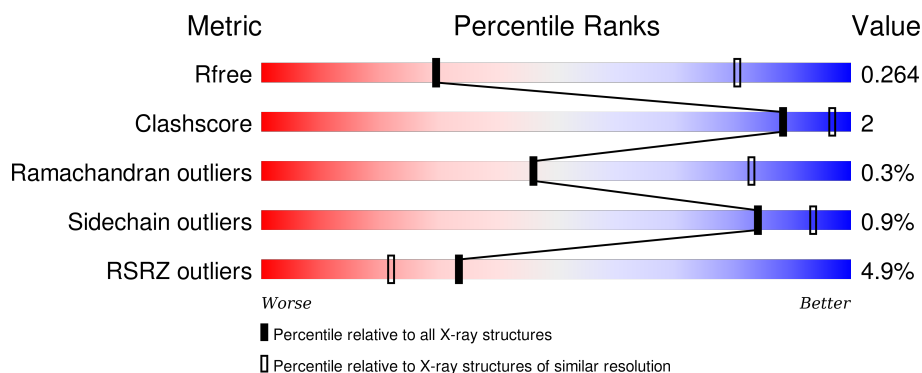
# 1 Overall quality at a glance

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))
$R_{free}$	91344	1101 (3.90-3.50)
Clashscore	102246	1224 (3.90-3.50)
Ramachandran outliers	100387	1172 (3.90-3.50)
Sidechain outliers	100360	1170 (3.90-3.50)
RSRZ outliers	91569	1108 (3.90-3.50)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>2%</div> <div>80% 6% 14%</div> </div>
1	E	1044	<div> <div>5%</div> <div>80% 5% 16%</div> </div>
2	B	1436	<div> <div>2%</div> <div>87% 8% 5%</div> </div>
2	F	1436	<div> <div>4%</div> <div>89% 5% 6%</div> </div>
3	C	397	<div> <div>90% 8% ..</div> </div>

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Mol	Chain	Length	Quality of chain
3	D	397	
3	G	397	
3	H	397	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	A	2004	-	-	-	X
4	SO4	C	1002	-	-	-	X
4	SO4	D	1001	-	-	-	X
4	SO4	D	1002	-	-	-	X
4	SO4	G	1001	-	-	-	X
4	SO4	G	1002	-	-	-	X

## 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			

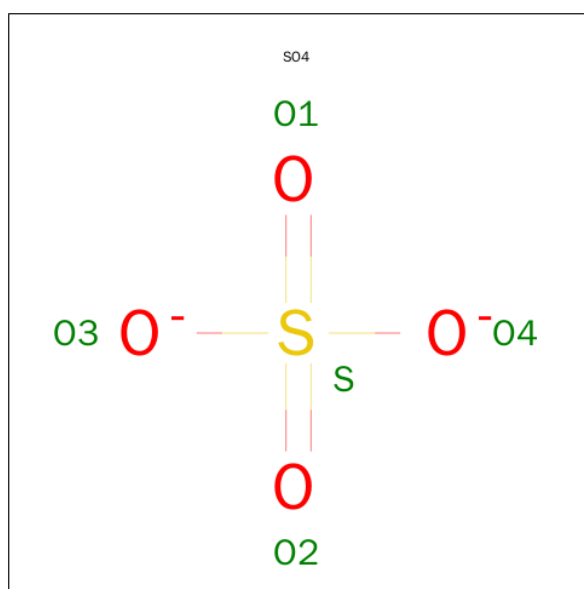
There are 8 discrepancies between the modelled and reference sequences:

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 (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



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

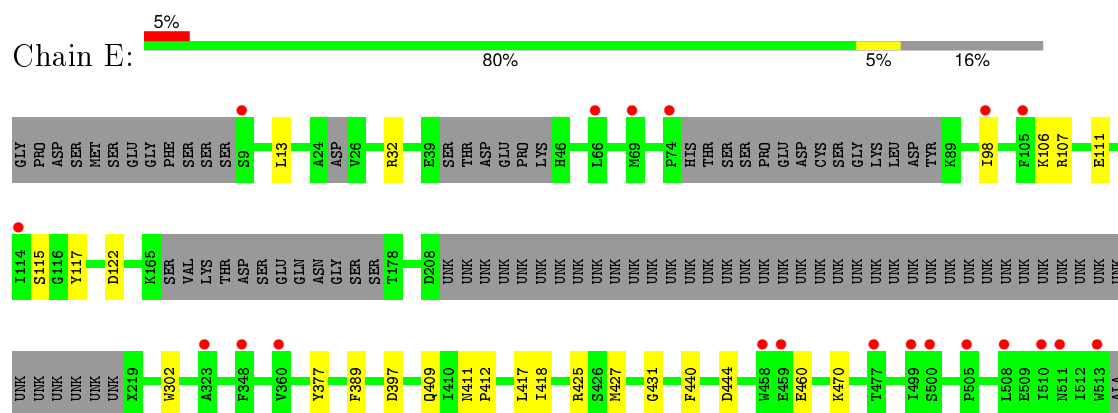
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0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

