



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:38 AM UTC

PDB ID : 3TGW / pdb_00003tgw
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)

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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

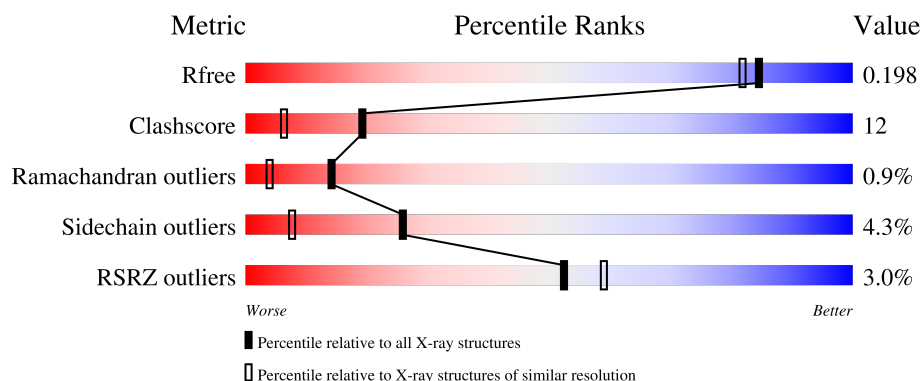
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

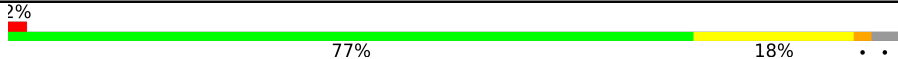
The reported resolution of this entry is 1.75 Å.

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}	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (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 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	A	462	-	-	X	-
2	GOL	A	464	-	-	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:

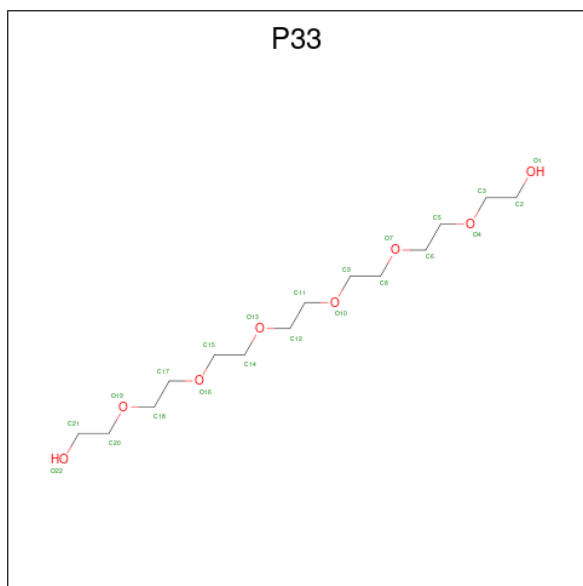
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	ALA	SEE REMARK 999	UNP Q60187
A	156	ALA	HIS	engineered mutation	UNP Q60187
B	2	VAL	ALA	SEE REMARK 999	UNP Q60187
B	156	ALA	HIS	engineered mutation	UNP Q60187

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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		

- Molecule 3 is 3,6,9,12,15,18-HEXAOXAICOSANE-1,20-DIOL (CCD ID: P33) (formula: $C_{14}H_{30}O_8$).

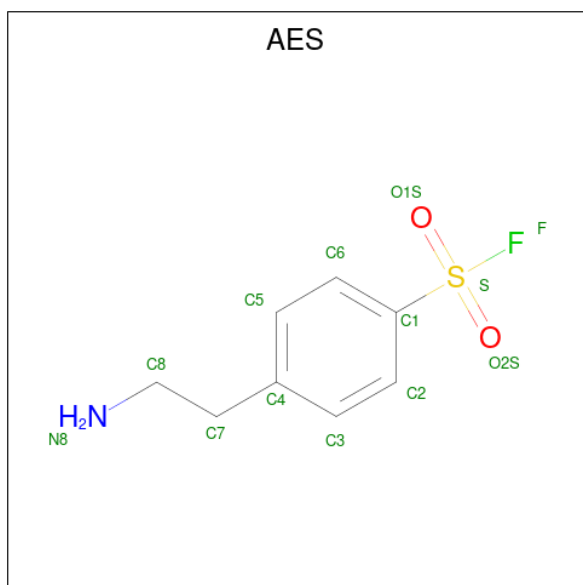


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			22	14	8		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

