



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:18 PM GMT

PDB ID : 2OVQ
Title : Structure of the Skp1-Fbw7-CyclinEdegCcomplex
Authors : Hao, B.; Oehlmann, S.; Sowa, M.E.; Harper, J.W.; Pavletich, N.P.
Deposited on : 2007-02-14
Resolution : 2.60 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

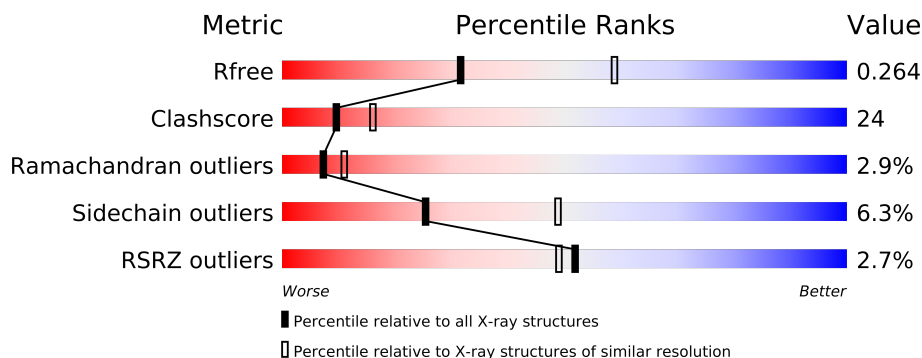
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.60 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	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	12	

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	906	-	X
4	SO4	B	907	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4896 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	134	Total	C	N	O	S	0	0	0
			1073	686	174	208	5			

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

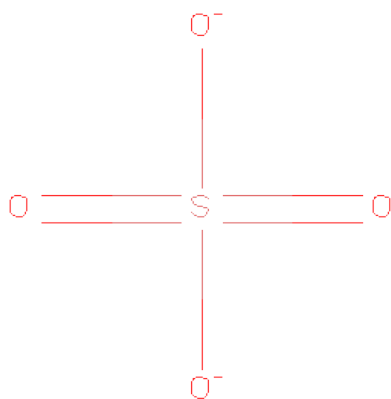
- Molecule 2 is a protein called F-box/WD repeat protein 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	444	Total	C	N	O	S	0	0	0
			3515	2205	637	651	22			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	12	Total	C	N	O	P	0	0	0
			90	52	13	23	2			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	7	Total	O	0	0
			7	7		

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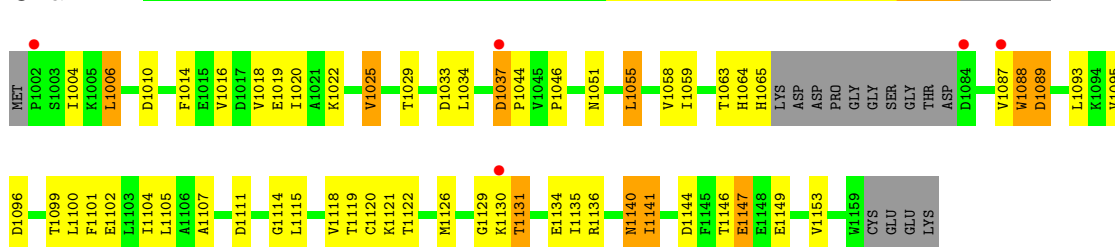
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	168	Total 168	O 168	0	0
5	C	3	Total 3	O 3	0	0

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.

