



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 07:26 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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : trunk28620

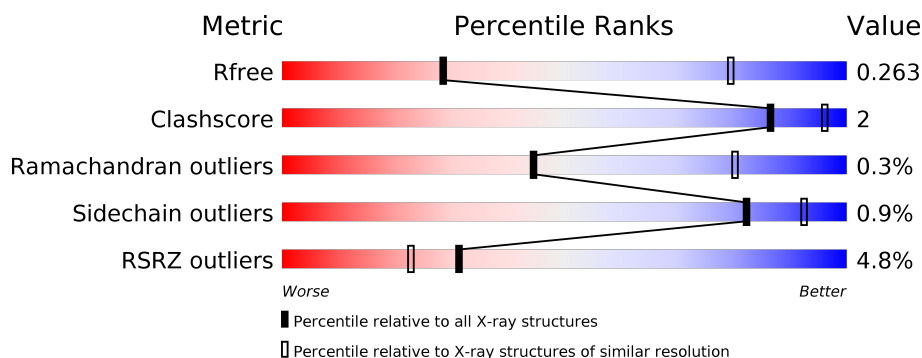
# 1 Overall quality at a glance

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))
$R_{free}$	100719	1234 (3.90-3.50)
Clashscore	112137	1377 (3.90-3.50)
Ramachandran outliers	110173	1323 (3.90-3.50)
Sidechain outliers	110143	1320 (3.90-3.50)
RSRZ outliers	101464	1262 (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></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></div> <div>90% 8% ..</div> </div>
3	D	397	<div> <div>2%</div> <div>89% 7% .</div> </div>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
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			

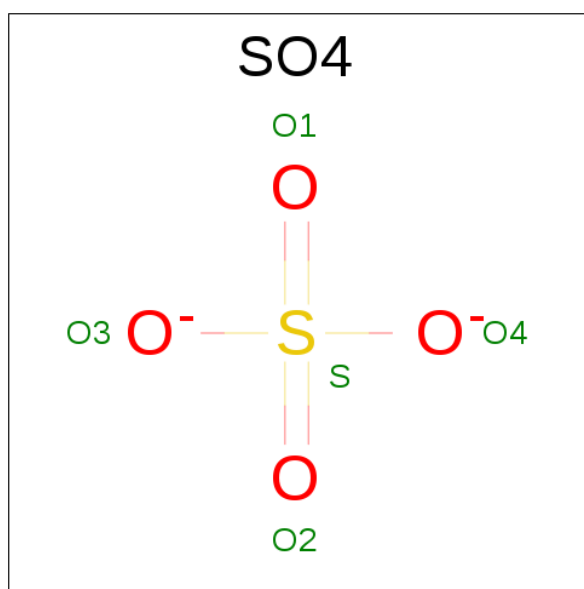
There are 8 discrepancies between the modelled and reference sequences:

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: SO4) (formula: O<sub>4</sub>S).



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

*Continued on next page...*

*Continued from previous page...*

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		

These plots are drawn for all protein, RNA and DNA 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 ( $\text{RSRZ} > 2$ ). 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.

Chain A:

Sequence logo for Chain A. The y-axis represents information content in bits (0.00 to 1.73). The x-axis shows positions 1 to 1000. Amino acids are color-coded: yellow for common, green for conserved, and red for rare. The sequence is: GLY, PRO, ASP, SER, MET, SER, GLU, GLY, PHE, SER, SER, SER, S8, Y14, K18, A24, ASP, V26, E39, SER, THR, ASP, GLU, PRO, K45, W64, V70, P74, S78, PRO, GLU, ASP, CYS, SER, G84, E111, Y117, I162, V167, THR, ASP, SER, GLN, ASN, GLY, SER, D397, L417, L434, E445, V446, H447, Y448, V449, R454, F471, L472, L473, L474, S475, A476, T477, L488, P502, L512, W513, A514, K535, H536, L539, L540, H541, GLY, GLU, SER, ALA, LYS, GLY, ALA, PRO, LYS, THR, ASP, ASN, ARG, GLY, GLY, ARG, GLY, GLY, H638, E639, I702, F715, F720, L737, F738, D745, G746, G765, S782, P783, Y808, L820, H833, ALA, GLY, SER, ARG, G1085, L1089, P1090, R1095, V1098, F1104, L1112, L1113, K1114, G1124, F1125, E1126, L1127, S1151, V1152, L1171, M1185, V1188, R1208, M1212, H1213, V1214, W1218, F1224, L1237.

