



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:47 PM GMT

PDB ID : 3UR0
Title : Crystal structures of murine norovirus RNA-dependent RNA polymerase in complex with Suramin
Authors : Milani, M.; Mastrangelo, E.; Bolognesi, M.
Deposited on : 2011-11-21
Resolution : 2.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

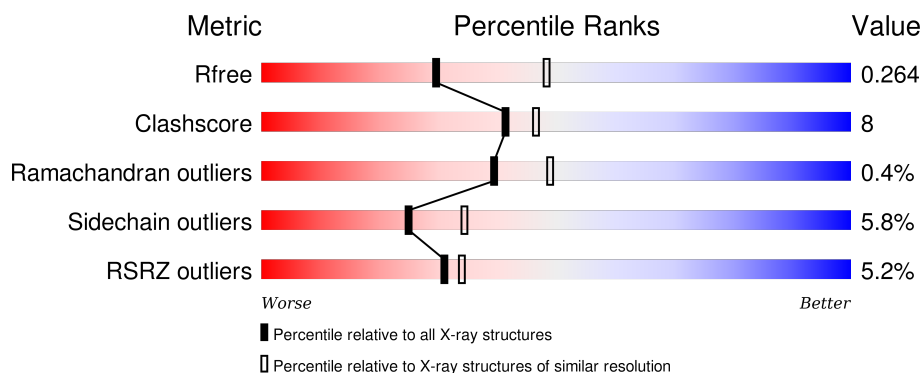
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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. 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	515	<div> <div>6%</div> <div> <div></div> <div>74%</div> <div>16%</div> <div>• 8%</div> </div> </div>
1	B	515	<div> <div>6%</div> <div> <div></div> <div>74%</div> <div>17%</div> <div>• 8%</div> </div> </div>
1	C	515	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>15%</div> <div>• 8%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12050 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 RNA-dependent RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	475	Total	C	N	O	S	0	1	0
			3785	2395	666	699	25			
1	B	476	Total	C	N	O	S	0	2	0
			3792	2402	665	700	25			
1	C	474	Total	C	N	O	S	0	2	0
			3776	2388	663	700	25			

There are 24 discrepancies between the modelled and reference sequences:

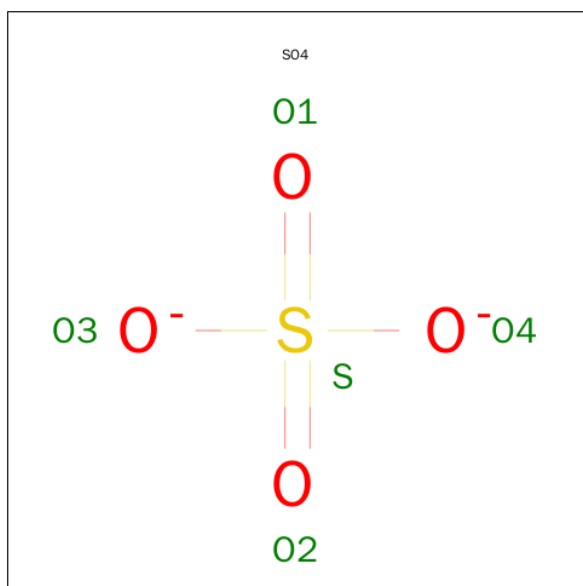
Chain	Residue	Modelled	Actual	Comment	Reference
A	508	LEU	-	EXPRESSION TAG	UNP Q80J95
A	509	GLU	-	EXPRESSION TAG	UNP Q80J95
A	510	HIS	-	EXPRESSION TAG	UNP Q80J95
A	511	HIS	-	EXPRESSION TAG	UNP Q80J95
A	512	HIS	-	EXPRESSION TAG	UNP Q80J95
A	513	HIS	-	EXPRESSION TAG	UNP Q80J95
A	514	HIS	-	EXPRESSION TAG	UNP Q80J95
A	515	HIS	-	EXPRESSION TAG	UNP Q80J95
B	508	LEU	-	EXPRESSION TAG	UNP Q80J95
B	509	GLU	-	EXPRESSION TAG	UNP Q80J95
B	510	HIS	-	EXPRESSION TAG	UNP Q80J95
B	511	HIS	-	EXPRESSION TAG	UNP Q80J95
B	512	HIS	-	EXPRESSION TAG	UNP Q80J95
B	513	HIS	-	EXPRESSION TAG	UNP Q80J95
B	514	HIS	-	EXPRESSION TAG	UNP Q80J95
B	515	HIS	-	EXPRESSION TAG	UNP Q80J95
C	508	LEU	-	EXPRESSION TAG	UNP Q80J95
C	509	GLU	-	EXPRESSION TAG	UNP Q80J95
C	510	HIS	-	EXPRESSION TAG	UNP Q80J95
C	511	HIS	-	EXPRESSION TAG	UNP Q80J95
C	512	HIS	-	EXPRESSION TAG	UNP Q80J95
C	513	HIS	-	EXPRESSION TAG	UNP Q80J95
C	514	HIS	-	EXPRESSION TAG	UNP Q80J95

Continued on next page...

