Full wwPDB X-ray Structure Validation Report (i)

Nov 13, 2016 – 04:28 AM EST

PDB ID	:	4MUN
Title	:	Crystal structure of pantothenate synthetase in complex with 2-(5-methoxy-2-(2-nitro-4-(trifluoromethyl)phenylsulfonylcarbamoyl)-1H-indol-1-yl)acetic acid
Authors	:	Silvestre, H.L.; Blundell, T.L.
Deposited on	:	2013-09-22
Resolution	:	1.57 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 (i) symbol.

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

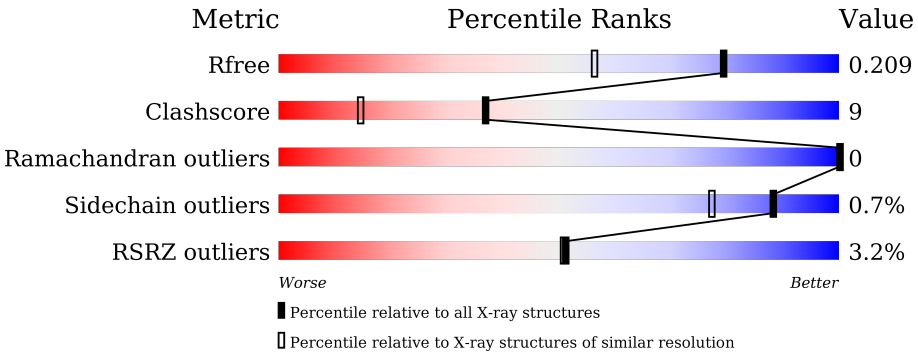
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028320
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028320

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.57 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	3815 (1.60-1.56)
Clashscore	102246	4131 (1.60-1.56)
Ramachandran outliers	100387	4021 (1.60-1.56)
Sidechain outliers	100360	4018 (1.60-1.56)
RSRZ outliers	91569	3823 (1.60-1.56)

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 <=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	300	2% 80% 13% • 6%
1	B	300	4% 80% 10% • 9%

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	EOH	A	401	-	-	-	X
3	2DZ	A	405	-	-	-	X
4	EDO	B	402	-	-	-	X
5	GOL	A	407	-	-	-	X
5	GOL	A	408	-	-	X	-
5	GOL	A	412	-	-	X	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4908 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.

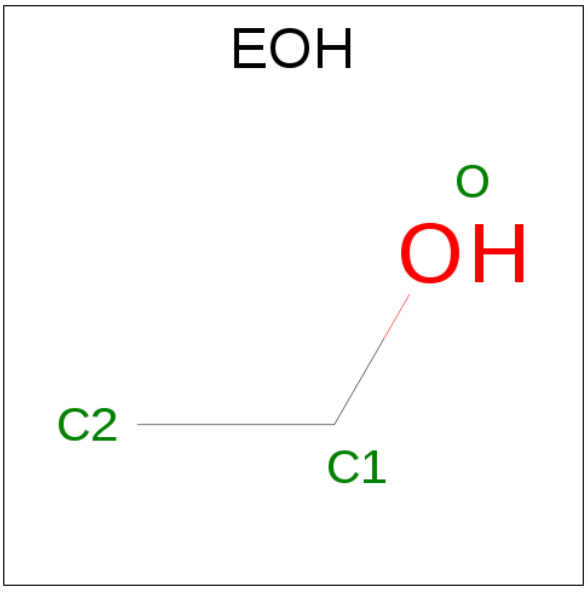
- Molecule 1 is a protein called Pantothenate synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	9	0
			2148	1356	382	404	6			
1	B	272	Total	C	N	O	S	0	7	0
			2048	1298	367	377	6			

There are 4 discrepancies between the modelled and reference sequences:

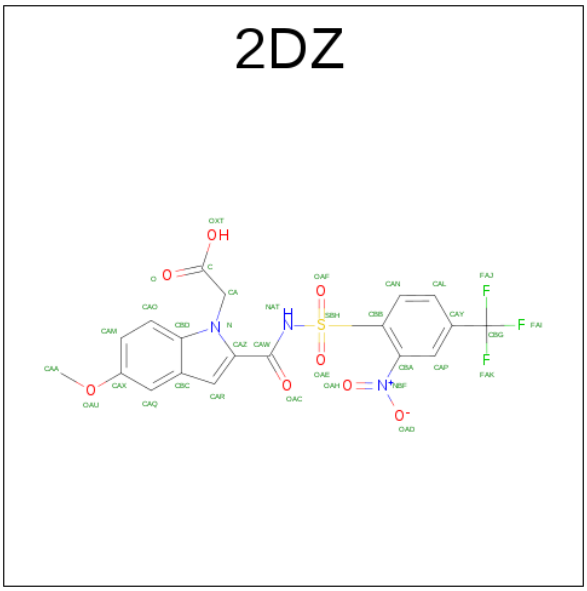
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	THR	ENGINEERED MUTATION	UNP P0A5R0
A	77	GLY	GLU	ENGINEERED MUTATION	UNP P0A5R0
B	2	ALA	THR	ENGINEERED MUTATION	UNP P0A5R0
B	77	GLY	GLU	ENGINEERED MUTATION	UNP P0A5R0

