



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2023 – 12:36 PM EDT

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 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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

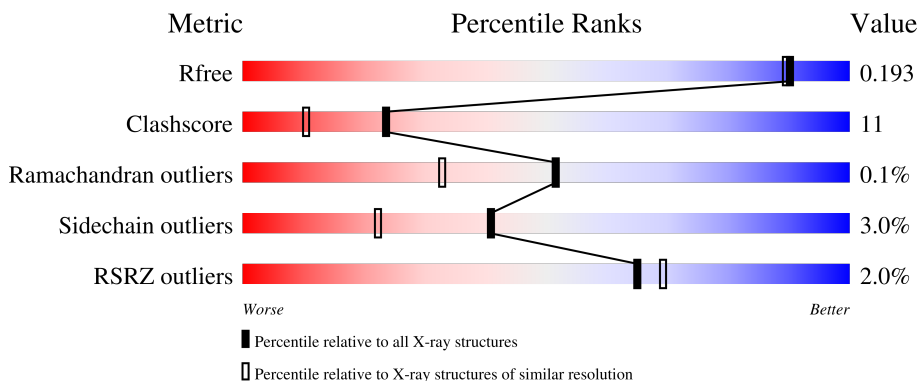
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (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 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 $\leq 5\%$. 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	460	
1	B	460	

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	GOL	B	463	-	X	X	-
2	GOL	B	466	-	-	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 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 V-type ATP synthase beta chain.

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

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
			Total	C	O		
2	A	1	6	3	3	0	0

Continued on next page...

Continued from previous page...

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

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

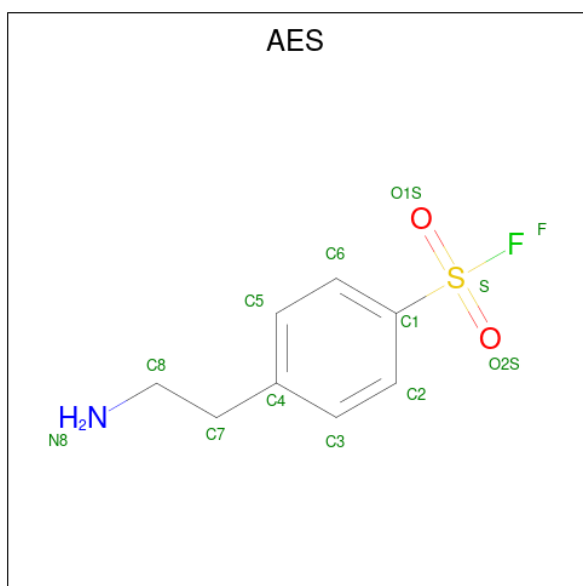
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	2	Total	Cl	0	0
			2	2		

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



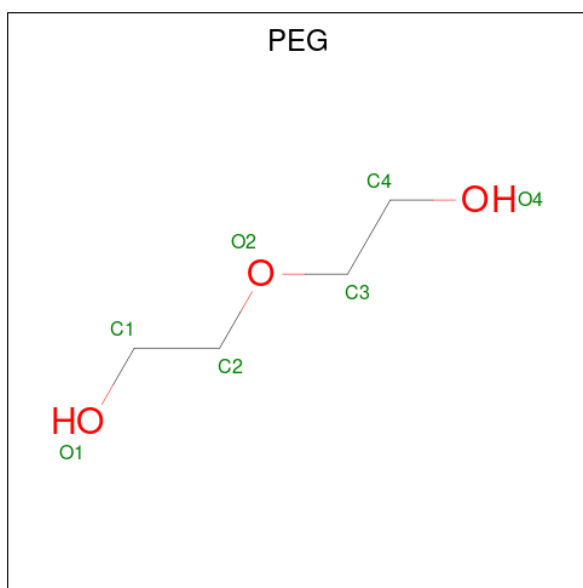
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			16	10	6		
4	A	1	Total	C	O	0	0
			13	8	5		