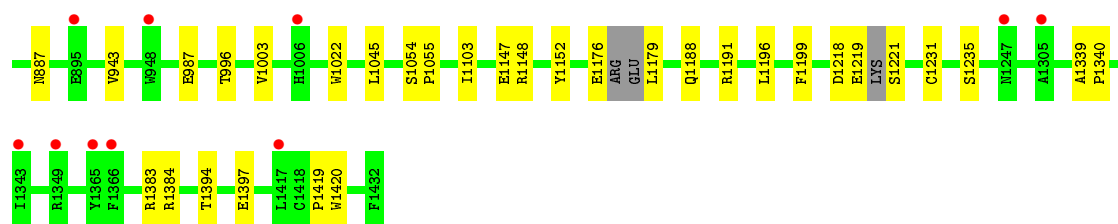


- Molecule 1: ANTIVIRAL HELICASE SKI2



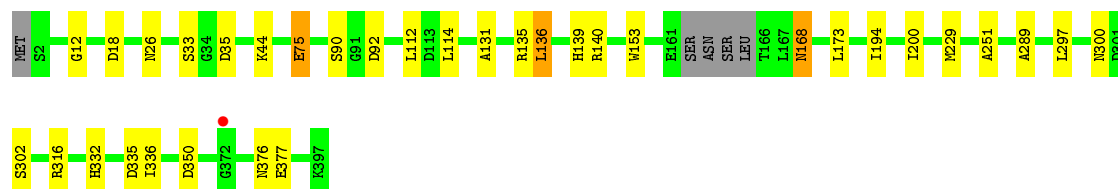






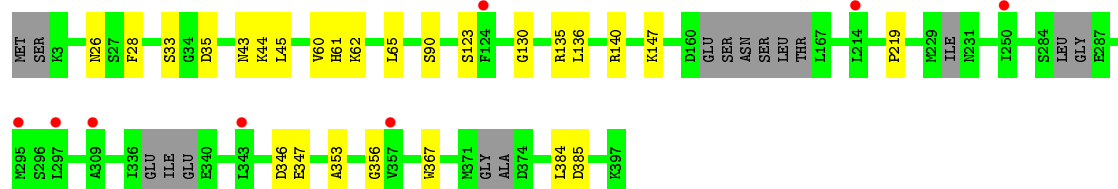
• Molecule 3: ANTIVIRAL PROTEIN SKI8

Chain C: 90% 8% ..



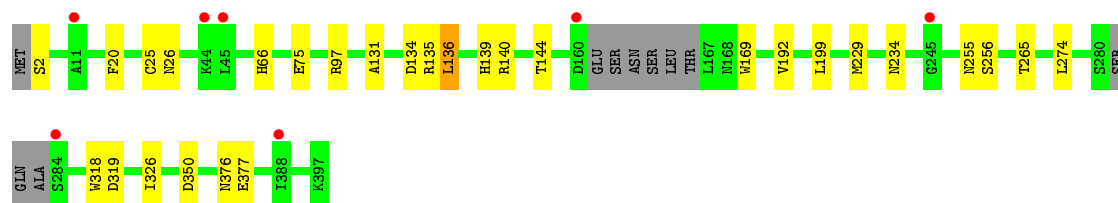
• Molecule 3: ANTIVIRAL PROTEIN SKI8

Chain D: 2% 89% 7% .



