



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 03:02 AM GMT

PDB ID : 2OVR  
Title : Structure of the Skp1-Fbw7-CyclinEdegNcomplex  
Authors : Hao, B.; Oehlmann, S.; Sowa, M.E.; Harper, J.W.; Pavletich, N.P.  
Deposited on : 2007-02-14  
Resolution : 2.50 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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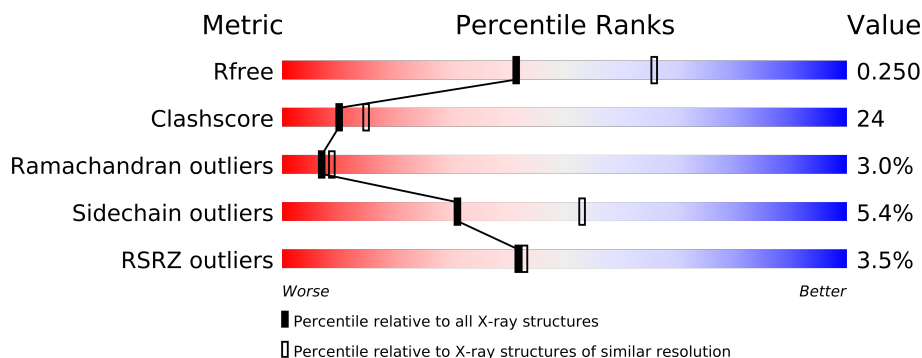
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.50 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))
$R_{free}$	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	149	
2	B	445	
3	C	8	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	SO4	B	902	-	X
4	SO4	B	909	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4907 atoms, of which 0 are hydrogen and 0 are deuterium.

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 S-phase kinase-associated protein 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	136	Total	C	N	O	S	0	0	0
			1087	693	176	212	6			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASP	DELETION	UNP P63208
A	?	-	ASP	DELETION	UNP P63208
A	?	-	GLU	DELETION	UNP P63208
A	?	-	GLY	DELETION	UNP P63208
A	?	-	ASP	DELETION	UNP P63208
A	?	-	ASP	DELETION	UNP P63208
A	?	-	PRO	DELETION	UNP P63208
A	?	-	PRO	DELETION	UNP P63208
A	?	-	PRO	DELETION	UNP P63208
A	?	-	GLU	DELETION	UNP P63208
A	?	-	ASP	DELETION	UNP P63208
A	?	-	ASP	DELETION	UNP P63208
A	?	-	GLU	DELETION	UNP P63208
A	?	-	ASN	DELETION	UNP P63208
A	1078	GLY	LYS	LINKER	UNP P63208
A	1079	GLY	GLU	LINKER	UNP P63208
A	1080	SER	LYS	LINKER	UNP P63208
A	1081	GLY	ARG	LINKER	UNP P63208

- Molecule 2 is a protein called F-box/WD repeat protein 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	442	Total	C	N	O	S	0	0	0
			3495	2193	631	649	22			

- Molecule 3 is a protein called cyclinE N-terminal degron.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	8	Total	C	N	O	P	0	0	0
			65	39	9	16	1			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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

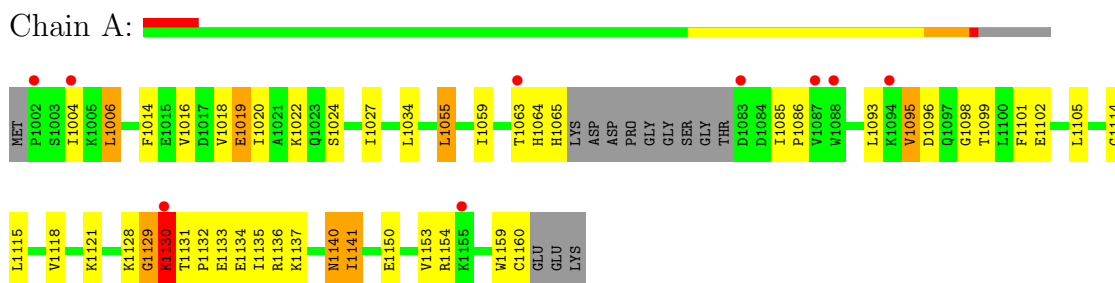
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	17	Total	O	0	0
			17	17		
5	B	182	Total	O	0	0
			182	182		
5	C	1	Total	O	0	0
			1	1		

