



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:11 PM UTC

PDB ID : 3OSV / pdb_00003osv
Title : The crystal structure of FLGD from P. Aeruginosa
Authors : Wang, D.; Luo, M.; Niu, S.
Deposited on : 2010-09-10
Resolution : 2.35 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
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

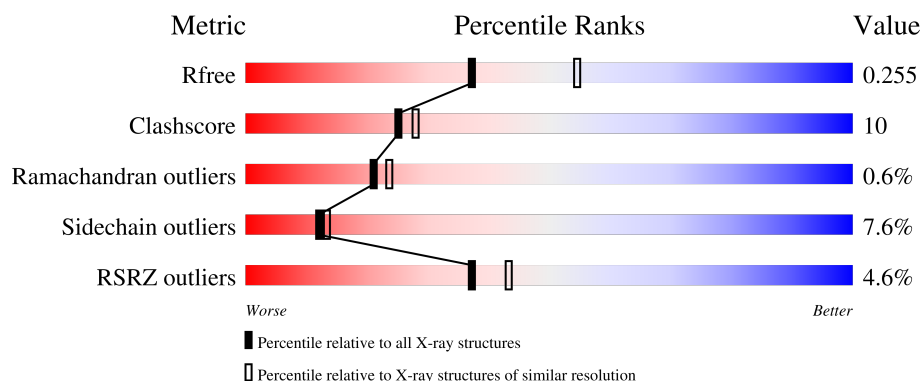
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	138	 4% 69% 22% • • 5%
1	B	138	 4% 72% 16% 6% • 5%
1	C	138	 6% 75% 17% • • •
1	D	138	 4% 70% 20% • • 7%

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	140	-	-	X	-
2	GOL	D	139	-	-	X	-

2 Entry composition [i](#)

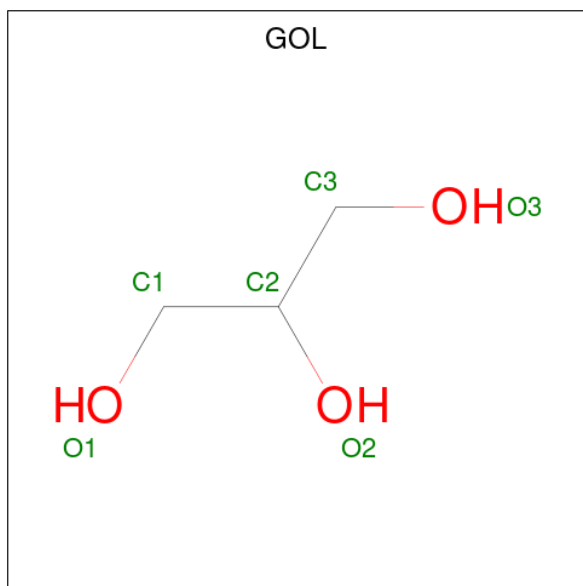
There are 3 unique types of molecules in this entry. The entry contains 4112 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Flagellar basal-body rod modification protein FlgD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	131	Total	C	N	O	S	11	0	0
			970	612	161	194	3			
1	B	131	Total	C	N	O	S	10	0	0
			963	607	161	192	3			
1	C	132	Total	C	N	O	S	12	0	0
			970	612	162	193	3			
1	D	129	Total	C	N	O	S	11	0	0
			957	605	159	190	3			

- 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		

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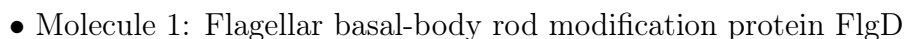
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	41	Total O 41 41	0	0
3	B	48	Total O 48 48	0	0
3	C	56	Total O 56 56	0	0
3	D	47	Total O 47 47	0	0

- Molecule 1: Flagellar basal-body rod modification protein FlgD



M118	L119	M120	L129	Q133	I134	I135	GLY	GLN
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4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	114.83Å 118.38Å 118.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.07 – 2.35 48.07 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.07-2.35) 99.8 (48.07-2.35)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.211 , 0.268 0.203 , 0.255	Depositor DCC
R_{free} test set	1724 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	40.8	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.049 for -h,-l,-k 0.000 for k,h,-l 0.000 for -l,-k,-h 0.000 for l,-h,-k 0.000 for -k,-l,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4112	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.35 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0043e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 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	1.33	4/983 (0.4%)	1.27	7/1333 (0.5%)
1	B	1.62	6/976 (0.6%)	1.37	15/1324 (1.1%)
1	C	1.45	8/983 (0.8%)	1.27	7/1333 (0.5%)
1	D	1.44	5/970 (0.5%)	1.34	9/1316 (0.7%)
All	All	1.46	23/3912 (0.6%)	1.31	38/5306 (0.7%)