Continued from previous page...

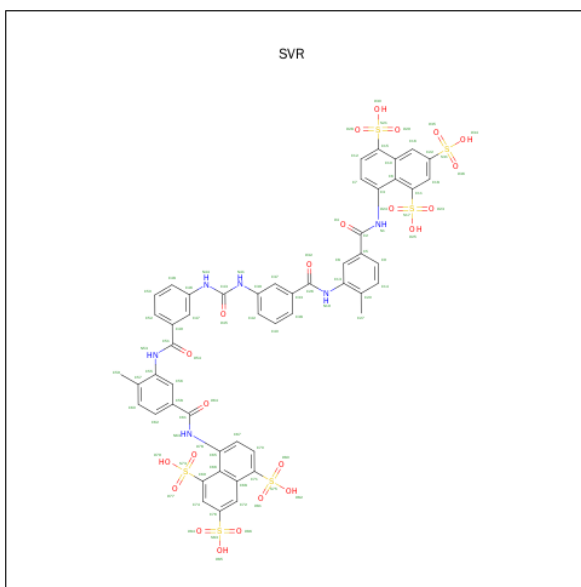
Chain	Residue	Modelled	Actual	Comment	Reference
C	515	HIS	-	EXPRESSION TAG	UNP Q80J95

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

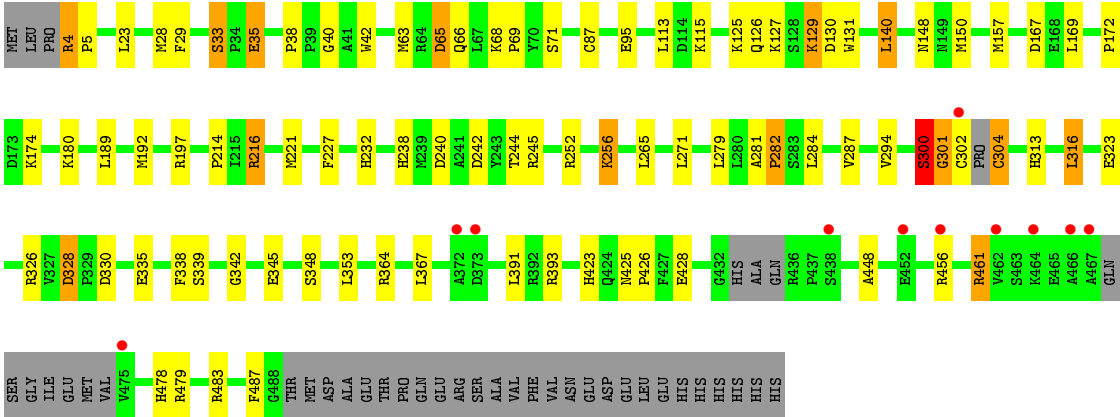
- Molecule 3 is 8,8'-[CARBONYLBIS[IMINO-3,1-PHENYLENECARBONYLIMINO(4-METHYL-3,1-PHENYLENE)CARBONYLIMINO]]BIS-1,3,5-NAPHTHALENETRISULFONIC ACID (three-letter code: SVR) (formula: C₅₁H₄₀N₆O₂₃S₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	0
			26	12	1	10	3		
3	C	1	Total	C	N	O	S	0	0
			26	12	1	10	3		
3	C	1	Total	C	N	O	S	0	0
			54	33	5	13	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	173	Total	O	0	0
			173	173		
4	B	166	Total	O	0	0
			166	166		
4	C	217	Total	O	0	0
			217	217		



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	120.84Å 196.51Å 109.07Å 90.00° 114.55° 90.00°	Depositor
Resolution (Å)	48.00 – 2.45 48.08 – 2.45	Depositor EDS
% Data completeness (in resolution range)	97.4 (48.00-2.45) 97.4 (48.08-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.199 , 0.268 0.199 , 0.264	Depositor DCC
R_{free} test set	4102 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	47.8	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 59.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 82297 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12050	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SVR, 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	0.58	0/3879	0.71	2/5250 (0.0%)
1	B	0.54	0/3890	0.64	0/5267
1	C	0.62	0/3872	0.71	1/5241 (0.0%)
All	All	0.58	0/11641	0.69	3/15758 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	279	LEU	CA-CB-CG	5.86	128.78	115.30
1	A	65	ASP	CB-CG-OD1	5.26	123.03	118.30
1	C	65	ASP	CB-CG-OD1	5.06	122.85	118.30

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	3785	0	3745	66	0
1	B	3792	0	3760	51	0
1	C	3776	0	3734	68	0
2	A	15	0	0	0	0
2	B	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	15	0	0	0	0
3	B	26	0	6	2	0
3	C	80	0	31	17	0
4	A	173	0	0	6	0
4	B	166	0	0	2	0
4	C	217	0	0	3	0
All	All	12050	0	11276	192	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 8.