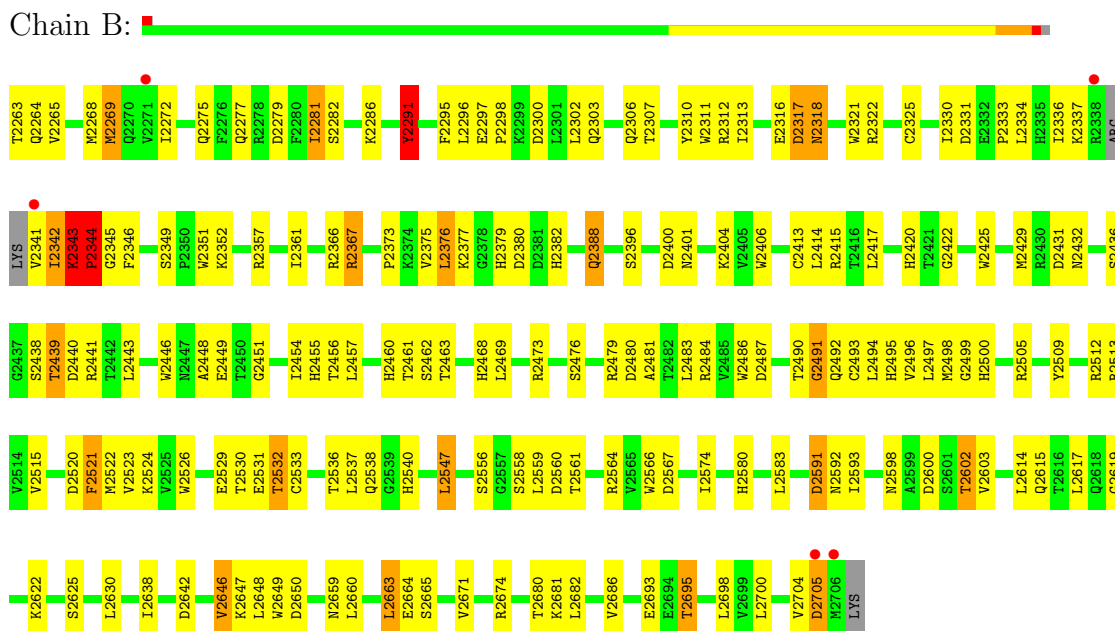
### 3 Residue-property plots

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

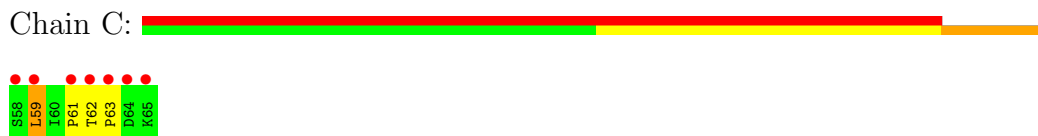
#### • Molecule 1: S-phase kinase-associated protein 1A



#### • Molecule 2: F-box/WD repeat protein 7



#### • Molecule 3: cyclinE N-terminal degnon



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	232.56Å 232.56Å 107.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.75 – 2.50 49.96 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.8 (19.75-2.50) 96.8 (49.96-2.50)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.99 (at 2.51Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.225 , 0.251 0.226 , 0.250	Depositor DCC
$R_{free}$ test set	1966 reflections (3.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	43.0	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 34.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 50355 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4907	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, 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	0.50	1/1105 (0.1%)	0.90	5/1495 (0.3%)
2	B	0.49	1/3565 (0.0%)	0.78	2/4829 (0.0%)
3	C	0.53	0/54	1.04	0/69
All	All	0.50	2/4724 (0.0%)	0.81	7/6393 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1129	GLY	CA-C	-7.20	1.40	1.51
2	B	2291	TYR	CD1-CE1	6.48	1.49	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1130	LYS	N-CA-C	15.86	153.82	111.00
1	A	1129	GLY	CA-C-N	-10.88	93.27	117.20
1	A	1129	GLY	O-C-N	9.44	137.80	122.70
1	A	1128	LYS	C-N-CA	-8.71	104.00	122.30
1	A	1130	LYS	N-CA-CB	-7.69	96.75	110.60
2	B	2646	VAL	N-CA-C	-5.42	96.36	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2547	LEU	CA-CB-CG	5.06	126.93	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1129	GLY	Mainchain
1	A	1130	LYS	Mainchain
2	B	2291	TYR	Sidechain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1087	0	1092	49	0
2	B	3495	0	3481	180	0
3	C	65	0	62	10	0
4	B	60	0	0	1	0
5	A	17	0	0	0	0
5	B	182	0	0	18	0
5	C	1	0	0	0	0
All	All	4907	0	4635	221	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 24.

