W O R L D W I D E

wwPDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:17 PM GMT

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PDB ID	:	3TGW
Title	:	Crystal structure of subunit B mutant H156A of the A1AO ATP synthase
Authors	:	Tadwal, V.S.; Manimekalai, M.S.S.; Jeyakanthan, J.; Gruber, G.
Deposited on	:	2011-08-18
Resolution	:	1.75 Å(reported)

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 1.75 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.
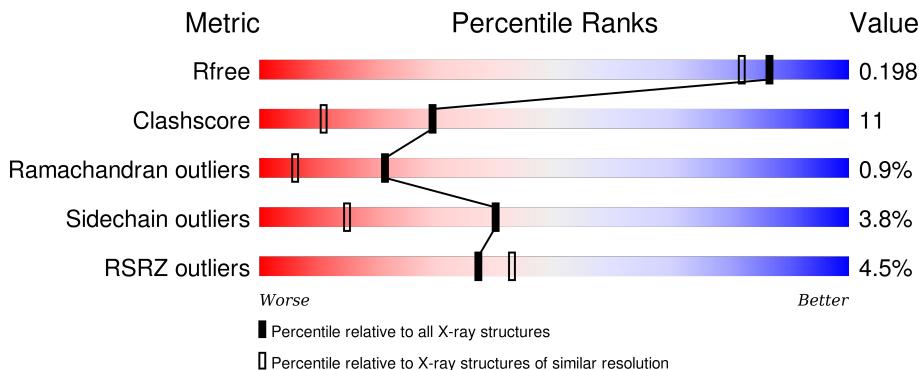
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (1.76-1.76)

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	460	
1	B	460	
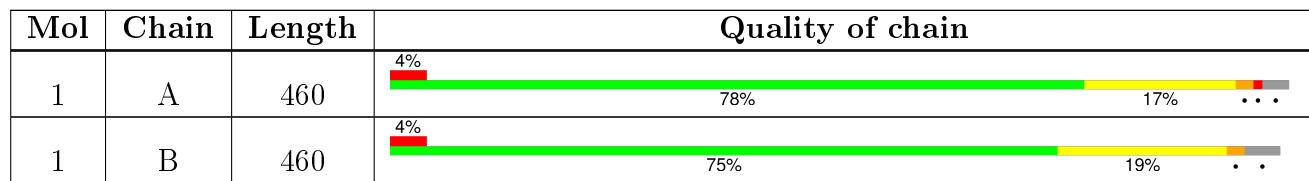
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	462	-	-	X	X
2	GOL	A	463	-	-	-	X
2	GOL	A	464	-	-	X	X
2	GOL	A	465	-	-	-	X
2	GOL	B	462	-	-	-	X
2	GOL	B	463	-	-	-	X
3	P33	A	5936	-	-	-	X
6	PG4	B	6112	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 8180 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
1	A	445	Total	C	N	O	S	0	13	0
			3483	2205	603	663	12			
1	B	441	Total	C	N	O	S	0	14	0
			3458	2188	596	663	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	ALA	SEE REMARK 999	UNP Q60187
A	156	ALA	HIS	ENGINEERED MUTATION	UNP Q60187
B	2	VAL	ALA	SEE REMARK 999	UNP Q60187
B	156	ALA	HIS	ENGINEERED MUTATION	UNP Q60187

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
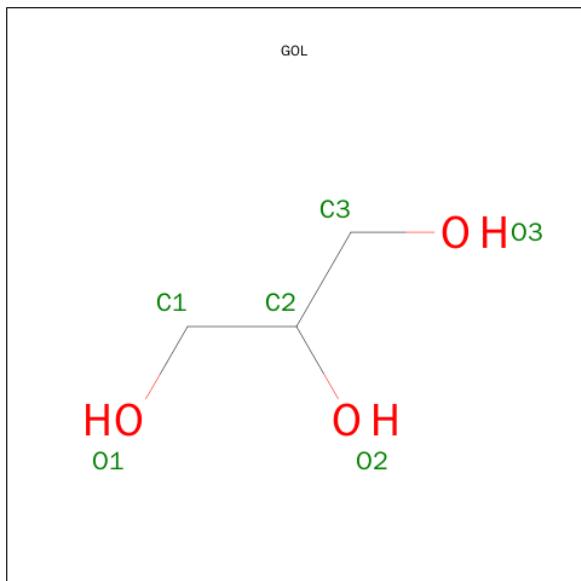
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 6	C 3	O 3	0	0
2	A	1	Total 6	C 3	O 3	0	0
2	A	1	Total 6	C 3	O 3	0	0
2	A	1	Total 6	C 3	O 3	0	0
2	A	1	Total 6	C 3	O 3	0	0
2	A	1	Total 6	C 3	O 3	0	0
2	B	1	Total 6	C 3	O 3	0	0
2	B	1	Total 6	C 3	O 3	0	0
2	B	1	Total 6	C 3	O 3	0	0