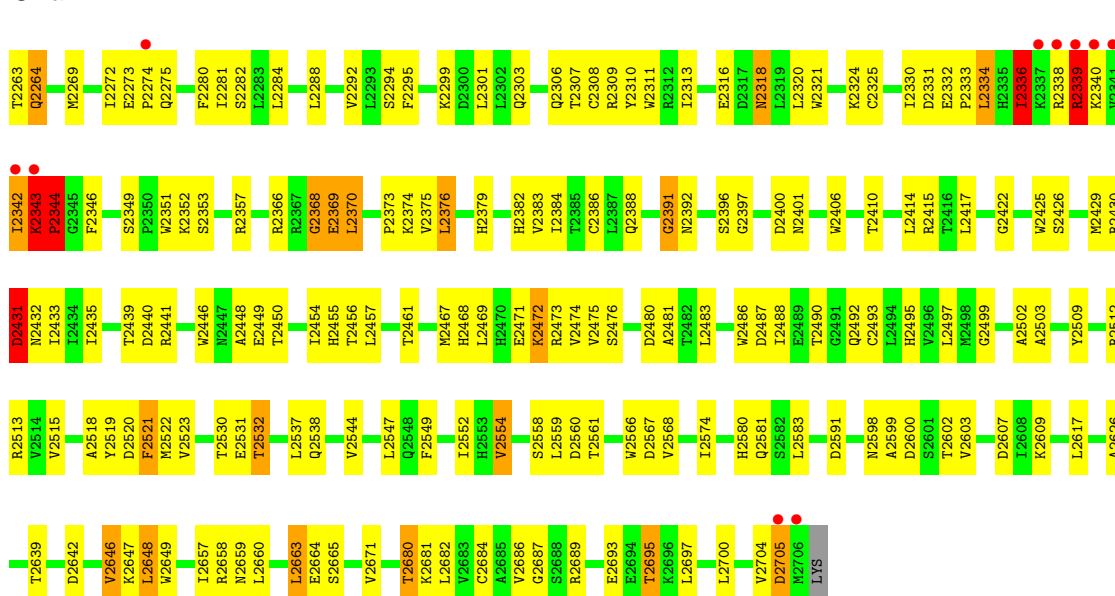
• Molecule 1: S-phase kinase-associated protein 1A

Chain A:



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

Chain B:



• Molecule 3: cyclinE C-terminal degon

Chain C:



4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	233.07Å 233.07Å 107.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.76 – 2.60 19.76 – 2.60	Depositor EDS
% Data completeness (in resolution range)	93.9 (19.76-2.60) 93.9 (19.76-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.15 (at 2.59Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.232 , 0.266 0.231 , 0.264	Depositor DCC
R_{free} test set	1488 reflections (3.61%)	DCC
Wilson B-factor (Å ²)	46.5	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 30.5	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 44757 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4896	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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, SEP

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	0.31	0/1091	0.61	0/1476
2	B	0.39	0/3586	0.75	4/4857 (0.1%)
3	C	0.46	0/69	0.74	0/89
All	All	0.38	0/4746	0.72	4/6422 (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
3	C	1	0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2339	ARG	N-CA-C	7.53	131.32	111.00
2	B	2342	ILE	N-CA-C	-6.13	94.46	111.00
2	B	2336	ILE	N-CA-C	5.23	125.12	111.00
2	B	2646	VAL	N-CA-C	-5.01	97.47	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	380	TPO	CB

There are no planarity outliers.

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	1073	0	1083	64	0
2	B	3515	0	3508	181	0
3	C	90	0	80	8	0
4	B	40	0	0	0	0
5	A	7	0	0	0	0
5	B	168	0	0	2	1
5	C	3	0	0	0	0
All	All	4896	0	4671	229	1

