



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 06:21 AM GMT

PDB ID : 3SSA
Title : Crystal structure of subunit B mutant N157T of the A1AO ATP synthase
Authors : Sundararaman, L.; Manimekalai, M.S.S.; Jeyakanthan, J.; Gruber, G.
Deposited on : 2011-07-08
Resolution : 1.70 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>

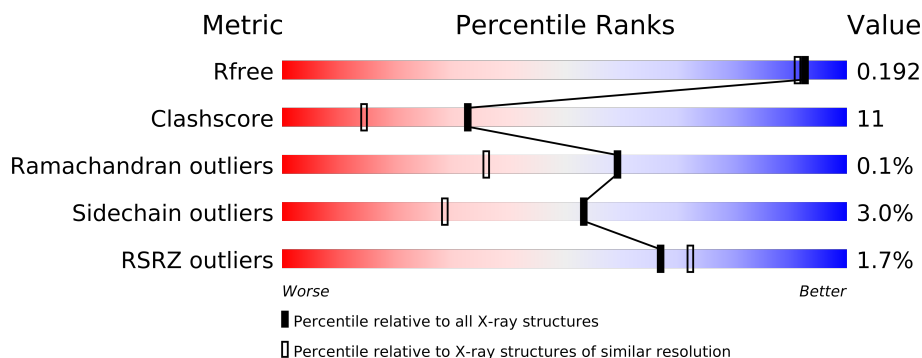
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.70 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	2456 (1.70-1.70)
Clashscore	79885	2929 (1.70-1.70)
Ramachandran outliers	78287	2878 (1.70-1.70)
Sidechain outliers	78261	2878 (1.70-1.70)
RSRZ outliers	66119	2456 (1.70-1.70)

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	460	
1	B	460	

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

Mol	Type	Chain	Res	Geometry	Electron density
2	GOL	A	461	-	X
2	GOL	A	463	-	X
2	GOL	A	465	-	X
2	GOL	A	467	-	X
2	GOL	B	462	-	X
2	GOL	B	463	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Geometry	Electron density
2	GOL	B	466	-	X
2	GOL	B	467	-	X
2	GOL	B	469	-	X
4	1PE	A	464	-	X
6	PEG	B	465	-	X
6	PEG	B	6073	-	X

2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 8124 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.

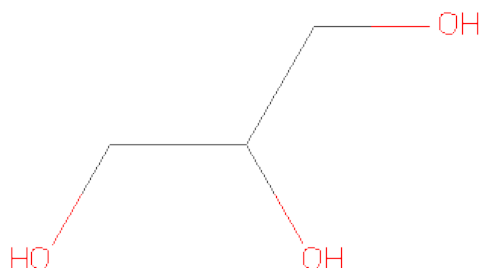
- Molecule 1 is a protein called V-type ATP synthase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	22	0
			3480	2207	601	660	12			
1	B	427	Total	C	N	O	S	0	16	0
			3383	2151	581	639	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	157	THR	ASN	ENGINEERED MUTATION	UNP Q60187
B	157	THR	ASN	ENGINEERED MUTATION	UNP Q60187

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

Continued on next page...

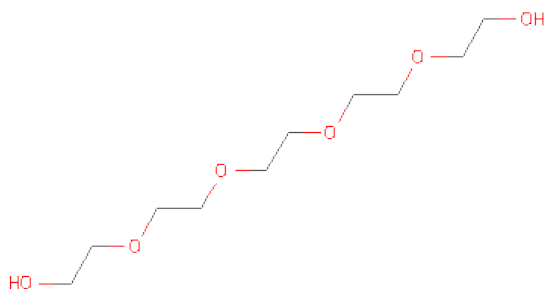
Continued from previous page...

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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

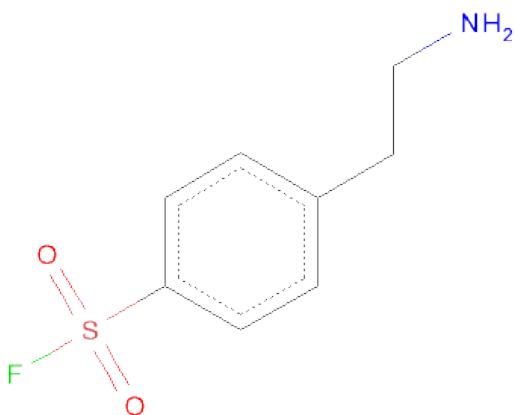
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Cl 2 2	0	0
3	A	1	Total Cl 1 1	0	0

- Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



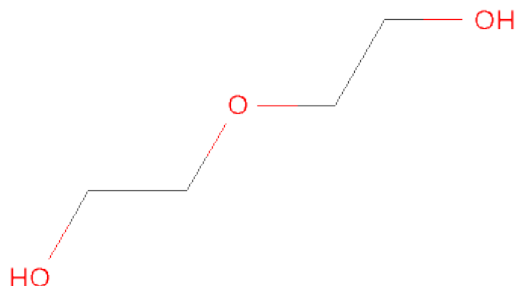
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			16	10	6		
4	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 5 is 4-(2-AMINOETHYL)BENZENESULFONYLFLUORIDE (three-letter code: AES) (formula: C₈H₁₀FNO₂S).