All (221) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:2439:THR:HA	5:B:181:HOH:O	1.45	1.17
2:B:2343:LYS:HB3	2:B:2344:PRO:CD	1.83	1.09
2:B:2463:THR:HA	5:B:181:HOH:O	1.60	1.01
1:A:1095:VAL:HG12	1:A:1096:ASP:H	1.25	1.01
2:B:2468:HIS:HD2	2:B:2509:TYR:H	1.07	0.94
1:A:1016:VAL:HG11	1:A:1059:ILE:HD12	1.52	0.91
2:B:2479:ARG:NH2	3:C:63:PRO:HD2	1.85	0.91

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:2560:ASP:O	2:B:2561:THR:HB	1.72	0.89
2:B:2388:GLN:HB3	2:B:2429:MET:HE2	1.54	0.87
2:B:2479:ARG:HH22	3:C:63:PRO:HD2	1.41	0.86
2:B:2343:LYS:HB3	2:B:2344:PRO:HD3	1.59	0.82
2:B:2479:ARG:NH2	3:C:62:TPO:HG22	1.96	0.81
1:A:1020:ILE:HG21	1:A:1063:THR:HG22	1.61	0.80
2:B:2336:ILE:HG22	2:B:2337:LYS:H	1.46	0.80
1:A:1095:VAL:HG11	1:A:1099:THR:HG21	1.63	0.78
2:B:2559:LEU:HD23	2:B:2559:LEU:O	1.83	0.77
2:B:2343:LYS:O	2:B:2344:PRO:C	2.22	0.76
2:B:2468:HIS:HD2	2:B:2509:TYR:N	1.84	0.75
2:B:2468:HIS:CD2	2:B:2509:TYR:H	1.99	0.75
2:B:2487:ASP:HB2	2:B:2494:LEU:HD11	1.72	0.71
2:B:2505:ARG:NE	3:C:62:TPO:O3P	2.23	0.71
2:B:2316:GLU:O	2:B:2316:GLU:HG3	1.89	0.71
1:A:1141:ILE:HD13	2:B:2307:THR:HG21	1.73	0.70
1:A:1020:ILE:HD13	1:A:1063:THR:HG22	1.74	0.70
1:A:1131:THR:O	1:A:1135:ILE:HG13	1.91	0.70
2:B:2343:LYS:HB3	2:B:2344:PRO:HD2	1.68	0.70
1:A:1095:VAL:HG12	1:A:1096:ASP:N	2.03	0.70
1:A:1114:GLY:O	1:A:1118:VAL:HG23	1.91	0.69
2:B:2520:ASP:OD1	2:B:2522:MET:HB2	1.93	0.69
2:B:2336:ILE:HG22	2:B:2337:LYS:N	2.08	0.68
2:B:2463:THR:CA	5:B:181:HOH:O	2.27	0.68
2:B:2441:ARG:HG2	2:B:2461:THR:O	1.92	0.68
2:B:2522:MET:SD	2:B:2538:GLN:HG2	2.34	0.68
2:B:2454:ILE:HG22	2:B:2455:HIS:CD2	2.29	0.68
1:A:1130:LYS:HG2	2:B:2303:GLN:HE21	1.59	0.68
2:B:2425:TRP:CD2	3:C:63:PRO:HG3	2.28	0.68
2:B:2647:LYS:HG2	2:B:2659:ASN:HD22	1.59	0.67
1:A:1006:LEU:HD12	1:A:1014:PHE:HB2	1.76	0.67
2:B:2530:THR:O	2:B:2532:THR:HG22	1.94	0.67
2:B:2439:THR:HG22	2:B:2463:THR:OG1	1.96	0.66
2:B:2373:PRO:HB3	2:B:2700:LEU:CD2	2.26	0.66
2:B:2665:SER:OG	2:B:2693:GLU:HG2	1.95	0.66
2:B:2647:LYS:HG2	2:B:2659:ASN:ND2	2.09	0.66
2:B:2512:ARG:NH1	5:B:10:HOH:O	2.28	0.66
1:A:1131:THR:HB	1:A:1134:GLU:HG3	1.77	0.66
2:B:2530:THR:OG1	2:B:2532:THR:CG2	2.43	0.66
2:B:2438:SER:O	5:B:181:HOH:O	2.15	0.65
2:B:2695:THR:HG22	5:B:66:HOH:O	1.97	0.65
1:A:1141:ILE:HG21	2:B:2307:THR:CG2	2.26	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:2325:CYS:HB3	2:B:2330:ILE:HB	1.79	0.64
2:B:2282:SER:HA	2:B:2310:TYR:CE2	2.34	0.63
2:B:2342:ILE:HG12	2:B:2343:LYS:N	2.13	0.63
1:A:1121:LYS:HE2	2:B:2295:PHE:HE2	1.63	0.63
2:B:2530:THR:OG1	2:B:2532:THR:HG23	1.97	0.63
2:B:2382:HIS:O	2:B:2695:THR:HG21	1.99	0.63