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

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1037:ASP:HB2	1:A:1044:PRO:HD3	1.41	1.00
1:A:1130:LYS:HG3	2:B:2303:GLN:HG3	1.46	0.96
2:B:2554:VAL:HG12	2:B:2568:VAL:HG22	1.45	0.95
2:B:2468:HIS:CD2	2:B:2509:TYR:H	1.85	0.94
2:B:2549:PHE:HE1	2:B:2568:VAL:HG21	1.32	0.93
2:B:2468:HIS:HD2	2:B:2509:TYR:H	0.92	0.89
2:B:2338:ARG:O	2:B:2339:ARG:HB2	1.75	0.87
1:A:1095:VAL:HG12	1:A:1096:ASP:H	1.42	0.85
2:B:2560:ASP:O	2:B:2561:THR:HB	1.76	0.84
1:A:1037:ASP:CB	1:A:1044:PRO:HD3	2.07	0.83
2:B:2343:LYS:HB3	2:B:2344:PRO:CD	2.07	0.83
1:A:1130:LYS:HG2	2:B:2303:GLN:HE21	1.45	0.81
2:B:2388:GLN:HB3	2:B:2429:MET:HE1	1.62	0.80
2:B:2334:LEU:HD13	2:B:2336:ILE:HG23	1.64	0.80
2:B:2468:HIS:HD2	2:B:2509:TYR:N	1.76	0.79
1:A:1037:ASP:HB2	1:A:1044:PRO:CD	2.14	0.78
2:B:2343:LYS:HD2	2:B:2343:LYS:H	1.48	0.78
1:A:1006:LEU:HD12	1:A:1014:PHE:HB2	1.68	0.76
1:A:1020:ILE:HG21	1:A:1063:THR:HG22	1.67	0.76
2:B:2343:LYS:HB3	2:B:2344:PRO:HD3	1.67	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:375:PRO:HG2	3:C:378:LEU:HD22	1.66	0.75
1:A:1025:VAL:HG13	1:A:1111:ASP:HB3	1.70	0.74
2:B:2425:TRP:CD2	3:C:381:PRO:HG3	2.23	0.73
2:B:2559:LEU:HD23	2:B:2559:LEU:O	1.89	0.72
2:B:2333:PRO:HD3	2:B:2351:TRP:CH2	2.25	0.71
2:B:2647:LYS:HG2	2:B:2659:ASN:ND2	2.05	0.71
2:B:2435:ILE:HD13	2:B:2474:VAL:HG21	1.72	0.70
2:B:2472:LYS:HD3	2:B:2472:LYS:H	1.55	0.70
1:A:1121:LYS:HE2	2:B:2295:PHE:CE2	2.26	0.70
2:B:2472:LYS:HE3	2:B:2473:ARG:HG3	1.74	0.70
2:B:2383:VAL:HG11	3:C:379:LEU:HD13	1.74	0.70
2:B:2391:GLY:O	2:B:2392:ASN:HB2	1.92	0.69
1:A:1020:ILE:HD13	1:A:1063:THR:HG22	1.73	0.69
1:A:1141:ILE:HD13	2:B:2307:THR:HG21	1.75	0.69
1:A:1153:VAL:HG12	2:B:2306:GLN:HG2	1.74	0.69
2:B:2415:ARG:HE	2:B:2450:THR:C	1.96	0.69
2:B:2642:ASP:HA	2:B:2671:VAL:HG23	1.75	0.68
1:A:1121:LYS:HE2	2:B:2295:PHE:HE2	1.58	0.68
2:B:2342:ILE:O	2:B:2343:LYS:O	2.12	0.68
2:B:2647:LYS:NZ	2:B:2659:ASN:HD21	1.91	0.68
2:B:2373:PRO:HB3	2:B:2700:LEU:HD22	1.75	0.68
2:B:2343:LYS:CB	2:B:2344:PRO:CD	2.71	0.67
2:B:2530:THR:OG1	2:B:2532:THR:HG22	1.95	0.67
2:B:2334:LEU:HD23	2:B:2357:ARG:HD2	1.76	0.67
1:A:1131:THR:HG21	1:A:1134:GLU:HG3	1.77	0.67
2:B:2603:VAL:HG21	2:B:2639:THR:HG21	1.77	0.66
2:B:2334:LEU:HD12	2:B:2334:LEU:O	1.95	0.66
2:B:2474:VAL:CG2	2:B:2488:ILE:HD11	2.26	0.65
1:A:1130:LYS:CG	2:B:2303:GLN:HE21	2.10	0.65
1:A:1018:VAL:O	1:A:1019:GLU:HB2	1.95	0.65
2:B:2549:PHE:CE1	2:B:2568:VAL:HG21	2.23	0.64
2:B:2414:LEU:O	2:B:2415:ARG:HG2	1.97	0.64
2:B:2343:LYS:CD	2:B:2343:LYS:H	2.11	0.63
1:A:1020:ILE:HG21	1:A:1063:THR:CG2	2.29	0.62
2:B:2334:LEU:HD13	2:B:2336:ILE:CG2	2.30	0.62
2:B:2425:TRP:CG	3:C:381:PRO:HG3	2.35	0.62
