

Full wwPDB X-ray Structure Validation Report (i)

Apr 30, 2024 - 07:47 pm BST

PDB ID	:	4CI8
Title	:	Crystal structure of the tandem atypical beta-propeller domain of EML1
Authors	:	Richards, M.W.; Bayliss, R.
Deposited on	:	2013-12-06
Resolution	:	2.60 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 https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

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.



Motria	Whole archive	Similar resolution
wietric	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	А	655	% 68%	28%	•••
1	В	655	3% 69%	27%	•••

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
2	SO4	А	1819	-	-	Х	-
2	SO4	А	1824	-	_	Х	-



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10193 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 ECHINODERM MICROTUBULE-ASSOCIATED PROTEIN-LIKE 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	А	640	Total 4936	C 3131	N 850	O 933	S 22	0	0	0
1	В	640	Total 4924	C 3124	N 843	O 935	S 22	0	0	0

Chain	Residue	Modelled	Actual	Comment	Reference
А	161	GLY	-	expression tag	UNP 000423
А	162	PRO	-	expression tag	UNP 000423
А	163	HIS	-	expression tag	UNP 000423
А	164	MET	-	expression tag	UNP 000423
А	165	SER	-	expression tag	UNP 000423
А	166	MET	-	expression tag	UNP 000423
В	161	GLY	-	expression tag	UNP 000423
В	162	PRO	-	expression tag	UNP 000423
В	163	HIS	-	expression tag	UNP 000423
В	164	MET	-	expression tag	UNP 000423
В	165	SER	-	expression tag	UNP 000423
В	166	MET	-	expression tag	UNP 000423

There are 12 discrepancies between the modelled and reference sequences:

• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	116	Total O 116 116	0	0
3	В	92	Total O 92 92	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 (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: ECHINODERM MICROTUBULE-ASSOCIATED PROTEIN-LIKE 1



D571 A572 V573 3523 537 538 539 540 541 K581 I582 .531 5532 5533 1542 1543 K616 H566 P57 **C**56 **R57** V61 F61 <mark>R714</mark> D715 1716 E717 G659 N683 S684 D685 Y634 0000 0657 WT 63 HT 64 HT 64 FT 65 ST 67 ST 77 ST 77</ Q811 W812 R813 V814 V815 I815 H798 L799 D806 T807



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	91.98Å 83.98Å 115.52Å	Depositor
a, b, c, α , β , γ	90.00° 96.61° 90.00°	Depositor
Bosolution (Å)	47.38 - 2.60	Depositor
	47.37 - 2.60	EDS
% Data completeness	99.2 (47.38-2.60)	Depositor
(in resolution range)	99.3 (47.37 - 2.60)	EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.86 (at 2.61 \text{\AA})$	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R R.	0.200 , 0.251	Depositor
II, II, <i>free</i>	0.195 , 0.245	DCC
R_{free} test set	2731 reflections $(5.09%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	42.4	Xtriage
Anisotropy	0.509	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34 , 44.4	EDS
L-test for $twinning^2$	$ < L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10193	wwPDB-VP
Average B, all atoms $(Å^2)$	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 29.03 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6635e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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).

Mal	Chain	Bond	lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.29	0/5064	0.48	0/6892	
1	В	0.28	0/5052	0.48	0/6879	
All	All	0.28	0/10116	0.48	0/13771	

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	А	4936	0	4716	152	0
1	В	4924	0	4687	140	0
2	А	65	0	0	5	0
2	В	60	0	0	2	0
3	А	116	0	0	3	0
3	В	92	0	0	2	0
All	All	10193	0	9403	291	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 15.

All (291) close contacts within the same asymmetric unit are listed below, sorted by their clash



magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:321:ILE:H	1:A:321:ILE:HD12	1.33	0.93
1:A:240:LEU:HD23	1:A:512:GLY:HA2	1.52	0.90
1:A:616:LYS:NZ	2:A:1824:SO4:O4	2.03	0.90
1:B:531:LEU:HD12	1:B:531:LEU:H	1.39	0.86
1:A:517:ILE:HG13	1:A:531:LEU:HD13	1.60	0.83
1:B:321:ILE:HD12	1:B:321:ILE:H	1.45	0.82
1:B:671:HIS:CE1	1:B:695:GLU:HG3	2.15	0.82
1:A:482:ARG:HD3	1:A:505:PRO:HA	1.63	0.80
1:B:200:MET:HE2	1:B:204:GLN:HB2	1.64	0.79
1:A:334:SER:O	1:A:339:GLY:HA2	1.83	0.78
1:B:657:ASP:N	2:B:1826:SO4:O3	2.19	0.74
1:A:434:THR:HG22	3:A:2047:HOH:O	1.89	0.73
1:A:277:LEU:HD12	1:A:278:ALA:N	2.02	0.73
1:B:694:TYR:CZ	1:B:739:GLY:HA3	2.23	0.73
1:A:398:TRP:CZ3	1:A:407:LYS:HB3	2.24	0.72
1:A:505:PRO:HG2	1:A:522:THR:HB	1.72	0.71
1:A:733:TRP:HE3	1:A:737:SER:HG	1.39	0.70
1:B:398:TRP:CE3	1:B:407:LYS:HB3	2.26	0.70
1:A:530:THR:HG23	1:A:532:SER:H	1.54	0.70
1:A:688:VAL:HG22	1:A:718:TRP:CZ3	2.27	0.69
1:B:392:LYS:HG2	1:B:420:PHE:CE2	2.27	0.69
1:A:813:ARG:HD2	3:A:2009:HOH:O	1.93	0.69
1:B:530:THR:HG23	1:B:532:SER:H	1.58	0.69
1:A:616:LYS:CE	2:A:1824:SO4:O4	2.41	0.68
1:A:383:ASP:HB3	1:A:386:ILE:HD11	1.74	0.68
1:B:476:SER:HB2	1:B:487:TRP:HE1	1.56	0.67
1:B:505:PRO:HG2	1:B:522:THR:HB	1.75	0.67
1:B:532:SER:HB2	1:B:533:GLY:HA2	1.76	0.67
1:B:250:ILE:HD11	1:B:807:THR:HG22	1.76	0.67
1:A:190:PHE:CE1	1:A:195:PRO:HB3	2.30	0.66
1:A:671:HIS:NE2	1:A:689:SER:HB3	2.09	0.66
1:A:290:GLN:HG2	1:A:291:VAL:O	1.95	0.66
1:A:482:ARG:CD	1:A:505:PRO:HA	2.26	0.66
1:A:321:ILE:HD12	1:A:321:ILE:N	2.09	0.66
1:A:421:VAL:HG13	1:A:434:THR:HG23	1.77	0.66
1:B:200:MET:HE3	1:B:208:TYR:CD2	2.30	0.66
1:A:390:CYS:HA	1:A:394:HIS:HD2	1.61	0.65
1:B:334:SER:O	1:B:339:GLY:HA2	1.96	0.65
1:A:200:MET:HE2	1:A:204:GLN:HB3	1.78	0.65
1:A:297:ASP:HB2	1:A:298:GLY:HA2	1.78	0.65
1:B:200:MET:HE2	1:B:204:GLN:CB	2.26	0.65



	lo uo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:321:ILE:H	1:A:321:ILE:CD1	2.08	0.64
1:A:551:ILE:HD13	1:A:791:ASP:HB3	1.80	0.64
1:B:403:SER:HB2	2:B:1825:SO4:O1	1.96	0.64
1:B:530:THR:HG23	1:B:532:SER:HB2	1.79	0.64
1:B:790:VAL:HG22	1:B:799:LEU:HD11	1.80	0.64
1:A:806:ASP:O	1:A:807:THR:HB	1.97	0.63
1:B:334:SER:O	1:B:339:GLY:CA	2.47	0.63
1:A:202:LYS:HG3	1:A:714:ARG:HD2	1.80	0.63
1:B:793:LEU:HD22	1:B:798:HIS:HB2	1.81	0.63
1:B:615:THR:O	1:B:616:LYS:HB3	1.99	0.63
1:B:277:LEU:HD12	1:B:288:THR:CG2	2.29	0.62
1:B:214:VAL:HG12	1:B:772:GLN:HB2	1.82	0.62
1:B:571:ASP:OD1	1:B:573:VAL:HG12	2.00	0.61
1:B:386:ILE:HG22	1:B:399:THR:HG23	1.82	0.61
1:B:530:THR:CG2	1:B:533:GLY:HA2	2.31	0.61
2:A:1819:SO4:O3	1:B:360:LYS:CE	2.49	0.60
1:B:280:HIS:CG	1:B:281:PRO:HD2	2.37	0.60
1:A:615:THR:O	1:A:616:LYS:HB3	2.00	0.60
1:A:763:VAL:HG22	1:A:780:TYR:HB2	1.83	0.60
1:B:530:THR:O	1:B:533:GLY:HA3	2.01	0.60
1:A:668:CYS:HB3	1:A:699:TRP:CE3	2.37	0.59
1:A:734:PRO:O	1:A:737:SER:HB2	2.01	0.59
1:B:505:PRO:HG2	1:B:522:THR:CG2	2.32	0.59
1:A:189:MET:HG2	1:A:196:VAL:CG1	2.33	0.59
1:B:790:VAL:CG2	1:B:799:LEU:HD11	2.32	0.59
1:A:688:VAL:HG22	1:A:718:TRP:CH2	2.37	0.59
1:B:292:ALA:HB2	1:B:303:PRO:HG3	1.85	0.59
1:A:200:MET:CE	1:A:204:GLN:HB3	2.31	0.59
1:B:217:PRO:HG3	1:B:766:PHE:C	2.22	0.59
1:B:221:LEU:HB2	1:B:780:TYR:CE2	2.37	0.59
1:B:671:HIS:HE1	1:B:695:GLU:HG3	1.67	0.59
1:B:190:PHE:CE1	1:B:195:PRO:HB3	2.38	0.58
1:B:503:PHE:CE1	1:B:537:PRO:HG3	2.37	0.58
1:B:548:GLY:HA3	1:B:561:CYS:SG	2.43	0.58
1:B:606:GLY:HA2	1:B:629:LEU:HD13	1.84	0.58
1:A:336:SER:OG	1:A:384:THR:HB	2.04	0.57
1:A:412:PHE:CZ	1:A:418:PRO:HD2	2.40	0.57
1:B:530:THR:HG23	1:B:533:GLY:HA2	1.86	0.57
1:B:531:LEU:H	1:B:531:LEU:CD1	2.15	0.57
1:A:348:SER:O	1:A:349:ASN:HB3	2.04	0.57
1:A:688:VAL:HG13	1:A:698:TYR:CE2	2.40	0.57