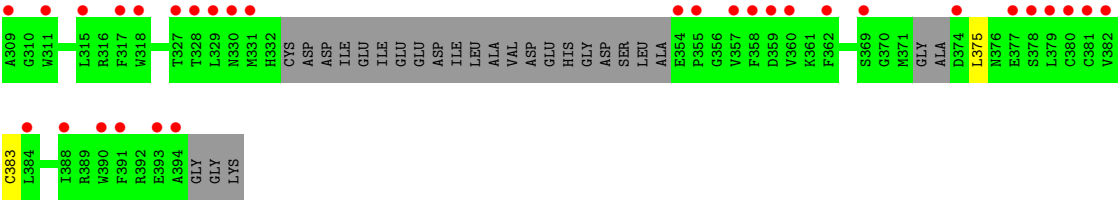
Chain E:

Amino Acid	Percentage
GLY	5%
PRO	80%
ASP	80%
MET	80%
SER	80%
GLU	80%
GLY	80%
PHE	80%
SER	80%
SER	80%
SER	80%
S9	80%
L13	5%
A24	80%
ASP	80%
V26	80%
R32	80%
F39	80%
SER	80%
THR	80%
ASP	80%
GLU	80%
PRO	80%
LYS	80%
H46	80%
L66	80%
M69	80%
P74	80%
HIS	80%
THR	80%
SER	80%
SER	80%
PRO	80%
GLU	80%
ASP	80%
CYS	80%
SER	80%
GLY	80%
LYS	80%
LEU	80%
ASP	80%
TYR	80%
R89	80%
I98	5%
F105	80%
K106	80%
R107	80%
E111	80%









## 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 , 0.263	Depositor DCC
$R_{free}$ test set	6658 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
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	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 <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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.28	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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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:1369:ASN:OD1	2:B:1391:ASN:ND2	2.37	0.55
2:B:735:ASP:OD2	2:B:738:SER:OG	2.18	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
2:B:324:TRP:CB	2:B:430:ILE:HD11	2.41	0.51
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
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
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
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: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
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:CD2	1:A:304:HIS:N	2.82	0.48

*Continued on next page...*

*Continued from previous page...*

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
1:A:1171:LEU:HB3	1:A:1212:MET:CE	2.45	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: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
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:427:MET:O	1:E:431:GLY:N	2.48	0.46
1:E:425:ARG:NE	1:E:460:GLU:OE1	2.47	0.46
2:B:729:LEU:HD11	2:B:738:SER:HB3	1.98	0.46
1:A:1152:VAL:O	1:A:1208:ARG:NH1	2.45	0.46
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: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:B:486:ALA:HB3	2:B:487:PRO:HD3	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
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:17:LEU:CD2	3:C:90:SER:HA	2.46	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:397:ASP:N	1:E:397:ASP:OD1	2.50	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: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
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
2:B:1191:ARG:HG2	2:B:1231:CYS:SG	2.58	0.43
2:B:815:MET:HE3	2:B:861:GLN:HB3	2.00	0.43
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: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:1210:GLN:O	2:B:1214:SER:N	2.50	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:252:LEU:HD21	2:B:263:PHE:HD1	1.85	0.42
3:C:332:HIS:N	3:C:335:ASP:OD2	2.47	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: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:1089:LEU:HB3	1:A:1090:PRO:HD3	2.02	0.41
1:A:445:GLU:N	1:A:474:LEU:O	2.53	0.41
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
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
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:F:735:ASP:OD2	2:F:738:SER:OG	2.38	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:A:1185:MET:HA	1:A:1188:VAL:HG12	2.02	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
2:B:729:LEU:HD11	2:B:738:SER:CB	2.50	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: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

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:B:1384:ARG:O	3:D:147:LYS:NZ	2.46	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%)	51	85
1	E	810/1044 (78%)	785 (97%)	24 (3%)	1 (0%)	55	88
2	B	1357/1436 (94%)	1298 (96%)	52 (4%)	7 (0%)	32	73
2	F	1333/1436 (93%)	1284 (96%)	48 (4%)	1 (0%)	55	88
3	C	388/397 (98%)	364 (94%)	23 (6%)	1 (0%)	44	80
3	D	369/397 (93%)	347 (94%)	17 (5%)	5 (1%)	13	55
3	G	381/397 (96%)	358 (94%)	22 (6%)	1 (0%)	44	80
3	H	337/397 (85%)	313 (93%)	23 (7%)	1 (0%)	44	80
All	All	5810/6548 (89%)	5546 (96%)	245 (4%)	19 (0%)	44	80