2:B:2521:PHE:N	2:B:2521:PHE:CD2	2.66	0.63
1:A:1132:PRO:HG2	1:A:1133:GLU:OE2	1.99	0.63
1:A:1098:GLY:O	1:A:1102:GLU:HG2	1.99	0.63
1:A:1018:VAL:O	1:A:1019:GLU:HB2	1.99	0.63
1:A:1006:LEU:HD13	1:A:1055:LEU:HD11	1.82	0.62
2:B:2479:ARG:HH22	3:C:62:TPO:HG22	1.64	0.62
2:B:2647:LYS:NZ	2:B:2659:ASN:HD21	1.97	0.61
2:B:2432:ASN:HD21	2:B:2449:GLU:HB2	1.65	0.61
2:B:2524:LYS:NZ	2:B:2536:THR:OG1	2.33	0.61
2:B:2366:ARG:HD2	5:B:108:HOH:O	1.99	0.61
2:B:2373:PRO:HB3	2:B:2700:LEU:HD22	1.83	0.61
2:B:2490:THR:O	2:B:2492:GLN:NE2	2.34	0.60
2:B:2469:LEU:HD12	2:B:2473:ARG:O	2.01	0.60
2:B:2521:PHE:HB3	2:B:2540:HIS:O	2.01	0.60
2:B:2455:HIS:ND1	2:B:2491:GLY:HA3	2.16	0.60
2:B:2400:ASP:O	2:B:2401:ASN:HB2	2.01	0.60
1:A:1153:VAL:HG12	2:B:2306:GLN:HG2	1.84	0.60
2:B:2425:TRP:CE2	3:C:63:PRO:HG3	2.37	0.59
2:B:2281:ILE:HG12	2:B:2311:TRP:CE2	2.37	0.59
2:B:2317:ASP:O	2:B:2318:ASN:HB2	2.01	0.59
2:B:2561:THR:HG23	2:B:2580:HIS:O	2.04	0.58
2:B:2521:PHE:N	2:B:2521:PHE:HD2	2.01	0.58
1:A:1121:LYS:HE2	2:B:2295:PHE:CE2	2.38	0.58
2:B:2500:HIS:HB2	5:B:14:HOH:O	2.03	0.58
1:A:1059:ILE:O	1:A:1063:THR:HG23	2.03	0.58
2:B:2559:LEU:CD2	2:B:2559:LEU:O	2.52	0.58
1:A:1150:GLU:O	1:A:1154:ARG:HG3	2.03	0.58
2:B:2367:ARG:HB3	2:B:2367:ARG:HH11	1.67	0.58
2:B:2263:THR:HG22	2:B:2264:GLN:N	2.18	0.57
2:B:2486:TRP:CZ3	2:B:2493:CYS:HB2	2.39	0.57
2:B:2664:GLU:HG3	5:B:2:HOH:O	2.04	0.57
2:B:2321:TRP:CE2	2:B:2352:LYS:HG3	2.40	0.57
2:B:2463:THR:HG23	5:B:181:HOH:O	2.05	0.57
2:B:2529:GLU:HG2	5:B:16:HOH:O	2.03	0.57
1:A:1136:ARG:O	1:A:1140:ASN:N	2.36	0.57
2:B:2495:HIS:HB3	2:B:2531:GLU:HG2	1.87	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:2436:SER:O	2:B:2443:LEU:HA	2.05	0.56
1:A:1093:LEU:C	1:A:1095:VAL:H	2.09	0.56
2:B:2333:PRO:HD3	2:B:2351:TRP:CH2	2.42	0.55
2:B:2558:SER:HB3	2:B:2560:ASP:OD1	2.06	0.55
1:A:1140:ASN:O	1:A:1141:ILE:O	2.25	0.55
1:A:1095:VAL:HG11	1:A:1099:THR:CG2	2.35	0.54
2:B:2318:ASN:ND2	2:B:2349:SER:OG	2.41	0.54
1:A:1006:LEU:CD1	1:A:1014:PHE:HB2	2.38	0.53
1:A:1018:VAL:O	1:A:1019:GLU:CB	2.56	0.53
1:A:1159:TRP:O	1:A:1160:CYS:HB2	2.08	0.53
2:B:2415:ARG:HD2	2:B:2451:GLY:HA3	1.89	0.53
1:A:1141:ILE:HD13	2:B:2307:THR:CG2	2.38	0.53
2:B:2375:VAL:C	2:B:2376:LEU:HD23	2.29	0.53
2:B:2522:MET:CE	2:B:2538:GLN:HG2	2.39	0.53
2:B:2415:ARG:HH11	2:B:2415:ARG:HG2	1.74	0.53
1:A:1137:LYS:HB3	1:A:1137:LYS:NZ	2.23	0.53
1:A:1018:VAL:CG2	1:A:1022:LYS:HE3	2.39	0.52
2:B:2291:TYR:CE2	2:B:2295:PHE:CE1	2.97	0.52
1:A:1130:LYS:CG	2:B:2303:GLN:HE21	2.21	0.52
2:B:2316:GLU:O	2:B:2317:ASP:O	2.27	0.52
1:A:1131:THR:HG22	1:A:1133:GLU:H	1.75	0.52
2:B:2564:ARG:NH1	5:B:88:HOH:O	2.42	0.52