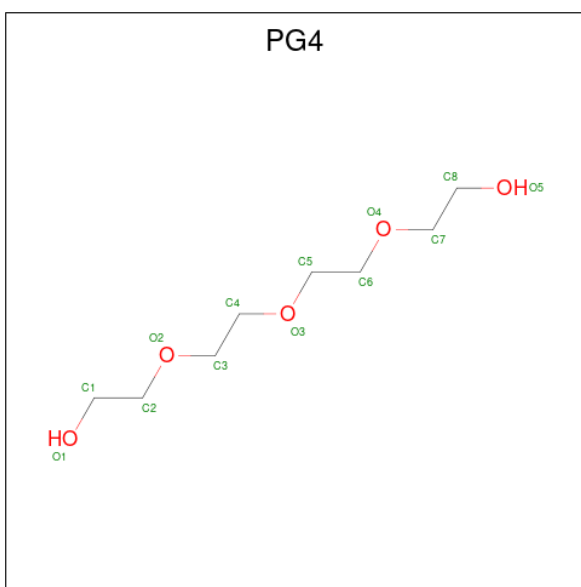
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0
4	B	1	Total Cl 1 1	0	0

- Molecule 5 is 4-(2-AMINOETHYL)BENZENESULFONYL FLUORIDE (CCD ID: AES) (formula: C₈H₁₀FNO₂S).



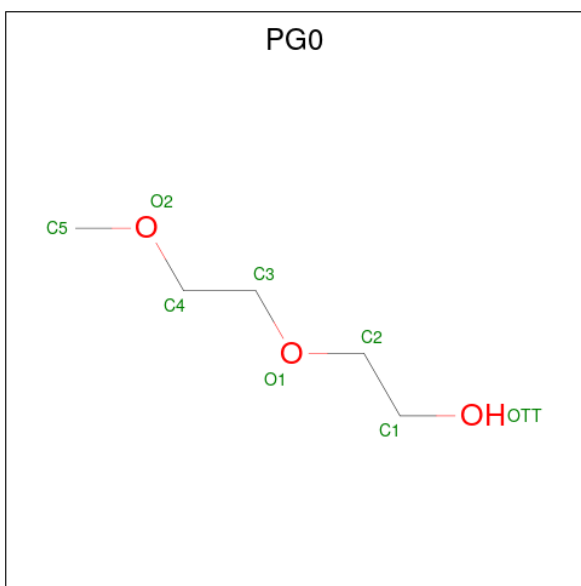
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C F N O S 13 8 1 1 2 1	0	0

- Molecule 6 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 7 is 2-(2-METHOXYETHOXY)ETHANOL (CCD ID: PG0) (formula: $C_5H_{12}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			8	5	3		

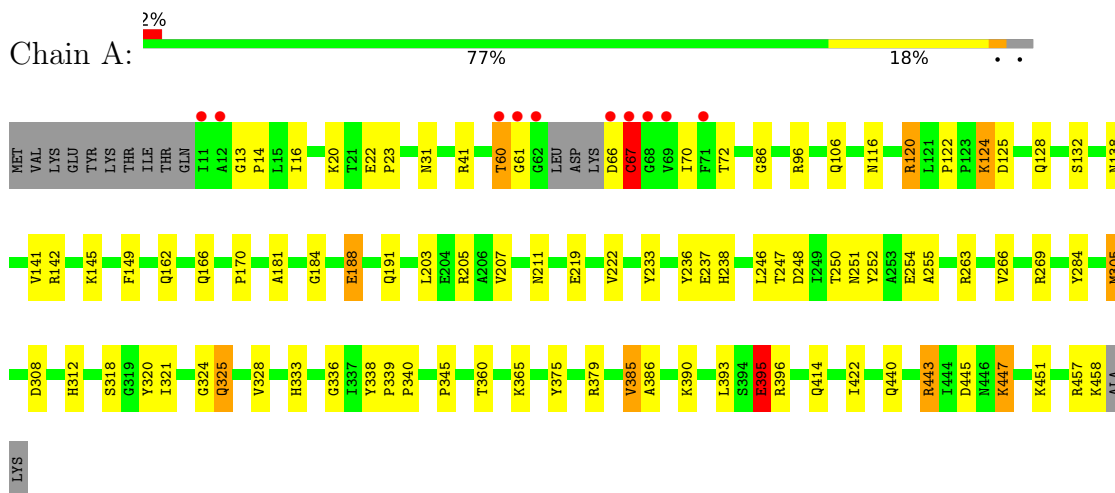
- Molecule 8 is water.