All (192) 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:C:301:GLY:HA3	1:C:302:CYS:CB	1.56	1.27
1:C:301:GLY:HA3	1:C:302:CYS:HB3	1.24	1.12
1:C:301:GLY:HA3	1:C:302:CYS:HB2	1.35	1.03
1:A:373:ASP:O	1:A:374:LYS:HB2	1.59	0.97
1:C:301:GLY:CA	1:C:302:CYS:CB	2.44	0.93
1:B:148:ASN:HD21	1:B:197:ARG:HH11	1.12	0.91
1:C:148:ASN:HD21	1:C:197:ARG:HH11	1.00	0.91
1:A:148:ASN:HD21	1:A:197:ARG:HH11	0.94	0.90
3:C:517:SVR:H44	3:C:517:SVR:H42	1.34	0.88
1:B:232:HIS:HE1	1:B:339:SER:OG	1.59	0.86
1:C:33:SER:OG	1:C:35:GLU:HG2	1.80	0.82
1:B:29:PHE:O	1:B:423:HIS:HE1	1.62	0.82
1:A:68:LYS:HB2	1:A:69:PRO:HD3	1.58	0.82
1:A:371:ARG:HD3	1:A:375:GLU:O	1.81	0.80
1:A:360[B]:MET:HA	1:A:360[B]:MET:HE3	1.61	0.80
1:C:301:GLY:CA	1:C:302:CYS:HB3	2.06	0.80
1:B:77:LEU:HD23	1:B:251:GLN:NE2	1.97	0.80
3:C:517:SVR:C26	3:C:517:SVR:H271	2.10	0.80
1:B:203[B]:CYS:SG	1:B:307:GLN:NE2	2.57	0.77
1:A:360[B]:MET:HA	1:A:360[B]:MET:CE	2.14	0.77
1:A:148:ASN:HD21	1:A:197:ARG:NH1	1.78	0.77
1:C:180:LYS:HB3	3:C:517:SVR:C27	2.15	0.77
1:C:238:HIS:HD2	1:C:348:SER:OG	1.66	0.77
1:C:302:CYS:O	1:C:304:CYS:N	2.18	0.75
1:B:77:LEU:HD23	1:B:251:GLN:HE22	1.51	0.75
1:C:216:ARG:HD2	1:C:216:ARG:N	2.02	0.75
1:A:148:ASN:ND2	1:A:197:ARG:HH11	1.78	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:ASN:ND2	1:C:197:ARG:HH11	1.82	0.74
1:B:232:HIS:CE1	1:B:339:SER:OG	2.39	0.74
1:A:313:HIS:HD2	1:A:342:GLY:O	1.73	0.72
1:B:29:PHE:O	1:B:423:HIS:CE1	2.44	0.71
1:B:313:HIS:HD2	1:B:342:GLY:O	1.74	0.70
1:C:180:LYS:HB3	3:C:517:SVR:H272	1.72	0.69
1:B:238:HIS:HD2	1:B:348:SER:OG	1.74	0.69
1:A:124:HIS:HE1	4:A:597:HOH:O	1.73	0.69
1:C:323:GLU:CD	1:C:364:ARG:HH22	1.96	0.69
1:C:328:ASP:HB3	1:C:330[A]:ASP:OD1	1.94	0.68
1:C:95:GLU:HG2	1:C:265:LEU:HD21	1.75	0.68
1:C:301:GLY:CA	1:C:302:CYS:HB2	2.20	0.67
1:C:244:THR:HG22	1:C:245:ARG:HG3	1.74	0.67
1:B:110:CYS:SG	4:B:617:HOH:O	2.52	0.67
1:A:335:GLU:OE1	1:C:326:ARG:NH1	2.29	0.65
1:C:28:MET:HG2	1:C:167:ASP:OD2	1.96	0.65
1:A:238:HIS:HD2	1:A:348:SER:OG	1.82	0.63
1:A:356:VAL:HG22	1:A:378:PRO:HB3	1.81	0.63
1:C:313:HIS:HD2	1:C:342:GLY:O	1.83	0.62
1:B:311:LEU:O	1:B:315:ILE:HG13	1.99	0.61
1:A:355:MET:HB3	1:A:379:LEU:O	2.00	0.61
1:A:68:LYS:HB2	1:A:69:PRO:CD	2.29	0.61
1:B:353:LEU:H	1:B:381:ARG:NH1	1.98	0.61
1:C:66:GLN:HE22	3:C:517:SVR:H37	1.65	0.61
1:A:182:ARG:HG3	4:A:541:HOH:O	2.02	0.60
1:B:40:GLY:HA2	1:B:172:PRO:HG3	1.84	0.59
1:B:69:PRO:HA	1:B:72:GLU:HG2	1.83	0.59
1:A:356:VAL:HA	1:A:378:PRO:HB3	1.85	0.59
3:C:517:SVR:C42	3:C:517:SVR:H44	2.12	0.58
1:A:214:PRO:HB3	1:A:338:PHE:HB2	1.84	0.58
3:C:516:SVR:N63	3:C:516:SVR:S73	2.70	0.58
1:A:313:HIS:HE1	1:A:345:GLU:OE2	1.87	0.58
1:C:238:HIS:CD2	1:C:348:SER:OG	2.55	0.58
1:B:84:ASP:OD1	1:B:257:ARG:NH2	2.35	0.57
1:B:371:ARG:HD3	1:B:375:GLU:O	2.04	0.57
1:C:180:LYS:CB	3:C:517:SVR:H272	2.35	0.57
1:B:214:PRO:HB3	1:B:338:PHE:HB2	1.86	0.56