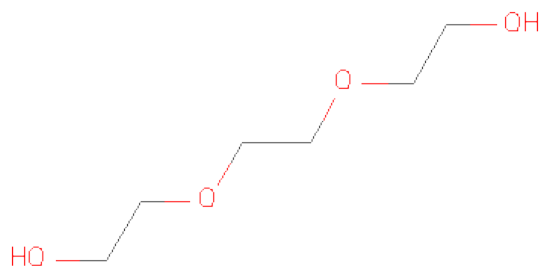
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	F	N	O	S	0	0
			13	8	1	1	2	1		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 8 is water.

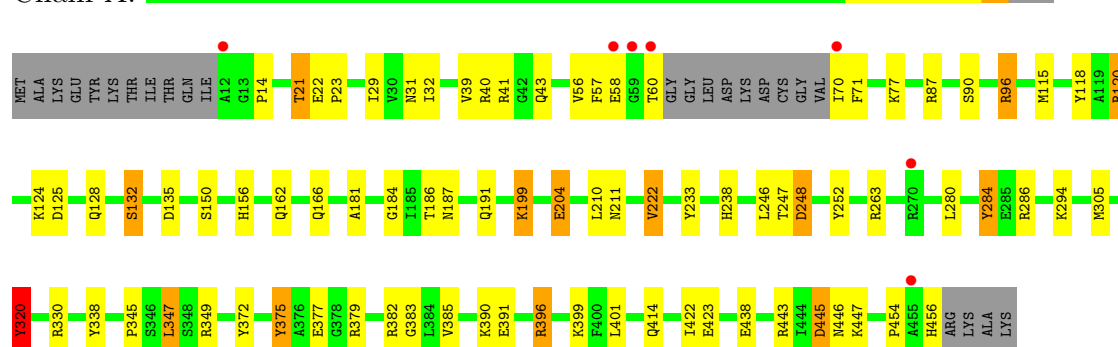
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	599	Total	O	0	0
			599	599		
8	B	507	Total	O	0	0
			507	507		

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.

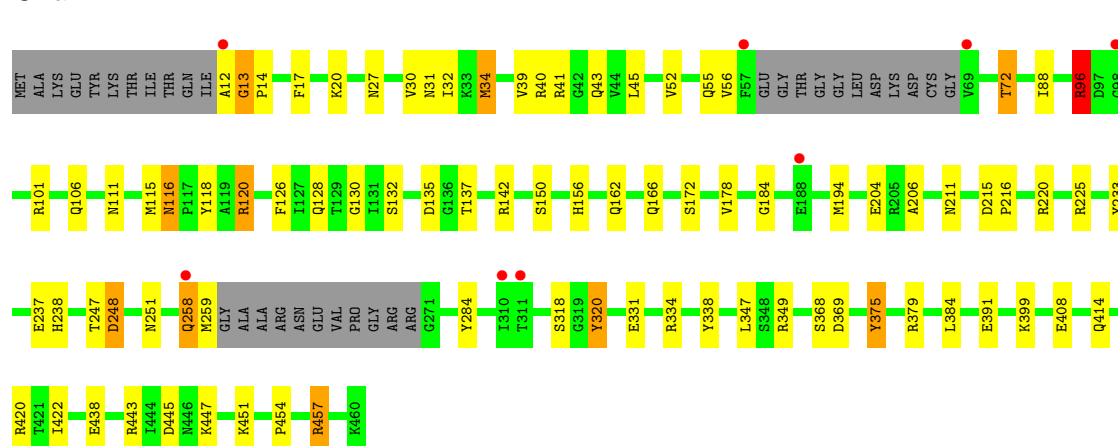
• Molecule 1: V-type ATP synthase beta chain

Chain A:



• Molecule 1: V-type ATP synthase beta chain

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.33Å 95.80Å 130.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	13.45 – 1.70 13.45 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (13.45-1.70) 99.7 (13.45-1.70)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.146 , 0.193 0.146 , 0.192	Depositor DCC
R_{free} test set	5072 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	19.5	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 58.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 101467 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8124	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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: GOL, AES, PGE, CL, 1PE, PEG