- Molecule 2 is ETHANOL (three-letter code: EOH) (formula: C_2H_6O).



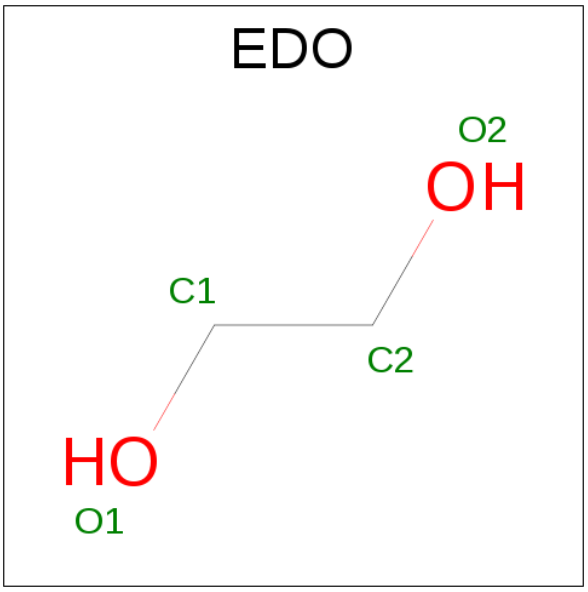
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 3 2 1	0	0
2	A	1	Total C O 3 2 1	0	0
2	A	1	Total C O 3 2 1	0	0

- Molecule 3 is [5-METHOXY-2-({[2-NITRO-4-(TRIFLUOROMETHYL)PHENYL]SULFONYL}CARBAMOYL)-1H-INDOL-1-YL]ACETIC ACID (three-letter code: 2DZ) (formula: $C_{19}H_{14}F_3N_3O_8S$).



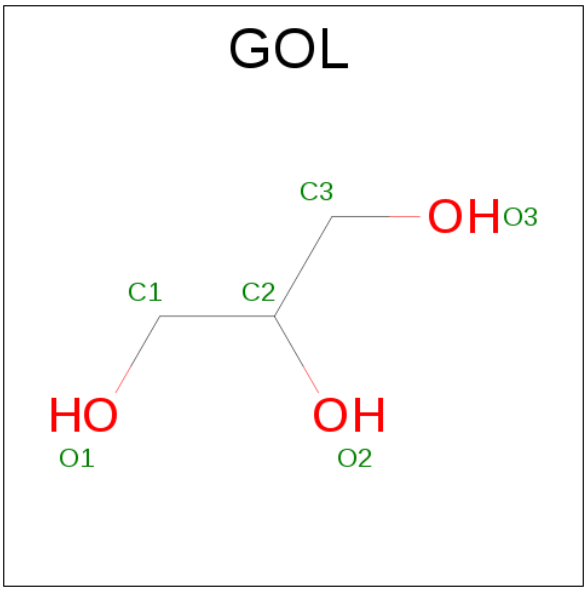
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C F N O S 34 19 3 3 8 1	0	0
3	A	1	Total C F N O S 34 19 3 3 8 1	0	0
3	A	1	Total C F N O S 34 19 3 3 8 1	0	0
3	B	1	Total C F N O S 68 38 6 6 16 2	0	1

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0

- Molecule 6 is water.

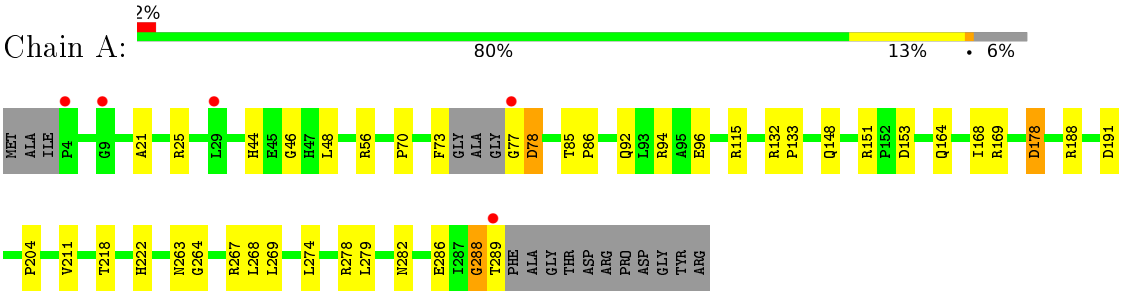
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	261	Total O 261 261	0	0
6	B	230	Total O 230 230	0	0

3 Residue-property plots (i)

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.