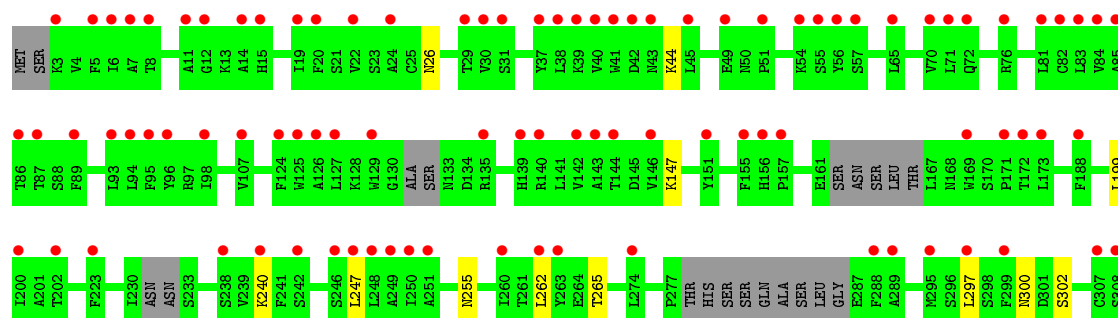
• Molecule 3: ANTIVIRAL PROTEIN SKI8

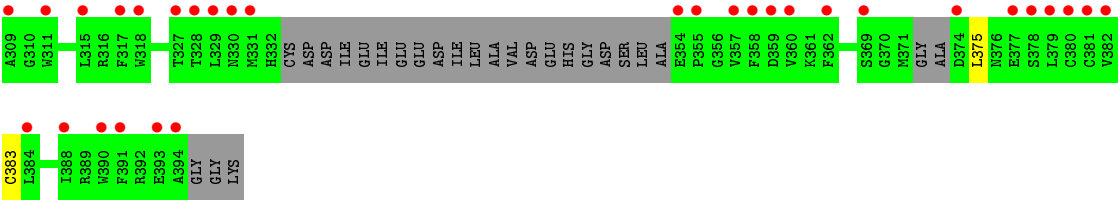
Chain G: 2% 90% 7% .



• Molecule 3: ANTIVIRAL PROTEIN SKI8

Chain H: 31% 85% 12% .





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 3.67Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.231 , 0.265 0.228 , 0.264	Depositor DCC
$R_{free}$ test set	6659 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	139.9	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 137.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	1 of 132490 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	43019	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.28	0/6488	0.47	0/8829
1	E	0.25	0/5886	0.43	0/8055
2	B	0.27	0/10000	0.44	0/13675
2	F	0.26	0/9511	0.41	0/13043
3	C	0.29	0/2999	0.49	0/4079
3	D	0.27	0/2855	0.47	0/3885
3	G	0.28	0/2972	0.50	0/4039
3	H	0.24	0/2588	0.43	0/3536
All	All	0.27	0/43299	0.45	0/59141

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6621	0	5996	41	0
1	E	6016	0	4947	25	0
2	B	9800	0	8525	61	0
2	F	9328	0	7703	38	0
3	C	2931	0	2691	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	2790	0	2487	11	0
3	G	2904	0	2658	14	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	199	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 2.