1:A:1055:LEU:O	1:A:1059:ILE:HG12	2.10	0.52
2:B:2647:LYS:HZ2	2:B:2659:ASN:HD21	1.57	0.51
2:B:2463:THR:HB	2:B:2479:ARG:HD2	1.92	0.51
2:B:2342:ILE:HG12	2:B:2343:LYS:H	1.74	0.51
1:A:1101:PHE:CE1	1:A:1105:LEU:HD11	2.45	0.51
2:B:2380:ASP:O	2:B:2382:HIS:HD2	1.93	0.51
2:B:2379:HIS:HE1	2:B:2396:SER:OG	1.94	0.51
2:B:2494:LEU:N	2:B:2494:LEU:HD12	2.27	0.50
2:B:2312:ARG:HG2	2:B:2346:PHE:CZ	2.46	0.50
2:B:2523:VAL:HB	2:B:2537:LEU:HB2	1.92	0.50
2:B:2580:HIS:HB3	2:B:2598:ASN:ND2	2.26	0.50
2:B:2476:SER:O	2:B:2483:LEU:HA	2.12	0.50
2:B:2484:ARG:HG2	2:B:2496:VAL:HG22	1.94	0.50
2:B:2291:TYR:CE2	2:B:2295:PHE:HE1	2.30	0.49
2:B:2463:THR:CB	5:B:181:HOH:O	2.56	0.49
2:B:2343:LYS:O	2:B:2345:GLY:N	2.44	0.49
2:B:2281:ILE:HG12	2:B:2311:TRP:CZ2	2.47	0.49
2:B:2336:ILE:CG2	2:B:2337:LYS:H	2.23	0.49
2:B:2600:ASP:OD1	2:B:2602:THR:HB	2.12	0.49
2:B:2298:PRO:O	2:B:2302:LEU:HG	2.13	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:2496:VAL:HG12	2:B:2498:MET:HG3	1.94	0.48
2:B:2665:SER:OG	2:B:2693:GLU:CG	2.60	0.48
2:B:2432:ASN:ND2	2:B:2449:GLU:HB2	2.29	0.47
2:B:2481:ALA:HB1	2:B:2500:HIS:O	2.13	0.47
2:B:2515:VAL:HG12	2:B:2547:LEU:HD11	1.95	0.47
2:B:2663:LEU:HD21	2:B:2686:VAL:HG13	1.95	0.47
2:B:2513:ARG:HG3	5:B:10:HOH:O	2.13	0.47
2:B:2281:ILE:HG12	2:B:2311:TRP:NE1	2.29	0.47
1:A:1141:ILE:HG21	2:B:2307:THR:HG22	1.96	0.47
2:B:2490:THR:O	2:B:2492:GLN:N	2.47	0.47
2:B:2414:LEU:O	2:B:2415:ARG:HG2	2.14	0.47
2:B:2404:LYS:HE3	2:B:2413:CYS:SG	2.54	0.47
2:B:2272:ILE:HD12	2:B:2313:ILE:HD11	1.97	0.47
2:B:2440:ASP:OD1	2:B:2440:ASP:C	2.53	0.47
1:A:1130:LYS:HG3	2:B:2303:GLN:HG3	1.97	0.47
2:B:2617:LEU:HD13	2:B:2649:TRP:CG	2.50	0.47
2:B:2479:ARG:HH21	3:C:62:TPO:HG22	1.78	0.47
2:B:2263:THR:CG2	2:B:2264:GLN:N	2.78	0.47
2:B:2593:ILE:HD13	5:B:22:HOH:O	2.15	0.46
2:B:2373:PRO:HB3	2:B:2700:LEU:HD23	1.97	0.46
2:B:2619:GLY:O	2:B:2622:LYS:HG2	2.15	0.46
2:B:2334:LEU:HD22	2:B:2357:ARG:HD2	1.98	0.46
2:B:2277:GLN:HB3	2:B:2279:ASP:OD1	2.14	0.46
2:B:2432:ASN:HD21	2:B:2449:GLU:CB	2.28	0.46
2:B:2646:VAL:HG11	2:B:2682:LEU:HD21	1.97	0.46
1:A:1095:VAL:CG1	1:A:1096:ASP:H	2.09	0.46
2:B:2333:PRO:HD3	2:B:2351:TRP:CZ2	2.51	0.46
2:B:2343:LYS:HA	2:B:2343:LYS:HD3	1.65	0.45
2:B:2336:ILE:CG2	2:B:2337:LYS:N	2.79	0.45
1:A:1018:VAL:HG23	1:A:1022:LYS:HE3	1.98	0.45
2:B:2480:ASP:O	2:B:2481:ALA:HB3	2.16	0.45
2:B:2366:ARG:NH2	2:B:2650:ASP:OD2	2.50	0.45
2:B:2456:THR:C	2:B:2457:LEU:HD23	2.37	0.45
2:B:2457:LEU:HB3	2:B:2486:TRP:CZ3	2.52	0.45
1:A:1055:LEU:HD23	1:A:1055:LEU:O	2.17	0.44
3:C:59:LEU:HA	3:C:59:LEU:HD22	1.69	0.44
2:B:2522:MET:HE1	2:B:2538:GLN:HG2	1.99	0.44