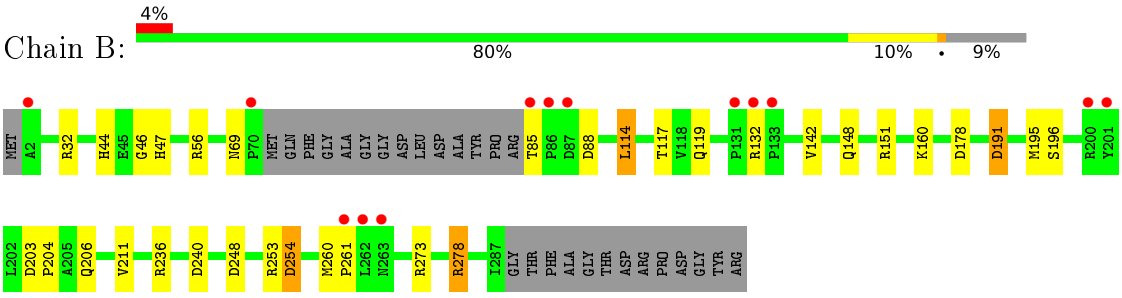
- Molecule 1: Pantothenate synthetase

Chain A:



- Molecule 1: Pantothenate synthetase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	48.37Å 70.81Å 81.78Å 90.00° 99.15° 90.00°	Depositor
Resolution (Å)	25.17 – 1.57 25.16 – 1.57	Depositor EDS
% Data completeness (in resolution range)	99.9 (25.17-1.57) 99.9 (25.16-1.57)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.09 (at 1.57Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.164 , 0.200 0.175 , 0.209	Depositor DCC
R_{free} test set	3816 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	17.6	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 47.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	4908	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.87% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, EOH, EDO, 2DZ

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	1.07	1/2186 (0.0%)	1.18	17/2986 (0.6%)
1	B	1.00	0/2088	1.11	9/2853 (0.3%)
All	All	1.04	1/4274 (0.0%)	1.15	26/5839 (0.4%)

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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	288	GLY	N-CA	5.16	1.53	1.46

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	278	ARG	NE-CZ-NH1	-10.45	115.08	120.30
1	A	133[A]	PRO	C-N-CA	8.37	142.62	121.70
1	A	133[B]	PRO	C-N-CA	8.37	142.62	121.70
1	B	32	ARG	NE-CZ-NH1	-7.49	116.55	120.30
1	A	278	ARG	NE-CZ-NH2	-7.47	116.57	120.30
1	B	236	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	B	56	ARG	NE-CZ-NH1	6.81	123.70	120.30
1	A	56	ARG	NE-CZ-NH2	6.48	123.54	120.30
1	B	191	ASP	CB-CG-OD1	6.26	123.94	118.30
1	A	153	ASP	CB-CG-OD2	6.15	123.84	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	178[A]	ASP	CB-CG-OD2	-6.15	112.77	118.30
1	A	178[B]	ASP	CB-CG-OD2	-6.15	112.77	118.30
1	A	188	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	A	169	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	A	267	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	B	253	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	A	178[A]	ASP	CB-CG-OD1	5.83	123.54	118.30
1	A	178[B]	ASP	CB-CG-OD1	5.83	123.54	118.30
1	B	56	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	267	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	B	240	ASP	CB-CG-OD1	5.45	123.20	118.30
1	A	115	ARG	NE-CZ-NH2	5.43	123.02	120.30
1	A	269	LEU	CB-CG-CD1	-5.24	102.09	111.00
1	A	94	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	B	254	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	A	73	PHE	CB-CG-CD1	5.07	124.35	120.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	288	GLY	Peptide

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	2148	0	2168	34	0
1	B	2048	0	2107	35	0
2	A	9	0	18	2	0
3	A	102	0	39	11	0
3	B	68	0	26	7	0
4	A	12	0	18	0	0
4	B	12	0	18	2	0
5	A	18	0	24	9	0
6	A	261	0	0	12	0
6	B	230	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4908	0	4418	83	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 9.