All (199) 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
2:B:1383:ARG:NH1	3:C:350:ASP:OD2	2.30	0.64
1:A:380:PRO:O	1:A:454:ARG:NH2	2.31	0.63
1:A:14:TYR:OH	2:B:1419:PRO:O	2.14	0.63
3:C:131:ALA:O	3:C:135:ARG:NH1	2.32	0.62
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:735:ASP:OD2	2:B:738:SER:OG	2.18	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
1:A:635:SER:OG	4:A:2002:SO4:O4	2.26	0.54
1:A:18:LYS:NZ	3:C:92:ASP:OD1	2.26	0.54
1:E:122:ASP:N	1:E:122:ASP:OD1	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:117:TYR:OH	2:B:803:GLU:OE1	2.29	0.51
1:A:111:GLU:HG2	2:B:737:GLU:HB2	1.93	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: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
2:F:486:ALA:HB3	2:F:487:PRO:HD3	1.92	0.50
1:E:1135:ASP:OD2	1:E:1177:ARG:NH2	2.44	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
3:H:240:LYS:NZ	3:H:297:LEU:O	2.40	0.49
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:E:810:MET:HE2	1:E:825:MET:HG2	1.94	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
1:A:702:ILE:HG21	1:A:1279:ILE:HD11	1.95	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
3:C:114:LEU:HD23	3:C:173:LEU:HG	1.94	0.48
2:B:84:TRP:HB3	2:B:113:TYR:CD2	2.48	0.48
1:A:304:HIS:CD2	1:A:304:HIS:N	2.82	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:1171:LEU:HB3	1:A:1212:MET:CE	2.45	0.47
2:B:623:LEU:CB	2:B:626:PHE:HB2	2.45	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:G:25:CYS:SG	3:G:26:ASN:N	2.89	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
1:E:427:MET:O	1:E:431:GLY:N	2.48	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:425:ARG:NE	1:E:460:GLU:OE1	2.47	0.46
1:E:389:PHE:HA	1:E:418:ILE:HD12	1.98	0.46
2:B:729:LEU:HD11	2:B:738:SER:HB3	1.98	0.46
2:B:1384:ARG:NH1	3:D:123:SER:OG	2.48	0.46
1:A:1152:VAL:O	1:A:1208:ARG:NH1	2.45	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
2:F:1022:TRP:HB2	2:F:1045:LEU:HD21	1.97	0.45
1:E:377:TYR:OH	1:E:444:ASP:OD2	2.35	0.45
2:B:1152:TYR:HB3	2:B:1196:LEU:HD12	1.98	0.45
2:B:486:ALA:HB3	2:B:487:PRO:HD3	1.98	0.45
3:G:136:LEU:HB3	3:G:140:ARG:HH12	1.81	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
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
2:B:84:TRP:HB3	2:B:113:TYR:HD2	1.82	0.45
1:A:17:LEU:CD2	3:C:90:SER:HA	2.46	0.45
3:C:136:LEU:HB3	3:C:140:ARG:HH12	1.81	0.45
2:B:1297:LEU:O	2:B:1300:THR:N	2.50	0.45
1:A:1151:SER:HA	1:A:1245:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1241:ASP:O	2:B:1243:ASP: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
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:1394:THR:HB	2:F:1397:GLU:HG3	2.00	0.44
2:F:782:ASP:OD1	2:F:816:ARG:NH1	2.50	0.44
1:E:397:ASP:N	1:E:397:ASP:OD1	2.50	0.44
1:E:1106:ASP:OD1	1:E:1107:GLN:N	2.51	0.44
3:C:112:LEU:HB3	3:C:114:LEU:HD11	1.99	0.44
1:A:64:TRP:CZ2	3:C:229:MET:HE1	2.53	0.44
2:F:519:ILE:HD11	2:F:531:LEU:HD11	1.98	0.44
2:B:461:ASP:OD1	2:B:462:LEU:N	2.49	0.44
3:G:75:GLU:OE1	3:G:139:HIS:NE2	2.51	0.44
1:A:417:LEU:HD11	1:A:434:LEU:HD11	1.99	0.44
2:F:1188:GLN:OE1	2:F:1191:ARG:NH2	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
2:B:815:MET:HE3	2:B:861:GLN:HB3	2.00	0.43
2:B:1191:ARG:HG2	2:B:1231:CYS:SG	2.58	0.43
2:F:1147:GLU:OE1	2:F:1188:GLN:NE2	2.50	0.43
2:B:511:LYS:NZ	2:B:533:GLN:OE1	2.51	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:G:199:LEU:HD22	3:G:265:THR:HG21	2.00	0.43
3:G:20:PHE:HB2	3:G:66:HIS:HA	2.00	0.43
2:F:1054:SER:N	2:F:1055:PRO:HD2	2.34	0.42
2:B:244:TRP:CE3	2:B:270:MET:HE1	2.54	0.42
3:G:256:SER:OG	3:G:256:SER:O	2.34	0.42
3:H:247:LEU:HD11	3:H:262:LEU:HB3	2.01	0.42
1:A:1171:LEU:HB3	1:A:1212:MET:HE2	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:332:HIS:N	3:C:335:ASP:OD2	2.47	0.42
2:B:1210:GLN:O	2:B:1214:SER:N	2.50	0.42
1:E:411:ASN:N	1:E:412:PRO:HD3	2.35	0.42
3:G:319:ASP:HB2	3:G:326:ILE:HD11	2.00	0.42
3:G:97:ARG:HD2	3:G:169:TRP:CZ2	2.55	0.42
2:B:285:TRP:HB3	2:B:308:TYR:CE1	2.55	0.42
3:C:33:SER:OG	3:C:35:ASP:OD1	2.37	0.42
2:B:1320:LEU:HD12	2:B:1346:ILE:HB	2.02	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
2:B:1413:ARG:NE	3:C:18:ASP:OD2	2.52	0.41
2:F:582:PHE:O	2:F:586:ASN:ND2	2.52	0.41
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:705:PHE:HB2	2:B:728:ALA:HB2	2.02	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
2:F:735:ASP:OD2	2:F:738:SER:OG	2.38	0.41
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
1:A:357:LYS:NZ	1:A:475:SER:O	2.47	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:E:107:ARG:HA	1:E:115:SER:H	1.86	0.41
2:B:729:LEU:HD11	2:B:738:SER:CB	2.50	0.41
1:A:1185:MET:HA	1:A:1188:VAL:HG12	2.02	0.41
2:F:255:MET:HB2	2:F:256:PRO:HD2	2.03	0.41
3:C:194:ILE:HG22	3:C:200:ILE:HG12	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:F:1191:ARG:HG2	2:F:1231:CYS:SG	2.61	0.41
2:F:860:SER:O	2:F:864:ARG:HG2	2.21	0.41
3:G:274:LEU:HB3	3:G:318:TRP:CE3	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:LEU:HD21	1:A:488:ILE:CD1	2.51	0.40
2:F:154:LEU:O	2:F:158:THR:N	2.54	0.40
2:F:151:PRO:HD3	2:F:170:LEU:HD11	2.02	0.40
1:A:535:LYS:O	1:A:539:ILE:HG13	2.21	0.40
2:B:1384:ARG:O	3:D:147:LYS:NZ	2.46	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
2:B:1388:ASN:H	3:D:147:LYS:HZ1	1.68	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