1:A:1087:VAL:O	1:A:1088:TRP:HB2	1.99	0.62
1:A:1114:GLY:O	1:A:1118:VAL:HG23	2.00	0.61
2:B:2521:PHE:N	2:B:2521:PHE:CD2	2.68	0.61
1:A:1095:VAL:HG12	1:A:1096:ASP:N	2.12	0.61
2:B:2282:SER:HA	2:B:2310:TYR:CE2	2.35	0.61
2:B:2321:TRP:CE2	2:B:2352:LYS:HG3	2.35	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:2382:HIS:O	2:B:2695:THR:HG21	2.01	0.61
1:A:1100:LEU:O	1:A:1104:ILE:HG12	2.01	0.61
1:A:1006:LEU:CD1	1:A:1014:PHE:HB2	2.30	0.60
2:B:2373:PRO:HB3	2:B:2700:LEU:CD2	2.30	0.60
2:B:2647:LYS:HZ2	2:B:2659:ASN:HD21	1.48	0.60
1:A:1131:THR:O	1:A:1135:ILE:HG13	2.02	0.60
2:B:2316:GLU:HG3	2:B:2346:PHE:CE2	2.38	0.59
2:B:2415:ARG:HH21	2:B:2450:THR:HA	1.67	0.59
2:B:2647:LYS:HG2	2:B:2659:ASN:HD22	1.67	0.59
2:B:2343:LYS:O	2:B:2344:PRO:C	2.40	0.59
2:B:2530:THR:OG1	2:B:2532:THR:CG2	2.51	0.58
2:B:2435:ILE:CD1	2:B:2474:VAL:HG21	2.33	0.58
2:B:2552:ILE:O	2:B:2568:VAL:HG23	2.03	0.58
2:B:2417:LEU:HB3	2:B:2446:TRP:CE3	2.39	0.57
2:B:2472:LYS:HD3	2:B:2472:LYS:N	2.20	0.57
2:B:2430:ARG:NH2	2:B:2471:GLU:O	2.37	0.57
2:B:2522:MET:SD	2:B:2538:GLN:HG2	2.45	0.57
2:B:2457:LEU:HB3	2:B:2486:TRP:CZ3	2.39	0.57
2:B:2272:ILE:HD12	2:B:2313:ILE:HD11	1.87	0.57
2:B:2665:SER:OG	2:B:2693:GLU:HG2	2.05	0.57
1:A:1131:THR:H	2:B:2303:GLN:HE21	1.53	0.56
2:B:2374:LYS:HE3	2:B:2410:THR:O	2.05	0.56
1:A:1016:VAL:HG11	1:A:1059:ILE:HD12	1.87	0.56
2:B:2325:CYS:HB3	2:B:2330:ILE:HB	1.87	0.56
2:B:2567:ASP:HB2	2:B:2574:ILE:HD11	1.87	0.55
2:B:2521:PHE:N	2:B:2521:PHE:HD2	2.04	0.55
2:B:2263:THR:HG22	2:B:2264:GLN:N	2.22	0.55
1:A:1136:ARG:O	1:A:1140:ASN:N	2.40	0.55
1:A:1006:LEU:HD13	1:A:1055:LEU:HD11	1.89	0.54
2:B:2417:LEU:HB3	2:B:2446:TRP:CZ3	2.42	0.54
2:B:2617:LEU:HD13	2:B:2649:TRP:CG	2.43	0.54
2:B:2523:VAL:HB	2:B:2537:LEU:HB2	1.88	0.54
1:A:1130:LYS:HG3	2:B:2303:GLN:CG	2.30	0.54
2:B:2486:TRP:CZ3	2:B:2493:CYS:HB2	2.42	0.54
2:B:2515:VAL:HG12	2:B:2547:LEU:CD1	2.38	0.54
2:B:2469:LEU:HD13	2:B:2474:VAL:HG22	1.88	0.54
1:A:1141:ILE:HG21	2:B:2307:THR:HG22	1.90	0.54
2:B:2474:VAL:HG23	2:B:2488:ILE:HD11	1.89	0.53
1:A:1141:ILE:HD13	2:B:2307:THR:CG2	2.38	0.53
2:B:2495:HIS:HB3	2:B:2531:GLU:HG2	1.90	0.53
2:B:2280:PHE:HE2	2:B:2284:LEU:HD11	1.74	0.53
2:B:2343:LYS:HE3	2:B:2343:LYS:N	2.24	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:2457:LEU:HB3	2:B:2486:TRP:CE3	2.45	0.52
2:B:2602:THR:CG2	2:B:2603:VAL:N	2.73	0.52
1:A:1018:VAL:O	1:A:1019:GLU:CB	2.56	0.51
2:B:2469:LEU:HD13	2:B:2474:VAL:CG2	2.40	0.51
1:A:1055:LEU:O	1:A:1058:VAL:HG22	2.11	0.51
2:B:2318:ASN:ND2	2:B:2349:SER:OG	2.42	0.51
2:B:2368:GLY:O	2:B:2369:GLU:HB2	2.09	0.51
1:A:1093:LEU:C	1:A:1095:VAL:H	2.14	0.51
2:B:2343:LYS:CD	2:B:2343:LYS:N	2.74	0.51