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

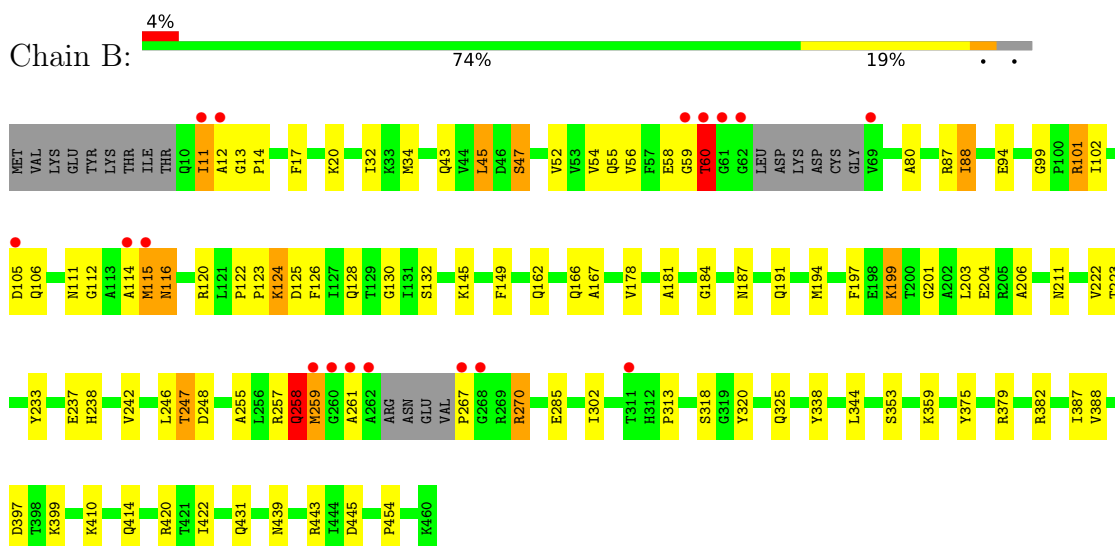
3 Residue-property plots

These plots are drawn for all protein, RNA, 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	73.93Å 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
$\langle I/\sigma(I) \rangle$ 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 (5.01%)	wwPDB-VP
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 , 55.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