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	1.36	13/3611 (0.4%)	1.25	20/4891 (0.4%)
1	B	1.36	9/3493 (0.3%)	1.20	13/4730 (0.3%)
All	All	1.36	22/7104 (0.3%)	1.23	33/9621 (0.3%)

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	1	4
1	B	0	3
All	All	1	7

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	375	TYR	CE1-CZ	8.56	1.49	1.38
1	A	118	TYR	CE2-CZ	7.48	1.48	1.38
1	A	132	SER	CB-OG	7.43	1.51	1.42
1	B	320	TYR	CE2-CZ	7.02	1.47	1.38
1	A	383	GLY	N-CA	6.62	1.55	1.46
1	B	408	GLU	CB-CG	6.47	1.64	1.52
1	A	320	TYR	CG-CD2	6.38	1.47	1.39
1	B	284	TYR	CD1-CE1	5.95	1.48	1.39
1	A	284	TYR	CD2-CE2	5.74	1.48	1.39
1	B	438	GLU	CB-CG	-5.73	1.41	1.52
1	A	77	LYS	CE-NZ	5.73	1.63	1.49
1	A	423[A]	GLU	CG-CD	5.62	1.60	1.51
1	A	423[B]	GLU	CG-CD	5.62	1.60	1.51
1	B	391	GLU	CG-CD	5.57	1.60	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	222	VAL	CB-CG1	-5.30	1.41	1.52
1	B	225	ARG	CG-CD	-5.26	1.38	1.51
1	B	30	VAL	CB-CG1	5.25	1.63	1.52
1	A	58	GLU	CG-CD	5.24	1.59	1.51
1	A	391	GLU	CG-CD	5.13	1.59	1.51
1	A	252	TYR	CE1-CZ	5.06	1.45	1.38
1	A	58	GLU	CB-CG	5.05	1.61	1.52
1	B	349	ARG	CZ-NH1	5.01	1.39	1.33

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96[A]	ARG	NE-CZ-NH1	-12.44	114.08	120.30
1	A	96[B]	ARG	NE-CZ-NH1	-12.44	114.08	120.30
1	A	96[A]	ARG	NE-CZ-NH2	10.63	125.61	120.30
1	A	96[B]	ARG	NE-CZ-NH2	10.63	125.61	120.30
1	A	248	ASP	CB-CG-OD1	-10.00	109.30	118.30
1	A	248	ASP	CB-CG-OD2	9.71	127.04	118.30
1	B	115	MET	CG-SD-CE	9.36	115.18	100.20
1	B	96	ARG	NE-CZ-NH1	-8.73	115.93	120.30
1	B	349	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	B	225	ARG	NE-CZ-NH2	-6.99	116.81	120.30
1	A	286	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	A	135	ASP	CB-CG-OD1	6.92	124.53	118.30
1	A	401	LEU	CB-CG-CD2	-6.74	99.53	111.00
1	B	349	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	B	126	PHE	CB-CG-CD2	-6.62	116.17	120.80
1	A	382	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	A	248	ASP	N-CA-C	-6.50	93.44	111.00
1	A	385	VAL	CA-CB-CG2	-6.39	101.31	110.90
1	A	21	THR	CA-CB-OG1	6.16	121.93	109.00
1	B	34	MET	CG-SD-CE	5.87	109.59	100.20
1	B	457[A]	ARG	NE-CZ-NH1	-5.81	117.40	120.30
1	B	457[B]	ARG	NE-CZ-NH1	-5.81	117.40	120.30
1	B	137	THR	CA-CB-CG2	-5.48	104.73	112.40
1	B	334	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	A	375	TYR	CB-CG-CD2	-5.36	117.78	121.00
1	A	347	LEU	CB-CG-CD1	-5.26	102.05	111.00
1	A	349	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	B	135	ASP	CB-CG-OD1	5.25	123.03	118.30
1	A	396	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	A	330	ARG	NE-CZ-NH1	5.20	122.90	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	87	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	B	126	PHE	CB-CG-CD1	5.06	124.34	120.80
1	A	372	TYR	CB-CG-CD2	-5.05	117.97	121.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	21	THR	CB

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	247	THR	Mainchain,Peptide
1	A	338	TYR	Mainchain,Peptide
1	B	248[A]	ASP	Mainchain
1	B	338	TYR	Mainchain,Peptide