1:A:371:ARG:NH2	1:A:373:ASP:OD1	2.27	0.56
1:C:339:SER:O	1:C:345:GLU:HA	2.05	0.56
1:B:211:ILE:O	1:B:216:ARG:NH2	2.38	0.56
1:A:86:VAL:HG13	1:A:318:LEU:HD23	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:517:SVR:O30	3:C:517:SVR:H16	2.05	0.56
1:A:386:GLN:HG3	1:A:402:TRP:HZ3	1.71	0.56
1:A:373:ASP:OD2	1:A:375:GLU:N	2.29	0.56
1:C:148:ASN:HD21	1:C:197:ARG:NH1	1.85	0.56
1:C:232:HIS:HD2	1:C:348:SER:OG	1.90	0.55
1:B:321:MET:HG2	1:B:353:LEU:HD11	1.88	0.55
1:C:448:ALA:O	1:C:478:HIS:HE1	1.89	0.55
1:C:323:GLU:OE2	1:C:364:ARG:NH2	2.31	0.55
1:C:180:LYS:HB3	3:C:517:SVR:H271	1.88	0.54
1:B:79:PRO:HG2	1:B:82:ILE:HB	1.88	0.54
1:A:326:ARG:NH1	1:C:335:GLU:OE1	2.40	0.54
1:B:217:VAL:HA	1:B:341:TYR:CE1	2.43	0.54
1:A:339:SER:O	1:A:345:GLU:HA	2.10	0.52
1:C:40:GLY:HA2	1:C:172:PRO:HG3	1.92	0.52
3:C:516:SVR:O64	3:C:516:SVR:H67	2.09	0.52
1:C:316:LEU:HG	1:C:367:LEU:HD11	1.92	0.52
1:B:104:TRP:CG	1:B:201:PRO:HD3	2.44	0.52
1:B:40:GLY:CA	1:B:172:PRO:HG3	2.40	0.52
3:C:517:SVR:O25	3:C:517:SVR:N1	2.43	0.52
1:B:201:PRO:HG2	4:B:532:HOH:O	2.08	0.52
1:C:29:PHE:O	1:C:423:HIS:HE1	1.91	0.52
1:B:458:VAL:O	1:B:462:VAL:HG23	2.09	0.52
3:C:517:SVR:N44	3:C:517:SVR:H42	2.11	0.52
1:C:216:ARG:NH1	1:C:339:SER:OG	2.41	0.52
1:A:373:ASP:O	1:A:374:LYS:CB	2.40	0.52
1:B:448:ALA:O	1:B:478:HIS:HE1	1.93	0.51
1:B:353:LEU:H	1:B:381:ARG:HH12	1.57	0.51
1:B:5:PRO:HD3	1:B:17:TYR:CE2	2.46	0.51
1:C:126:GLN:O	1:C:129:LYS:HB2	2.12	0.50
1:B:200:GLY:N	1:B:201:PRO:HD2	2.26	0.50
1:B:456:ARG:HA	1:B:459:ALA:HB3	1.94	0.50
1:C:214:PRO:HB3	1:C:338:PHE:HB2	1.94	0.50
1:A:4:ARG:HA	4:A:538:HOH:O	2.12	0.49
1:A:229:PHE:CZ	1:A:395:ILE:HG12	2.48	0.49
1:A:29:PHE:O	1:A:423:HIS:HE1	1.95	0.49
1:A:216:ARG:HD3	1:A:339:SER:OG	2.13	0.48
1:B:338:PHE:HE1	1:B:347:VAL:HG13	1.79	0.48
1:A:256:LYS:HA	1:A:280:LEU:CD1	2.43	0.48
1:C:300:SER:O	1:C:301:GLY:O	2.31	0.47
1:C:125:LYS:HD3	1:C:129:LYS:HE3	1.96	0.47
1:A:20:ALA:HB3	1:A:288:GLY:HA2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:HIS:HE1	1:C:339:SER:OG	1.97	0.47
1:A:355:MET:CE	1:A:379:LEU:HB3	2.44	0.47
1:A:174:LYS:O	1:A:179:ILE:HA	2.15	0.47
1:A:355:MET:HE3	1:A:379:LEU:CB	2.45	0.47
1:C:38:PRO:HG2	3:C:516:SVR:O77	2.14	0.47
3:C:517:SVR:S17	3:C:517:SVR:N1	2.88	0.47
1:A:130:ASP:HB2	1:A:140:LEU:HD22	1.97	0.47
1:A:386:GLN:HG3	1:A:402:TRP:CZ3	2.50	0.46
1:B:310:SER:O	1:B:313:HIS:HB3	2.14	0.46
1:B:158:ARG:NH2	1:B:284:LEU:HD13	2.30	0.46
1:A:345:GLU:OE2	4:A:653:HOH:O	2.21	0.46
1:A:115:LYS:HE2	1:A:131:TRP:CD2	2.50	0.46
1:A:323:GLU:OE2	1:A:364:ARG:NH2	2.49	0.46
1:B:338:PHE:CE1	1:B:347:VAL:HG13	2.51	0.46
1:C:40:GLY:CA	1:C:172:PRO:HG3	2.45	0.46
1:C:63:MET:HE3	1:C:287:VAL:HB	1.98	0.46
1:B:148:ASN:ND2	1:B:197:ARG:HH11	1.95	0.45
1:C:33:SER:OG	1:C:35:GLU:CG	2.59	0.45
1:A:215:ILE:HG12	1:A:310:SER:HB3	1.98	0.45
1:C:65:ASP:O	1:C:68:LYS:HB2	2.16	0.45
1:C:23:LEU:HD11	1:C:63:MET:HE2	1.98	0.45