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%)	85	93
1	E	466/832 (56%)	461 (99%)	5 (1%)	78	90
2	B	836/1282 (65%)	826 (99%)	10 (1%)	75	90
2	F	715/1282 (56%)	712 (100%)	3 (0%)	93	97
3	C	295/347 (85%)	293 (99%)	2 (1%)	87	94
3	D	266/347 (77%)	263 (99%)	3 (1%)	78	90
3	G	289/347 (83%)	285 (99%)	4 (1%)	71	89
3	H	240/347 (69%)	238 (99%)	2 (1%)	85	93
All	All	3721/5616 (66%)	3687 (99%)	34 (1%)	82	92

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	0.13	0	6,6,6	0.06	0
4	SO4	A	2002	-	4,4,4	0.17	0	6,6,6	0.07	0
4	SO4	A	2003	-	4,4,4	0.13	0	6,6,6	0.14	0
4	SO4	A	2004	-	4,4,4	0.15	0	6,6,6	0.06	0
4	SO4	B	2001	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	C	1001	-	4,4,4	0.13	0	6,6,6	0.07	0
4	SO4	C	1002	-	4,4,4	0.15	0	6,6,6	0.07	0
4	SO4	C	1003	-	4,4,4	0.12	0	6,6,6	0.07	0
4	SO4	C	1004	-	4,4,4	0.15	0	6,6,6	0.11	0
4	SO4	D	1001	-	4,4,4	0.13	0	6,6,6	0.05	0
4	SO4	D	1002	-	4,4,4	0.14	0	6,6,6	0.10	0
4	SO4	E	2001	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	E	2002	-	4,4,4	0.16	0	6,6,6	0.06	0
4	SO4	E	2003	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	G	1001	-	4,4,4	0.13	0	6,6,6	0.07	0
4	SO4	G	1002	-	4,4,4	0.15	0	6,6,6	0.10	0
4	SO4	G	1003	-	4,4,4	0.15	0	6,6,6	0.05	0
4	SO4	G	1004	-	4,4,4	0.16	0	6,6,6	0.08	0
4	SO4	H	1001	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	H	1002	-	4,4,4	0.14	0	6,6,6	0.06	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%)	0.19	15 (1%) 69 56	49, 86, 153, 361	0
1	E	832/1044 (79%)	0.26	53 (6%) 20 14	79, 150, 224, 363	0
2	B	1367/1436 (95%)	0.11	25 (1%) 69 56	51, 101, 164, 277	0
2	F	1351/1436 (94%)	0.18	52 (3%) 41 30	61, 128, 199, 310	0
3	C	392/397 (98%)	0.35	1 (0%) 93 90	40, 67, 140, 322	0
3	D	381/397 (95%)	0.32	8 (2%) 64 51	56, 92, 169, 265	0
3	G	387/397 (97%)	0.37	7 (1%) 69 56	45, 87, 151, 235	0
3	H	351/397 (88%)	1.50	124 (35%) 0 1	115, 180, 260, 351	0
All	All	5912/6548 (90%)	0.29	285 (4%) 31 23	40, 112, 203, 363	0