2:B:2264:GLN:O	2:B:2268:MET:HG2	2.18	0.44
1:A:1004:ILE:C	1:A:1004:ILE:HD12	2.37	0.44
2:B:2417:LEU:HB3	2:B:2446:TRP:CE3	2.53	0.44
1:A:1085:ILE:CG1	1:A:1121:LYS:HD2	2.48	0.44
2:B:2376:LEU:HB3	2:B:2406:TRP:CZ3	2.52	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:2642:ASP:HA	2:B:2671:VAL:HG22	2.00	0.44
2:B:2401:ASN:HA	2:B:2422:GLY:O	2.18	0.43
2:B:2526:TRP:CZ3	2:B:2533:CYS:HB2	2.53	0.43
2:B:2296:LEU:HB3	2:B:2300:ASP:HB2	2.00	0.43
2:B:2540:HIS:HE1	2:B:2556:SER:OG	2.01	0.43
2:B:2400:ASP:C	2:B:2400:ASP:OD1	2.57	0.43
1:A:1131:THR:HB	1:A:1134:GLU:CG	2.47	0.43
2:B:2417:LEU:HD13	2:B:2446:TRP:CG	2.53	0.43
3:C:62:TPO:HA	3:C:63:PRO:HD3	1.20	0.43
2:B:2462:SER:OG	2:B:2479:ARG:HB2	2.19	0.43
2:B:2379:HIS:HD2	2:B:2400:ASP:OD2	2.01	0.43
2:B:2457:LEU:N	2:B:2457:LEU:HD23	2.34	0.43
2:B:2512:ARG:HG2	2:B:2513:ARG:HG2	2.00	0.42
2:B:2361:ILE:HD13	2:B:2680:THR:HG22	2.01	0.42
2:B:2520:ASP:OD1	2:B:2522:MET:CB	2.64	0.42
2:B:2417:LEU:HB3	2:B:2446:TRP:CZ3	2.54	0.42
2:B:2341:VAL:O	2:B:2342:ILE:O	2.38	0.42
2:B:2614:LEU:C	2:B:2615:GLN:HG2	2.39	0.42
2:B:2537:LEU:HD13	2:B:2566:TRP:CG	2.53	0.42
2:B:2704:VAL:HG12	2:B:2705:ASP:N	2.33	0.42
2:B:2367:ARG:HB3	2:B:2367:ARG:NH1	2.34	0.42
2:B:2602:THR:HG23	2:B:2603:VAL:N	2.34	0.42
2:B:2286:LYS:HG2	4:B:908:SO4:O4	2.20	0.42
2:B:2342:ILE:CG1	2:B:2343:LYS:N	2.81	0.42
2:B:2440:ASP:O	2:B:2441:ARG:HB2	2.20	0.42
1:A:1064:HIS:HD2	1:A:1065:HIS:CE1	2.37	0.42
2:B:2439:THR:CA	5:B:181:HOH:O	2.29	0.42
1:A:1006:LEU:O	1:A:1006:LEU:HD12	2.20	0.42
2:B:2312:ARG:HG2	2:B:2346:PHE:HZ	1.85	0.42
1:A:1098:GLY:HA2	1:A:1101:PHE:HB3	2.02	0.41
2:B:2297:GLU:HA	2:B:2297:GLU:OE2	2.20	0.41
1:A:1085:ILE:HG13	1:A:1121:LYS:HD2	2.02	0.41
2:B:2630:LEU:HA	2:B:2638:ILE:O	2.20	0.41
1:A:1024:SER:OG	1:A:1027:ILE:HG13	2.20	0.41
2:B:2281:ILE:HG13	2:B:2282:SER:N	2.34	0.41
2:B:2460:HIS:O	5:B:103:HOH:O	2.22	0.41
2:B:2415:ARG:HG2	2:B:2415:ARG:NH1	2.35	0.41
2:B:2265:VAL:O	2:B:2269:MET:HG2	2.20	0.41
2:B:2591:ASP:O	2:B:2592:ASN:HB2	2.21	0.41
2:B:2375:VAL:HG12	2:B:2377:LYS:HD2	2.03	0.41
2:B:2343:LYS:CB	2:B:2344:PRO:CD	2.73	0.40
2:B:2457:LEU:HB3	2:B:2486:TRP:CE3	2.56	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:2567:ASP:HB2	2:B:2574:ILE:HD11	2.04	0.40
2:B:2420:HIS:ND1	2:B:2438:SER:HB3	2.37	0.40
2:B:2432:ASN:HA	2:B:2448:ALA:HB3	2.04	0.40
2:B:2674:ARG:NH1	5:B:196:HOH:O	2.48	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	132/149 (89%)	114 (86%)	12 (9%)	6 (4%)	4	4
2	B	438/445 (98%)	400 (91%)	28 (6%)	10 (2%)	10	14
3	C	5/8 (62%)	3 (60%)	1 (20%)	1 (20%)	0	0
All	All	575/602 (96%)	517 (90%)	41 (7%)	17 (3%)	7	9