All (83) 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)
3:B:401[B]:2DZ:OAD	3:B:401[B]:2DZ:NBF	1.56	1.37
3:B:401[A]:2DZ:NBF	3:B:401[A]:2DZ:OAD	1.60	1.34
3:B:401[A]:2DZ:NBF	3:B:401[A]:2DZ:OAC	1.88	1.06
3:B:401[A]:2DZ:OAC	3:B:401[A]:2DZ:OAH	1.82	0.95
1:A:263:ASN:ND2	1:A:264:GLY:H	1.65	0.94
1:A:263:ASN:CG	1:A:264:GLY:H	1.69	0.94
1:B:44:HIS:HD2	1:B:46:GLY:H	1.10	0.91
1:A:263:ASN:CG	1:A:264:GLY:N	2.28	0.83
1:B:248:ASP:OD1	6:B:663:HOH:O	1.95	0.82
1:A:44:HIS:HD2	1:A:46:GLY:H	1.29	0.81
1:A:286:GLU:OE1	6:A:645:HOH:O	2.05	0.74
1:A:21:ALA:HB1	5:A:412:GOL:H32	1.69	0.74
1:A:78:ASP:HB3	3:A:405:2DZ:OXT	1.87	0.73
1:B:151:ARG:NH2	6:B:508:HOH:O	2.26	0.68
1:B:44:HIS:HD2	1:B:46:GLY:N	1.89	0.68
1:B:44:HIS:CD2	1:B:46:GLY:H	2.03	0.66
1:B:85:THR:HB	1:B:88:ASP:HB2	1.78	0.65
1:B:195[B]:MET:HE3	1:B:196:SER:N	2.13	0.63
1:A:168:ILE:HD12	6:A:717:HOH:O	1.99	0.61
3:A:404:2DZ:CA	3:A:404:2DZ:H11	2.13	0.61
1:B:195[B]:MET:C	1:B:195[B]:MET:HE3	2.21	0.60
1:A:48:LEU:HD11	1:A:92:GLN:HE21	1.66	0.60
1:A:44:HIS:HE1	3:A:403:2DZ:OXT	1.85	0.59
1:B:278:ARG:HG2	1:B:278:ARG:NH1	2.18	0.59
1:A:218[B]:THR:HG21	2:A:401:EOH:H23	1.83	0.59
3:A:403:2DZ:OAE	5:A:408:GOL:H32	2.02	0.59
1:A:164:GLN:NE2	3:A:403:2DZ:OAD	2.35	0.58
1:A:44:HIS:HD2	1:A:46:GLY:N	1.99	0.58
1:A:132:ARG:HG3	3:A:405:2DZ:CAP	2.34	0.58
5:A:408:GOL:H11	6:A:585:HOH:O	2.04	0.58
1:A:85:THR:N	1:A:86:PRO:HD3	2.19	0.58
1:B:44:HIS:CD2	1:B:195[B]:MET:HE2	2.41	0.55
1:B:132:ARG:NH1	6:B:592:HOH:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:404:2DZ:H3	3:A:404:2DZ:OAH	2.10	0.52
1:A:77:GLY:N	6:A:556:HOH:O	2.43	0.51
1:B:211[B]:VAL:HG21	6:B:656:HOH:O	2.11	0.51
1:B:273:ARG:NH2	6:B:663:HOH:O	2.42	0.51
1:B:278:ARG:HG2	1:B:278:ARG:HH11	1.75	0.51
1:A:218[B]:THR:O	1:A:222:HIS:HD2	1.94	0.51
1:A:44:HIS:CD2	1:A:46:GLY:H	2.19	0.50
3:A:404:2DZ:H11	3:A:404:2DZ:C	2.24	0.50
1:B:69:ASN:CG	1:B:142[B]:VAL:HG21	2.32	0.50
5:A:412:GOL:H12	1:B:178[B]:ASP:OD2	2.11	0.49
1:B:203:ASP:HB2	1:B:204:PRO:CD	2.42	0.49
1:B:254:ASP:HB3	1:B:261:PRO:HD3	1.95	0.49
1:A:191:ASP:OD2	1:A:211[B]:VAL:HG22	2.14	0.48
1:B:44:HIS:CD2	1:B:195[B]:MET:CE	2.97	0.48
1:B:85:THR:HB	1:B:88:ASP:CB	2.42	0.48
1:A:191:ASP:OD2	1:A:211[B]:VAL:CG2	2.62	0.47
1:A:25:ARG:HB2	5:A:412:GOL:O2	2.15	0.47
1:B:114:LEU:HD21	1:B:117:THR:HG21	1.96	0.47
5:A:408:GOL:C1	6:A:585:HOH:O	2.63	0.47
1:A:178[B]:ASP:OD2	1:B:151:ARG:NE	2.48	0.47
3:A:403:2DZ:OAE	5:A:408:GOL:C3	2.64	0.46
1:A:70:PRO:HG3	6:A:757:HOH:O	2.15	0.46
1:A:289:THR:HG21	6:A:651:HOH:O	2.15	0.46
3:B:401[A]:2DZ:OAH	6:B:728:HOH:O	2.21	0.46
1:A:148:GLN:HE22	4:B:404:EDO:C2	2.28	0.46
1:B:69:ASN:OD1	1:B:142[B]:VAL:HG21	2.15	0.45
1:A:48:LEU:HD22	1:A:96:GLU:HG3	1.98	0.45
1:A:218[B]:THR:HG23	6:A:697:HOH:O	2.17	0.45
1:A:92:GLN:OE1	6:A:695:HOH:O	2.20	0.45
3:B:401[B]:2DZ:OAE	3:B:401[B]:2DZ:OAC	2.33	0.44
1:A:274:LEU:HD13	1:A:279:LEU:HD12	2.00	0.44
2:A:402:EOH:H23	6:A:617:HOH:O	2.17	0.44
1:B:148:GLN:HE22	4:B:404:EDO:H21	1.83	0.44
3:A:403:2DZ:OAH	3:A:403:2DZ:NAT	2.51	0.43
1:B:44:HIS:HE1	3:B:401[B]:2DZ:H3	1.83	0.43
1:B:160:LYS:HG3	6:B:712:HOH:O	2.18	0.43
1:B:248:ASP:HB3	6:B:534:HOH:O	2.18	0.43
1:B:191:ASP:OD2	1:B:211[B]:VAL:HG22	2.19	0.42
5:A:407:GOL:O1	1:B:119:GLN:HG2	2.19	0.42
1:A:77:GLY:CA	6:A:556:HOH:O	2.67	0.42
1:A:151:ARG:HG3	5:A:412:GOL:O1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:LYS:HE3	6:B:622:HOH:O	2.19	0.42
1:A:164:GLN:CD	3:A:403:2DZ:OAD	2.58	0.42
1:A:289:THR:CG2	6:A:651:HOH:O	2.68	0.41
1:A:268:LEU:O	1:A:282:ASN:HA	2.20	0.41
1:B:278:ARG:HH11	1:B:278:ARG:CG	2.29	0.41
1:B:206:GLN:HG2	6:B:725:HOH:O	2.21	0.41
1:B:44:HIS:CE1	1:B:47:HIS:CE1	3.09	0.41
1:B:260:MET:SD	1:B:261:PRO:HD2	2.61	0.40
1:B:69:ASN:ND2	1:B:142[B]:VAL:HG21	2.36	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	287/300 (96%)	277 (96%)	10 (4%)	0	100	100
1	B	275/300 (92%)	271 (98%)	4 (2%)	0	100	100
All	All	562/600 (94%)	548 (98%)	14 (2%)	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 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	220/223 (99%)	218 (99%)	2 (1%)	84 69
1	B	210/223 (94%)	209 (100%)	1 (0%)	92 84
All	All	430/446 (96%)	427 (99%)	3 (1%)	88 77