1:A:1087:VAL:O	1:A:1087:VAL:HG23	2.10	0.51
2:B:2320:LEU:O	2:B:2324:LYS:HG2	2.11	0.51
2:B:2600:ASP:OD1	2:B:2602:THR:HB	2.11	0.50
2:B:2333:PRO:HB3	2:B:2351:TRP:CD2	2.47	0.50
1:A:1004:ILE:C	1:A:1004:ILE:HD12	2.32	0.50
2:B:2425:TRP:CE2	3:C:381:PRO:HG3	2.46	0.49
2:B:2642:ASP:OD1	2:B:2671:VAL:HB	2.12	0.49
2:B:2379:HIS:HD2	2:B:2400:ASP:OD2	1.95	0.49
2:B:2520:ASP:OD1	2:B:2522:MET:HB2	2.12	0.49
1:A:1144:ASP:OD1	2:B:2308:CYS:HB2	2.12	0.49
1:A:1101:PHE:CE1	1:A:1105:LEU:HD11	2.47	0.49
2:B:2273:GLU:N	2:B:2274:PRO:HD3	2.27	0.49
2:B:2663:LEU:HD21	2:B:2686:VAL:HG13	1.94	0.49
1:A:1018:VAL:CG2	1:A:1022:LYS:HE3	2.42	0.49
2:B:2343:LYS:CB	2:B:2344:PRO:HD2	2.43	0.49
2:B:2375:VAL:C	2:B:2376:LEU:HD23	2.33	0.49
1:A:1141:ILE:HG21	2:B:2307:THR:CG2	2.43	0.49
2:B:2281:ILE:HG12	2:B:2311:TRP:CE2	2.48	0.49
2:B:2439:THR:C	2:B:2441:ARG:H	2.17	0.48
2:B:2440:ASP:OD1	2:B:2440:ASP:C	2.50	0.48
2:B:2490:THR:HB	2:B:2492:GLN:HE21	1.78	0.48
1:A:1029:THR:O	1:A:1033:ASP:HB2	2.13	0.48
1:A:1130:LYS:HD3	2:B:2299:LYS:HE2	1.94	0.48
2:B:2352:LYS:HB3	2:B:2352:LYS:NZ	2.28	0.48
1:A:1055:LEU:O	1:A:1059:ILE:HG12	2.14	0.48
2:B:2512:ARG:HG2	2:B:2513:ARG:HG2	1.96	0.48
2:B:2432:ASN:HA	2:B:2448:ALA:HB3	1.96	0.47
2:B:2602:THR:HG22	2:B:2603:VAL:N	2.30	0.47
2:B:2686:VAL:HG12	2:B:2687:GLY:N	2.30	0.47
2:B:2316:GLU:HG3	2:B:2346:PHE:HE2	1.78	0.47
1:A:1006:LEU:O	1:A:1006:LEU:HD12	2.15	0.46
2:B:2382:HIS:CG	2:B:2400:ASP:HB3	2.50	0.46
2:B:2476:SER:O	2:B:2483:LEU:HA	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:2269:MET:SD	2:B:2310:TYR:CE1	3.08	0.46
1:A:1104:ILE:HD13	1:A:1119:THR:OG1	2.14	0.46
2:B:2474:VAL:HG21	2:B:2488:ILE:HD11	1.96	0.46
1:A:1037:ASP:CB	1:A:1044:PRO:CD	2.82	0.46
2:B:2515:VAL:HG12	2:B:2547:LEU:HD11	1.98	0.46
2:B:2646:VAL:HG11	2:B:2682:LEU:HD21	1.97	0.46
2:B:2472:LYS:CD	2:B:2472:LYS:H	2.23	0.46
1:A:1018:VAL:HG22	1:A:1019:GLU:N	2.31	0.46
2:B:2648:LEU:HD13	2:B:2657:ILE:HD12	1.96	0.46
1:A:1149:GLU:O	1:A:1153:VAL:HG23	2.16	0.45
1:A:1131:THR:CG2	1:A:1134:GLU:HG3	2.44	0.45
2:B:2294:SER:HA	2:B:2320:LEU:HD11	1.99	0.45
1:A:1099:THR:O	1:A:1102:GLU:HB2	2.16	0.45
2:B:2383:VAL:HG11	3:C:379:LEU:CD1	2.46	0.45
2:B:2603:VAL:HG21	2:B:2639:THR:CG2	2.46	0.45
2:B:2502:ALA:HA	5:B:139:HOH:O	2.15	0.45
2:B:2441:ARG:HG2	2:B:2461:THR:O	2.17	0.45
2:B:2472:LYS:HE3	2:B:2473:ARG:CG	2.46	0.45
2:B:2456:THR:C	2:B:2457:LEU:HD23	2.37	0.45
2:B:2309:ARG:O	2:B:2313:ILE:HG13	2.17	0.45
2:B:2457:LEU:HD23	2:B:2457:LEU:N	2.32	0.45
2:B:2684:CYS:O	2:B:2697:LEU:HA	2.17	0.45
2:B:2561:THR:HG23	2:B:2580:HIS:O	2.17	0.44
2:B:2515:VAL:HG12	2:B:2547:LEU:HD13	1.99	0.44
2:B:2376:LEU:N	2:B:2376:LEU:HD23	2.32	0.44
2:B:2664:GLU:HG3	5:B:11:HOH:O	2.17	0.44