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



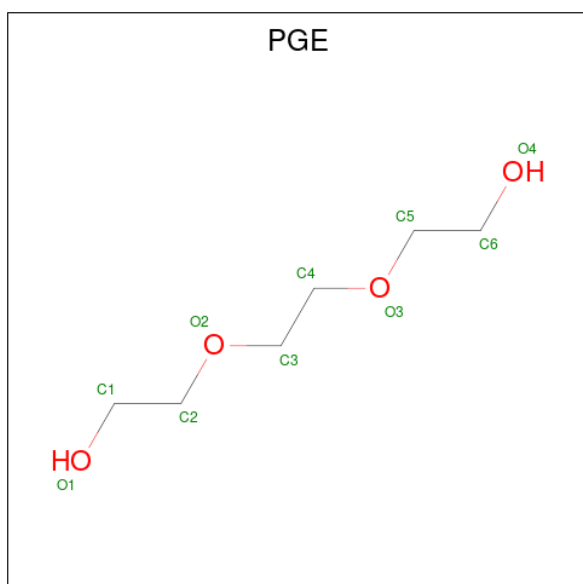
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
5	A	1	Total	C	F	N	O	S	0	0
			13	8	1	1	2	1		

- 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 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0

- 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		

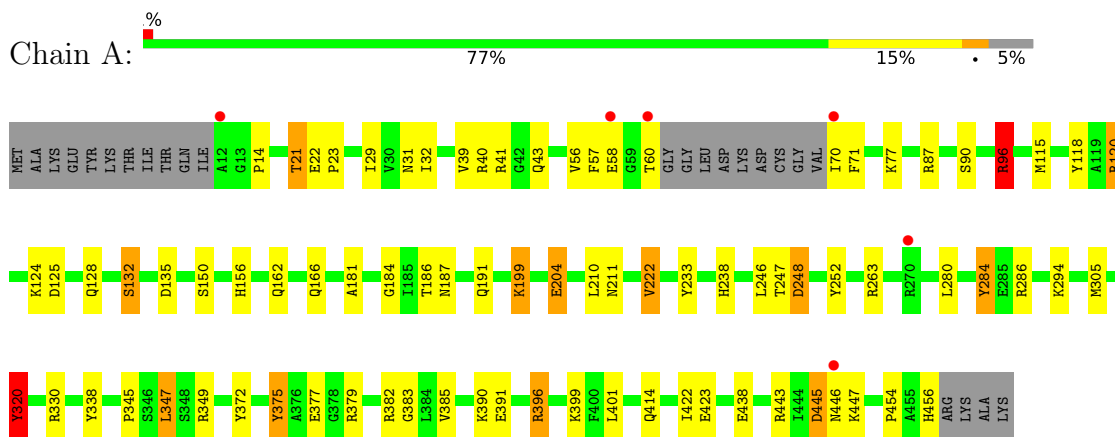
- Molecule 8 is water.

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

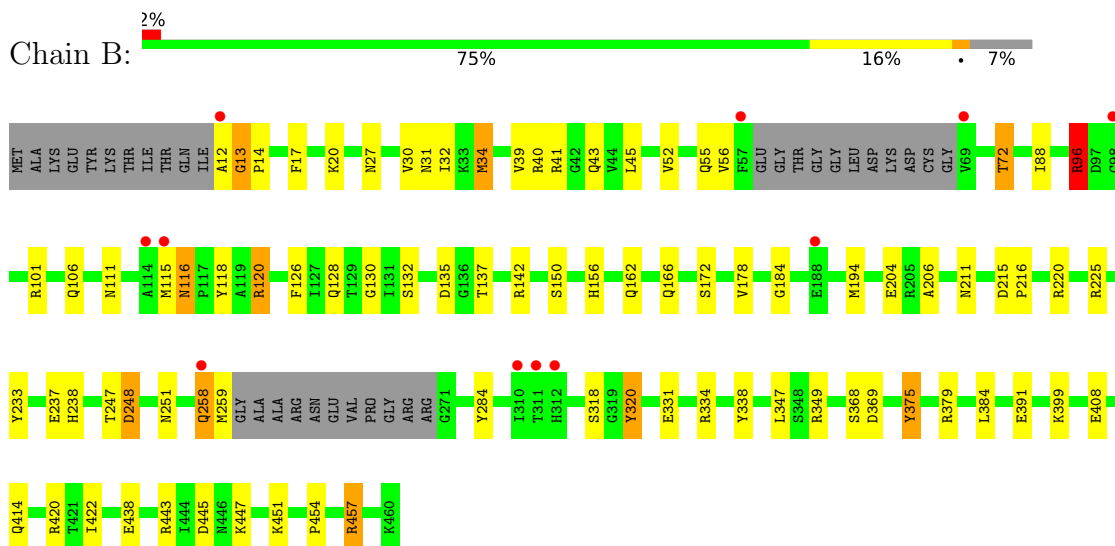
3 Residue-property plots [i](#)