1:B:199:PHE:CE1	1:B:272:ALA:HB1	2.50	0.45
1:A:63:MET:HE1	1:A:287:VAL:HB	1.98	0.45
1:C:4:ARG:HA	1:C:5:PRO:C	2.37	0.45
1:A:15:ALA:HB2	1:A:293:VAL:HG23	1.99	0.45
1:B:104:TRP:CD1	1:B:201:PRO:HD3	2.52	0.45
1:C:130:ASP:HB2	1:C:140:LEU:HB2	1.98	0.45
1:C:150:MET:HG3	1:C:157:MET:SD	2.56	0.45
1:A:373:ASP:OD2	1:A:375:GLU:HB2	2.15	0.44
1:A:338:PHE:CE1	1:A:347:VAL:HG13	2.53	0.44
1:C:252:ARG:O	1:C:256:LYS:HB2	2.17	0.44
1:A:374:LYS:HA	1:A:374:LYS:HD3	1.54	0.44
1:A:316:LEU:HG	1:A:367:LEU:HD11	1.98	0.44
1:A:358:TYR:CE2	1:A:362:LEU:HD11	2.53	0.44
1:C:68:LYS:N	1:C:69:PRO:CD	2.81	0.44
1:C:115:LYS:HE2	1:C:131:TRP:CD2	2.53	0.43
3:B:516:SVR:N63	3:B:516:SVR:S73	2.91	0.43
1:A:444:LEU:HD21	1:A:475:VAL:HG23	2.00	0.43
1:A:423:HIS:HD2	1:A:428:GLU:OE1	2.01	0.43
1:C:240:ASP:OD1	1:C:240:ASP:C	2.57	0.43
1:A:229:PHE:CE2	1:A:395:ILE:HG12	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ASP:C	1:A:240:ASP:OD1	2.56	0.43
1:C:221:MET:HG2	1:C:393:ARG:HG3	2.01	0.43
1:B:38:PRO:HG2	3:B:516:SVR:O77	2.18	0.43
1:A:105:THR:HB	4:A:680:HOH:O	2.18	0.43
1:C:174:LYS:HE2	3:C:517:SVR:O24	2.19	0.43
1:A:313:HIS:CD2	1:A:342:GLY:O	2.62	0.43
1:C:127:LYS:HE2	1:C:192:MET:SD	2.59	0.43
1:A:44:PRO:HG2	1:A:426:PRO:HB3	2.00	0.42
1:C:425:ASN:HA	1:C:426:PRO:HD2	1.82	0.42
1:C:313:HIS:HE1	1:C:345:GLU:OE2	2.02	0.42
1:A:330:ASP:OD1	1:A:330:ASP:N	2.52	0.42
1:C:87:CYS:SG	4:C:682:HOH:O	2.62	0.42
1:B:185:TRP:CD1	1:B:300:SER:HB2	2.54	0.42
1:C:281:ALA:O	1:C:282:PRO:C	2.57	0.42
1:B:358:TYR:CZ	1:B:362:LEU:HD11	2.55	0.42
1:C:42:TRP:HH2	3:C:517:SVR:C16	2.33	0.42
1:C:483:ARG:NH2	4:C:630:HOH:O	2.53	0.42
1:C:423:HIS:HD2	1:C:428:GLU:OE1	2.03	0.42
1:A:281:ALA:O	1:A:282:PRO:C	2.57	0.42
1:B:121:TYR:HA	1:B:122:PRO:HA	1.84	0.41
1:C:425:ASN:HB3	1:C:428:GLU:OE2	2.20	0.41
1:A:238:HIS:HD2	1:A:348:SER:CB	2.33	0.41
1:A:151:TYR:HB2	1:A:194:ARG:HG2	2.02	0.41
1:B:18:GLY:HA3	1:B:288:GLY:O	2.20	0.41
1:C:232:HIS:HD2	1:C:348:SER:CB	2.34	0.41
1:B:352:GLU:HA	1:B:381:ARG:HH12	1.86	0.41
1:A:126:GLN:HB3	1:A:129:LYS:HD2	2.01	0.41
1:C:35:GLU:H	1:C:35:GLU:HG2	1.55	0.41
1:B:386:GLN:HG3	1:B:402:TRP:CZ3	2.56	0.41
1:A:122:PRO:O	1:A:124:HIS:CD2	2.74	0.41
1:A:151:TYR:HA	4:A:598:HOH:O	2.21	0.41
1:B:391:LEU:O	1:B:392:ARG:HB2	2.21	0.41
1:C:461:ARG:NH2	4:C:706:HOH:O	2.54	0.40
1:A:334:GLN:HG2	1:B:399:GLN:CG	2.51	0.40
1:B:314:TRP:HA	1:B:340:PHE:CE2	2.56	0.40
1:B:386:GLN:HG3	1:B:402:TRP:HZ3	1.86	0.40
1:B:323:GLU:CD	1:B:364:ARG:HH22	2.24	0.40
1:A:302:CYS:HG	1:A:304:CYS:HG	1.40	0.40
1:A:219:MET:O	1:A:219:MET:HG3	2.21	0.40
1:A:211:ILE:O	1:A:216:ARG:NH2	2.54	0.40
1:B:20:ALA:HB3	1:B:288:GLY:HA2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	468/515 (91%)	451 (96%)	16 (3%)	1 (0%)	52	64
1	B	470/515 (91%)	449 (96%)	20 (4%)	1 (0%)	52	64
1	C	468/515 (91%)	452 (97%)	12 (3%)	4 (1%)	21	25
All	All	1406/1545 (91%)	1352 (96%)	48 (3%)	6 (0%)	39	49