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%)	52	87
1	E	810/1044 (78%)	785 (97%)	24 (3%)	1 (0%)	56	90
2	B	1357/1436 (94%)	1298 (96%)	52 (4%)	7 (0%)	34	77
2	F	1333/1436 (93%)	1284 (96%)	48 (4%)	1 (0%)	56	90
3	C	388/397 (98%)	364 (94%)	23 (6%)	1 (0%)	46	83
3	D	369/397 (93%)	347 (94%)	17 (5%)	5 (1%)	14	60
3	G	381/397 (96%)	358 (94%)	22 (6%)	1 (0%)	46	83
3	H	337/397 (85%)	313 (93%)	23 (7%)	1 (0%)	46	83
All	All	5810/6548 (89%)	5546 (96%)	245 (4%)	19 (0%)	46	83

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%)	609 (99%)	5 (1%)	86	94
1	E	466/832 (56%)	461 (99%)	5 (1%)	80	92
2	B	836/1282 (65%)	826 (99%)	10 (1%)	78	91
2	F	715/1282 (56%)	712 (100%)	3 (0%)	93	98
3	C	295/347 (85%)	293 (99%)	2 (1%)	88	95
3	D	266/347 (77%)	263 (99%)	3 (1%)	80	92
3	G	289/347 (83%)	285 (99%)	4 (1%)	74	91
3	H	240/347 (69%)	238 (99%)	2 (1%)	86	94
All	All	3721/5616 (66%)	3687 (99%)	34 (1%)	84	93

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	302	TRP
1	A	448	TYR
1	A	477	THR
1	A	536	HIS
1	A	1112	LEU
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	1189	PHE
2	B	1249	PHE
2	B	1402	TYR
3	C	136	LEU
3	C	168	ASN
3	D	28	PHE
3	D	62	LYS
3	D	136	LEU
1	E	13	LEU
1	E	32	ARG
1	E	117	TYR
1	E	302	TRP
1	E	417	LEU
2	F	594	TYR
2	F	815	MET
2	F	851	GLU
3	G	134	ASP
3	G	136	LEU
3	G	229	MET
3	G	234	ASN
3	H	375	LEU
3	H	383	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	A	2001	-	4,4,4	0.31	0	6,6,6	0.06	0
4	SO4	A	2002	-	4,4,4	0.21	0	6,6,6	0.06	0
4	SO4	A	2003	-	4,4,4	0.27	0	6,6,6	0.17	0
4	SO4	A	2004	-	4,4,4	0.19	0	6,6,6	0.08	0
4	SO4	B	2001	-	4,4,4	0.26	0	6,6,6	0.08	0
4	SO4	C	1001	-	4,4,4	0.28	0	6,6,6	0.09	0
4	SO4	C	1002	-	4,4,4	0.24	0	6,6,6	0.06	0
4	SO4	C	1003	-	4,4,4	0.25	0	6,6,6	0.09	0
4	SO4	C	1004	-	4,4,4	0.19	0	6,6,6	0.09	0
4	SO4	D	1001	-	4,4,4	0.31	0	6,6,6	0.07	0
4	SO4	D	1002	-	4,4,4	0.25	0	6,6,6	0.10	0
4	SO4	E	2001	-	4,4,4	0.25	0	6,6,6	0.07	0
4	SO4	E	2002	-	4,4,4	0.20	0	6,6,6	0.09	0
4	SO4	E	2003	-	4,4,4	0.26	0	6,6,6	0.09	0
4	SO4	G	1001	-	4,4,4	0.28	0	6,6,6	0.11	0
4	SO4	G	1002	-	4,4,4	0.21	0	6,6,6	0.11	0
4	SO4	G	1003	-	4,4,4	0.23	0	6,6,6	0.07	0
4	SO4	G	1004	-	4,4,4	0.20	0	6,6,6	0.11	0
4	SO4	H	1001	-	4,4,4	0.26	0	6,6,6	0.08	0
4	SO4	H	1002	-	4,4,4	0.25	0	6,6,6	0.08	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	A	2001	-	-	0/0/0/0	0/0/0/0
4	SO4	A	2002	-	-	0/0/0/0	0/0/0/0
4	SO4	A	2003	-	-	0/0/0/0	0/0/0/0
4	SO4	A	2004	-	-	0/0/0/0	0/0/0/0
4	SO4	B	2001	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1001	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1002	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1003	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1004	-	-	0/0/0/0	0/0/0/0
4	SO4	D	1001	-	-	0/0/0/0	0/0/0/0
4	SO4	D	1002	-	-	0/0/0/0	0/0/0/0
4	SO4	E	2001	-	-	0/0/0/0	0/0/0/0
4	SO4	E	2002	-	-	0/0/0/0	0/0/0/0
4	SO4	E	2003	-	-	0/0/0/0	0/0/0/0
4	SO4	G	1001	-	-	0/0/0/0	0/0/0/0
4	SO4	G	1002	-	-	0/0/0/0	0/0/0/0
4	SO4	G	1003	-	-	0/0/0/0	0/0/0/0
4	SO4	G	1004	-	-	0/0/0/0	0/0/0/0
4	SO4	H	1001	-	-	0/0/0/0	0/0/0/0
4	SO4	H	1002	-	-	0/0/0/0	0/0/0/0