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	ASP
1	A	204	PRO
1	B	114	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	HIS
1	A	92	GLN
1	A	119	GLN
1	A	148	GLN
1	A	164	GLN
1	A	222	HIS
1	B	44	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

17 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	EOH	A	401	-	2,2,2	0.75	0	1,1,1	0.37	0
2	EOH	A	402	-	2,2,2	0.47	0	1,1,1	0.54	0
3	2DZ	A	403	-	29,36,36	3.70	10 (34%)	41,55,55	2.30	6 (14%)
3	2DZ	A	404	-	29,36,36	3.46	11 (37%)	41,55,55	1.55	8 (19%)
3	2DZ	A	405	-	29,36,36	3.74	16 (55%)	41,55,55	1.98	9 (21%)
4	EDO	A	406	-	3,3,3	0.45	0	2,2,2	0.15	0
5	GOL	A	407	-	5,5,5	0.24	0	5,5,5	0.64	0
5	GOL	A	408	-	5,5,5	0.57	0	5,5,5	1.19	1 (20%)
4	EDO	A	409	-	3,3,3	0.68	0	2,2,2	0.64	0
2	EOH	A	410	-	2,2,2	0.40	0	1,1,1	0.83	0
4	EDO	A	411	-	3,3,3	0.32	0	2,2,2	0.56	0
5	GOL	A	412	-	5,5,5	0.33	0	5,5,5	0.83	0
3	2DZ	B	401[A]	-	29,36,36	3.61	12 (41%)	41,55,55	2.45	13 (31%)
3	2DZ	B	401[B]	-	29,36,36	3.12	9 (31%)	41,55,55	2.26	10 (24%)
4	EDO	B	402	-	3,3,3	0.47	0	2,2,2	0.48	0
4	EDO	B	403	-	3,3,3	0.36	0	2,2,2	1.19	0
4	EDO	B	404	-	3,3,3	0.51	0	2,2,2	0.63	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	EOH	A	401	-	-	0/0/0/0	0/0/0/0
2	EOH	A	402	-	-	0/0/0/0	0/0/0/0
3	2DZ	A	403	-	-	0/25/31/31	0/3/3/3
3	2DZ	A	404	-	-	0/25/31/31	0/3/3/3
3	2DZ	A	405	-	-	0/25/31/31	0/3/3/3
4	EDO	A	406	-	-	0/1/1/1	0/0/0/0
5	GOL	A	407	-	-	0/4/4/4	0/0/0/0
5	GOL	A	408	-	-	0/4/4/4	0/0/0/0
4	EDO	A	409	-	-	0/1/1/1	0/0/0/0
2	EOH	A	410	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	411	-	-	0/1/1/1	0/0/0/0
5	GOL	A	412	-	-	0/4/4/4	0/0/0/0
3	2DZ	B	401[A]	-	-	0/25/31/31	0/3/3/3
3	2DZ	B	401[B]	-	-	0/25/31/31	0/3/3/3
4	EDO	B	402	-	-	0/1/1/1	0/0/0/0
4	EDO	B	403	-	-	0/1/1/1	0/0/0/0
4	EDO	B	404	-	-	0/1/1/1	0/0/0/0

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401[A]	2DZ	CAW-NAT	-6.29	1.31	1.39
3	A	403	2DZ	CAW-NAT	-6.16	1.31	1.39
3	A	405	2DZ	CAR-CAZ	-4.74	1.34	1.38
3	A	405	2DZ	CBG-CAY	-4.59	1.40	1.49
3	A	404	2DZ	CAW-NAT	-4.20	1.33	1.39