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	3480	0	3535	68	0
1	B	3383	0	3439	75	0
2	A	36	0	47	6	0
2	B	36	0	48	16	0
3	A	1	0	0	1	0
3	B	2	0	0	0	0
4	A	29	0	39	2	0
5	A	13	0	10	2	0
6	A	14	0	20	3	0
6	B	14	0	20	10	0
7	A	10	0	14	2	0
8	A	599	0	0	19	0
8	B	507	0	0	15	0
All	All	8124	0	7172	159	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (159) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:90:SER:HA	1:A:96[A]:ARG:NH1	1.36	1.41
1:B:120:ARG:HG3	8:B:1048:HOH:O	1.47	1.14
1:B:40[B]:ARG:HH11	1:B:40[B]:ARG:HG2	1.19	1.06
6:B:6073:PEG:H11	8:B:1013:HOH:O	1.56	1.04
1:A:90:SER:CA	1:A:96[A]:ARG:NH1	2.21	1.04
1:A:90:SER:CA	1:A:96[A]:ARG:HH12	1.72	1.02
1:A:204[B]:GLU:HG3	8:A:847:HOH:O	1.61	1.00
1:A:39:VAL:O	1:A:40[B]:ARG:HD2	1.65	0.96
6:B:6073:PEG:H32	8:B:594:HOH:O	1.66	0.93
1:A:120[A]:ARG:HG2	1:A:120[A]:ARG:HH11	1.34	0.93
1:B:96:ARG:HG3	1:B:96:ARG:NH1	1.86	0.91
1:A:120[A]:ARG:CG	1:A:120[A]:ARG:HH11	1.86	0.87
1:A:280[B]:LEU:HD11	1:A:320:TYR:CD1	2.10	0.87
1:A:445[B]:ASP:OD2	1:A:447:LYS:HG2	1.77	0.83
1:A:90:SER:HA	1:A:96[A]:ARG:HH12	0.93	0.82
1:B:31:ASN:HD21	1:B:41:ARG:HH11	1.24	0.82
1:B:96:ARG:HH11	1:B:96:ARG:HG3	1.45	0.82
1:B:12:ALA:O	1:B:13:GLY:O	1.98	0.80
1:B:220:ARG:HD3	1:B:251[A]:ASN:ND2	1.96	0.80
1:A:90:SER:HA	1:A:96[A]:ARG:HH11	1.44	0.79
1:B:184:GLY:H	1:B:211:ASN:HD22	1.26	0.79
4:A:464:1PE:H121	6:A:6073:PEG:H31	1.66	0.77
2:B:469:GOL:H31	8:B:634:HOH:O	1.85	0.77
1:A:120[A]:ARG:CG	1:A:120[A]:ARG:NH1	2.47	0.77
1:B:17:PHE:H	1:B:111:ASN:HD21	1.33	0.76
1:B:204[B]:GLU:CB	2:B:463:GOL:H12	2.16	0.75
1:A:280[B]:LEU:HD12	1:A:284:TYR:CD2	2.21	0.75
1:B:204[B]:GLU:HB2	2:B:463:GOL:H12	1.69	0.75
1:A:184:GLY:H	1:A:211:ASN:HD22	1.34	0.75
1:A:280[B]:LEU:CD1	1:A:284:TYR:HD2	1.99	0.74
1:B:31:ASN:HB2	1:B:72:THR:HB	1.70	0.74
1:B:40[B]:ARG:HG2	1:B:40[B]:ARG:NH1	2.00	0.74
1:B:368:SER:OG	2:B:466:GOL:H32	1.87	0.73
1:B:220:ARG:HD3	1:B:251[A]:ASN:HD22	1.53	0.73
1:A:454:PRO:HA	6:A:470:PEG:H21	1.70	0.73
1:B:369:ASP:OD1	2:B:466:GOL:H31	1.89	0.73
1:B:96:ARG:HH11	1:B:96:ARG:CG	2.00	0.72
1:B:45[B]:LEU:HD11	1:B:55:GLN:HG3	1.72	0.72
1:A:280[B]:LEU:CD1	1:A:284:TYR:CD2	2.73	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:377[B]:GLU:OE1	1:A:396:ARG:NH1	2.20	0.71
8:A:1027:HOH:O	2:B:466:GOL:H12	1.90	0.71
1:A:280[B]:LEU:HD12	1:A:284:TYR:CE2	2.26	0.70
1:A:29:ILE:HD13	1:A:43[B]:GLN:HG2	1.72	0.70
1:A:31:ASN:OD1	1:A:41:ARG:HG2	1.92	0.69
1:A:187:ASN:O	1:A:191[A]:GLN:HG3	1.93	0.67
2:B:461:GOL:H12	8:B:820:HOH:O	1.93	0.67
1:B:451:LYS:O	1:B:457[B]:ARG:HG3	1.94	0.67
1:B:132:SER:H	1:B:414:GLN:HE22	1.44	0.66
1:A:96[A]:ARG:NH1	1:A:210:LEU:O	2.29	0.66
1:A:96[B]:ARG:NH2	8:A:568:HOH:O	2.27	0.66
1:B:204[A]:GLU:HB2	2:B:463:GOL:H12	1.77	0.65
1:A:96[B]:ARG:HD3	8:A:628:HOH:O	1.96	0.65
1:B:31:ASN:ND2	1:B:41:ARG:HD3	2.12	0.64
1:B:72:THR:CG2	8:B:1080:HOH:O	2.45	0.64
1:A:43[B]:GLN:HG3	1:A:57:PHE:CZ	2.33	0.64
1:B:45[B]:LEU:CD1	1:B:55:GLN:HG3	2.27	0.63
1:A:90:SER:CB	1:A:96[A]:ARG:NH1	2.62	0.62
1:A:399[B]:LYS:HE3	8:A:627:HOH:O	1.98	0.62
1:B:12:ALA:O	1:B:55:GLN:NE2	2.33	0.62
1:A:186:THR:HA	2:A:469:GOL:H12	1.82	0.62
1:A:132:SER:H	1:A:414:GLN:HE22	1.47	0.61
1:A:280[B]:LEU:HD11	1:A:320:TYR:HD1	1.65	0.61
1:B:142:ARG:NH1	6:B:6073:PEG:H42	2.16	0.60
1:B:184:GLY:H	1:B:211:ASN:ND2	1.99	0.60
1:B:31:ASN:HD21	1:B:41:ARG:HD3	1.68	0.59
5:A:1474:AES:N8	8:A:898:HOH:O	2.22	0.58
1:A:43[B]:GLN:HG3	1:A:57:PHE:HZ	1.69	0.58
1:A:60:THR:HG22	8:A:647:HOH:O	2.03	0.58
1:B:172:SER:OG	6:B:6073:PEG:H41	2.03	0.57
1:B:106:GLN:NE2	1:B:237:GLU:OE1	2.32	0.57
1:B:259:MET:O	1:B:259:MET:HG2	2.04	0.57
1:A:90:SER:CB	1:A:96[A]:ARG:HH12	2.19	0.56
1:B:17:PHE:H	1:B:111:ASN:ND2	2.03	0.56
1:A:263[A]:ARG:NH2	8:A:751:HOH:O	2.37	0.56
1:B:258[A]:GLN:HE21	1:B:258[A]:GLN:HA	1.69	0.56
1:A:345:PRO:HG3	1:B:318:SER:HB2	1.87	0.56
1:A:21:THR:HG1	1:A:71:PHE:HE2	1.54	0.56
1:B:72:THR:HG22	8:B:1080:HOH:O	2.06	0.55
1:B:375:TYR:CZ	1:B:379:ARG:HD2	2.41	0.55
1:B:150:SER:OG	1:B:156:HIS:HD2	1.90	0.54
1:B:384:LEU:HD21	2:B:467:GOL:H32	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:469:GOL:H12	8:B:1000:HOH:O	2.07	0.53
1:B:178:VAL:O	1:B:206:ALA:HA	2.08	0.53
1:A:128:GLN:NE2	1:A:422:ILE:H	2.07	0.53
1:B:32:ILE:HG22	1:B:34:MET:CE	2.39	0.53
1:B:204[B]:GLU:HB3	2:B:463:GOL:H12	1.91	0.53
1:A:184:GLY:H	1:A:211:ASN:ND2	2.07	0.52
1:A:120[A]:ARG:HG3	1:A:120[A]:ARG:NH1	2.24	0.52
2:B:462:GOL:H32	6:B:465:PEG:H21	1.92	0.52
1:A:162:GLN:HE21	1:A:166:GLN:HE22	1.57	0.51
1:A:263[A]:ARG:CZ	8:A:751:HOH:O	2.59	0.51
1:B:116:ASN:HD22	1:B:118:TYR:H	1.59	0.50
1:A:150:SER:OG	1:A:156:HIS:HD2	1.94	0.50
1:A:377[A]:GLU:OE1	1:B:120:ARG:NH2	2.43	0.50
1:A:347:LEU:HD22	1:B:347:LEU:HD22	1.93	0.50
1:A:22:GLU:HB2	1:A:23[B]:PRO:HD2	1.93	0.50
3:A:462:CL:CL	8:A:756:HOH:O	2.56	0.50
1:B:88:ILE:HD13	1:B:194:MET:HG2	1.95	0.49
6:B:6073:PEG:H21	8:B:1013:HOH:O	2.11	0.49
1:B:331:GLU:OE2	8:B:811:HOH:O	2.20	0.49
1:A:199:LYS:HD3	8:A:704:HOH:O	2.12	0.49
1:A:96[A]:ARG:CZ	1:A:210:LEU:O	2.61	0.49
1:B:258[A]:GLN:HE21	1:B:258[A]:GLN:CA	2.23	0.49
1:B:132:SER:H	1:B:414:GLN:NE2	2.11	0.48
1:B:233:TYR:OH	1:B:238:HIS:HE1	1.96	0.48
1:A:238:HIS:HD2	8:A:1081:HOH:O	1.97	0.48
1:B:27:ASN:HA	1:B:43:GLN:HG3	1.95	0.48
1:A:375:TYR:CZ	1:A:379:ARG:HD2	2.49	0.48
1:A:115:MET:O	7:A:471:PGE:H12	2.14	0.48
1:A:443:ARG:HG2	1:A:443:ARG:HH21	1.79	0.48
6:B:6073:PEG:C1	8:B:1013:HOH:O	2.33	0.48
1:A:40[A]:ARG:NH1	8:A:513:HOH:O	2.32	0.47
1:B:369:ASP:OD1	2:B:466:GOL:C3	2.62	0.47
1:B:156:HIS:HE1	8:B:768:HOH:O	1.97	0.47
1:B:14:PRO:HG2	1:B:56[B]:VAL:CG1	2.45	0.47
1:A:443:ARG:HD2	8:A:1091:HOH:O	2.14	0.46
1:B:120:ARG:HD2	1:B:120:ARG:HA	1.80	0.46
1:B:150:SER:OG	1:B:156:HIS:CD2	2.69	0.46
4:A:464:1PE:H262	8:A:767:HOH:O	2.15	0.46
1:B:45[B]:LEU:HD11	1:B:55:GLN:CG	2.42	0.45
1:B:204[B]:GLU:HB3	2:B:463:GOL:C1	2.47	0.45
2:B:462:GOL:H32	6:B:465:PEG:C2	2.47	0.45
1:A:31:ASN:O	1:A:32:ILE:HD13	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:20:LYS:NZ	1:B:52:VAL:HG22	2.32	0.45
1:B:20:LYS:HZ3	1:B:52:VAL:HG22	1.81	0.45
6:A:470:PEG:C4	8:A:590:HOH:O	2.66	0.44
2:A:469:GOL:H11	8:A:968:HOH:O	2.17	0.44
1:B:128:GLN:NE2	1:B:422:ILE:H	2.16	0.44
1:B:258[A]:GLN:NE2	1:B:258[A]:GLN:HA	2.32	0.44
1:B:399[B]:LYS:HE2	8:B:1086:HOH:O	2.17	0.44
1:A:23[B]:PRO:HG2	2:A:461:GOL:H2	1.98	0.44
1:A:156:HIS:HE1	2:A:465:GOL:O3	2.01	0.43
1:B:443:ARG:NH1	8:B:583:HOH:O	2.51	0.43
1:A:305[A]:MET:HE3	8:A:995:HOH:O	2.19	0.43
5:A:1474:AES:H81	5:A:1474:AES:H3	1.36	0.43
1:B:130:GLY:HA2	1:B:420:ARG:O	2.18	0.43
1:B:162:GLN:HE21	1:B:166:GLN:HE22	1.67	0.43
1:A:438:GLU:CD	1:A:456:HIS:HE2	2.22	0.43
1:B:40[A]:ARG:NH2	1:B:56[A]:VAL:HG11	2.35	0.42
1:B:20:LYS:HB2	1:B:20:LYS:HE2	1.47	0.42
1:A:132:SER:H	1:A:414:GLN:NE2	2.16	0.42
1:A:248:ASP:HB2	2:A:465:GOL:C3	2.50	0.42
1:A:233:TYR:OH	1:A:238:HIS:HE1	2.02	0.42
7:A:471:PGE:H2	8:A:578:HOH:O	2.20	0.42
2:B:462:GOL:C3	6:B:465:PEG:H21	2.49	0.42
1:B:211:ASN:ND2	1:B:220:ARG:HG3	2.35	0.41
1:A:186:THR:CA	2:A:469:GOL:H12	2.48	0.41
1:B:142:ARG:HH11	6:B:6073:PEG:H42	1.84	0.41
1:B:194:MET:HE2	8:B:638:HOH:O	2.20	0.41
1:A:124:LYS:O	1:A:125:ASP:HB2	2.20	0.41
1:B:34:MET:HE2	1:B:34:MET:HA	2.03	0.41
1:B:215:ASP:O	1:B:216:PRO:C	2.59	0.41
1:A:181:ALA:HB3	1:A:246:LEU:HD23	2.04	0.41
1:A:14:PRO:HD2	1:A:56:VAL:CG2	2.51	0.40
1:B:14:PRO:HG2	1:B:56[B]:VAL:HG13	2.02	0.40
1:B:247:THR:HA	1:B:248[A]:ASP:HA	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	454/460 (99%)	444 (98%)	10 (2%)	0	100	100
1	B	437/460 (95%)	427 (98%)	9 (2%)	1 (0%)	56	33
All	All	891/920 (97%)	871 (98%)	19 (2%)	1 (0%)	59	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	13	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	377/374 (101%)	364 (97%)	13 (3%)	49	23
1	B	366/374 (98%)	354 (97%)	12 (3%)	50	25
All	All	743/748 (99%)	718 (97%)	25 (3%)	53	23