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:530:THR:CG2	1:B:532:SER:HB2	2.33	0.57
1:A:348:SER:C	1:A:350:ASP:H	2.08	0.57
1:A:747:ARG:NH2	1:A:752:LYS:HD3	2.20	0.57
1:B:396:TYR:CD2	1:B:407:LYS:HD3	2.39	0.57
1:A:379:PHE:CE2	1:A:387:ILE:HD11	2.40	0.57
1:A:277:LEU:HD12	1:A:277:LEU:C	2.24	0.57
1:A:412:PHE:CE2	1:A:418:PRO:CD	2.88	0.57
1:A:680:TRP:CZ3	1:A:701:PRO:HG2	2.39	0.56
1:B:216:LEU:HG	1:B:217:PRO:HD2	1.86	0.56
1:B:398:TRP:CZ3	1:B:407:LYS:HB3	2.40	0.56
1:A:461:GLY:HA3	1:A:480:LYS:HB2	1.87	0.56
1:B:348:SER:C	1:B:350:ASP:H	2.10	0.56
1:B:484:LEU:HD22	1:B:519:ILE:HD11	1.88	0.55
1:A:694:TYR:CZ	1:A:739:GLY:HA3	2.41	0.55
1:A:321:ILE:HG12	1:B:318:VAL:HG21	1.88	0.55
1:A:441:ILE:HB	1:A:455:VAL:HB	1.89	0.55
1:B:201:PRO:HD2	1:B:204:GLN:HG3	1.88	0.55
1:B:610:VAL:HB	1:B:620:THR:HG22	1.88	0.55
1:A:530:THR:HG22	1:A:533:GLY:HA2	1.89	0.55
1:B:531:LEU:HD12	1:B:531:LEU:N	2.17	0.54
1:B:717:GLU:O	1:B:717:GLU:HG2	2.07	0.54
1:A:647:ASP:O	1:A:648:ASN:HB2	2.07	0.54
1:A:671:HIS:CE1	1:A:697:LEU:HD22	2.43	0.54
1:B:275:LYS:HG3	1:B:291:VAL:HG13	1.89	0.54
1:A:443:VAL:HB	1:A:453:TYR:HB2	1.90	0.54
1:B:647:ASP:O	1:B:648:ASN:HB2	2.06	0.54
1:B:458:ALA:HB1	1:B:487:TRP:CZ2	2.43	0.53
1:A:766:PHE:CE2	1:A:777:SER:HB3	2.43	0.53
1:A:220:ARG:NH1	2:A:1819:SO4:O2	2.41	0.53
1:B:505:PRO:HG2	1:B:522:THR:CB	2.38	0.53
1:B:691:SER:OG	1:B:695:GLU:HG2	2.08	0.53
1:A:476:SER:HB2	1:A:487:TRP:HE1	1.73	0.53
1:B:422:LEU:HB2	1:B:463:ILE:O	2.08	0.53
1:A:192:ARG:NH2	1:A:736:GLY:O	2.42	0.53
1:B:683:ASN:HD21	1:B:685:GLN:HB3	1.72	0.53
1:B:723:CYS:O	1:B:729:VAL:HG21	2.08	0.53
1:B:768:TYR:CG	1:B:769:PRO:HA	2.44	0.53
1:A:334:SER:O	1:A:339:GLY:CA	2.56	0.53
1:A:200:MET:HE2	1:A:204:GLN:CB	2.39	0.52
1:A:480:LYS:HD2	1:A:480:LYS:N	2.24	0.52
1:A:517:ILE:HG13	1:A:531:LEU:CD1	2.35	0.52