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	2001	SO4	1	0
4	A	2002	SO4	1	0

## 5.7 Other polymers ⓘ

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 ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	851/1044 (81%)	0.22	17 (1%) 68 53	49, 86, 153, 361	0
1	E	832/1044 (79%)	0.28	53 (6%) 23 13	79, 150, 224, 363	0
2	B	1367/1436 (95%)	0.14	25 (1%) 71 57	51, 101, 164, 277	0
2	F	1351/1436 (94%)	0.21	53 (3%) 43 29	61, 128, 199, 310	0
3	C	392/397 (98%)	0.38	1 (0%) 94 90	40, 67, 140, 322	0
3	D	381/397 (95%)	0.34	8 (2%) 67 52	56, 92, 169, 265	0
3	G	387/397 (97%)	0.40	7 (1%) 71 57	45, 87, 151, 235	0
3	H	351/397 (88%)	1.52	124 (35%) 0 1	115, 180, 260, 351	0
All	All	5912/6548 (90%)	0.31	288 (4%) 33 22	40, 112, 203, 363	0

All (288) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	11	ALA	8.6
3	H	12	GLY	6.7
3	H	355	PRO	6.6
3	H	24	ALA	6.6
3	H	394	ALA	6.0
3	H	71	LEU	5.9
3	H	38	LEU	5.8
3	H	41	TRP	5.8
3	H	3	LYS	5.8
3	H	5	PHE	5.7
3	H	42	ASP	5.5
3	H	289	ALA	5.4
3	H	56	TYR	5.3
3	H	31	SER	5.3
3	H	360	VAL	5.3
3	H	14	ALA	5.1