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	ILE
1	A	120[A]	ARG
1	A	120[B]	ARG
1	A	199	LYS
1	A	204[A]	GLU
1	A	204[B]	GLU
1	A	222	VAL
1	A	294	LYS
1	A	320	TYR
1	A	390	LYS
1	A	445[A]	ASP
1	A	445[B]	ASP
1	A	446	ASN
1	B	39	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	72	THR
1	B	96	ARG
1	B	101	ARG
1	B	116	ASN
1	B	120	ARG
1	B	258[A]	GLN
1	B	258[B]	GLN
1	B	320	TYR
1	B	445	ASP
1	B	447	LYS
1	B	454	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	128	GLN
1	A	138	ASN
1	A	156	HIS
1	A	166	GLN
1	A	211	ASN
1	A	238	HIS
1	A	264	ASN
1	A	299	GLN
1	A	312	HIS
1	A	414	GLN
1	A	417	ASN
1	A	431	GLN
1	B	31	ASN
1	B	111	ASN
1	B	116	ASN
1	B	128	GLN
1	B	156	HIS
1	B	166	GLN
1	B	211	ASN
1	B	238	HIS
1	B	299	GLN
1	B	312	HIS
1	B	414	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 23 ligands modelled in this entry, 3 are monoatomic - leaving 20 for Mogul analysis.