	lo uo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:245:GLU:OE2	1:B:265:ARG:HD3	2.10	0.52
1:B:412:PHE:CE2	1:B:418:PRO:HD2	2.44	0.52
1:A:571:ASP:OD1	1:A:573:VAL:HG12	2.10	0.52
1:B:768:TYR:CD1	1:B:769:PRO:HA	2.44	0.52
1:B:814:VAL:O	1:B:815:ILE:HG23	2.10	0.52
1:B:526:VAL:HB	1:B:539:THR:HG22	1.92	0.51
1:A:280:HIS:CG	1:A:281:PRO:HD2	2.46	0.51
1:B:668:CYS:HB3	1:B:699:TRP:CE3	2.45	0.51
1:A:709:SER:O	1:A:712:THR:HG23	2.11	0.51
1:B:321:ILE:H	1:B:321:ILE:CD1	2.21	0.51
1:A:616:LYS:HE2	2:A:1824:SO4:O4	2.10	0.51
1:A:482:ARG:HG3	1:A:501:GLU:OE1	2.11	0.51
1:A:412:PHE:CE2	1:A:418:PRO:HD3	2.45	0.51
1:A:768:TYR:CG	1:A:769:PRO:HA	2.45	0.51
1:B:277:LEU:HD12	1:B:288:THR:HG23	1.92	0.51
1:A:189:MET:HG2	1:A:196:VAL:HG12	1.92	0.50
1:B:321:ILE:HD12	1:B:321:ILE:N	2.21	0.50
1:A:730:PHE:O	1:A:770:CYS:O	2.30	0.50
1:A:280:HIS:HB3	1:A:282:ASP:OD1	2.11	0.50
1:B:806:ASP:OD1	1:B:806:ASP:C	2.49	0.50
1:A:479:GLY:O	1:A:505:PRO:HB3	2.11	0.49
1:B:380:HIS:HB2	1:B:386:ILE:HD11	1.94	0.49
1:B:679:ASP:HB2	1:B:688:VAL:HG13	1.92	0.49
1:A:686:PHE:HE1	1:A:707:VAL:HG21	1.77	0.49
1:A:624:ASP:HB3	1:A:651:TYR:CD2	2.47	0.49
1:A:301:LEU:HD12	1:A:301:LEU:N	2.27	0.49
1:A:590:SER:HB2	1:A:600:ALA:O	2.13	0.49
1:B:683:ASN:ND2	1:B:685:GLN:HB3	2.28	0.49
1:B:236:ASN:H	1:B:508:THR:HG22	1.78	0.49
1:B:384:THR:HG22	3:B:2024:HOH:O	2.12	0.49
1:B:561:CYS:HB2	1:B:587:ALA:CB	2.42	0.49
1:A:655:VAL:CG1	1:A:659:GLY:HA2	2.42	0.48
1:B:576:ARG:HB2	1:B:577:PRO:HD2	1.95	0.48
1:A:297:ASP:CB	1:A:298:GLY:HA2	2.38	0.48
1:A:650:ILE:HB	1:A:668:CYS:HB2	1.96	0.48
1:B:780:TYR:HB3	1:B:812:TRP:CZ3	2.48	0.48
1:A:703:ALA:O	1:A:705:LYS:HG3	2.14	0.48
1:B:239:TYR:CE2	1:B:277:LEU:HD23	2.49	0.48
1:B:250:ILE:HD11	1:B:807:THR:CG2	2.42	0.48
1:A:395:LEU:HD22	1:A:444:TRP:CZ2	2.48	0.48
1:B:336:SER:HB3	1:B:384:THR:HB	1.95	0.48