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

5.1 Standard geometry

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

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	1.43	13/3586 (0.4%)	1.31	9/4857 (0.2%)
1	B	1.43	13/3562 (0.4%)	1.30	17/4822 (0.4%)
All	All	1.43	26/7148 (0.4%)	1.30	26/9679 (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 (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	116	ASN	C-O	-9.97	1.19	1.23
1	B	125	ASP	C-O	-8.48	1.14	1.23
1	B	125	ASP	N-CA	8.32	1.55	1.45
1	B	242	VAL	N-CA	7.33	1.54	1.46
1	A	124	LYS	C-O	-6.79	1.15	1.24
1	B	124	LYS	C-O	-6.51	1.15	1.24
1	B	47	SER	N-CA	-6.48	1.38	1.46
1	A	124	LYS	C-N	-6.33	1.22	1.33
1	A	395	GLU	CB-CG	-6.21	1.33	1.52
1	A	122	PRO	C-O	-5.93	1.17	1.24
1	A	360	THR	CA-CB	5.91	1.62	1.53
1	A	125	ASP	C-O	-5.78	1.16	1.24
1	A	125	ASP	N-CA	5.63	1.52	1.45
1	B	123	PRO	C-O	-5.54	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	16	ILE	C-O	-5.49	1.17	1.23
1	B	60	THR	CA-CB	5.48	1.62	1.53
1	A	395	GLU	C-O	-5.47	1.17	1.24
1	A	252	TYR	C-O	5.37	1.30	1.24
1	B	116	ASN	CA-C	-5.36	1.46	1.52
1	A	255	ALA	CA-CB	5.34	1.61	1.53
1	A	248	ASP	N-CA	5.31	1.52	1.46
1	B	88	ILE	C-O	5.24	1.29	1.24
1	B	222	VAL	CA-CB	5.18	1.61	1.54
1	B	126	PHE	C-O	-5.18	1.17	1.23
1	B	122	PRO	C-O	-5.17	1.18	1.24
1	B	359	LYS	CA-C	-5.04	1.46	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	LYS	CA-C-N	-13.20	97.38	122.73
1	A	124	LYS	C-N-CA	-13.20	97.38	122.73
1	B	124	LYS	CA-C-N	-9.40	105.57	122.12
1	B	124	LYS	C-N-CA	-9.40	105.57	122.12
1	A	248	ASP	N-CA-C	-8.48	93.22	108.48
1	A	124	LYS	N-CA-C	7.21	126.17	110.80
1	B	116	ASN	N-CA-CB	6.65	122.20	110.37
1	A	124	LYS	O-C-N	-6.39	114.09	122.59
1	B	115	MET	CG-SD-CE	6.22	114.58	100.90
1	B	124	LYS	N-CA-C	6.08	123.76	110.80
1	B	247	THR	N-CA-C	6.00	121.21	107.48
1	A	305	MET	CA-C-N	-5.95	113.84	119.85
1	A	305	MET	C-N-CA	-5.95	113.84	119.85
1	B	11	ILE	N-CA-C	5.70	114.95	106.85
1	A	385	VAL	CB-CA-C	-5.67	104.48	112.14
1	B	223	THR	CA-C-N	-5.50	113.36	119.19
1	B	223	THR	C-N-CA	-5.50	113.36	119.19
1	B	99	GLY	CA-C-N	5.49	125.44	119.78
1	B	99	GLY	C-N-CA	5.49	125.44	119.78
1	B	258	GLN	CB-CA-C	-5.37	100.99	111.03
1	B	247	THR	CB-CA-C	-5.29	103.72	111.77
1	B	248[A]	ASP	N-CA-CB	5.22	119.39	110.57
1	B	248[B]	ASP	N-CA-CB	5.22	119.39	110.57
1	A	207	VAL	CB-CA-C	-5.22	103.06	110.83
1	B	258	GLN	N-CA-C	5.10	119.37	111.56
1	B	12	ALA	N-CA-C	5.04	119.07	111.96

There are no chirality outliers.

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	B	247	THR	Peptide,Mainchain
1	B	338	TYR	Peptide,Mainchain

5.2 Too-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 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	74	0
1	B	3458	0	3487	83	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	28	0
8	B	539	0	0	25	0
All	All	8180	0	7144	166	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 12.