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	$\# Z > 2$
5	AES	A	1474	-	13,13,13	2.27	3 (23%)	18,18,18	2.44	10 (55%)
2	GOL	A	461	-	5,5,5	0.48	0	5,5,5	0.76	0
2	GOL	A	463	-	5,5,5	0.41	0	5,5,5	0.74	0
4	1PE	A	464	-	15,15,15	0.61	0	14,14,14	0.75	0
2	GOL	A	465	-	5,5,5	0.58	0	5,5,5	1.08	0
4	1PE	A	466	-	12,12,15	0.51	0	11,11,14	0.97	1 (9%)
2	GOL	A	467	-	5,5,5	0.37	0	5,5,5	0.83	0
2	GOL	A	468	-	5,5,5	0.40	0	5,5,5	0.35	0
2	GOL	A	469	-	5,5,5	0.85	0	5,5,5	1.66	1 (20%)
6	PEG	A	470	-	6,6,6	0.77	0	5,5,5	0.96	0
7	PGE	A	471	-	9,9,9	0.99	0	8,8,8	0.96	1 (12%)
6	PEG	A	6073	-	6,6,6	0.73	0	5,5,5	0.31	0
2	GOL	B	461	-	5,5,5	0.73	0	5,5,5	1.55	1 (20%)
2	GOL	B	462	-	5,5,5	0.45	0	5,5,5	0.98	0
2	GOL	B	463	-	5,5,5	0.80	0	5,5,5	1.70	3 (60%)
6	PEG	B	465	-	6,6,6	0.63	0	5,5,5	1.45	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	B	466	-	5,5,5	1.02	0	5,5,5	0.89	0
2	GOL	B	467	-	5,5,5	0.56	0	5,5,5	1.54	1 (20%)
2	GOL	B	469	-	5,5,5	0.26	0	5,5,5	1.29	0
6	PEG	B	6073	-	6,6,6	1.18	0	5,5,5	0.88	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
5	AES	A	1474	-	-	0/9/9/9	0/1/1/1
2	GOL	A	461	-	-	0/4/4/4	0/0/0/0
2	GOL	A	463	-	-	0/4/4/4	0/0/0/0
4	1PE	A	464	-	-	0/13/13/13	0/0/0/0
2	GOL	A	465	-	-	0/4/4/4	0/0/0/0
4	1PE	A	466	-	-	0/10/10/13	0/0/0/0
2	GOL	A	467	-	-	0/4/4/4	0/0/0/0
2	GOL	A	468	-	-	0/4/4/4	0/0/0/0
2	GOL	A	469	-	-	0/4/4/4	0/0/0/0
6	PEG	A	470	-	-	0/4/4/4	0/0/0/0
7	PGE	A	471	-	-	0/7/7/7	0/0/0/0
6	PEG	A	6073	-	-	0/4/4/4	0/0/0/0
2	GOL	B	461	-	-	0/4/4/4	0/0/0/0
2	GOL	B	462	-	-	0/4/4/4	0/0/0/0
2	GOL	B	463	-	-	0/4/4/4	0/0/0/0
6	PEG	B	465	-	-	0/4/4/4	0/0/0/0
2	GOL	B	466	-	-	0/4/4/4	0/0/0/0
2	GOL	B	467	-	-	0/4/4/4	0/0/0/0
2	GOL	B	469	-	-	0/4/4/4	0/0/0/0
6	PEG	B	6073	-	-	0/4/4/4	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1474	AES	C1-S	-6.12	1.63	1.74
5	A	1474	AES	O1S-S	3.44	1.50	1.42
5	A	1474	AES	O2S-S	-3.28	1.34	1.42