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	301	GLY
1	A	300	SER
1	B	437	PRO
1	C	242	ASP
1	C	300	SER
1	C	282	PRO

5.3.2 Protein sidechains [i](#)

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	407/441 (92%)	387 (95%)	20 (5%)	31	43
1	B	409/441 (93%)	385 (94%)	24 (6%)	24	34
1	C	406/441 (92%)	380 (94%)	26 (6%)	22	29

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1222/1323 (92%)	1152 (94%)	70 (6%)	25	35

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	8	THR
1	A	91	GLU
1	A	111	GLU
1	A	140	LEU
1	A	216	ARG
1	A	279	LEU
1	A	294	VAL
1	A	302	CYS
1	A	304	CYS
1	A	311	LEU
1	A	316	LEU
1	A	353	LEU
1	A	374	LYS
1	A	389	SER
1	A	429	THR
1	A	444	LEU
1	A	453	LYS
1	A	460	SER
1	A	461	ARG
1	B	21	PRO
1	B	71	SER
1	B	92	ASN
1	B	108	LYS
1	B	113	LEU
1	B	129	LYS
1	B	140	LEU
1	B	169	LEU
1	B	216	ARG
1	B	227	PHE
1	B	236	ARG
1	B	264	ARG
1	B	271	LEU
1	B	279	LEU
1	B	294	VAL
1	B	298	LEU
1	B	306	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	316	LEU
1	B	352	GLU
1	B	375	GLU
1	B	403	TYR
1	B	423	HIS
1	B	461	ARG
1	B	475	VAL
1	C	4	ARG
1	C	33	SER
1	C	35	GLU
1	C	71	SER
1	C	113	LEU
1	C	129	LYS
1	C	140	LEU
1	C	169	LEU
1	C	189	LEU
1	C	216	ARG
1	C	227	PHE
1	C	256	LYS
1	C	271	LEU
1	C	279	LEU
1	C	284	LEU
1	C	294	VAL
1	C	300	SER
1	C	304	CYS
1	C	316	LEU
1	C	328	ASP
1	C	353	LEU
1	C	391	LEU
1	C	456	ARG
1	C	461	ARG
1	C	479	ARG
1	C	487	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	92	ASN
1	A	124	HIS
1	A	148	ASN
1	A	222	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	232	HIS
1	A	234	ASN
1	A	238	HIS
1	A	313	HIS
1	A	334	GLN
1	A	399	GLN
1	A	423	HIS
1	B	80	GLN
1	B	148	ASN
1	B	232	HIS
1	B	238	HIS
1	B	251	GLN
1	B	307	GLN
1	B	313	HIS
1	B	423	HIS
1	B	478	HIS
1	C	60	GLN
1	C	66	GLN
1	C	124	HIS
1	C	148	ASN
1	C	232	HIS
1	C	238	HIS
1	C	251	GLN
1	C	313	HIS
1	C	423	HIS
1	C	478	HIS