1:A:1044:PRO:O	1:A:1046:PRO:HD3	2.17	0.44
2:B:2558:SER:HB3	2:B:2560:ASP:OD1	2.18	0.44
2:B:2433:ILE:HG21	2:B:2488:ILE:HG21	2.00	0.44
2:B:2281:ILE:HG12	2:B:2311:TRP:NE1	2.33	0.44
2:B:2379:HIS:HE1	2:B:2396:SER:OG	2.01	0.44
2:B:2426:SER:HB2	2:B:2467:MET:HG2	1.99	0.44
2:B:2366:ARG:O	2:B:2658:ARG:HD2	2.18	0.44
1:A:1130:LYS:HG2	2:B:2303:GLN:NE2	2.22	0.43
2:B:2559:LEU:CD2	2:B:2559:LEU:O	2.64	0.43
2:B:2316:GLU:OE2	2:B:2352:LYS:HE3	2.19	0.43
2:B:2680:THR:HG22	2:B:2681:LYS:HG2	2.00	0.43
2:B:2401:ASN:OD1	2:B:2422:GLY:C	2.57	0.43
2:B:2269:MET:CE	2:B:2313:ILE:HD12	2.48	0.43
2:B:2519:TYR:OH	3:C:380:TPO:O3P	2.36	0.43
2:B:2487:ASP:HB3	2:B:2490:THR:OG1	2.18	0.43
3:C:374:LEU:O	3:C:375:PRO:C	2.57	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:2665:SER:OG	2:B:2693:GLU:CG	2.66	0.43
2:B:2432:ASN:HD21	2:B:2449:GLU:H	1.65	0.43
2:B:2376:LEU:HB3	2:B:2406:TRP:CZ3	2.54	0.42
2:B:2607:ASP:OD1	2:B:2609:LYS:HB2	2.19	0.42
2:B:2700:LEU:N	2:B:2700:LEU:HD23	2.35	0.42
1:A:1146:THR:O	1:A:1147:GLU:C	2.58	0.42
2:B:2343:LYS:CE	2:B:2343:LYS:N	2.83	0.42
2:B:2454:ILE:HG13	2:B:2455:HIS:CD2	2.55	0.42
2:B:2383:VAL:HG12	2:B:2384:ILE:N	2.33	0.42
2:B:2281:ILE:HG13	2:B:2282:SER:N	2.34	0.42
1:A:1104:ILE:HG22	2:B:2288:LEU:HD13	2.02	0.42
2:B:2401:ASN:OD1	2:B:2422:GLY:O	2.38	0.42
2:B:2386:CYS:SG	2:B:2397:GLY:HA3	2.60	0.42
2:B:2580:HIS:HB3	2:B:2598:ASN:ND2	2.35	0.42
2:B:2357:ARG:HH11	2:B:2357:ARG:HG3	1.84	0.42
2:B:2430:ARG:O	2:B:2431:ASP:C	2.57	0.42
2:B:2599:ALA:HA	2:B:2626:ALA:CB	2.50	0.42
2:B:2334:LEU:HD11	2:B:2353:SER:HB2	2.02	0.41
2:B:2316:GLU:HG3	2:B:2346:PHE:CZ	2.54	0.41
1:A:1131:THR:HB	1:A:1134:GLU:HB2	2.03	0.41
1:A:1025:VAL:HG13	1:A:1111:ASP:CB	2.45	0.41
1:A:1064:HIS:HD2	1:A:1065:HIS:CE1	2.39	0.41
2:B:2275:GLN:HE21	2:B:2275:GLN:HB2	1.64	0.41
2:B:2467:MET:HA	2:B:2475:VAL:O	2.20	0.41
1:A:1120:CYS:HB3	2:B:2292:VAL:HG22	2.02	0.41
2:B:2301:LEU:H	2:B:2301:LEU:HD22	1.86	0.41
1:A:1095:VAL:CG1	1:A:1096:ASP:H	2.23	0.41
1:A:1107:ALA:O	1:A:1111:ASP:N	2.53	0.41
1:A:1131:THR:H	2:B:2303:GLN:NE2	2.18	0.41
1:A:1089:ASP:HB3	1:A:1118:VAL:HG11	2.01	0.41
2:B:2480:ASP:O	2:B:2481:ALA:HB3	2.19	0.41
2:B:2663:LEU:HD21	2:B:2686:VAL:CG1	2.51	0.41
2:B:2503:ALA:O	2:B:2518:ALA:HB1	2.20	0.41
2:B:2370:LEU:N	2:B:2370:LEU:HD13	2.35	0.41
2:B:2554:VAL:HG22	2:B:2566:TRP:CD1	2.56	0.40
2:B:2639:THR:O	2:B:2646:VAL:HA	2.21	0.40
2:B:2330:ILE:C	2:B:2332:GLU:H	2.24	0.40
2:B:2704:VAL:HG12	2:B:2705:ASP:N	2.35	0.40
2:B:2686:VAL:CG1	2:B:2687:GLY:N	2.84	0.40
1:A:1122:THR:O	1:A:1126:MET:HG3	2.21	0.40
1:A:1010:ASP:OD2	1:A:1051:ASN:HB2	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:B:173:HOH:O	5:B:173:HOH:O[6_555]	1.01	1.19