	louis page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:530:THR:O	1:A:533:GLY:HA3	2.14	0.48
1:B:221:LEU:HD21	1:B:799:LEU:HD22	1.95	0.48
1:B:358:TRP:CZ3	1:B:359:GLN:HG2	2.49	0.48
1:A:768:TYR:CD2	1:A:769:PRO:HA	2.48	0.47
1:B:646:HIS:ND1	1:B:674:PHE:HB2	2.29	0.47
1:A:307:ILE:HD12	1:A:307:ILE:N	2.28	0.47
1:A:331:ILE:HD11	1:A:342:LEU:HD21	1.95	0.47
1:A:412:PHE:CE2	1:A:418:PRO:HD2	2.49	0.47
1:B:671:HIS:ND1	1:B:695:GLU:HG3	2.29	0.47
1:B:217:PRO:HG2	1:B:765:LEU:O	2.14	0.47
1:B:275:LYS:CG	1:B:291:VAL:HG13	2.44	0.47
1:A:506:ILE:HG23	1:A:519:ILE:HG23	1.97	0.47
1:A:227:TYR:HB2	1:A:809:ILE:HB	1.96	0.47
1:A:192:ARG:HE	1:A:192:ARG:HA	1.79	0.47
1:B:655:VAL:CG1	1:B:659:GLY:HA2	2.44	0.47
1:B:261:GLU:HA	1:B:261:GLU:OE1	2.15	0.47
1:B:680:TRP:CZ3	1:B:701:PRO:HG2	2.50	0.47
1:B:353:LEU:HB3	1:B:369:CYS:HB2	1.95	0.47
1:B:365:ALA:HB2	1:B:403:SER:HA	1.95	0.47
1:A:581:LYS:HA	1:A:616:LYS:HE3	1.97	0.46
1:A:558:PHE:CE1	1:A:570:TRP:CD1	3.04	0.46
1:B:209:SER:HB3	1:B:212:ALA:HB2	1.96	0.46
1:B:530:THR:HG23	1:B:532:SER:CB	2.44	0.46
1:B:530:THR:C	1:B:532:SER:H	2.18	0.46
1:A:559:LEU:HD22	1:A:568:THR:O	2.16	0.46
1:A:762:LYS:HG3	1:A:779:ILE:HD11	1.96	0.46
1:B:185:GLY:O	1:B:200:MET:HG2	2.16	0.46
1:A:307:ILE:HD13	1:A:319:ILE:HD13	1.96	0.46
1:B:273:ASP:N	1:B:273:ASP:OD1	2.48	0.46
1:B:751:LYS:HD2	1:B:751:LYS:N	2.30	0.46
1:B:581:LYS:HE2	1:B:611:PHE:CE1	2.51	0.46
1:A:192:ARG:NH1	1:A:738:ASP:HB2	2.30	0.46
1:B:766:PHE:CE2	1:B:777:SER:HB3	2.51	0.46
1:A:221:LEU:HB2	1:A:780:TYR:CE2	2.51	0.46
1:B:186:TYR:CD1	1:B:186:TYR:C	2.90	0.46
1:A:495:ARG:HH21	1:A:532:SER:HA	1.80	0.46
1:A:421:VAL:HG13	1:A:434:THR:CG2	2.46	0.45
1:A:606:GLY:HA2	1:A:629:LEU:HD13	1.98	0.45
1:A:618:LEU:HD21	1:A:621:VAL:HG23	1.99	0.45
1:A:647:ASP:O	1:A:648:ASN:CB	2.64	0.45
1:A:806:ASP:C	1:A:806:ASP:OD1	2.55	0.45



	lo do pagom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:745:VAL:HG22	1:B:746:CYS:N	2.31	0.45
1:B:697:LEU:HD23	1:B:699:TRP:CZ2	2.51	0.45
1:A:412:PHE:HA	1:A:451:ILE:CD1	2.46	0.45
1:A:512:GLY:HA3	1:A:516:VAL:HG12	1.98	0.45
1:B:813:ARG:NH1	1:B:815:ILE:HG21	2.32	0.45
1:A:192:ARG:HB3	1:A:193:GLY:H	1.59	0.45
1:A:709:SER:HB3	1:A:712:THR:CG2	2.45	0.45
1:A:476:SER:CB	1:A:487:TRP:HE1	2.30	0.45
1:A:186:TYR:CD1	1:A:186:TYR:C	2.91	0.45
1:A:559:LEU:HD13	1:A:560:THR:N	2.32	0.45
1:B:212:ALA:O	1:B:772:GLN:HB3	2.17	0.45
1:A:394:HIS:CD2	1:A:394:HIS:C	2.90	0.45
1:B:240:LEU:CD2	1:B:512:GLY:HA2	2.46	0.44
1:B:389:THR:HG1	1:B:394:HIS:CE1	2.35	0.44
1:B:427:SER:HB3	1:B:433:ILE:HD11	1.99	0.44
1:B:334:SER:OG	1:B:339:GLY:HA2	2.17	0.44
1:B:540:GLN:HG2	3:B:2047:HOH:O	2.16	0.44
1:A:190:PHE:CD1	1:A:195:PRO:HB3	2.52	0.44
1:A:302:PRO:HA	1:A:303:PRO:HD3	1.82	0.44
1:B:351:HIS:O	1:B:369:CYS:HB3	2.18	0.44
1:B:476:SER:CB	1:B:487:TRP:HE1	2.27	0.44
1:A:488:SER:HB3	1:A:494:LEU:HD13	1.99	0.44
1:B:273:ASP:OD1	1:B:784:SER:HB3	2.18	0.44
1:A:307:ILE:O	1:A:316:LEU:HB2	2.18	0.43
1:A:530:THR:CG2	1:A:533:GLY:HA2	2.47	0.43
1:A:700:VAL:HG23	1:A:707:VAL:HG23	2.00	0.43
1:B:793:LEU:CD2	1:B:798:HIS:HB2	2.46	0.43
1:A:191:LEU:HD12	1:A:191:LEU:HA	1.86	0.43
1:A:353:LEU:HB3	1:A:369:CYS:HB2	2.00	0.43
1:A:292:ALA:HB2	1:A:303:PRO:HG3	2.01	0.43
1:B:647:ASP:O	1:B:648:ASN:CB	2.67	0.43
1:A:331:ILE:HA	1:A:343:CYS:O	2.19	0.43
1:A:394:HIS:CE1	1:A:396:TYR:CD1	3.07	0.43
1:A:394:HIS:CE1	1:A:396:TYR:HD1	2.37	0.43
1:B:634:TYR:CE2	1:B:641:LEU:HD13	2.54	0.43
3:A:2038:HOH:O	1:B:268:ALA:HB1	2.18	0.43
1:A:309:ASP:OD2	1:A:311:VAL:HB	2.19	0.43
1:A:713:THR:HA	1:A:716:ILE:CD1	2.49	0.43
1:B:503:PHE:O	1:B:523:ARG:HB2	2.18	0.43
1:B:806:ASP:O	1:B:807:THR:HB	2.18	0.43
1:A:348:SER:O	1:A:349:ASN:CB	2.67	0.43