All (166) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:43:GLN:CD	8:B:1055:HOH:O	2.34	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:A:132:SER:H	1:A:414:GLN:HE22	1.44	0.65
1:B:149:PHE:CG	8:B:932:HOH:O	2.50	0.65
1:B:20:LYS:NZ	5:B:1474:AES:O1S	2.29	0.65
1:A:120:ARG:NH2	1:B:397:ASP:OD1	2.30	0.64
1:A:443:ARG:HH21	1:A:443:ARG:CG	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:258:GLN:O	1:B:259:MET:C	2.45	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
1:A:386:ALA:HB1	1:B:14:PRO:HB3	1.84	0.60
3:A:5936:P33:H212	8:A:727:HOH:O	2.01	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
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:HG2	1:B:270:ARG:NH1	2.19	0.57
6:B:6112:PG4:H51	8:B:932:HOH:O	2.03	0.57
1:A:149[A]:PHE:CZ	1:A:305:MET:HE2	2.39	0.57
1:B:178:VAL:O	1:B:206:ALA:HA	2.05	0.57
1:A:324:GLY:C	1:A:325[A]:GLN:HE21	2.12	0.57
1:A:188:GLU:CD	1:A:188:GLU:H	2.12	0.56
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: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:410:LYS:NZ	8:B:618:HOH:O	2.34	0.54
1:B:106:GLN:NE2	1:B:237:GLU:OE1	2.40	0.54
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:N8	5:B:1474:AES:H3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ARG:NH1	8:A:983:HOH:O	2.42	0.52
8:A:806:HOH:O	1:B:120:ARG:HD2	2.10	0.52
1:A:120:ARG:NH1	1:A:120:ARG:CG	2.72	0.52
1:A:191:GLN:NE2	8:A:735:HOH:O	2.26	0.52
1:A:142:ARG:NH1	2:A:462:GOL:H32	2.25	0.52
1:B:45:LEU:HG	1:B:55:GLN:HG3	1.91	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
1:A:451:LYS:NZ	8:A:667:HOH:O	2.45	0.50
2:A:465:GOL:H2	1:B:388:VAL:HA	1.93	0.49
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:34:MET:HA	1:B:34:MET:HE2	1.96	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:A:266:VAL:HB	1:A:269:ARG:HG3	1.97	0.47
1:A:305:MET:HE3	8:A:971:HOH:O	2.14	0.47
1:B:88:ILE:HD13	1:B:194:MET:HG2	1.96	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: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:A:365[A]:LYS:CE	8:A:858:HOH:O	2.63	0.46
1:B:255:ALA:O	1:B:258:GLN:HB2	2.16	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:188:GLU:CD	1:A:188:GLU:N	2.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:GLN:OE1	1:A:237:GLU:OE2	2.33	0.45
1:A:149[B]:PHE:CE2	6:B:6112:PG4:H62	2.51	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:199:LYS:HB3	1:B:199:LYS:HE2	1.76	0.45
1:B:344:LEU:CD1	1:B:379[A]:ARG:HD3	2.46	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: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
1:A:86:GLY:HA2	1:A:203:LEU:O	2.19	0.42
1:A:318:SER:HA	1:A:321:ILE:HD12	2.02	0.42
1:B:11:ILE:HG23	1:B:55:GLN:CD	2.45	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:A:219:GLU:HG3	8:A:793:HOH:O	2.20	0.42
1:B:11:ILE:HG21	1:B:45:LEU:HD11	2.02	0.42
1:B:379[B]:ARG:HD3	1:B:382:ARG:NH1	2.35	0.42
1:A:128:GLN:NE2	1:A:422:ILE:H	2.18	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:379[B]:ARG:HD2	1:B:379[B]:ARG:HA	1.90	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:142:ARG:NH2	2:A:462:GOL:H32	2.36	0.40
1:B:128:GLN:O	1:B:167:ALA:HA	2.21	0.40
1:B:445[B]:ASP:CB	8:B:1100:HOH:O	2.39	0.40
1:A:375:TYR:CZ	1:A:379:ARG:HD2	2.57	0.40
1:B:43:GLN:NE2	8:B:1055:HOH:O	2.48	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%)	18	7
1	B	449/460 (98%)	432 (96%)	12 (3%)	5 (1%)	11	2
All	All	903/920 (98%)	870 (96%)	25 (3%)	8 (1%)	14	4

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%)	352 (94%)	21 (6%)	19	4
1	B	370/374 (99%)	357 (96%)	13 (4%)	32	12
All	All	743/748 (99%)	709 (95%)	34 (5%)	26	6

All (34) 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	222	VAL
1	A	320	TYR
1	A	325[A]	GLN
1	A	325[B]	GLN
1	A	385	VAL
1	A	393	LEU
1	A	395	GLU
1	A	443	ARG
1	A	445	ASP
1	A	447	LYS
1	A	458	LYS
1	B	45	LEU
1	B	60	THR
1	B	101	ARG
1	B	115	MET
1	B	145	LYS
1	B	191	GLN
1	B	199	LYS
1	B	258	GLN
1	B	270	ARG
1	B	302	ILE
1	B	320	TYR
1	B	439	ASN
1	B	454	PRO