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	130/149 (87%)	108 (83%)	16 (12%)	6 (5%)	4	4
2	B	442/445 (99%)	396 (90%)	35 (8%)	11 (2%)	9	14
3	C	8/12 (67%)	8 (100%)	0	0	100	100
All	All	580/606 (96%)	512 (88%)	51 (9%)	17 (3%)	7	11

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1088	TRP
2	B	2339	ARG
2	B	2343	LYS
2	B	2369	GLU
2	B	2431	ASP
1	A	1141	ILE
2	B	2340	LYS
2	B	2368	GLY
2	B	2391	GLY
2	B	2344	PRO
1	A	1131	THR
1	A	1140	ASN
1	A	1147	GLU
2	B	2331	ASP
2	B	2336	ILE
1	A	1129	GLY
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	122/134 (91%)	115 (94%)	7 (6%)	29	54
2	B	394/395 (100%)	369 (94%)	25 (6%)	25	49
3	C	8/8 (100%)	7 (88%)	1 (12%)	7	12
All	All	524/537 (98%)	491 (94%)	33 (6%)	25	49

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1006	LEU
1	A	1025	VAL
1	A	1034	LEU
1	A	1037	ASP
1	A	1055	LEU
1	A	1089	ASP
1	A	1115	LEU
2	B	2264	GLN
2	B	2318	ASN
2	B	2334	LEU
2	B	2339	ARG
2	B	2343	LYS
2	B	2344	PRO
2	B	2370	LEU
2	B	2376	LEU
2	B	2431	ASP
2	B	2472	LYS
2	B	2497	LEU
2	B	2521	PHE
2	B	2532	THR
2	B	2544	VAL
2	B	2554	VAL
2	B	2581	GLN
2	B	2583	LEU
2	B	2591	ASP
2	B	2648	LEU
2	B	2660	LEU