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

10 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	$\# Z > 2$
2	SO4	A	516	-	4,4,4	0.15	0	6,6,6	0.37	0
2	SO4	A	517	-	4,4,4	0.21	0	6,6,6	0.19	0
2	SO4	A	518	-	4,4,4	0.12	0	6,6,6	0.11	0
3	SVR	B	516	-	27,27,93	1.53	2 (7%)	37,44,145	1.64	8 (21%)
2	SO4	B	517	-	4,4,4	0.19	0	6,6,6	0.21	0
3	SVR	C	516	-	27,27,93	1.41	4 (14%)	37,44,145	1.36	3 (8%)
3	SVR	C	517	-	58,58,93	2.73	15 (25%)	82,88,145	1.91	14 (17%)
2	SO4	C	518	-	4,4,4	0.27	0	6,6,6	0.58	0
2	SO4	C	519	-	4,4,4	0.36	0	6,6,6	0.27	0
2	SO4	C	520	-	4,4,4	0.20	0	6,6,6	0.16	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
2	SO4	A	516	-	-	0/0/0/0	0/0/0/0
2	SO4	A	517	-	-	0/0/0/0	0/0/0/0
2	SO4	A	518	-	-	0/0/0/0	0/0/0/0
3	SVR	B	516	-	-	0/22/22/76	0/2/2/8
2	SO4	B	517	-	-	0/0/0/0	0/0/0/0
3	SVR	C	516	-	-	0/22/22/76	0/2/2/8
3	SVR	C	517	-	-	0/46/46/76	0/5/5/8
2	SO4	C	518	-	-	0/0/0/0	0/0/0/0
2	SO4	C	519	-	-	0/0/0/0	0/0/0/0
2	SO4	C	520	-	-	0/0/0/0	0/0/0/0

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	517	SVR	C27-C20	-7.13	1.36	1.51
3	C	517	SVR	C49-C51	-6.23	1.40	1.50
3	B	516	SVR	C69-S73	-5.24	1.70	1.78
3	C	517	SVR	C5-C2	-5.15	1.39	1.50
3	C	517	SVR	C33-C26	-4.33	1.41	1.50
3	C	517	SVR	C39-N41	-3.29	1.35	1.41
3	C	517	SVR	C46-N44	-3.26	1.35	1.41
3	C	517	SVR	C3-N1	-2.76	1.33	1.41
3	C	516	SVR	C69-S73	-2.68	1.74	1.78
3	C	517	SVR	C13-N19	-2.49	1.37	1.41
3	C	516	SVR	C65-N63	-2.10	1.35	1.41
3	C	516	SVR	C71-C68	-2.08	1.40	1.43
3	B	516	SVR	C72-C76	2.00	1.40	1.36
3	C	517	SVR	O35-S31	2.06	1.53	1.43
3	C	517	SVR	O36-S31	2.09	1.53	1.43
3	C	517	SVR	O24-S17	2.09	1.53	1.43
3	C	517	SVR	O29-S21	2.17	1.54	1.43
3	C	517	SVR	C18-C11	2.18	1.40	1.37
3	C	517	SVR	O28-S21	2.20	1.54	1.43
3	C	516	SVR	C58-C61	2.25	1.55	1.50
3	C	517	SVR	O54-C51	13.94	1.53	1.24