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

Mol	Chain	Res	Type
1	A	166	GLN
1	A	211	ASN
1	A	238	HIS
1	A	299	GLN
1	A	312	HIS

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Mol	Chain	Res	Type
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	414	GLN
1	B	439	ASN
1	B	446	ASN
1	B	450	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 oligosaccharides 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	464	-	5,5,5	0.70	0	5,5,5	1.56	2 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PG4	B	6112	-	12,12,12	0.90	1 (8%)	11,11,11	1.34	2 (18%)
2	GOL	A	465	-	5,5,5	0.38	0	5,5,5	0.59	0
2	GOL	B	462	-	5,5,5	0.37	0	5,5,5	0.93	0
2	GOL	B	461	-	5,5,5	0.68	0	5,5,5	1.13	1 (20%)
2	GOL	B	463	-	5,5,5	0.55	0	5,5,5	1.36	1 (20%)
7	PG0	B	6108	-	7,7,7	1.08	0	6,6,6	1.09	0
2	GOL	A	466	-	5,5,5	0.31	0	5,5,5	0.85	0
2	GOL	A	463	-	5,5,5	0.77	0	5,5,5	1.09	0
3	P33	A	5936	-	21,21,21	1.42	1 (4%)	20,20,20	1.94	4 (20%)
2	GOL	A	462	-	5,5,5	0.70	0	5,5,5	1.50	2 (40%)
5	AES	B	1474	-	12,13,13	0.88	1 (8%)	17,18,18	2.38	7 (41%)
2	GOL	A	461	-	5,5,5	0.54	0	5,5,5	0.63	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	464	-	-	2/4/4/4	-
6	PG4	B	6112	-	-	5/10/10/10	-
2	GOL	A	465	-	-	1/4/4/4	-
2	GOL	B	462	-	-	1/4/4/4	-
2	GOL	B	461	-	-	3/4/4/4	-
2	GOL	B	463	-	-	3/4/4/4	-
7	PG0	B	6108	-	-	4/5/5/5	-
2	GOL	A	466	-	-	0/4/4/4	-
2	GOL	A	463	-	-	2/4/4/4	-
3	P33	A	5936	-	-	14/19/19/19	-
2	GOL	A	462	-	-	2/4/4/4	-
5	AES	B	1474	-	-	4/9/9/9	0/1/1/1
2	GOL	A	461	-	-	1/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1474	AES	O2S-S	-2.30	1.35	1.42
3	A	5936	P33	O10-C11	2.28	1.52	1.42
6	B	6112	PG4	O3-C5	2.24	1.51	1.42

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	5936	P33	O10-C9-C8	5.11	133.64	110.35
3	A	5936	P33	O10-C11-C12	4.54	131.02	110.35
5	B	1474	AES	O2S-S-O1S	-4.41	105.92	119.18
5	B	1474	AES	F-S-O1S	-3.76	97.96	106.35
5	B	1474	AES	F-S-O2S	3.72	114.64	106.35
5	B	1474	AES	C6-C1-S	3.70	121.87	119.25
3	A	5936	P33	O16-C17-C18	3.29	125.36	110.35
5	B	1474	AES	C6-C5-C4	-3.21	116.78	121.00
5	B	1474	AES	C5-C6-C1	3.19	122.55	119.44
3	A	5936	P33	O13-C14-C15	3.17	124.79	110.35
5	B	1474	AES	C5-C4-C3	2.77	122.35	118.23
6	B	6112	PG4	O3-C5-C6	2.56	122.00	110.35
2	B	463	GOL	O1-C1-C2	-2.48	99.21	110.38
2	A	462	GOL	C3-C2-C1	-2.20	103.72	111.80
2	A	464	GOL	O2-C2-C1	-2.19	100.09	109.18
6	B	6112	PG4	C5-O3-C4	-2.14	103.87	113.26
2	A	462	GOL	O2-C2-C1	2.14	118.05	109.18
2	B	461	GOL	O2-C2-C1	2.14	118.02	109.18
2	A	464	GOL	O1-C1-C2	-2.01	101.31	110.38