- Molecule 3 is 3,6,9,12,15,18-HEXAOXAICOSANE-1,20-DIOL (three-letter code: P33) (formula: $C_{14}H_{30}O_8$).
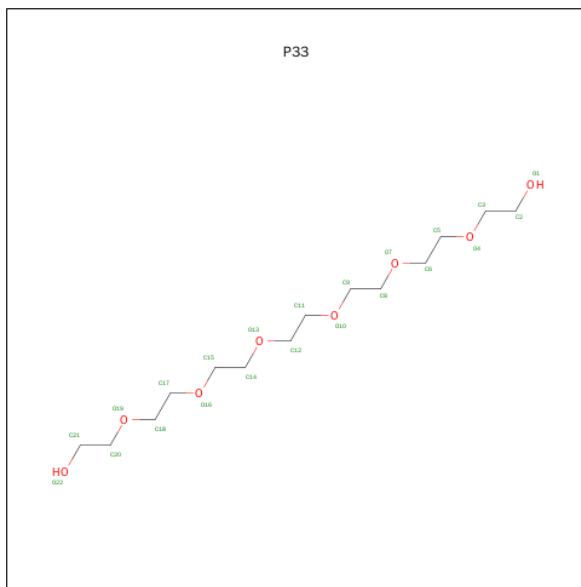
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 22	C 14	O 8	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is 4-(2-AMINOETHYL)BENZENESULFONYL FLUORIDE (three-letter code: AES) (formula: $C_8H_{10}FNO_2S$).
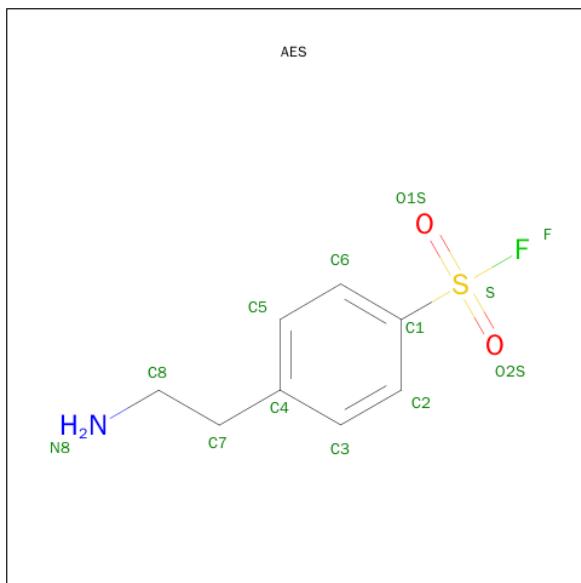
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	B	1	Total 13	C 8	F 1	N 1	O 2	S 1	0	0

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).
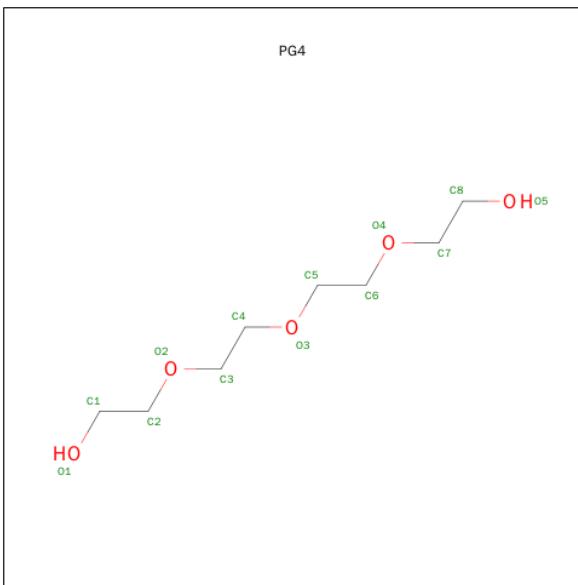
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total 13	C 8	O 5	0	0

- Molecule 7 is 2-(2-METHOXYETHOXY)ETHANOL (three-letter code: PG0) (formula: $C_5H_{12}O_3$).
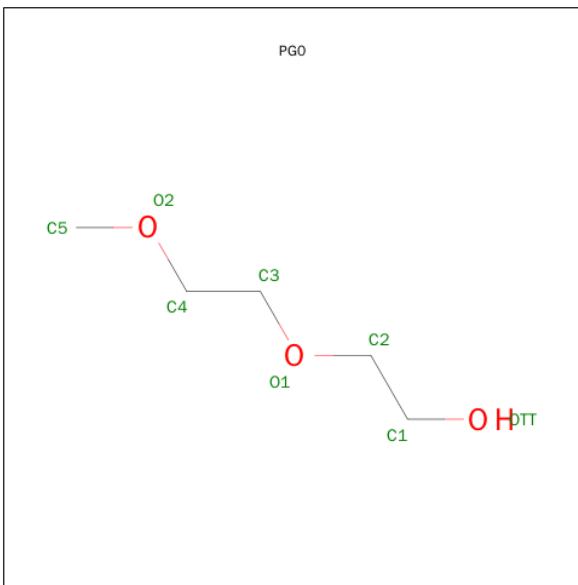
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total 8	C 5	O 3	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	588	Total 588	O 588	0	0
8	B	539	Total 539	O 539	0	0