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	517	SVR	C3-N1-C2	-5.86	110.40	128.87
3	C	517	SVR	C16-C10-C15	-4.98	117.49	123.23
3	C	517	SVR	O45-C43-N41	-3.72	117.94	123.58
3	B	516	SVR	C74-C69-S73	-3.56	111.65	117.82
3	C	516	SVR	C72-C68-C71	-3.41	119.30	123.23
3	B	516	SVR	C72-C68-C71	-3.38	119.34	123.23
3	C	517	SVR	C46-N44-C43	-3.22	120.44	126.65
3	C	517	SVR	C7-C12-C15	-2.48	118.86	121.77
3	C	517	SVR	O54-C51-N53	-2.38	119.24	122.59
3	C	517	SVR	O4-C2-C5	-2.24	117.14	120.97
3	B	516	SVR	C67-C65-N63	-2.19	116.91	123.10
3	C	517	SVR	O45-C43-N44	-2.02	120.51	123.58
3	B	516	SVR	C66-C65-N63	2.02	123.72	120.58
3	B	516	SVR	C72-C76-S83	2.32	124.13	119.96
3	C	516	SVR	O81-S75-C71	2.77	109.34	106.20
3	C	517	SVR	C49-C51-N53	2.90	120.99	117.82
3	C	517	SVR	C15-C10-C6	3.06	121.81	118.11
3	B	516	SVR	O80-S75-C71	3.16	109.78	106.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	516	SVR	O81-S75-C71	3.46	110.12	106.20
3	C	517	SVR	O28-S21-C15	3.61	110.29	106.20
3	B	516	SVR	O78-S73-C69	3.61	110.29	106.20
3	C	516	SVR	O77-S73-C69	4.09	110.83	106.20
3	C	517	SVR	O24-S17-C11	4.64	111.46	106.20
3	C	517	SVR	N44-C43-N41	5.74	121.55	112.53
3	C	517	SVR	C14-C20-C13	6.73	122.67	117.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	516	SVR	2	0
3	C	516	SVR	3	0
3	C	517	SVR	14	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	475/515 (92%)	0.20	33 (6%)	20 21	30, 50, 105, 124	7 (1%)
1	B	476/515 (92%)	0.25	30 (6%)	23 25	36, 58, 102, 124	7 (1%)
1	C	474/515 (92%)	0.00	11 (2%)	64 66	25, 44, 83, 120	7 (1%)
All	All	1425/1545 (92%)	0.15	74 (5%)	31 34	25, 51, 99, 124	21 (1%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	481	VAL	7.2
1	A	454	TYR	7.1
1	B	378	PRO	6.1
1	A	39	PRO	6.0
1	A	474	VAL	5.9
1	A	476	PRO	5.6
1	B	479	ARG	5.6
1	A	478	HIS	5.2
1	B	2	LEU	5.1
1	A	475	VAL	5.0
1	A	480	SER	5.0
1	A	484	TRP	4.9
1	B	303	PRO	4.9
1	A	455	TYR	4.7
1	B	484	TRP	4.4
1	A	444	LEU	4.3
1	B	103	PRO	4.3
1	B	455	TYR	4.1
1	B	464	LYS	4.1
1	C	302	CYS	4.0
1	C	466	ALA	3.9
1	A	477	ARG	3.9
1	A	443	LEU	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	479	ARG	3.9
1	A	379	LEU	3.8
1	B	456	ARG	3.8
1	B	3	PRO	3.7
1	C	456	ARG	3.6
1	B	463	SER	3.6
1	B	488	GLY	3.5
1	A	438	SER	3.5
1	A	452	GLU	3.4
1	A	437	PRO	3.4
1	A	459	ALA	3.3
1	B	474	VAL	3.3
1	A	378	PRO	3.2
1	C	464	LYS	3.2
1	C	467	ALA	3.1
1	B	454	TYR	3.1
1	B	478	HIS	3.0
1	B	452	GLU	3.0
1	C	372	ALA	3.0
1	C	475	VAL	2.9
1	B	475	VAL	2.9
1	A	458	VAL	2.9
1	A	483	ARG	2.9
1	A	302	CYS	2.9
1	A	433	HIS	2.9
1	A	457	THR	2.8
1	A	488	GLY	2.7
1	B	476	PRO	2.7
1	B	465	GLU	2.6
1	B	438	SER	2.6
1	B	108	LYS	2.5
1	A	464	LYS	2.5
1	B	54	VAL	2.4
1	C	438	SER	2.4
1	B	462	VAL	2.3
1	B	432	GLY	2.3
1	C	452	GLU	2.3
1	A	192	MET	2.2
1	B	4	ARG	2.2
1	B	481	VAL	2.2
1	A	441	MET	2.2
1	A	439	GLN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	54	VAL	2.2
1	B	373	ASP	2.2
1	C	373	ASP	2.2
1	A	456	ARG	2.1
1	B	99	GLU	2.1
1	B	39	PRO	2.1
1	C	462	VAL	2.1
1	A	451	GLY	2.0
1	B	483	ARG	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	A	518	5/5	0.95	0.23	1.68	124,124,125,127	0
3	SVR	C	516	26/86	0.94	0.20	1.53	82,96,102,104	0
3	SVR	C	517	54/86	0.85	0.22	1.46	87,95,127,130	0
3	SVR	B	516	26/86	0.89	0.21	1.03	112,121,130,131	0
2	SO4	C	519	5/5	0.94	0.15	0.56	92,94,97,98	0
2	SO4	C	518	5/5	0.98	0.13	-0.43	72,79,86,88	0
2	SO4	C	520	5/5	0.95	0.12	-1.22	93,94,96,96	0
2	SO4	A	516	5/5	0.86	0.20	-	112,115,116,116	0
2	SO4	B	517	5/5	0.87	0.19	-	133,134,135,135	0
2	SO4	A	517	5/5	0.84	0.18	-	155,155,155,156	0

6.5 Other polymers [i](#)

There are no such residues in this entry.