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: V-type ATP synthase beta chain



- Molecule 1: V-type ATP synthase beta chain



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) 99.6 (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)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.146 , 0.193 0.146 , 0.193	Depositor DCC
R_{free} test set	5072 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	19.5	Xtrriage
Anisotropy	0.080	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 67.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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.

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.

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: PEG, GOL, PGE, AES, CL, 1PE

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	6
1	B	0	3
All	All	1	9

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 (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	247	THR	Peptide,Mainchain
1	A	338	TYR	Peptide,Mainchain
1	A	96[A]	ARG	Sidechain
1	A	96[B]	ARG	Sidechain
1	B	248[A]	ASP	Mainchain
1	B	338	TYR	Peptide,Mainchain

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	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

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 11.

All (159) 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: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:HG2	1:B:40[B]:ARG:HH11	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:HH11	1:A:120[A]:ARG:HG2	1.34	0.93
1:B:96:ARG:HG3	1:B:96:ARG:NH1	1.86	0.91
1:A:120[A]:ARG:HH11	1:A:120[A]:ARG:CG	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:HG3	1:B:96:ARG:HH11	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:HG2	1:B:259:MET:O	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:178:VAL:O	1:B:206:ALA:HA	2.08	0.53
2:B:469:GOL:H12	8:B:1000:HOH:O	2.07	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:NH1	1:A:120[A]:ARG:HG3	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:22:GLU:HB2	1:A:23[B]:PRO:HD2	1.93	0.50
1:A:347:LEU:HD22	1:B:347:LEU:HD22	1.93	0.50
1:A:377[A]:GLU:OE1	1:B:120:ARG:NH2	2.43	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
1:B:331:GLU:OE2	8:B:811:HOH:O	2.20	0.49
6:B:6073:PEG:H21	8:B:1013:HOH:O	2.11	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:115:MET:O	7:A:471:PGE:H12	2.14	0.48
1:A:375:TYR:CZ	1:A:379:ARG:HD2	2.49	0.48
1:A:443:ARG:HH21	1:A:443:ARG:HG2	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:156:HIS:HE1	8:B:768:HOH:O	1.97	0.47
1:B:369:ASP:OD1	2:B:466:GOL:C3	2.62	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:HA	1:B:120:ARG:HD2	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:A:469:GOL:H11	8:A:968:HOH:O	2.17	0.44
6:A:470:PEG:C4	8:A:590:HOH:O	2.66	0.44
1:B:128:GLN:NE2	1:B:422:ILE:H	2.16	0.44
1:B:258[A]:GLN:HA	1:B:258[A]:GLN:NE2	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:H3	5:A:1474:AES:H81	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:20:LYS:HB2	1:B:20:LYS:HE2	1.47	0.42
1:B:40[A]:ARG:NH2	1:B:56[A]:VAL:HG11	2.35	0.42
1:A:132:SER:H	1:A:414:GLN:NE2	2.16	0.42
1:A:233:TYR:OH	1:A:238:HIS:HE1	2.02	0.42
1:A:248:ASP:HB2	2:A:465:GOL:C3	2.50	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:A:124:LYS:O	1:A:125:ASP:HB2	2.20	0.41
1:B:194:MET:HE2	8:B:638:HOH:O	2.20	0.41
1:B:34:MET:HA	1:B:34:MET:HE2	2.03	0.41
1:A:181:ALA:HB3	1:A:246:LEU:HD23	2.04	0.41
1:B:215:ASP:O	1:B:216:PRO:C	2.59	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 [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	454/460 (99%)	444 (98%)	10 (2%)	0	100	100
1	B	437/460 (95%)	427 (98%)	9 (2%)	1 (0%)	47	30
All	All	891/920 (97%)	871 (98%)	19 (2%)	1 (0%)	51	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	13	GLY