3	B	401[B]	2DZ	CBG-CAY	-4.09	1.41	1.49
3	A	404	2DZ	CAR-CAZ	-3.84	1.35	1.38
3	B	401[B]	2DZ	CAR-CAZ	-3.60	1.35	1.38
3	A	404	2DZ	CBC-CBD	-3.53	1.33	1.41
3	A	405	2DZ	CAQ-CBC	-3.45	1.33	1.42
3	B	401[A]	2DZ	CAR-CAZ	-3.39	1.35	1.38
3	B	401[B]	2DZ	CAW-NAT	-3.35	1.34	1.39
3	A	405	2DZ	FAI-CBG	-3.26	1.21	1.32
3	A	405	2DZ	CBB-SBH	-3.20	1.72	1.77
3	A	405	2DZ	CBC-CBD	-3.04	1.34	1.41
3	A	404	2DZ	CAO-CBD	-3.00	1.34	1.41
3	B	401[B]	2DZ	CAQ-CBC	-2.80	1.35	1.42
3	B	401[A]	2DZ	CBG-CAY	-2.79	1.44	1.49
3	B	401[A]	2DZ	CAQ-CBC	-2.74	1.35	1.42
3	A	403	2DZ	CA-N	-2.65	1.44	1.49
3	A	403	2DZ	CBC-CBD	-2.64	1.35	1.41
3	B	401[A]	2DZ	CAO-CBD	-2.59	1.35	1.41
3	B	401[A]	2DZ	CBC-CBD	-2.50	1.35	1.41
3	A	405	2DZ	CAW-NAT	-2.45	1.36	1.39
3	A	403	2DZ	CAZ-CAW	-2.32	1.36	1.50
3	A	405	2DZ	CAO-CBD	-2.20	1.36	1.41
3	A	405	2DZ	FAK-CBG	-2.14	1.25	1.32
3	A	404	2DZ	CAZ-CAW	-2.13	1.37	1.50
3	A	404	2DZ	CAQ-CBC	-2.13	1.37	1.42
3	B	401[B]	2DZ	CAZ-CAW	-2.06	1.37	1.50
3	B	401[B]	2DZ	CBC-CBD	-2.06	1.36	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	405	2DZ	CAZ-CAW	-2.01	1.38	1.50
3	B	401[A]	2DZ	CA-N	2.49	1.54	1.49
3	B	401[A]	2DZ	FAI-CBG	2.67	1.42	1.32
3	A	404	2DZ	CBB-SBH	2.80	1.81	1.77
3	A	403	2DZ	CAQ-CAX	3.36	1.43	1.37
3	A	403	2DZ	CBA-CBB	3.76	1.43	1.40
3	A	405	2DZ	CAN-CBB	3.85	1.43	1.39
3	A	404	2DZ	CAQ-CAX	3.89	1.44	1.37
3	A	405	2DZ	FAJ-CBG	4.05	1.47	1.32
3	A	403	2DZ	FAI-CBG	4.32	1.48	1.32
3	A	405	2DZ	SBH-NAT	4.91	1.74	1.64
3	A	403	2DZ	OAH-NBF	5.37	1.33	1.22
3	B	401[A]	2DZ	OAE-SBH	5.50	1.49	1.43
3	A	405	2DZ	OAH-NBF	6.12	1.34	1.22
3	A	405	2DZ	OAE-SBH	6.60	1.50	1.43
3	B	401[A]	2DZ	SBH-NAT	6.80	1.78	1.64
3	B	401[B]	2DZ	SBH-NAT	7.05	1.78	1.64
3	A	404	2DZ	OAE-SBH	7.65	1.52	1.43
3	B	401[A]	2DZ	OAH-NBF	7.72	1.38	1.22
3	A	404	2DZ	CA-N	7.77	1.64	1.49
3	B	401[B]	2DZ	OAF-SBH	8.71	1.53	1.43
3	B	401[B]	2DZ	OAE-SBH	8.72	1.53	1.43
3	A	403	2DZ	OAE-SBH	10.03	1.54	1.43
3	A	404	2DZ	OAF-SBH	11.04	1.55	1.43
3	B	401[A]	2DZ	OAF-SBH	11.42	1.56	1.43
3	A	405	2DZ	OAF-SBH	12.06	1.56	1.43
3	A	403	2DZ	OAF-SBH	12.20	1.57	1.43