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
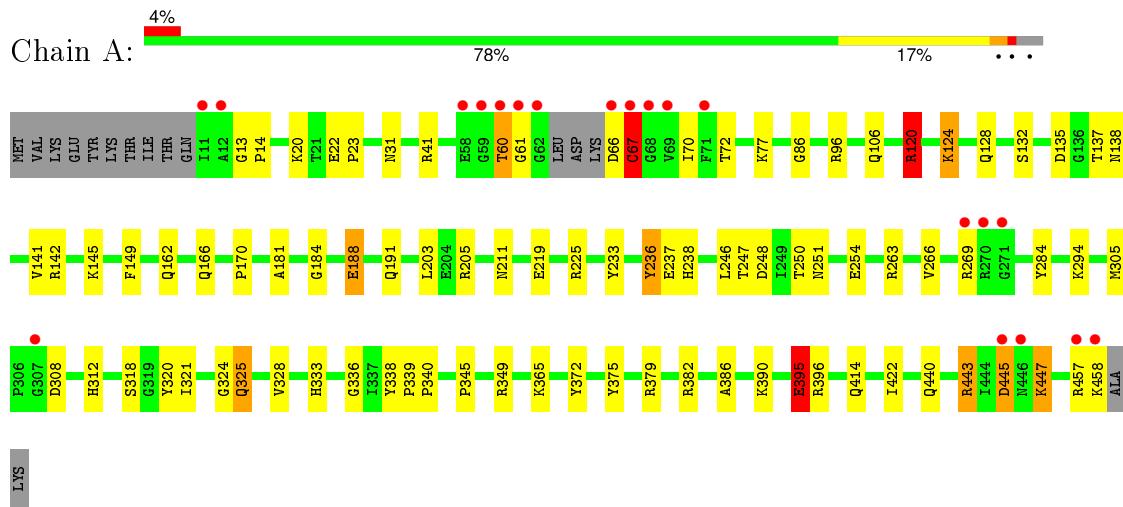
• Molecule 1: V-type ATP synthase beta chain
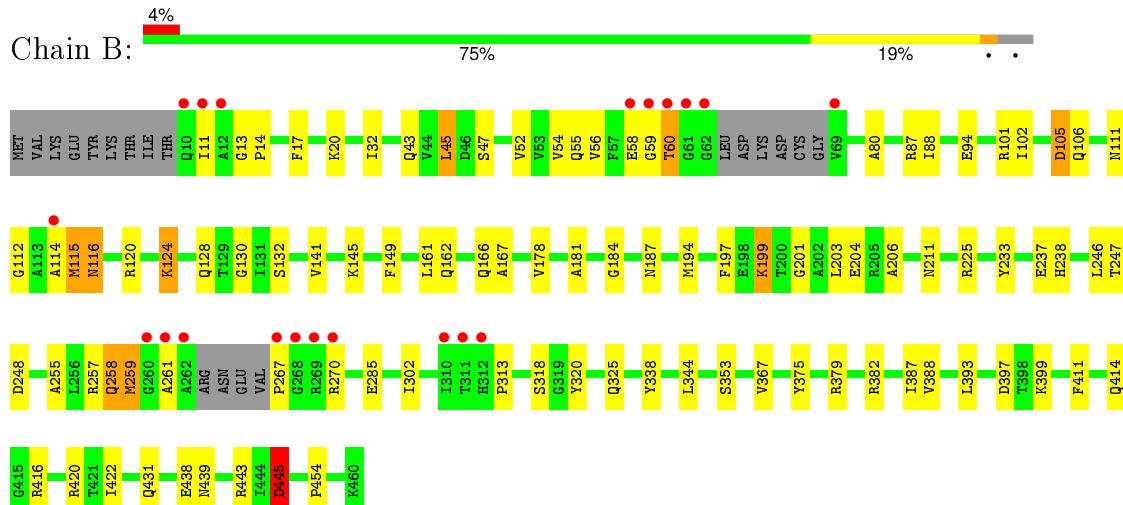
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	73.93Å 95.80Å 130.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.10 – 1.75 20.10 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.4 (20.10-1.75) 99.4 (20.10-1.75)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.61 (at 1.74Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.147 , 0.197 0.149 , 0.198	Depositor DCC
R_{free} test set	4682 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	19.0	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 59.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \mid L \mid > = 0.50, < L^2 > = 0.34$	Xtriage
Outliers	1 of 93384 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	8180	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, AES, CL, PG4, PG0, P33

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	1.20	6/3586 (0.2%)	1.12	16/4857 (0.3%)
1	B	1.21	4/3562 (0.1%)	1.10	12/4822 (0.2%)
All	All	1.21	10/7148 (0.1%)	1.11	28/9679 (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	0	4
1	B	0	5
All	All	0	9