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	377/374 (101%)	364 (97%)	13 (3%)	37	18
1	B	366/374 (98%)	354 (97%)	12 (3%)	38	19
All	All	743/748 (99%)	718 (97%)	25 (3%)	41	18

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Sometimes 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 [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](#)

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	$\# Z > 2$
2	GOL	A	467	-	5,5,5	0.37	0	5,5,5	0.90	0
2	GOL	B	466	-	5,5,5	1.05	0	5,5,5	0.91	0
4	1PE	A	464	-	15,15,15	0.60	0	14,14,14	0.78	0
2	GOL	A	465	-	5,5,5	0.62	0	5,5,5	1.19	0
6	PEG	A	470	-	6,6,6	0.77	0	5,5,5	1.00	0
6	PEG	B	6073	-	6,6,6	1.19	0	5,5,5	0.97	0
2	GOL	B	461	-	5,5,5	0.72	0	5,5,5	1.57	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	B	463	-	5,5,5	0.86	0	5,5,5	1.72	2 (40%)
5	AES	A	1474	-	11,13,13	1.76	2 (18%)	16,18,18	2.22	7 (43%)
2	GOL	B	462	-	5,5,5	0.47	0	5,5,5	0.98	0
2	GOL	B	467	-	5,5,5	0.58	0	5,5,5	1.76	1 (20%)
6	PEG	B	465	-	6,6,6	0.63	0	5,5,5	1.59	2 (40%)
2	GOL	A	463	-	5,5,5	0.47	0	5,5,5	0.62	0
2	GOL	B	469	-	5,5,5	0.28	0	5,5,5	1.42	2 (40%)
2	GOL	A	468	-	5,5,5	0.42	0	5,5,5	0.37	0
2	GOL	A	469	-	5,5,5	0.91	0	5,5,5	1.82	1 (20%)
7	PGE	A	471	-	9,9,9	0.99	0	8,8,8	1.05	1 (12%)
6	PEG	A	6073	-	6,6,6	0.73	0	5,5,5	0.39	0
2	GOL	A	461	-	5,5,5	0.54	0	5,5,5	0.69	0
4	1PE	A	466	-	12,12,15	0.34	0	11,11,14	0.90	1 (9%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	467	-	-	4/4/4/4	-
2	GOL	B	466	-	-	2/4/4/4	-
4	1PE	A	464	-	-	6/13/13/13	-
2	GOL	A	465	-	-	3/4/4/4	-
6	PEG	A	470	-	-	3/4/4/4	-
6	PEG	B	6073	-	-	2/4/4/4	-
2	GOL	B	461	-	-	4/4/4/4	-
2	GOL	B	463	-	-	4/4/4/4	-
5	AES	A	1474	-	-	6/9/9/9	0/1/1/1
2	GOL	B	462	-	-	0/4/4/4	-
2	GOL	B	467	-	-	4/4/4/4	-
6	PEG	B	465	-	-	1/4/4/4	-
2	GOL	A	463	-	-	2/4/4/4	-
2	GOL	B	469	-	-	0/4/4/4	-
2	GOL	A	468	-	-	2/4/4/4	-
2	GOL	A	469	-	-	0/4/4/4	-
7	PGE	A	471	-	-	7/7/7/7	-
6	PEG	A	6073	-	-	3/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	461	-	-	1/4/4/4	-
4	1PE	A	466	-	-	7/10/10/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1474	AES	O1S-S	3.76	1.50	1.42
5	A	1474	AES	O2S-S	-3.57	1.34	1.42