	A h o	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:343:CYS:HA	1:B:354:SER:O	2.18	0.43
1:B:558:PHE:CE2	1:B:572:ALA:HB2	2.54	0.43
1:B:200:MET:CE	1:B:208:TYR:CD2	3.01	0.43
1:B:204:GLN:C	1:B:206:ASP:H	2.22	0.42
1:B:713:THR:HA	1:B:716:ILE:CD1	2.49	0.42
1:A:551:ILE:HG13	1:A:793:LEU:HD23	2.01	0.42
1:B:348:SER:O	1:B:349:ASN:CB	2.66	0.42
1:A:439:GLY:HA2	1:A:463:ILE:HG13	2.01	0.42
1:B:635:SER:HB2	1:B:684:SER:OG	2.19	0.42
1:A:327:ALA:O	1:A:346:ASP:HA	2.19	0.42
1:A:542:HIS:O	1:A:807:THR:HG23	2.19	0.42
1:A:604:LEU:HD23	1:A:628:GLN:HG3	2.02	0.42
1:A:668:CYS:HB3	1:A:699:TRP:CZ3	2.55	0.42
1:B:205:VAL:O	1:B:205:VAL:HG22	2.20	0.42
1:B:230:ARG:HD3	1:B:234:CYS:SG	2.59	0.42
1:B:798:HIS:CD2	1:B:811:GLN:HE21	2.37	0.42
1:A:681:SER:HA	1:A:718:TRP:HA	2.01	0.42
1:A:609:PHE:CD2	1:A:621:VAL:HG22	2.55	0.42
1:A:694:TYR:CE1	1:A:739:GLY:HA3	2.55	0.42
1:A:815:ILE:HG13	1:A:815:ILE:O	2.20	0.42
1:B:624:ASP:HB3	1:B:651:TYR:CE2	2.55	0.42
1:A:377:ALA:HA	1:A:388:VAL:O	2.20	0.42
1:A:295:SER:HB3	1:A:301:LEU:HD11	2.02	0.41
1:A:479:GLY:O	1:A:505:PRO:CB	2.68	0.41
1:A:700:VAL:HG23	1:A:707:VAL:CG2	2.50	0.41
1:A:717:GLU:HG3	1:A:717:GLU:O	2.20	0.41
1:B:379:PHE:CE1	1:B:387:ILE:HD11	2.55	0.41
1:B:754:LEU:HD12	1:B:770:CYS:HB2	2.02	0.41
1:A:282:ASP:O	1:A:283:ARG:HB2	2.20	0.41
1:B:561:CYS:HA	1:B:566:HIS:O	2.19	0.41
1:A:297:ASP:N	1:A:298:GLY:HA2	2.34	0.41
1:A:399:THR:OG1	1:A:408:LYS:HE2	2.19	0.41
1:A:353:LEU:CB	1:A:369:CYS:HB2	2.51	0.41
1:B:542:HIS:CD2	1:B:546:LEU:HD22	2.55	0.41
1:B:240:LEU:HD22	1:B:512:GLY:HA2	2.03	0.41
1:B:380:HIS:HB2	1:B:386:ILE:CD1	2.51	0.41
1:A:337:ASN:OD1	1:A:337:ASN:N	2.49	0.41
1:A:462:GLY:H	1:A:480:LYS:HD3	1.85	0.41
1:A:619:VAL:O	1:A:620:THR:HB	2.20	0.40
1:A:790:VAL:HG22	1:A:799:LEU:HD11	2.03	0.40
1:B:624:ASP:HB3	1:B:651:TYR:CD2	2.56	0.40