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	462	GOL	C1-C2-C3-O3
2	A	463	GOL	O1-C1-C2-O2
2	A	463	GOL	O1-C1-C2-C3
2	A	464	GOL	C1-C2-C3-O3
2	B	461	GOL	O1-C1-C2-C3
6	B	6112	PG4	O2-C3-C4-O3
3	A	5936	P33	O4-C5-C6-O7
3	A	5936	P33	O19-C20-C21-O22
7	B	6108	PG0	C3-C4-O2-C5
6	B	6112	PG4	O3-C5-C6-O4
2	A	464	GOL	O2-C2-C3-O3
3	A	5936	P33	C11-C12-O13-C14
2	B	463	GOL	C1-C2-C3-O3
2	A	462	GOL	O2-C2-C3-O3
2	B	461	GOL	O1-C1-C2-O2
7	B	6108	PG0	OTT-C1-C2-O1
2	A	465	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	B	1474	AES	C5-C4-C7-C8
5	B	1474	AES	C3-C4-C7-C8
6	B	6112	PG4	O1-C1-C2-O2
6	B	6112	PG4	O4-C7-C8-O5
2	B	462	GOL	O1-C1-C2-O2
3	A	5936	P33	C12-C11-O10-C9
3	A	5936	P33	C2-C3-O4-C5
7	B	6108	PG0	C4-C3-O1-C2
7	B	6108	PG0	C1-C2-O1-C3
3	A	5936	P33	C8-C9-O10-C11
3	A	5936	P33	C21-C20-O19-C18
3	A	5936	P33	C17-C18-O19-C20
2	B	463	GOL	O2-C2-C3-O3
5	B	1474	AES	C2-C1-S-O1S
5	B	1474	AES	C6-C1-S-O1S
2	B	463	GOL	O1-C1-C2-O2
3	A	5936	P33	O1-C2-C3-O4
2	A	461	GOL	C1-C2-C3-O3
2	B	461	GOL	C1-C2-C3-O3
3	A	5936	P33	C6-C5-O4-C3
6	B	6112	PG4	C8-C7-O4-C6
3	A	5936	P33	O16-C17-C18-O19
3	A	5936	P33	O7-C8-C9-O10
3	A	5936	P33	O10-C11-C12-O13
3	A	5936	P33	O13-C14-C15-O16

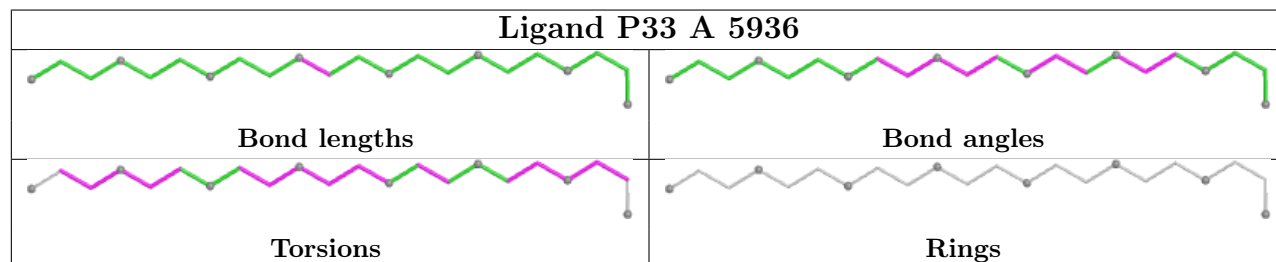
There are no ring outliers.

9 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	464	GOL	5	0
6	B	6112	PG4	6	0
2	A	465	GOL	3	0
2	B	462	GOL	2	0
2	B	461	GOL	1	0
2	A	466	GOL	3	0
3	A	5936	P33	7	0
2	A	462	GOL	6	0
5	B	1474	AES	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	445/460 (96%)	-0.36	10 (2%) 62 69	8, 19, 39, 82	13 (2%)
1	B	441/460 (95%)	-0.38	17 (3%) 43 49	8, 18, 41, 77	14 (3%)
All	All	886/920 (96%)	-0.37	27 (3%) 52 59	8, 18, 40, 82	27 (3%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	60	THR	4.7
1	A	11	ILE	4.4
1	B	114	ALA	4.2
1	B	61	GLY	4.2
1	A	12	ALA	4.1
1	B	262	ALA	3.8
1	A	62	GLY	3.5
1	B	261	ALA	3.0
1	A	67	CYS	3.0
1	A	69	VAL	2.9
1	B	268	GLY	2.8
1	A	66	ASP	2.8
1	B	260	GLY	2.8
1	B	59	GLY	2.6
1	B	11	ILE	2.6
1	B	62	GLY	2.5
1	B	12	ALA	2.5
1	A	60	THR	2.4
1	B	69	VAL	2.4
1	B	115	MET	2.3
1	B	105	ASP	2.2
1	B	267	PRO	2.2
1	B	259	MET	2.1
1	B	311	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	71	PHE	2.1
1	A	61	GLY	2.1
1	A	68	GLY	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](#)