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	395	GLU	CB-CG	-9.64	1.33	1.52
1	A	395	GLU	CG-CD	-6.56	1.42	1.51
1	B	438	GLU	CB-CG	-6.43	1.40	1.52
1	B	411	PHE	CE1-CZ	6.17	1.49	1.37
1	A	77	LYS	CE-NZ	5.70	1.63	1.49
1	A	372	TYR	CD1-CE1	5.14	1.47	1.39
1	B	367	VAL	CB-CG2	5.12	1.63	1.52
1	A	236	TYR	CD2-CE2	5.06	1.47	1.39
1	A	124	LYS	C-N	-5.03	1.22	1.34
1	B	141	VAL	CB-CG2	-5.01	1.42	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	124	LYS	C-N-CA	-9.73	97.38	121.70
1	B	115	MET	CG-SD-CE	8.99	114.58	100.20
1	A	135	ASP	CB-CG-OD1	7.61	125.14	118.30
1	A	120	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	A	248	ASP	CB-CG-OD1	6.98	124.58	118.30
1	B	225	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	B	445[A]	ASP	CB-CG-OD2	6.77	124.39	118.30
1	B	445[B]	ASP	CB-CG-OD2	6.77	124.39	118.30
1	A	248	ASP	N-CA-C	-6.59	93.22	111.00
1	A	382	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	B	124	LYS	C-N-CA	-6.45	105.57	121.70
1	B	116	ASN	N-CA-CB	6.45	122.20	110.60
1	B	248[A]	ASP	N-CA-CB	6.39	122.10	110.60
1	B	248[B]	ASP	N-CA-CB	6.39	122.10	110.60
1	A	225	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	B	393	LEU	CB-CG-CD2	-6.28	100.33	111.00
1	A	225	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	A	135	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	A	120	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	A	248	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	A	349	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	A	124	LYS	N-CA-C	5.62	126.17	111.00
1	A	445	ASP	CB-CG-OD2	5.55	123.30	118.30
1	B	416	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	124	LYS	O-C-N	-5.38	114.09	122.70
1	B	105	ASP	CB-CG-OD1	5.30	123.07	118.30
1	B	161	LEU	CB-CG-CD1	-5.17	102.20	111.00
1	A	137	THR	CA-CB-CG2	-5.06	105.31	112.40