All (285) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	11	ALA	8.6
3	H	12	GLY	6.8
3	H	355	PRO	6.7
3	H	24	ALA	6.6
3	H	394	ALA	6.0
3	H	71	LEU	5.9
3	H	3	LYS	5.9
3	H	38	LEU	5.9
3	H	41	TRP	5.7
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	360	VAL	5.3
3	H	31	SER	5.2
3	H	14	ALA	5.1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	H	379	LEU	4.9
3	H	30	VAL	4.9
3	H	391	PHE	4.7
3	H	135	ARG	4.6
3	H	309	ALA	4.6
3	H	288	PHE	4.5
1	E	783	PRO	4.4
3	H	327	THR	4.4
1	E	521	VAL	4.4
1	E	508	LEU	4.4
3	H	354	GLU	4.4
1	E	510	ILE	4.3
2	B	641	TYR	4.3
3	H	173	LEU	4.3
1	E	715	PHE	4.3
3	H	381	CYS	4.3
3	H	329	LEU	4.3
2	F	641	TYR	4.1
3	H	81	LEU	4.1
2	F	84	TRP	4.1
3	H	155	PHE	4.1
3	H	84	VAL	4.0
2	F	83	ALA	4.0
3	H	139	HIS	3.9
2	F	482	THR	3.9
1	E	820	LEU	3.9
3	H	295	MET	3.8
3	H	29	THR	3.8
3	H	94	LEU	3.8
3	H	8	THR	3.8
1	E	825	MET	3.8
3	C	372	GLY	3.7
1	E	505	PRO	3.7
1	E	739	SER	3.7
3	H	317	PHE	3.6
3	H	388	ILE	3.6
1	E	782	SER	3.5
3	H	297	LEU	3.5
3	H	380	CYS	3.5
3	H	249	ALA	3.4
3	H	358	PHE	3.4
1	A	765	GLY	3.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	H	126	ALA	3.4
3	H	157	PRO	3.4
3	H	146	VAL	3.3
3	G	160	ASP	3.3
3	H	40	VAL	3.3
2	F	1366	PHE	3.3
3	H	39	LYS	3.2
3	H	240	LYS	3.2
3	H	384	LEU	3.2
3	H	49	GLU	3.2
3	H	248	LEU	3.2
2	B	43	PHE	3.2
3	H	378	SER	3.2
1	A	192	GLY	3.2
3	H	251	ALA	3.2
2	F	571	GLY	3.2
3	H	45	LEU	3.2
3	H	247	LEU	3.2
3	H	20	PHE	3.1
3	H	328	THR	3.1
1	E	499	ILE	3.1
3	H	82	CYS	3.1
3	H	96	TYR	3.1
1	E	716	ILE	3.1
3	D	309	ALA	3.1
1	A	8	SER	3.1
3	H	140	ARG	3.1
1	E	500	SER	3.1
2	F	550	TRP	3.1
2	B	106	TYR	3.0
2	B	279	HIS	3.0
2	B	595	ILE	3.0
2	B	971	ALA	3.0
3	H	382	VAL	3.0
2	F	514	LYS	3.0
2	F	626	PHE	3.0
3	H	390	TRP	3.0
2	B	640	TYR	3.0
3	H	359	ASP	3.0
1	E	74	PRO	2.9
1	E	741	ILE	2.9
3	H	85	ALA	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	715	PHE	2.9
3	H	51	PRO	2.9
2	B	41	HIS	2.9
2	F	853	GLN	2.9
1	E	520	PRO	2.9
1	E	609	PRO	2.9
3	H	15	HIS	2.9
3	H	263	TYR	2.9
3	G	245	GLY	2.8
2	B	967	TYR	2.8
2	F	27	SER	2.8
3	H	57	SER	2.8
3	H	95	PHE	2.8
1	E	1196	LEU	2.8
3	H	86	THR	2.8
3	H	19	ILE	2.8
3	H	250	ILE	2.8
1	E	761	ALA	2.8
3	H	98	ILE	2.8
3	H	125	TRP	2.8
1	E	808	TYR	2.8
3	H	87	THR	2.8
1	E	731	LEU	2.8
3	H	374	ASP	2.8
1	E	721	ALA	2.8
1	E	522	ILE	2.7
3	H	83	LEU	2.7
3	H	274	LEU	2.7
2	F	586	ASN	2.7
3	H	223	PHE	2.7
3	H	89	PHE	2.7
3	H	357	VAL	2.7
2	F	547	GLU	2.7
2	F	948	TRP	2.7
2	F	637	TYR	2.7
3	H	242	SER	2.6
3	H	369	SER	2.6
2	F	530	LEU	2.6
3	G	45	LEU	2.6
1	E	738	PHE	2.6
3	H	202	THR	2.6
2	B	630	PHE	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	F	1349	ARG	2.6
1	A	688	LEU	2.6
3	H	172	THR	2.6
2	B	37	ASN	2.6
3	H	171	PRO	2.6
2	B	613	PHE	2.6
2	F	1365	TYR	2.6
2	B	48	LEU	2.6