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:551:ILE:HG23	1:B:793:LEU:HD12	2.03	0.40
1:A:297:ASP:HB2	1:A:298:GLY:CA	2.48	0.40
1:A:286:ILE:HG22	1:A:287:ALA:N	2.37	0.40
1:A:551:ILE:HG12	1:A:792:PHE:O	2.21	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	Perce	ntiles
1	А	638/655~(97%)	599~(94%)	39~(6%)	0	100	100
1	В	638/655~(97%)	592 (93%)	46 (7%)	0	100	100
All	All	1276/1310~(97%)	1191 (93%)	85 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	А	532/562~(95%)	505~(95%)	27~(5%)	24 46
1	В	530/562~(94%)	492 (93%)	38 (7%)	14 29
All	All	1062/1124~(94%)	997 (94%)	65(6%)	18 38



All	(65)	residues	with a	non-rotameric	sidechain	are listed	below:
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Mol	Chain	Res	Type
1	А	187	VAL
1	А	191	LEU
1	А	192	ARG
1	А	214	VAL
1	А	235	ARG
1	А	277	LEU
1	А	283	ARG
1	А	294	THR
1	А	335	LYS
1	А	347	ASP
1	А	374	VAL
1	А	386	ILE
1	А	403	SER
1	А	422	LEU
1	А	424	VAL
1	А	469	LEU
1	А	522	THR
1	А	531	LEU
1	А	556	SER
1	А	629	LEU
1	А	688	VAL
1	А	712	THR
1	А	730	PHE
1	А	759	ASP
1	А	763	VAL
1	А	785	SER
1	А	807	THR
1	В	186	TYR
1	В	191	LEU
1	В	194	ARG
1	В	214	VAL
1	В	221	LEU
1	В	224	GLU
1	В	229	TYR
1	В	235	ARG
1	В	273	ASP
1	В	277	LEU
1	В	295	SER
1	В	335	LYS
1	В	342	LEU
1	В	371	ASN
1	В	374	VAL



Mol	Chain	Res	Type
1	В	392	LYS
1	В	394	HIS
1	В	399	THR
1	В	428	GLU
1	В	522	THR
1	В	531	LEU
1	В	543	THR
1	В	582	ILE
1	В	603	THR
1	В	628	GLN
1	В	646	HIS
1	В	669	SER
1	В	671	HIS
1	В	693	ASP
1	В	710	VAL
1	В	715	ASP
1	В	738	ASP
1	В	763	VAL
1	В	767	SER
1	В	785	SER
1	В	793	LEU
1	В	806	ASP
1	В	807	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	В	575	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.



5.6 Ligand geometry (i)

25 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).

Mal	Mol Type Ch		Thain Bos I		В	Bond lengths		Bond angles		
WIOI	Type	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
2	SO4	A	1818	-	4,4,4	0.12	0	$6,\!6,\!6$	0.08	0
2	SO4	В	1826	-	4,4,4	0.15	0	$6,\!6,\!6$	0.06	0
2	SO4	А	1827	-	4,4,4	0.13	0	$6,\!6,\!6$	0.10	0
2	SO4	A	1828	-	4,4,4	0.14	0	$6,\!6,\!6$	0.10	0
2	SO4	В	1816	-	4,4,4	0.16	0	$6,\!6,\!6$	0.22	0
2	SO4	А	1820	-	4,4,4	0.14	0	$6,\!6,\!6$	0.05	0
2	SO4	В	1819	-	4,4,4	0.15	0	$6,\!6,\!6$	0.06	0
2	SO4	А	1823	-	4,4,4	0.13	0	$6,\!6,\!6$	0.08	0
2	SO4	В	1822	-	4,4,4	0.13	0	$6,\!6,\!6$	0.08	0
2	SO4	В	1821	-	4,4,4	0.13	0	$6,\!6,\!6$	0.08	0
2	SO4	А	1816	-	4,4,4	0.16	0	$6,\!6,\!6$	0.13	0
2	SO4	А	1826	-	4,4,4	0.15	0	$6,\!6,\!6$	0.05	0
2	SO4	В	1824	-	4,4,4	0.14	0	$6,\!6,\!6$	0.05	0
2	SO4	A	1822	-	4,4,4	0.14	0	$6,\!6,\!6$	0.06	0
2	SO4	В	1827	-	4,4,4	0.14	0	$6,\!6,\!6$	0.08	0
2	SO4	А	1819	-	4,4,4	0.15	0	6,6,6	0.09	0
2	SO4	А	1821	-	4,4,4	0.16	0	$6,\!6,\!6$	0.04	0
2	SO4	А	1824	-	4,4,4	0.15	0	$6,\!6,\!6$	0.08	0
2	SO4	В	1817	-	4,4,4	0.15	0	$6,\!6,\!6$	0.06	0
2	SO4	В	1823	-	4,4,4	0.13	0	$6,\!6,\!6$	0.08	0
2	SO4	A	1825	-	4,4,4	0.13	0	6,6,6	0.07	0
2	SO4	В	1820	-	4,4,4	0.12	0	$6,\!6,\!6$	0.09	0
2	SO4	A	1817	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	В	1825	-	4,4,4	0.14	0	$6,\!6,\!6$	0.13	0
2	SO4	В	1818	-	4,4,4	0.13	0	$6,\!6,\!6$	0.07	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.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	1826	SO4	1	0
2	А	1819	SO4	2	0
2	А	1824	SO4	3	0
2	В	1825	SO4	1	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 (i)