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	247	THR	Mainchain,Peptide
1	A	338	TYR	Mainchain,Peptide
1	B	247	THR	Mainchain,Peptide
1	B	338	TYR	Mainchain,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	3483	0	3516	72	0
1	B	3458	0	3487	80	0
2	A	36	0	47	17	0
2	B	18	0	24	3	0
3	A	22	0	30	7	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	B	13	0	10	4	0
6	B	13	0	18	6	0
7	B	8	0	12	0	0
8	A	588	0	0	26	0
8	B	539	0	0	24	0
All	All	8180	0	7144	161	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 (161) 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:339:PRO:HG2	8:A:571:HOH:O	1.47	1.12
2:B:462:GOL:H2	8:B:1056:HOH:O	1.49	1.09
1:B:445[B]:ASP:HB3	8:B:1100:HOH:O	1.56	1.02
1:A:447:LYS:HD3	8:A:921:HOH:O	1.66	0.93
6:B:6112:PG4:H42	8:B:932:HOH:O	1.67	0.93
1:B:379[B]:ARG:HH11	1:B:382:ARG:HH11	1.21	0.89
1:B:20:LYS:HE3	1:B:52:VAL:HG22	1.61	0.82
1:A:60:THR:HG22	1:A:61:GLY:H	1.41	0.82
1:A:443:ARG:HH21	1:A:443:ARG:HG2	1.46	0.81
1:A:184:GLY:H	1:A:211:ASN:HD22	1.30	0.79
1:B:11:ILE:HG22	1:B:55:GLN:NE2	1.97	0.79
8:A:806:HOH:O	1:B:120:ARG:HG3	1.84	0.77
1:B:17:PHE:H	1:B:111:ASN:HD21	1.31	0.77
1:B:184:GLY:H	1:B:211:ASN:HD22	1.31	0.77
1:B:325[B]:GLN:NE2	6:B:6112:PG4:H52	2.01	0.76
1:B:112:GLY:CA	8:B:886:HOH:O	2.34	0.75
1:B:132:SER:H	1:B:414:GLN:HE22	1.34	0.75
8:A:806:HOH:O	1:B:120:ARG:CG	2.33	0.75
1:B:20:LYS:HE3	1:B:52:VAL:CG2	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:466:GOL:H12	8:A:991:HOH:O	1.86	0.74
1:B:112:GLY:HA2	8:B:886:HOH:O	1.87	0.73
1:B:379[B]:ARG:NH1	1:B:382:ARG:HH11	1.87	0.71
1:B:270:ARG:HH11	1:B:270:ARG:HG2	1.55	0.71
1:B:238:HIS:HD2	8:B:657:HOH:O	1.73	0.70
3:A:5936:P33:H32	8:A:934:HOH:O	1.90	0.70
1:A:251:ASN:ND2	8:A:652:HOH:O	2.24	0.70
1:A:14:PRO:HG2	2:A:465:GOL:H12	1.73	0.70
1:A:22:GLU:HA	2:A:464:GOL:O3	1.90	0.70
2:B:461:GOL:H12	8:B:489:HOH:O	1.91	0.69
1:A:20:LYS:HE2	2:A:464:GOL:C2	2.23	0.69
1:B:399:LYS:NZ	8:B:902:HOH:O	2.26	0.68
1:B:445[A]:ASP:HB3	8:B:1100:HOH:O	1.93	0.68
1:B:11:ILE:HG12	1:B:45:LEU:HD21	1.75	0.67
1:A:20:LYS:HE2	2:A:464:GOL:H2	1.78	0.66
1:B:11:ILE:CG2	1:B:55:GLN:NE2	2.58	0.66
1:B:43:GLN:CD	8:B:1055:HOH:O	2.34	0.65
1:B:149:PHE:CG	8:B:932:HOH:O	2.50	0.65
1:A:132:SER:H	1:A:414:GLN:HE22	1.44	0.65
1:B:20:LYS:NZ	5:B:1474:AES:O1S	2.29	0.65
1:A:443:ARG:HH21	1:A:443:ARG:CG	2.10	0.64
1:A:120:ARG:NH2	1:B:397:ASP:OD1	2.30	0.64
1:A:120:ARG:HG2	1:A:120:ARG:NH1	2.12	0.63
2:B:462:GOL:C2	8:B:1056:HOH:O	2.22	0.62
1:A:263:ARG:NH2	8:A:740:HOH:O	2.33	0.62
1:B:443:ARG:HD2	8:B:712:HOH:O	2.00	0.62
1:B:325[B]:GLN:NE2	6:B:6112:PG4:C5	2.63	0.61
1:A:120:ARG:CG	1:A:120:ARG:HH11	2.14	0.60
1:B:47:SER:O	5:B:1474:AES:H81	2.01	0.60
1:A:22:GLU:CA	2:A:464:GOL:O3	2.49	0.60
1:B:379[B]:ARG:HD2	1:B:382:ARG:HD2	1.82	0.60
1:B:184:GLY:H	1:B:211:ASN:ND2	2.00	0.60
3:A:5936:P33:H212	8:A:727:HOH:O	2.01	0.60
1:A:386:ALA:HB1	1:B:14:PRO:HB3	1.84	0.60
1:A:23:PRO:HD3	2:A:464:GOL:H32	1.83	0.59
1:A:263:ARG:HD3	8:A:1079:HOH:O	2.01	0.59
1:A:120:ARG:HG2	1:A:120:ARG:HH11	1.66	0.59
1:B:162:GLN:HE21	1:B:166:GLN:HE22	1.50	0.59
1:A:41:ARG:NH1	1:A:67:CYS:HA	2.17	0.58
1:B:124:LYS:O	1:B:353:SER:O	2.21	0.58
1:B:132:SER:H	1:B:414:GLN:NE2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ARG:HH12	2:A:462:GOL:H32	1.68	0.58
1:B:32:ILE:HD11	1:B:54:VAL:HG11	1.85	0.58
1:B:11:ILE:HG22	1:B:55:GLN:HE22	1.68	0.57
1:B:270:ARG:NH1	1:B:270:ARG:HG2	2.19	0.57
6:B:6112:PG4:H51	8:B:932:HOH:O	2.03	0.57
1:B:178:VAL:O	1:B:206:ALA:HA	2.05	0.57
1:B:285:GLU:HG2	8:B:481:HOH:O	2.06	0.56
1:A:325[A]:GLN:NE2	8:A:618:HOH:O	2.33	0.55
1:B:258:GLN:O	1:B:259:MET:C	2.45	0.55
1:A:184:GLY:H	1:A:211:ASN:ND2	2.03	0.55
3:A:5936:P33:H62	8:A:570:HOH:O	2.07	0.55
1:B:20:LYS:CE	5:B:1474:AES:O1S	2.55	0.55
2:A:466:GOL:C1	8:A:991:HOH:O	2.50	0.54
1:A:162:GLN:HE21	1:A:166:GLN:HE22	1.55	0.54
1:B:106:GLN:NE2	1:B:237:GLU:OE1	2.40	0.54
1:A:324:GLY:C	1:A:325[A]:GLN:HE21	2.12	0.53