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1141	ILE
2	B	2275	GLN
2	B	2317	ASP
2	B	2318	ASN
2	B	2342	ILE
2	B	2343	LYS
2	B	2344	PRO
2	B	2431	ASP
1	A	1130	LYS
2	B	2491	GLY
1	A	1140	ASN
1	A	1019	GLU
3	C	61	PRO
2	B	2331	ASP
1	A	1095	VAL

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Mol	Chain	Res	Type
1	A	1086	PRO
2	B	2499	GLY

### 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	124/134 (92%)	120 (97%)	4 (3%)	51	77
2	B	392/395 (99%)	369 (94%)	23 (6%)	28	48
3	C	7/7 (100%)	6 (86%)	1 (14%)	5	8
All	All	523/536 (98%)	495 (95%)	28 (5%)	31	53

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1006	LEU
1	A	1034	LEU
1	A	1055	LEU
1	A	1115	LEU
2	B	2269	MET
2	B	2281	ILE
2	B	2322	ARG
2	B	2343	LYS
2	B	2344	PRO
2	B	2367	ARG
2	B	2376	LEU
2	B	2388	GLN
2	B	2439	THR
2	B	2497	LEU
2	B	2521	PHE
2	B	2532	THR
2	B	2583	LEU
2	B	2591	ASP
2	B	2602	THR
2	B	2625	SER
2	B	2648	LEU

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Mol	Chain	Res	Type
2	B	2660	LEU
2	B	2663	LEU
2	B	2681	LYS
2	B	2695	THR
2	B	2698	LEU
2	B	2705	ASP
3	C	59	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1060	GLN
1	A	1064	HIS
2	B	2275	GLN
2	B	2303	GLN
2	B	2318	ASN
2	B	2348	HIS
2	B	2379	HIS
2	B	2382	HIS
2	B	2392	ASN
2	B	2432	ASN
2	B	2468	HIS
2	B	2470	HIS
2	B	2492	GLN
2	B	2540	HIS
2	B	2572	ASN
2	B	2612	GLN
2	B	2615	GLN
2	B	2659	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z  > 2$
3	TPO	C	62	3	10,10,11	5.85	3 (30%)	12,14,16	3.68	3 (25%)