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Mol	Chain	Res	Type
2	B	2663	LEU
2	B	2680	THR
2	B	2689	ARG
2	B	2695	THR
2	B	2705	ASP
3	C	379	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1060	GLN
1	A	1064	HIS
1	A	1097	GLN
2	B	2275	GLN
2	B	2303	GLN
2	B	2318	ASN
2	B	2348	HIS
2	B	2364	ASN
2	B	2379	HIS
2	B	2382	HIS
2	B	2388	GLN
2	B	2392	ASN
2	B	2432	ASN
2	B	2468	HIS
2	B	2492	GLN
2	B	2540	HIS
2	B	2572	ASN
2	B	2581	GLN
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 ⓘ

2 non-standard protein/DNA/RNA residues 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$
3	TPO	C	380	3	10,10,11	5.76	2 (20%)	12,14,16	1.62	2 (16%)
3	SEP	C	384	3	9,9,10	6.66	5 (55%)	10,12,14	4.57	4 (40%)

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	380	3	1/1/3/4	0/9/11/13	0/0/0/0
3	SEP	C	384	3	-	0/6/8/10	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	384	SEP	O-C	18.22	1.24	1.11
3	C	380	TPO	O-C	17.55	1.23	1.11
3	C	384	SEP	OG-CB	-6.78	1.16	1.44
3	C	380	TPO	OG1-CB	-4.00	1.37	1.45
3	C	384	SEP	CA-C	2.58	1.53	1.48
3	C	384	SEP	P-O1P	2.24	1.58	1.51
3	C	384	SEP	P-O3P	2.09	1.62	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	384	SEP	OG-CB-CA	8.76	121.09	108.69
3	C	384	SEP	P-OG-CB	-7.09	97.70	118.19
3	C	384	SEP	OG-P-O1P	6.58	125.99	106.71
3	C	384	SEP	O2P-P-OG	-5.48	91.51	106.65
3	C	380	TPO	C-CA-N	-3.89	105.61	111.94
3	C	380	TPO	OG1-CB-CG2	-2.95	105.20	110.13

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	380	TPO	CB

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

8 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	0.23	0	6,6,6	0.10	0
4	SO4	B	902	-	4,4,4	0.29	0	6,6,6	0.10	0
4	SO4	B	903	-	4,4,4	0.31	0	6,6,6	0.11	0
4	SO4	B	904	-	4,4,4	0.24	0	6,6,6	0.21	0
4	SO4	B	905	-	4,4,4	0.34	0	6,6,6	0.08	0
4	SO4	B	906	-	4,4,4	0.26	0	6,6,6	0.14	0
4	SO4	B	907	-	4,4,4	0.30	0	6,6,6	0.06	0
4	SO4	B	908	-	4,4,4	0.39	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	134/149 (89%)	0.12	5 (3%) 39 35	52, 73, 95, 101	0
2	B	444/445 (99%)	-0.23	10 (2%) 57 54	22, 42, 87, 101	0
3	C	12/12 (100%)	0.82	1 (8%) 11 8	51, 67, 87, 88	0
All	All	590/606 (97%)	-0.13	16 (2%) 52 49	22, 48, 90, 101	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	2339	ARG	6.7
3	C	385	GLY	5.3
2	B	2340	LYS	5.1
2	B	2343	LYS	4.3
2	B	2338	ARG	3.9
2	B	2337	LYS	3.5
1	A	1087	VAL	3.4
2	B	2706	MET	3.2
2	B	2274	PRO	3.1
2	B	2705	ASP	3.1
2	B	2342	ILE	2.9
1	A	1002	PRO	2.7
1	A	1084	ASP	2.4
1	A	1037	ASP	2.3
2	B	2341	VAL	2.2
1	A	1130	LYS	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	SEP	C	384	10/11	0.22	0.05	77,86,88,88	0
3	TPO	C	380	11/12	0.15	-0.18	45,50,52,53	0

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	SO4	B	906	5/5	0.21	4.70	98,99,99,100	0
4	SO4	B	907	5/5	0.27	3.15	99,100,100,100	0
4	SO4	B	902	5/5	0.19	2.49	97,97,98,98	0
4	SO4	B	904	5/5	0.19	1.77	91,91,92,92	0
4	SO4	B	905	5/5	0.24	1.41	98,100,100,100	0
4	SO4	B	901	5/5	0.10	-1.05	52,53,55,55	0
4	SO4	B	903	5/5	0.12	-1.06	59,61,63,63	0
4	SO4	B	908	5/5	0.28	-	100,100,100,100	0

6.5 Other polymers [i](#)

There are no such residues in this entry.