1:A:142:ARG:HH22	2:A:462:GOL:C3	2.21	0.53
1:A:60:THR:HG22	1:A:61:GLY:N	2.19	0.53
5:B:1474:AES:H3	5:B:1474:AES:N8	2.23	0.53
1:A:96:ARG:HG2	8:A:983:HOH:O	2.08	0.53
1:B:120:ARG:NH1	8:B:491:HOH:O	2.41	0.53
1:B:313:PRO:HB3	8:B:1011:HOH:O	2.08	0.53
1:A:233:TYR:OH	1:A:238:HIS:HE1	1.92	0.52
8:A:806:HOH:O	1:B:120:ARG:CD	2.55	0.52
8:A:806:HOH:O	1:B:120:ARG:HD2	2.10	0.52
1:A:96:ARG:NH1	8:A:983:HOH:O	2.42	0.52
1:A:120:ARG:CG	1:A:120:ARG:NH1	2.72	0.52
1:A:191:GLN:NE2	8:A:735:HOH:O	2.26	0.52
1:A:188:GLU:CD	1:A:188:GLU:H	2.12	0.52
1:B:45:LEU:HG	1:B:55:GLN:HG3	1.91	0.52
1:A:142:ARG:NH1	2:A:462:GOL:H32	2.25	0.52
1:B:112:GLY:N	8:B:886:HOH:O	2.41	0.52
1:B:261:ALA:HB1	1:B:267:PRO:HB2	1.91	0.52
1:B:128:GLN:NE2	1:B:422:ILE:H	2.09	0.51
1:B:187[A]:ASN:ND2	8:B:1002:HOH:O	2.42	0.51
1:A:390:LYS:HE3	8:A:1058:HOH:O	2.10	0.51
1:A:333:HIS:O	3:A:5936:P33:H92	2.12	0.50
1:B:14:PRO:HG2	1:B:56:VAL:CG2	2.41	0.50
1:B:94:GLU:OE1	1:B:101:ARG:HD2	2.12	0.50
1:A:145[B]:LYS:HD3	1:A:284:TYR:O	2.12	0.50
2:A:465:GOL:H2	1:B:388:VAL:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:ALA:O	1:B:105:ASP:OD2	2.30	0.49
1:A:365[A]:LYS:HD2	8:A:1052:HOH:O	2.11	0.49
1:A:336:GLY:HA2	3:A:5936:P33:C9	2.43	0.49
1:B:233:TYR:OH	1:B:238:HIS:HE1	1.96	0.49
1:A:181:ALA:HB3	1:A:246:LEU:HD23	1.95	0.48
1:B:17:PHE:H	1:B:111:ASN:ND2	2.06	0.48
1:A:443:ARG:CG	1:A:443:ARG:NH2	2.75	0.48
1:A:336:GLY:HA2	3:A:5936:P33:H92	1.97	0.47
1:A:447:LYS:HG2	8:A:884:HOH:O	2.14	0.47
1:B:431[B]:GLN:NE2	1:B:431[B]:GLN:HA	2.29	0.47
1:B:88:ILE:HD13	1:B:194:MET:HG2	1.96	0.47
1:A:266:VAL:HB	1:A:269:ARG:HG3	1.97	0.47
1:B:130:GLY:HA2	1:B:420:ARG:O	2.14	0.47
1:A:250:THR:O	1:A:254:GLU:HG2	2.15	0.47
1:A:345:PRO:HG3	1:B:318:SER:HB2	1.97	0.46
1:B:43:GLN:NE2	8:B:1055:HOH:O	2.48	0.46
1:A:236:TYR:OH	2:A:466:GOL:H31	2.15	0.46
1:B:116:ASN:ND2	8:B:936:HOH:O	2.48	0.46
1:B:255:ALA:O	1:B:258:GLN:HB2	2.16	0.46
1:A:365[A]:LYS:CE	8:A:858:HOH:O	2.63	0.46
1:B:13:GLY:N	8:B:801:HOH:O	2.48	0.46
2:A:465:GOL:H31	1:B:387:ILE:O	2.16	0.46
1:A:149[B]:PHE:CE2	6:B:6112:PG4:H62	2.51	0.45
1:A:106:GLN:OE1	1:A:237:GLU:OE2	2.33	0.45
1:A:149[B]:PHE:CZ	1:A:321:ILE:HD13	2.52	0.45
1:B:375:TYR:CZ	1:B:379[A]:ARG:HD2	2.52	0.45
1:B:344:LEU:CD1	1:B:379[A]:ARG:HD3	2.46	0.45
1:B:199:LYS:HB3	1:B:199:LYS:HE2	1.76	0.45
1:A:395:GLU:OE2	1:A:395:GLU:CA	2.54	0.44
3:A:5936:P33:H141	8:A:569:HOH:O	2.17	0.44
1:B:201:GLY:O	1:B:204[B]:GLU:HG3	2.18	0.44
1:A:96:ARG:CZ	8:A:983:HOH:O	2.65	0.44
1:A:305:MET:HE3	1:A:305:MET:HB2	1.87	0.44
1:A:13:GLY:HA3	1:A:14:PRO:HD3	1.72	0.43
1:A:396:ARG:HE	1:A:440:GLN:NE2	2.16	0.43
1:A:170:PRO:O	2:A:462:GOL:O3	2.37	0.43
1:A:308:ASP:OD2	1:A:312:HIS:HD2	2.02	0.43
1:A:328:VAL:HG13	1:A:340:PRO:HG2	2.00	0.43
1:A:66:ASP:O	1:A:67:CYS:HB2	2.18	0.43
1:A:142:ARG:HH22	2:A:462:GOL:H32	1.83	0.43
1:B:344:LEU:HD11	1:B:379[A]:ARG:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:SER:HA	1:A:321:ILE:HD12	2.02	0.42
1:A:86:GLY:HA2	1:A:203:LEU:O	2.19	0.42
1:A:31:ASN:O	1:A:72:THR:HA	2.20	0.42
1:B:87:ARG:HG3	1:B:102:ILE:HD11	2.01	0.42
1:B:114:ALA:HB2	8:B:603:HOH:O	2.19	0.42
1:B:379[B]:ARG:HD3	1:B:382:ARG:NH1	2.35	0.42
1:B:11:ILE:HG21	1:B:45:LEU:HD11	2.02	0.42
1:A:219:GLU:HG3	8:A:793:HOH:O	2.20	0.42
1:A:128:GLN:NE2	1:A:422:ILE:H	2.18	0.41
1:B:379[B]:ARG:HA	1:B:379[B]:ARG:HD2	1.90	0.41
1:A:365[A]:LYS:HE2	8:A:858:HOH:O	2.20	0.41
1:B:181:ALA:HB3	1:B:246:LEU:HD23	2.02	0.41
1:B:197:PHE:HB3	1:B:203:LEU:HB2	2.01	0.41
1:B:325[B]:GLN:NE2	6:B:6112:PG4:O3	2.53	0.41
1:A:188:GLU:N	1:A:188:GLU:CD	2.75	0.41
1:A:142:ARG:NH2	2:A:462:GOL:H32	2.36	0.40
1:B:445[B]:ASP:CB	8:B:1100:HOH:O	2.39	0.40
1:B:128:GLN:O	1:B:167:ALA:HA	2.21	0.40
1:A:375:TYR:CZ	1:A:379:ARG:HD2	2.57	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%)	438 (96%)	13 (3%)	3 (1%)	26	10
1	B	449/460 (98%)	432 (96%)	12 (3%)	5 (1%)	17	4
All	All	903/920 (98%)	870 (96%)	25 (3%)	8 (1%)	21	6