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Mol	Chain	Res	Type	RSRZ
3	H	379	LEU	4.9
3	H	30	VAL	4.8
3	H	391	PHE	4.7
3	H	309	ALA	4.6
3	H	381	CYS	4.5
3	H	135	ARG	4.5
3	H	288	PHE	4.5
3	H	354	GLU	4.4
3	H	327	THR	4.4
1	E	783	PRO	4.4
1	E	521	VAL	4.3
1	E	508	LEU	4.3
2	B	641	TYR	4.3
3	H	173	LEU	4.3
1	E	715	PHE	4.3
1	E	510	ILE	4.3
3	H	329	LEU	4.2
2	F	641	TYR	4.1
2	F	84	TRP	4.1
3	H	81	LEU	4.1
3	H	155	PHE	4.1
3	H	84	VAL	4.0
2	F	83	ALA	4.0
2	F	482	THR	3.9
1	E	820	LEU	3.8
3	H	295	MET	3.8
3	H	29	THR	3.8
3	H	8	THR	3.8
3	H	139	HIS	3.8
1	E	739	SER	3.8
3	H	94	LEU	3.8
1	E	825	MET	3.7
3	H	380	CYS	3.7
1	E	505	PRO	3.7
3	C	372	GLY	3.7
1	E	782	SER	3.6
3	H	317	PHE	3.6
3	H	388	ILE	3.5
3	H	249	ALA	3.5
3	H	297	LEU	3.5
3	H	358	PHE	3.5
3	H	126	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
3	G	160	ASP	3.4
1	A	765	GLY	3.4
3	H	82	CYS	3.3
3	H	157	PRO	3.3
3	H	146	VAL	3.3
3	H	49	GLU	3.3
2	F	1366	PHE	3.3
3	H	378	SER	3.3
3	H	40	VAL	3.3
3	H	251	ALA	3.2
2	B	43	PHE	3.2
3	H	384	LEU	3.2
3	H	248	LEU	3.2
3	H	39	LYS	3.2
3	H	240	LYS	3.2
1	A	192	GLY	3.2
3	H	328	THR	3.2
3	H	20	PHE	3.2
3	H	45	LEU	3.1
1	A	8	SER	3.1
3	H	96	TYR	3.1
3	H	247	LEU	3.1
2	F	571	GLY	3.1
1	E	500	SER	3.1
2	F	550	TRP	3.1
3	D	309	ALA	3.1
1	E	499	ILE	3.1
1	E	716	ILE	3.1
2	B	106	TYR	3.1
2	B	971	ALA	3.0
3	H	390	TRP	3.0
3	H	359	ASP	3.0
3	H	382	VAL	3.0
2	B	595	ILE	3.0
3	H	140	ARG	3.0
2	F	626	PHE	3.0
2	B	640	TYR	3.0
3	H	85	ALA	2.9
2	F	853	GLN	2.9
1	E	74	PRO	2.9
2	B	279	HIS	2.9
1	A	715	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
2	F	27	SER	2.9
3	H	57	SER	2.9
2	F	514	LYS	2.9
1	E	741	ILE	2.9
3	H	51	PRO	2.9
3	H	263	TYR	2.9
1	E	520	PRO	2.9
2	B	967	TYR	2.9
3	H	125	TRP	2.9
1	E	609	PRO	2.8
3	H	95	PHE	2.8
3	H	86	THR	2.8
2	B	41	HIS	2.8
3	G	245	GLY	2.8
1	E	761	ALA	2.8
3	H	374	ASP	2.8
1	E	1196	LEU	2.8
1	E	808	TYR	2.8
3	H	87	THR	2.8
1	E	721	ALA	2.8
3	H	19	ILE	2.8
3	H	250	ILE	2.8
3	H	15	HIS	2.8
2	F	586	ASN	2.8
3	H	98	ILE	2.8
1	E	731	LEU	2.7
2	F	547	GLU	2.7
2	F	948	TRP	2.7
3	H	242	SER	2.7
3	H	369	SER	2.7
3	H	83	LEU	2.7
1	E	522	ILE	2.7
3	H	223	PHE	2.7
3	H	274	LEU	2.7
3	H	89	PHE	2.7
3	H	357	VAL	2.7
2	F	637	TYR	2.7
2	B	37	ASN	2.6
1	E	738	PHE	2.6
3	H	202	THR	2.6
2	F	530	LEU	2.6
3	G	45	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	630	PHE	2.6
3	H	172	THR	2.6
3	H	307	CYS	2.6
1	A	688	LEU	2.6
2	F	1365	TYR	2.6
2	B	613	PHE	2.6
2	F	895	GLU	2.6
2	F	551	SER	2.6
2	F	1305	ALA	2.6
3	H	171	PRO	2.6
2	F	107	PHE	2.6
3	H	393	GLU	2.6
2	B	48	LEU	2.6
2	F	1349	ARG	2.5
3	H	169	TRP	2.5
3	H	37	TYR	2.5
2	B	127	LEU	2.5
2	B	587	LEU	2.5
2	F	106	TYR	2.5
2	F	515	GLY	2.5
3	H	6	ILE	2.5
3	H	22	VAL	2.5
2	B	47	ALA	2.5
3	D	343	LEU	2.5
3	H	127	LEU	2.5
2	F	39	PHE	2.5
3	G	11	ALA	2.5
3	H	246	SER	2.5
2	F	507	ASN	2.5
2	F	1247	ASN	2.5
3	H	188	PHE	2.5
1	E	717	LYS	2.5
1	E	732	PRO	2.5
2	F	152	GLY	2.5
2	F	707	VAL	2.5
3	G	284	SER	2.5
3	H	377	GLU	2.4
3	H	70	VAL	2.4
3	H	308	SER	2.4
2	F	434	TYR	2.4
3	D	124	PHE	2.4
1	E	348	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	44	LEU	2.4