3	H	6	ILE	2.6
2	F	515	GLY	2.6
2	F	107	PHE	2.6
2	F	1305	ALA	2.5
2	B	127	LEU	2.5
2	B	587	LEU	2.5
1	E	717	LYS	2.5
3	D	343	LEU	2.5
3	H	127	LEU	2.5
3	H	22	VAL	2.5
3	H	37	TYR	2.5
2	F	106	TYR	2.5
2	F	895	GLU	2.5
2	F	551	SER	2.5
2	F	39	PHE	2.5
3	H	393	GLU	2.5
2	B	47	ALA	2.5
1	E	732	PRO	2.5
3	H	169	TRP	2.5
2	F	152	GLY	2.5
3	G	11	ALA	2.5
3	H	188	PHE	2.5
2	F	707	VAL	2.5
2	F	507	ASN	2.4
2	F	1247	ASN	2.4
3	H	70	VAL	2.4
3	H	246	SER	2.4
3	H	307	CYS	2.4
2	F	44	LEU	2.4
3	D	124	PHE	2.4
2	F	434	TYR	2.4
3	H	262	LEU	2.4
1	E	348	PHE	2.4
2	B	44	LEU	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	H	93	LEU	2.4
3	G	284	SER	2.4
3	H	377	GLU	2.4
3	H	308	SER	2.4
2	F	284	ALA	2.4
2	F	484	VAL	2.4
3	H	299	PHE	2.4
2	B	39	PHE	2.3
2	F	43	PHE	2.3
3	G	44	LYS	2.3
2	F	429	ARG	2.3
2	B	569	ILE	2.3
2	B	999	ILE	2.3
1	E	614	TRP	2.3
2	F	289	PHE	2.3
2	F	544	VAL	2.3
1	E	742	ARG	2.3
1	E	66	LEU	2.3
2	B	648	PHE	2.3
1	A	737	ILE	2.3
3	H	107	VAL	2.3
1	A	651	PHE	2.3
1	A	514	ALA	2.3
3	H	55	SER	2.3
1	E	9	SER	2.2
1	E	1238	VAL	2.2
3	H	43	ASN	2.2
3	H	72	GLN	2.2
2	B	284	ALA	2.2
3	D	297	LEU	2.2
1	A	512	ILE	2.2
1	E	718	VAL	2.2
3	H	156	HIS	2.2
3	H	362	PHE	2.2
1	A	689	GLU	2.2
1	E	519	ILE	2.2
2	F	516	ILE	2.2
2	F	124	GLN	2.2
3	G	388	ILE	2.2
1	A	720	PHE	2.2
3	H	330	ASN	2.2
3	H	144	THR	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	694	VAL	2.2
2	F	441	TYR	2.2
3	H	151	TYR	2.2
2	F	1006	HIS	2.2
1	A	783	PRO	2.2
2	F	291	TRP	2.2
1	A	782	SER	2.2
1	E	105	PHE	2.2
2	B	20	TYR	2.2
2	F	324	TRP	2.2
3	H	318	TRP	2.2
3	H	238	SER	2.2
1	E	360	VAL	2.2
1	E	98	ILE	2.2
1	E	477	THR	2.2
3	H	7	ALA	2.2
1	E	631	VAL	2.2
2	F	590	GLN	2.2
2	F	636	ILE	2.2
1	E	778	MET	2.1
2	F	469	THR	2.1
3	H	129	TRP	2.1
1	E	1232	PRO	2.1
1	E	114	ILE	2.1
1	E	458	TRP	2.1
1	E	650	ASN	2.1
3	D	214	LEU	2.1
3	D	250	ILE	2.1
3	D	357	VAL	2.1
3	H	311	TRP	2.1
1	E	69	MET	2.1
3	H	76	ARG	2.1
3	H	54	LYS	2.1
3	H	124	PHE	2.1
2	B	38	TYR	2.1
2	F	739	TRP	2.1
2	F	1343	ILE	2.1
3	H	200	ILE	2.1
2	F	45	GLY	2.1
1	E	459	GLU	2.1
3	H	260	ILE	2.1
1	A	738	PHE	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	693	ALA	2.1
1	E	645	TRP	2.1
3	H	143	ALA	2.1
1	E	1200	GLU	2.1
2	F	110	CYS	2.1
2	F	668	ILE	2.1
1	E	511	ASN	2.1
2	B	1250	GLN	2.1
2	F	1417	LEU	2.1
3	H	331	MET	2.0
3	H	315	LEU	2.0
3	H	65	LEU	2.0
3	H	142	VAL	2.0
1	E	513	TRP	2.0
1	A	614	TRP	2.0
3	D	295	MET	2.0
1	E	695	HIS	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( $\text{\AA}^2$ )	Q<0.9
4	SO4	C	1002	5/5	0.83	0.79	6.52	162,162,162,162	0
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

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
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

There are no such residues in this entry.