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	CYS
1	A	60	THR
1	A	457	ARG
1	B	59	GLY
1	B	60	THR
1	B	58	GLU
1	B	257	ARG
1	B	259	MET

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	373/374 (100%)	354 (95%)	19 (5%)	29	8
1	B	370/374 (99%)	358 (97%)	12 (3%)	46	20
All	All	743/748 (99%)	712 (96%)	31 (4%)	40	12

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	CYS
1	A	70	ILE
1	A	120	ARG
1	A	124	LYS
1	A	138[A]	ASN
1	A	138[B]	ASN
1	A	141	VAL
1	A	188	GLU
1	A	205[A]	ARG
1	A	205[B]	ARG
1	A	294	LYS
1	A	320	TYR
1	A	325[A]	GLN
1	A	325[B]	GLN
1	A	395	GLU
1	A	443	ARG

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Mol	Chain	Res	Type
1	A	445	ASP
1	A	447	LYS
1	A	458	LYS
1	B	45	LEU
1	B	60	THR
1	B	115	MET
1	B	145	LYS
1	B	199	LYS
1	B	258	GLN
1	B	302	ILE
1	B	320	TYR
1	B	439	ASN
1	B	445[A]	ASP
1	B	445[B]	ASP
1	B	454	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	A	166	GLN
1	A	211	ASN
1	A	238	HIS
1	A	299	GLN
1	A	312	HIS
1	A	414	GLN
1	A	417	ASN
1	A	431	GLN
1	A	440	GLN
1	B	111	ASN
1	B	128	GLN
1	B	166	GLN
1	B	211	ASN
1	B	238	HIS
1	B	299	GLN
1	B	414	GLN
1	B	439	ASN

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)

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 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	461	-	5,5,5	0.48	0	5,5,5	0.57	0
2	GOL	A	462	-	5,5,5	0.68	0	5,5,5	1.35	1 (20%)
2	GOL	A	463	-	5,5,5	0.76	0	5,5,5	0.92	0
2	GOL	A	464	-	5,5,5	0.72	0	5,5,5	1.42	0
2	GOL	A	465	-	5,5,5	0.32	0	5,5,5	0.62	0
2	GOL	A	466	-	5,5,5	0.32	0	5,5,5	0.73	0
3	P33	A	5936	-	21,21,21	1.44	3 (14%)	20,20,20	1.99	4 (20%)
5	AES	B	1474	-	11,13,13	1.05	1 (9%)	17,18,18	2.41	7 (41%)
2	GOL	B	461	-	5,5,5	0.62	0	5,5,5	1.03	1 (20%)
2	GOL	B	462	-	5,5,5	0.36	0	5,5,5	0.90	0
2	GOL	B	463	-	5,5,5	0.57	0	5,5,5	1.25	1 (20%)
7	PG0	B	6108	-	7,7,7	1.05	0	6,6,6	1.01	0
6	PG4	B	6112	-	12,12,12	0.91	1 (8%)	11,11,11	1.37	2 (18%)

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	GOL	A	461	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	462	-	-	0/4/4/4	0/0/0/0
2	GOL	A	463	-	-	0/4/4/4	0/0/0/0
2	GOL	A	464	-	-	0/4/4/4	0/0/0/0
2	GOL	A	465	-	-	0/4/4/4	0/0/0/0
2	GOL	A	466	-	-	0/4/4/4	0/0/0/0
3	P33	A	5936	-	-	0/19/19/19	0/0/0/0
5	AES	B	1474	-	-	0/9/9/9	0/1/1/1
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
7	PG0	B	6108	-	-	0/5/5/5	0/0/0/0
6	PG4	B	6112	-	-	0/10/10/10	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1474	AES	O2S-S	-2.81	1.35	1.42
3	A	5936	P33	O7-C8	2.03	1.50	1.42
3	A	5936	P33	O13-C12	2.03	1.50	1.42
6	B	6112	PG4	O3-C5	2.29	1.51	1.42
3	A	5936	P33	O10-C11	2.33	1.52	1.42