3	H	262	LEU	2.4
2	B	44	LEU	2.4
3	H	93	LEU	2.4
2	F	284	ALA	2.4
3	H	299	PHE	2.4
1	E	614	TRP	2.4
2	B	39	PHE	2.4
2	F	43	PHE	2.4
2	F	484	VAL	2.4
3	H	55	SER	2.3
1	E	9	SER	2.3
2	F	289	PHE	2.3
1	A	514	ALA	2.3
2	B	648	PHE	2.3
2	B	569	ILE	2.3
2	F	544	VAL	2.3
3	G	44	LYS	2.3
1	A	651	PHE	2.3
2	B	999	ILE	2.3
1	E	66	LEU	2.3
1	A	689	GLU	2.3
3	H	43	ASN	2.3
3	H	107	VAL	2.3
2	F	429	ARG	2.3
3	H	72	GLN	2.3
2	B	284	ALA	2.3
1	A	737	ILE	2.3
1	A	782	SER	2.2
2	F	291	TRP	2.2
3	H	330	ASN	2.2
1	E	742	ARG	2.2
2	F	124	GLN	2.2
2	F	324	TRP	2.2
3	H	318	TRP	2.2
1	E	1238	VAL	2.2
3	H	238	SER	2.2
3	H	362	PHE	2.2
3	D	297	LEU	2.2
2	F	110	CYS	2.2
1	A	720	PHE	2.2
3	H	144	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	718	VAL	2.2
2	F	441	TYR	2.2
3	H	151	TYR	2.2
3	H	129	TRP	2.2
1	E	458	TRP	2.2
2	B	20	TYR	2.2
1	E	105	PHE	2.2
1	E	694	VAL	2.2
1	A	512	ILE	2.2
2	F	590	GLN	2.2
3	H	7	ALA	2.2
1	E	519	ILE	2.2
2	F	516	ILE	2.2
1	E	650	ASN	2.2
1	E	477	THR	2.2
3	G	388	ILE	2.2
1	A	783	PRO	2.2
3	H	311	TRP	2.2
1	E	360	VAL	2.2
2	F	469	THR	2.2
1	E	631	VAL	2.2
2	F	739	TRP	2.2
1	E	778	MET	2.2
3	H	156	HIS	2.1
1	E	459	GLU	2.1
1	E	98	ILE	2.1
1	E	1232	PRO	2.1
2	F	636	ILE	2.1
3	D	214	LEU	2.1
2	F	1006	HIS	2.1
1	E	645	TRP	2.1
1	E	1200	GLU	2.1
3	D	357	VAL	2.1
3	H	124	PHE	2.1
2	B	38	TYR	2.1
1	E	69	MET	2.1
1	E	114	ILE	2.1
3	D	250	ILE	2.1
1	E	511	ASN	2.1
1	E	693	ALA	2.1
3	H	143	ALA	2.1
1	A	738	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	1250	GLN	2.1
1	E	513	TRP	2.1
1	A	614	TRP	2.1
3	H	54	LYS	2.1
2	F	45	GLY	2.1
2	F	1343	ILE	2.1
3	H	200	ILE	2.1
3	H	76	ARG	2.1
3	H	260	ILE	2.1
3	H	331	MET	2.1
2	F	1417	LEU	2.0
3	H	315	LEU	2.0
2	F	668	ILE	2.0
3	H	142	VAL	2.0
3	H	65	LEU	2.0
1	E	323	ALA	2.0
1	A	513	TRP	2.0
1	A	632	PHE	2.0
2	F	619	SER	2.0
3	D	295	MET	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	SO4	C	1002	5/5	0.83	0.79	6.52	162,162,162,162	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	A	2004	5/5	0.44	0.60	3.50	205,205,205,205	0
4	SO4	G	1002	5/5	0.77	0.69	3.08	151,151,151,151	0
4	SO4	G	1001	5/5	0.86	0.44	1.53	178,178,178,178	0
4	SO4	G	1004	5/5	0.68	0.37	1.46	191,191,191,191	0
4	SO4	C	1001	5/5	0.84	0.39	0.75	173,173,173,173	0
4	SO4	D	1001	5/5	0.77	0.46	0.52	174,174,174,174	0
4	SO4	D	1002	5/5	0.87	0.48	0.30	142,142,142,142	0
4	SO4	E	2003	5/5	0.80	0.28	0.06	252,252,252,252	0
4	SO4	G	1003	5/5	0.85	0.30	-0.24	142,142,142,142	0
4	SO4	A	2003	5/5	0.94	0.21	-0.67	97,97,97,97	0
4	SO4	A	2001	5/5	0.84	0.22	-0.77	175,175,175,175	0
4	SO4	C	1004	5/5	0.89	0.26	-0.92	182,182,182,182	0
4	SO4	E	2001	5/5	0.81	0.16	-1.50	238,238,238,238	0
4	SO4	H	1001	5/5	0.37	0.22	-1.50	256,256,256,256	0
4	SO4	A	2002	5/5	0.91	0.16	-	133,133,133,133	0
4	SO4	B	2001	5/5	0.87	0.40	-	212,212,212,212	0
4	SO4	E	2002	5/5	0.92	0.13	-	208,208,208,208	0
4	SO4	H	1002	5/5	0.77	0.18	-	267,267,267,267	0
4	SO4	C	1003	5/5	0.89	0.24	-	122,122,122,122	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.