6.1 Protein, DNA and RNA chains (i)

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^{th} 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	А	640/655~(97%)	-0.13	5 (0%) 86 84	27, 44, 71, 95	0
1	В	640/655~(97%)	-0.00	18 (2%) 53 46	29, 48, 78, 94	0
All	All	1280/1310~(97%)	-0.07	23 (1%) 68 64	27, 46, 74, 95	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	206	ASP	4.0
1	В	180	PHE	3.3
1	В	207	SER	3.1
1	В	209	SER	3.1
1	В	212	ALA	3.0
1	А	348	SER	2.9
1	В	179	VAL	2.8
1	В	773	PHE	2.8
1	В	393	SER	2.7
1	В	619	VAL	2.7
1	В	215	GLU	2.7
1	А	300	GLN	2.6
1	А	412	PHE	2.5
1	В	214	VAL	2.5
1	А	206	ASP	2.4
1	В	582	ILE	2.4
1	В	660	ARG	2.3
1	В	420	PHE	2.3
1	В	184	GLU	2.2
1	В	211	GLU	2.1
1	В	618	LEU	2.1
1	В	396	TYR	2.0
1	А	369	CYS	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 monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} 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	$B-factors(A^2)$	Q<0.9
2	SO4	В	1822	5/5	0.84	0.36	86,94,118,119	0
2	SO4	А	1825	5/5	0.86	0.27	66,88,116,121	0
2	SO4	В	1818	5/5	0.89	0.18	85,86,102,115	0
2	SO4	В	1827	5/5	0.90	0.45	83,84,108,118	0
2	SO4	А	1817	5/5	0.91	0.19	58,69,107,112	0
2	SO4	А	1828	5/5	0.92	0.43	82,84,110,113	0
2	SO4	А	1820	5/5	0.92	0.27	74,88,96,103	0
2	SO4	В	1819	5/5	0.92	0.20	68,69,89,107	0
2	SO4	А	1818	5/5	0.92	0.15	76,78,95,101	0
2	SO4	А	1827	5/5	0.92	0.33	72,80,100,106	0
2	SO4	А	1824	5/5	0.93	0.28	66,84,102,105	0
2	SO4	А	1822	5/5	0.93	0.22	84,92,101,120	0
2	SO4	А	1821	5/5	0.94	0.19	87,90,105,114	0
2	SO4	В	1824	5/5	0.94	0.21	73,78,94,96	0
2	SO4	А	1819	5/5	0.94	0.17	64,81,90,98	0
2	SO4	В	1826	5/5	0.95	0.30	93,99,111,126	0
2	SO4	А	1823	5/5	0.95	0.29	68,73,97,98	0
2	SO4	А	1826	5/5	0.96	0.28	70,86,110,110	0
2	SO4	В	1823	5/5	0.96	0.20	80,92,103,110	0
2	SO4	В	1817	5/5	0.96	0.19	54,72,91,102	0
2	SO4	В	1820	5/5	0.96	0.13	44,52,74,88	0
2	SO4	В	1821	5/5	0.96	0.27	75,78,104,107	0
2	SO4	В	1825	5/5	0.97	0.17	53,69,74,83	0
2	SO4	В	1816	5/5	0.99	0.13	31,41,46,47	0
2	SO4	А	1816	5/5	0.99	0.14	35,35,40,42	0



6.5 Other polymers (i)

There are no such residues in this entry.