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	401[A]	2DZ	CAW-NAT-SBH	-8.93	113.14	123.34
3	B	401[B]	2DZ	CAW-NAT-SBH	-8.46	113.68	123.34
3	A	405	2DZ	CBA-CBB-SBH	-6.55	116.65	124.37
3	A	403	2DZ	OAE-SBH-OAF	-5.91	111.70	119.54
3	B	401[A]	2DZ	CAN-CBB-SBH	-4.83	111.24	117.35
3	A	404	2DZ	OAE-SBH-CBB	-4.23	100.81	107.64
3	B	401[A]	2DZ	OAC-CAW-NAT	-3.75	116.46	120.80
3	B	401[A]	2DZ	OAF-SBH-NAT	-3.60	96.46	106.73
3	B	401[B]	2DZ	OAE-SBH-OAF	-3.40	115.03	119.54
3	A	405	2DZ	FAJ-CBG-CAY	-3.30	105.97	112.92
3	A	403	2DZ	CAN-CBB-SBH	-3.29	113.19	117.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	401[A]	2DZ	CAR-CAZ-CAW	-3.15	121.55	129.81
3	A	405	2DZ	CAP-CAY-CBG	-3.14	115.38	119.58
3	B	401[B]	2DZ	CAN-CBB-SBH	-3.04	113.51	117.35
3	B	401[B]	2DZ	CAR-CAZ-CAW	-3.02	121.88	129.81
3	A	404	2DZ	CBA-CBB-SBH	-2.93	120.92	124.37
3	A	404	2DZ	CAO-CAM-CAX	-2.93	116.27	120.19
3	B	401[A]	2DZ	CAM-CAX-CAQ	-2.82	116.80	120.81
3	B	401[A]	2DZ	OAF-SBH-CBB	-2.75	103.20	107.64
3	A	403	2DZ	CAW-NAT-SBH	-2.74	120.21	123.34
3	B	401[B]	2DZ	CAP-CAY-CBG	-2.44	116.31	119.58
3	B	401[A]	2DZ	CAP-CBA-CBB	-2.43	118.89	122.40
3	B	401[B]	2DZ	OAC-CAW-NAT	-2.19	118.27	120.80
3	A	404	2DZ	CAL-CAN-CBB	-2.18	116.66	120.14
3	A	404	2DZ	CAO-CBD-N	-2.12	129.09	132.06
3	B	401[B]	2DZ	CAM-CAX-CAQ	-2.06	117.87	120.81
3	A	404	2DZ	CAA-OAU-CAX	-2.02	112.83	117.51
3	B	401[A]	2DZ	CAM-CAO-CBD	2.08	122.92	119.42
5	A	408	GOL	O1-C1-C2	2.14	120.83	109.97
3	A	405	2DZ	CBB-SBH-NAT	2.16	108.88	106.31
3	A	404	2DZ	CAM-CAO-CBD	2.20	123.13	119.42
3	A	403	2DZ	CBA-CBB-SBH	2.24	127.00	124.37
3	A	404	2DZ	OAF-SBH-NAT	2.29	113.26	106.73
3	A	405	2DZ	CAL-CAY-CBG	2.48	123.67	119.99
3	A	405	2DZ	FAJ-CBG-FAK	2.65	115.26	105.75
3	B	401[A]	2DZ	OAE-SBH-NAT	2.77	114.64	106.73
3	B	401[B]	2DZ	CAL-CAY-CBG	2.92	124.32	119.99
3	B	401[A]	2DZ	CAP-CAY-CBG	3.04	123.66	119.58
3	B	401[B]	2DZ	CBA-CBB-SBH	3.18	128.12	124.37
3	A	405	2DZ	OAC-CAW-NAT	3.21	124.52	120.80
3	A	403	2DZ	CBB-SBH-NAT	3.46	110.43	106.31
3	A	405	2DZ	CAR-CBC-CBD	3.83	109.61	106.27
3	B	401[A]	2DZ	CBA-CBB-SBH	3.86	128.92	124.37
3	B	401[A]	2DZ	CBB-SBH-NAT	4.27	111.39	106.31
3	A	405	2DZ	CAN-CBB-SBH	4.33	122.84	117.35
3	B	401[B]	2DZ	CBB-SBH-NAT	6.64	114.22	106.31
3	A	403	2DZ	C-CA-N	10.67	128.46	114.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	EOH	1	0
2	A	402	EOH	1	0
3	A	403	2DZ	6	0
3	A	404	2DZ	3	0
3	A	405	2DZ	2	0
5	A	407	GOL	1	0
5	A	408	GOL	4	0
5	A	412	GOL	4	0
3	B	401[A]	2DZ	4	0
3	B	401[B]	2DZ	3	0
4	B	404	EDO	2	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, 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	A	283/300 (94%)	-0.16	5 (1%) 71 72	10, 17, 38, 52	1 (0%)
1	B	272/300 (90%)	0.07	13 (4%) 34 32	12, 19, 43, 74	1 (0%)
All	All	555/600 (92%)	-0.05	18 (3%) 51 51	10, 18, 40, 74	2 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	262	LEU	8.2
1	B	86	PRO	5.8
1	B	85	THR	5.6
1	B	87	ASP	5.2
1	B	201	TYR	4.0
1	B	261	PRO	3.9
1	A	77	GLY	3.7
1	B	70	PRO	3.7
1	B	263	ASN	3.3
1	B	200	ARG	2.9
1	A	289	THR	2.9
1	A	4	PRO	2.8
1	A	9	GLY	2.6
1	B	132	ARG	2.6
1	B	131	PRO	2.4
1	B	2	ALA	2.3
1	A	29	LEU	2.2
1	B	133	PRO	2.2