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
3	TPO	C	62	3	-	0/9/11/13	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	62	TPO	O-C	18.00	1.23	1.11
3	C	62	TPO	OG1-CB	-3.10	1.39	1.45
3	C	62	TPO	P-O1P	2.28	1.58	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	62	TPO	C-CA-N	-10.94	94.15	111.94
3	C	62	TPO	OG1-CB-CA	-4.67	99.72	107.55
3	C	62	TPO	CB-CA-N	-3.50	104.70	109.60

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

12 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	B	901	-	4,4,4	0.24	0	6,6,6	0.08	0
4	SO4	B	902	-	4,4,4	0.30	0	6,6,6	0.15	0
4	SO4	B	903	-	4,4,4	0.39	0	6,6,6	0.24	0
4	SO4	B	904	-	4,4,4	0.27	0	6,6,6	0.09	0
4	SO4	B	905	-	4,4,4	0.25	0	6,6,6	0.12	0
4	SO4	B	906	-	4,4,4	0.30	0	6,6,6	0.19	0
4	SO4	B	907	-	4,4,4	0.23	0	6,6,6	0.20	0
4	SO4	B	908	-	4,4,4	0.26	0	6,6,6	0.12	0
4	SO4	B	909	-	4,4,4	0.27	0	6,6,6	0.09	0
4	SO4	B	910	-	4,4,4	0.34	0	6,6,6	0.08	0
4	SO4	B	911	-	4,4,4	0.21	0	6,6,6	0.11	0
4	SO4	B	912	-	4,4,4	0.27	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	B	901	-	-	0/0/0/0	0/0/0/0
4	SO4	B	902	-	-	0/0/0/0	0/0/0/0
4	SO4	B	903	-	-	0/0/0/0	0/0/0/0
4	SO4	B	904	-	-	0/0/0/0	0/0/0/0
4	SO4	B	905	-	-	0/0/0/0	0/0/0/0
4	SO4	B	906	-	-	0/0/0/0	0/0/0/0
4	SO4	B	907	-	-	0/0/0/0	0/0/0/0
4	SO4	B	908	-	-	0/0/0/0	0/0/0/0
4	SO4	B	909	-	-	0/0/0/0	0/0/0/0
4	SO4	B	910	-	-	0/0/0/0	0/0/0/0
4	SO4	B	911	-	-	0/0/0/0	0/0/0/0
4	SO4	B	912	-	-	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.

## 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	136/149 (91%)	0.46	9 (6%) 18 17	44, 66, 93, 107	0
2	B	442/445 (99%)	0.00	5 (1%) 77 79	19, 40, 80, 115	0
3	C	8/8 (100%)	3.65	7 (87%) 0 0	96, 106, 112, 114	0
All	All	586/602 (97%)	0.16	21 (3%) 42 42	19, 46, 87, 115	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	2338	ARG	6.7
3	C	58	SER	5.5
3	C	59	LEU	5.2
3	C	64	ASP	4.4
1	A	1087	VAL	4.3
3	C	62	TPO	3.9
1	A	1002	PRO	3.6
3	C	65	LYS	3.6
1	A	1130	LYS	3.1
3	C	63	PRO	3.0
1	A	1088	TRP	3.0
2	B	2341	VAL	2.9
2	B	2705	ASP	2.8
2	B	2706	MET	2.7
2	B	2271	VAL	2.2
3	C	61	PRO	2.2
1	A	1063	THR	2.2
1	A	1004	ILE	2.1
1	A	1155	LYS	2.1
1	A	1094	LYS	2.0
1	A	1083	ASP	2.0

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

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	TPO	C	62	11/12	0.27	0.49	89,96,100,101	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	SO4	B	909	5/5	0.21	5.09	111,112,112,113	0
4	SO4	B	902	5/5	0.20	3.93	114,115,116,116	0
4	SO4	B	905	5/5	0.20	1.52	97,97,99,100	0
4	SO4	B	904	5/5	0.15	0.89	79,83,84,84	0
4	SO4	B	910	5/5	0.19	0.86	110,111,113,113	0
4	SO4	B	908	5/5	0.21	0.74	110,110,110,110	0
4	SO4	B	907	5/5	0.16	0.18	86,86,87,88	0
4	SO4	B	906	5/5	0.12	-0.13	89,89,90,90	0
4	SO4	B	911	5/5	0.17	-0.23	97,98,100,102	0
4	SO4	B	912	5/5	0.19	-0.40	135,135,135,136	0
4	SO4	B	901	5/5	0.12	-0.94	98,99,99,100	0
4	SO4	B	903	5/5	0.11	-2.17	64,67,69,71	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.