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1474	AES	O2S-S-C1	4.16	114.99	110.74
2	B	467	GOL	C3-C2-C1	-3.57	97.84	111.70
5	A	1474	AES	F-S-O1S	-3.33	98.92	106.49
2	A	469	GOL	O2-C2-C1	-3.25	94.82	109.12
5	A	1474	AES	C5-C4-C3	3.12	123.07	118.17
5	A	1474	AES	C8-C7-C4	-3.02	105.90	112.85
2	B	461	GOL	O2-C2-C1	2.81	121.49	109.12
5	A	1474	AES	C6-C1-S	2.75	123.05	119.44
6	B	465	PEG	O2-C2-C1	2.33	120.29	110.07
7	A	471	PGE	O3-C5-C6	2.32	120.26	110.07
5	A	1474	AES	C2-C3-C4	-2.29	117.88	121.03
2	B	463	GOL	C3-C2-C1	2.17	120.14	111.70
2	B	463	GOL	O2-C2-C3	2.12	118.47	109.12
5	A	1474	AES	O2S-S-O1S	-2.11	112.48	119.07
4	A	466	1PE	OH5-C25-C15	-2.08	101.01	110.39
2	B	469	GOL	C3-C2-C1	-2.05	103.73	111.70
2	B	469	GOL	O1-C1-C2	-2.02	100.54	110.20
6	B	465	PEG	O2-C3-C4	-2.01	101.22	110.07

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	463	GOL	O1-C1-C2-C3
2	A	465	GOL	O1-C1-C2-C3
2	A	467	GOL	C1-C2-C3-O3
2	B	461	GOL	O1-C1-C2-C3
2	B	463	GOL	O1-C1-C2-C3
2	B	463	GOL	C1-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	467	GOL	O1-C1-C2-C3
5	A	1474	AES	C4-C7-C8-N8
7	A	471	PGE	C6-C5-O3-C4
6	A	6073	PEG	O2-C3-C4-O4
2	B	466	GOL	O2-C2-C3-O3
6	B	6073	PEG	O1-C1-C2-O2
7	A	471	PGE	O2-C3-C4-O3
4	A	466	1PE	OH5-C14-C24-OH4
4	A	464	1PE	OH2-C12-C22-OH3
4	A	466	1PE	OH7-C16-C26-OH6
4	A	464	1PE	C25-C15-OH6-C26
2	A	468	GOL	O1-C1-C2-C3
2	B	461	GOL	C1-C2-C3-O3
2	B	466	GOL	C1-C2-C3-O3
2	A	465	GOL	O1-C1-C2-O2
2	A	467	GOL	O2-C2-C3-O3
2	A	468	GOL	O1-C1-C2-O2
2	B	463	GOL	O1-C1-C2-O2
2	B	463	GOL	O2-C2-C3-O3
2	B	467	GOL	O1-C1-C2-O2
5	A	1474	AES	C3-C4-C7-C8
4	A	466	1PE	OH6-C15-C25-OH5
6	A	470	PEG	O2-C3-C4-O4
6	B	465	PEG	O2-C3-C4-O4
7	A	471	PGE	O1-C1-C2-O2
2	A	463	GOL	O1-C1-C2-O2
2	B	461	GOL	O1-C1-C2-O2
4	A	464	1PE	OH5-C14-C24-OH4
5	A	1474	AES	C5-C4-C7-C8
5	A	1474	AES	C2-C1-S-O1S
5	A	1474	AES	C6-C1-S-O1S
2	A	467	GOL	O1-C1-C2-O2
7	A	471	PGE	C4-C3-O2-C2
7	A	471	PGE	C1-C2-O2-C3
5	A	1474	AES	C2-C1-S-F
4	A	464	1PE	C13-C23-OH3-C22
4	A	466	1PE	C14-C24-OH4-C13
6	A	470	PEG	C4-C3-O2-C2
2	A	465	GOL	O2-C2-C3-O3
4	A	464	1PE	C12-C22-OH3-C23
6	B	6073	PEG	O2-C3-C4-O4
4	A	466	1PE	C25-C15-OH6-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	A	6073	PEG	C1-C2-O2-C3
2	A	461	GOL	O1-C1-C2-O2
7	A	471	PGE	C3-C4-O3-C5
2	B	461	GOL	O2-C2-C3-O3
4	A	466	1PE	C23-C13-OH4-C24
4	A	464	1PE	OH6-C15-C25-OH5
2	A	467	GOL	O1-C1-C2-C3
4	A	466	1PE	C24-C14-OH5-C25
2	B	467	GOL	O2-C2-C3-O3
6	A	470	PEG	C1-C2-O2-C3
2	B	467	GOL	C1-C2-C3-O3
6	A	6073	PEG	O1-C1-C2-O2
7	A	471	PGE	O3-C5-C6-O4