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{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	LLDF	B-factors(Å^2)	Q<0.9
2	EOH	A	401	3/3	0.88	0.16	6.94	29,29,30,33	0
5	GOL	A	407	6/6	0.91	0.15	4.40	23,36,45,54	0
3	2DZ	A	405	34/34	0.89	0.19	3.54	22,30,37,43	34
5	GOL	A	412	6/6	0.81	0.27	3.30	43,52,53,57	0
4	EDO	B	402	4/4	0.98	0.12	2.27	23,24,26,26	0
5	GOL	A	408	6/6	0.88	0.15	1.99	33,40,45,52	0
3	2DZ	B	401[B]	34/34	0.94	0.12	0.96	22,30,38,44	34
3	2DZ	B	401[A]	34/34	0.94	0.12	0.92	17,24,28,30	34
4	EDO	A	409	4/4	0.90	0.09	0.73	29,29,32,33	0
4	EDO	A	406	4/4	0.96	0.08	0.62	21,21,22,23	0
3	2DZ	A	403	34/34	0.94	0.08	0.27	15,21,40,51	0
3	2DZ	A	404	34/34	0.95	0.09	0.19	18,26,35,38	0
4	EDO	B	404	4/4	0.87	0.11	0.08	36,37,37,42	0
4	EDO	A	411	4/4	0.89	0.10	-0.29	43,43,43,44	0
2	EOH	A	410	3/3	0.90	0.07	-0.46	39,39,39,39	0
2	EOH	A	402	3/3	0.93	0.10	-	34,34,41,42	0
4	EDO	B	403	4/4	0.84	0.22	-	34,38,41,42	0

6.5 Other polymers (i)

There are no such residues in this entry.