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1474	AES	O2S-S-C1	5.59	114.99	111.02
5	A	1474	AES	F-S-C1	4.06	112.16	102.39
5	A	1474	AES	F-S-O1S	-3.14	98.92	106.44
2	B	467	GOL	C3-C2-C1	-3.04	97.84	111.26
2	A	469	GOL	O2-C2-C1	-2.94	94.82	108.22
5	A	1474	AES	C5-C4-C3	2.91	123.07	118.16
2	B	461	GOL	O2-C2-C1	2.91	121.49	108.22
5	A	1474	AES	O1S-S-C1	-2.62	109.16	111.02
5	A	1474	AES	C7-C8-N8	-2.52	105.98	112.31
2	B	463	GOL	O2-C2-C3	2.25	118.47	108.22
5	A	1474	AES	C8-C7-C4	-2.18	105.90	112.58
5	A	1474	AES	C2-C3-C4	-2.15	117.88	121.05
5	A	1474	AES	C6-C1-S	2.11	123.05	119.61
4	A	466	1PE	OH5-C25-C15	-2.08	101.01	110.47
2	B	463	GOL	O3-C3-C2	2.02	119.56	109.71
2	B	463	GOL	C3-C2-C1	2.01	120.14	111.26
6	B	465	PEG	O2-C2-C1	2.01	120.29	110.61
7	A	471	PGE	O3-C5-C6	2.01	120.26	110.61
5	A	1474	AES	O2S-S-O1S	-2.00	112.48	118.98