There are no ring outliers.

16 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	466	GOL	4	0
4	A	464	1PE	2	0
2	A	465	GOL	2	0
6	A	470	PEG	2	0
6	B	6073	PEG	7	0
2	B	461	GOL	1	0
2	B	463	GOL	5	0
5	A	1474	AES	2	0
2	B	462	GOL	3	0
2	B	467	GOL	1	0
6	B	465	PEG	3	0
2	B	469	GOL	2	0
2	A	469	GOL	3	0
7	A	471	PGE	2	0
6	A	6073	PEG	1	0
2	A	461	GOL	1	0

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 [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, 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%)	-0.47	6 (1%) 75 79	12, 20, 36, 53	0
1	B	427/460 (92%)	-0.45	11 (2%) 56 60	12, 19, 36, 47	0
All	All	863/920 (93%)	-0.46	17 (1%) 65 69	12, 19, 36, 53	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	12	ALA	7.4
1	A	270	ARG	4.6
1	A	60	THR	4.4
1	B	69	VAL	4.4
1	B	258[A]	GLN	3.9
1	A	70	ILE	3.7
1	B	12	ALA	3.6
1	A	58	GLU	2.6
1	B	188	GLU	2.6
1	B	311	THR	2.5
1	B	57	PHE	2.4
1	B	98	GLY	2.4
1	B	115	MET	2.3
1	B	310	ILE	2.2
1	B	312	HIS	2.1
1	B	114	ALA	2.1
1	A	446	ASN	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, 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	B-factors(\AA^2)	Q<0.9
6	PEG	A	6073	7/7	0.63	0.19	63,66,69,69	0
2	GOL	A	468	6/6	0.70	0.24	75,76,77,78	0
6	PEG	B	465	7/7	0.70	0.21	49,53,58,59	0
2	GOL	B	469	6/6	0.77	0.20	52,55,56,57	0
2	GOL	A	465	6/6	0.80	0.17	47,49,50,51	0
6	PEG	A	470	7/7	0.81	0.18	46,48,50,51	0
2	GOL	A	461	6/6	0.81	0.15	39,44,48,51	0
2	GOL	A	463	6/6	0.83	0.21	61,65,66,70	0
4	1PE	A	464	16/16	0.84	0.16	37,50,66,66	0
2	GOL	B	463	6/6	0.85	0.22	37,46,50,53	0
7	PGE	A	471	10/10	0.87	0.14	40,51,60,60	0
2	GOL	B	462	6/6	0.88	0.15	44,52,57,57	0
3	CL	B	464	1/1	0.90	0.10	54,54,54,54	0
2	GOL	B	467	6/6	0.90	0.22	25,50,54,55	0
2	GOL	A	467	6/6	0.90	0.16	24,49,52,53	0
2	GOL	A	469	6/6	0.91	0.15	24,35,39,43	0
2	GOL	B	466	6/6	0.91	0.15	31,34,41,44	0
6	PEG	B	6073	7/7	0.92	0.17	21,32,34,35	0
4	1PE	A	466	13/16	0.95	0.08	41,44,51,53	0
5	AES	A	1474	13/13	0.96	0.10	18,24,34,42	13
2	GOL	B	461	6/6	0.96	0.07	16,22,36,40	0
3	CL	A	462	1/1	0.99	0.03	20,20,20,20	0
3	CL	B	468	1/1	0.99	0.05	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.