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^\circ$)	Ideal($^\circ$)
5	B	1474	AES	O2S-S-O1S	-4.11	105.92	118.95
5	B	1474	AES	F-S-O1S	-3.61	97.96	106.52
5	B	1474	AES	C6-C5-C4	-3.11	116.78	121.04
2	B	463	GOL	O1-C1-C2	-2.26	99.21	110.18
6	B	6112	PG4	C5-O3-C4	-2.19	103.87	113.31
2	B	461	GOL	O2-C2-C1	2.04	118.02	108.65
2	A	462	GOL	O2-C2-C1	2.05	118.05	108.65
6	B	6112	PG4	O3-C5-C6	2.62	122.00	110.36
5	B	1474	AES	C5-C4-C3	2.63	122.35	118.13
5	B	1474	AES	C5-C6-C1	2.78	122.55	119.48
3	A	5936	P33	O13-C14-C15	3.25	124.79	110.36
3	A	5936	P33	O16-C17-C18	3.37	125.36	110.36
5	B	1474	AES	F-S-O2S	3.43	114.64	106.52
5	B	1474	AES	F-S-C1	4.62	113.04	102.39
3	A	5936	P33	O10-C11-C12	4.65	131.02	110.36
3	A	5936	P33	O10-C9-C8	5.24	133.64	110.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	462	GOL	6	0
2	A	464	GOL	5	0
2	A	465	GOL	3	0
2	A	466	GOL	3	0
3	A	5936	P33	7	0
5	B	1474	AES	4	0
2	B	461	GOL	1	0
2	B	462	GOL	2	0
6	B	6112	PG4	6	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, 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(Å²)	Q<0.9
1	A	445/460 (96%)	-0.08	20 (4%)	37	43	11, 19, 39, 82	0
1	B	441/460 (95%)	-0.04	20 (4%)	37	43	11, 18, 41, 77	0
All	All	886/920 (96%)	-0.06	40 (4%)	37	43	11, 19, 40, 82	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	268	GLY	11.6
1	A	11	ILE	10.7
1	A	67	CYS	10.5
1	B	267	PRO	8.8
1	B	262	ALA	8.8
1	A	66	ASP	8.8
1	A	69	VAL	8.2
1	B	261	ALA	8.2
1	A	12	ALA	8.1
1	B	11	ILE	7.9
1	B	10	GLN	7.6
1	B	60	THR	7.3
1	B	269	ARG	7.2
1	A	62	GLY	7.1
1	A	61	GLY	6.4
1	B	270	ARG	6.2
1	A	68	GLY	6.1
1	A	270	ARG	5.9
1	A	60	THR	5.7
1	B	12	ALA	5.7
1	B	62	GLY	5.6
1	B	59	GLY	5.5
1	B	61	GLY	5.2
1	B	311	THR	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	69	VAL	4.8
1	B	310	ILE	3.9
1	B	260	GLY	3.7
1	A	458	LYS	3.5
1	B	114	ALA	3.3
1	B	312	HIS	3.1
1	B	58	GLU	3.0
1	A	269	ARG	2.9
1	A	71	PHE	2.7
1	A	58	GLU	2.5
1	A	59	GLY	2.3
1	A	457	ARG	2.2
1	A	445	ASP	2.2
1	A	307	GLY	2.1
1	A	446	ASN	2.1
1	A	271	GLY	2.1

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
3	P33	A	5936	22/22	0.84	0.21	6.61	32,47,62,63	0
2	GOL	B	462	6/6	0.88	0.18	5.28	18,32,33,38	0
2	GOL	A	465	6/6	0.86	0.18	5.13	41,45,46,49	0
2	GOL	A	463	6/6	0.90	0.15	4.89	26,39,41,44	0
2	GOL	B	463	6/6	0.87	0.15	4.75	37,46,48,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
2	GOL	A	462	6/6	0.78	0.19	3.08	40,47,49,49	0
2	GOL	A	464	6/6	0.86	0.22	2.76	36,42,48,50	0
6	PG4	B	6112	13/13	0.88	0.15	2.08	47,51,58,60	0
2	GOL	A	461	6/6	0.95	0.16	1.83	24,35,39,43	0
5	AES	B	1474	13/13	0.94	0.12	1.39	16,22,32,37	13
2	GOL	B	461	6/6	0.93	0.12	0.72	16,25,35,40	0
2	GOL	A	466	6/6	0.80	0.14	0.56	58,60,63,66	0
7	PG0	B	6108	8/8	0.91	0.10	0.11	45,47,50,51	0
4	CL	B	464	1/1	0.98	0.04	-2.49	22,22,22,22	0
4	CL	A	467	1/1	0.99	0.03	-5.29	21,21,21,21	0

6.5 Other polymers (i)

There are no such residues in this entry.