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	436/460 (94%)	-0.42	7 (1%) 68 74	12, 20, 36, 53	0
1	B	427/460 (92%)	-0.40	8 (1%) 64 69	12, 19, 36, 47	0
All	All	863/920 (93%)	-0.41	15 (1%) 67 72	12, 19, 36, 53	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	12	ALA	6.4
1	A	270	ARG	4.3
1	B	258[A]	GLN	4.1
1	B	69	VAL	3.9
1	B	12	ALA	3.8
1	A	60	THR	3.5
1	A	70	ILE	3.4
1	A	58	GLU	2.7
1	B	57	PHE	2.5
1	B	98	GLY	2.5
1	B	311	THR	2.4
1	B	188	GLU	2.4
1	A	455	ALA	2.1
1	A	59	GLY	2.0
1	B	310	ILE	2.0

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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
2	GOL	B	469	6/6	0.21	18.05	52,55,56,57	0
2	GOL	A	463	6/6	0.20	5.17	61,65,66,70	0
2	GOL	A	465	6/6	0.16	4.76	47,49,50,51	0
2	GOL	B	466	6/6	0.15	4.08	31,34,41,44	0
2	GOL	A	467	6/6	0.15	3.95	24,49,52,53	0
4	1PE	A	464	16/16	0.15	3.66	37,50,66,66	0
2	GOL	B	463	6/6	0.21	3.59	37,46,50,53	0
2	GOL	B	467	6/6	0.23	3.53	25,50,54,55	0
6	PEG	B	6073	7/7	0.17	3.47	21,32,34,35	0
2	GOL	A	461	6/6	0.15	2.97	39,44,48,51	0
2	GOL	B	462	6/6	0.14	2.58	44,52,57,57	0
6	PEG	B	465	7/7	0.20	2.29	49,53,58,59	0
6	PEG	A	6073	7/7	0.18	1.59	63,66,69,69	0
6	PEG	A	470	7/7	0.18	1.56	46,48,50,51	0
4	1PE	A	466	13/16	0.09	1.36	41,44,51,53	0
2	GOL	A	468	6/6	0.25	1.35	75,76,77,78	0
2	GOL	A	469	6/6	0.13	1.30	24,35,39,43	0
5	AES	A	1474	13/13	0.10	1.24	18,24,34,42	13
7	PGE	A	471	10/10	0.13	0.85	40,51,60,60	0
3	CL	B	464	1/1	0.11	0.73	54,54,54,54	0
2	GOL	B	461	6/6	0.07	-0.33	16,22,36,40	0
3	CL	B	468	1/1	0.06	-0.38	23,23,23,23	0
3	CL	A	462	1/1	0.04	-2.63	20,20,20,20	0

6.5 Other polymers ⓘ

There are no such residues in this entry.