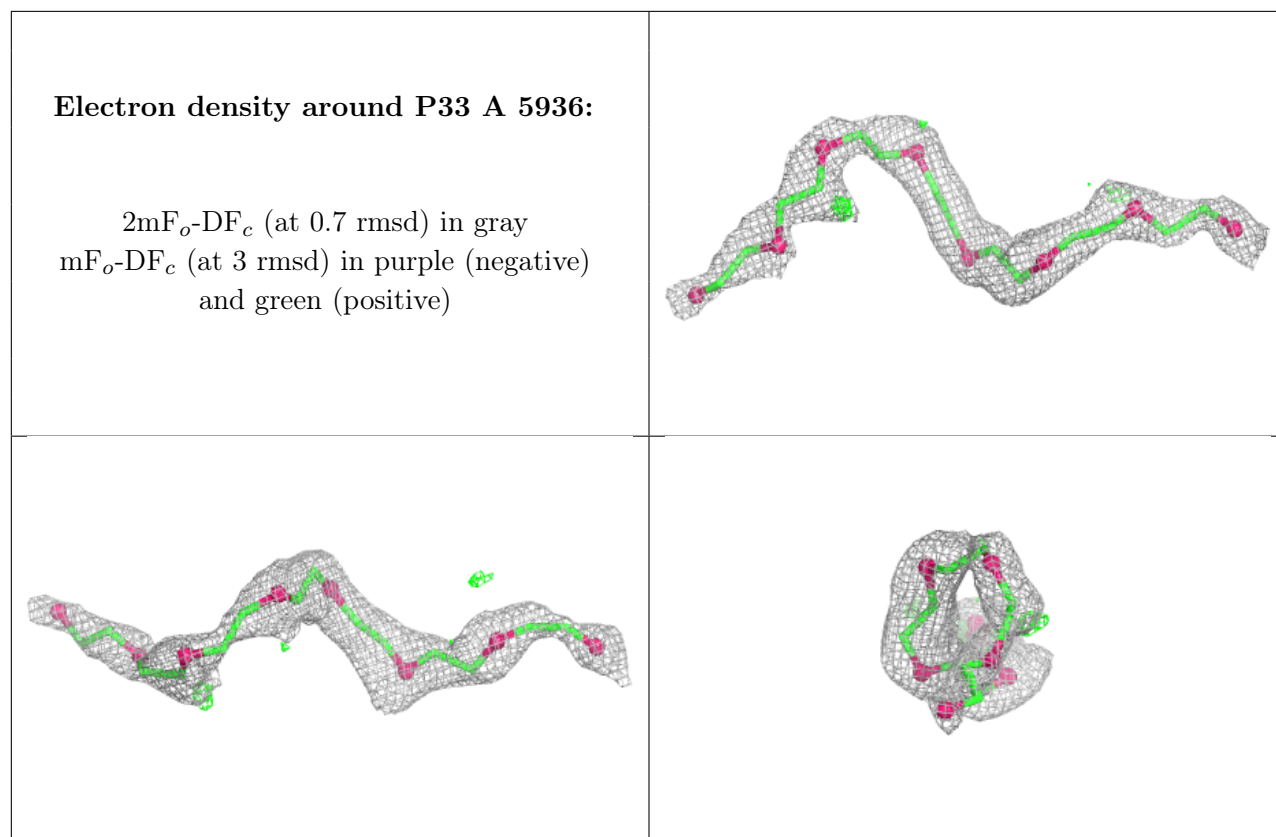
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
2	GOL	A	462	6/6	0.82	0.13	40,47,49,49	0
2	GOL	A	464	6/6	0.83	0.14	36,42,48,50	0
2	GOL	A	466	6/6	0.83	0.14	58,60,63,66	0
2	GOL	B	462	6/6	0.85	0.15	18,32,33,38	0
2	GOL	B	463	6/6	0.85	0.13	37,46,48,54	0
6	PG4	B	6112	13/13	0.85	0.11	47,51,58,60	0
7	PG0	B	6108	8/8	0.86	0.11	45,47,50,51	0
2	GOL	A	465	6/6	0.87	0.10	41,45,46,49	0
3	P33	A	5936	22/22	0.87	0.11	32,47,62,63	0
2	GOL	B	461	6/6	0.89	0.12	16,25,35,40	0
2	GOL	A	463	6/6	0.90	0.09	26,39,41,44	0
2	GOL	A	461	6/6	0.92	0.10	24,35,39,43	0
5	AES	B	1474	13/13	0.94	0.09	16,22,32,37	13
4	CL	B	464	1/1	0.98	0.09	22,22,22,22	0
4	CL	A	467	1/1	0.98	0.05	21,21,21,21	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.