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	B	0	1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	133	GLN	CA-CB	-24.90	1.16	1.53
1	D	46	LYS	CD-CE	-16.04	1.04	1.52
1	C	46	LYS	CG-CD	-14.90	1.07	1.52
1	B	133	GLN	CG-CD	-11.78	1.22	1.52
1	D	9	LYS	CG-CD	-10.24	1.21	1.52
1	C	16	LYS	CD-CE	-9.77	1.23	1.52
1	B	9	LYS	CE-NZ	8.57	1.75	1.49
1	A	9	LYS	CB-CG	-8.13	1.28	1.52
1	D	93	LYS	CG-CD	-8.10	1.28	1.52
1	B	22	LYS	CG-CD	-7.25	1.30	1.52
1	C	9	LYS	CG-CD	-7.09	1.31	1.52
1	D	12	VAL	CA-CB	7.09	1.64	1.54
1	D	27	ALA	C-O	-6.89	1.17	1.24
1	B	105	VAL	CA-CB	6.88	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	19	VAL	CA-CB	6.40	1.61	1.54
1	C	93	LYS	CG-CD	-6.28	1.33	1.52
1	A	110	LEU	CG-CD2	-5.89	1.33	1.52
1	A	93	LYS	CG-CD	-5.85	1.34	1.52
1	C	27	ALA	C-O	-5.75	1.18	1.24
1	A	112	GLN	CA-CB	-5.74	1.42	1.53
1	B	78	PRO	CA-C	5.33	1.55	1.52
1	C	108	VAL	C-O	-5.32	1.18	1.24
1	C	33	VAL	N-CA	5.17	1.52	1.46

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	LEU	CD1-CG-CD2	11.72	136.58	110.80
1	D	133	GLN	CG-CD-NE2	-11.54	99.08	116.40
1	B	133	GLN	CG-CD-OE1	-9.75	101.29	120.80
1	D	9	LYS	CG-CD-CE	8.80	131.55	111.30
1	C	46	LYS	CB-CG-CD	8.30	130.38	111.30
1	D	133	GLN	CG-CD-OE1	7.92	136.65	120.80
1	A	112	GLN	CB-CA-C	-7.90	95.09	110.10
1	A	16	LYS	CG-CD-CE	-7.69	93.60	111.30
1	B	133	GLN	N-CA-CB	7.49	121.56	109.95
1	B	49	VAL	CB-CA-C	-7.31	99.40	111.32
1	D	46	LYS	CG-CD-CE	7.29	128.08	111.30
1	B	133	GLN	CG-CD-NE2	6.72	126.48	116.40
1	B	105	VAL	CB-CA-C	6.46	118.77	110.96
1	D	16	LYS	CG-CD-CE	-6.27	96.88	111.30
1	A	50	VAL	CB-CA-C	-6.22	105.33	111.30
1	B	22	LYS	CB-CG-CD	6.19	125.53	111.30
1	B	9	LYS	CB-CG-CD	5.88	124.83	111.30
1	C	91	ASP	CB-CA-C	-5.86	103.57	111.89
1	C	3	SER	N-CA-C	5.76	117.01	108.60
1	D	91	ASP	CA-C-N	-5.73	107.81	122.78
1	D	91	ASP	C-N-CA	-5.73	107.81	122.78
1	A	101	LEU	CA-C-N	5.70	125.46	119.76
1	A	101	LEU	C-N-CA	5.70	125.46	119.76
1	B	9	LYS	CG-CD-CE	5.69	124.38	111.30
1	A	109	THR	N-CA-C	5.55	115.62	108.34
1	C	9	LYS	CG-CD-CE	5.51	123.98	111.30
1	B	133	GLN	CB-CA-C	5.41	118.65	109.84
1	D	19	VAL	N-CA-C	5.40	115.73	108.17
1	C	109	THR	CB-CA-C	-5.38	99.70	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	129	LEU	CA-CB-CG	-5.38	97.46	116.30
1	D	129	LEU	CA-CB-CG	-5.27	97.86	116.30
1	C	18	VAL	CA-C-N	-5.26	116.66	123.19
1	C	18	VAL	C-N-CA	-5.26	116.66	123.19
1	B	104	ASN	CA-C-N	-5.20	115.87	122.37
1	B	104	ASN	C-N-CA	-5.20	115.87	122.37
1	B	78	PRO	CA-C-N	-5.19	114.44	119.78
1	B	78	PRO	C-N-CA	-5.19	114.44	119.78
1	B	50	VAL	N-CA-C	-5.04	107.89	112.12

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	133	GLN	Sidechain

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	970	0	978	24	0
1	B	963	0	968	23	0
1	C	970	0	980	14	0
1	D	957	0	969	23	0
2	A	24	0	32	8	0
2	B	18	0	24	0	0
2	C	6	0	8	0	0
2	D	12	0	16	4	0
3	A	41	0	0	1	0
3	B	48	0	0	2	0
3	C	56	0	0	0	0
3	D	47	0	0	0	0
All	All	4112	0	3975	75	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 10.

All (75) 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:D:109:THR:HG22	1:D:110:LEU:H	1.24	1.02
1:A:51:ASN:HD21	2:A:139:GOL:H31	1.28	0.95
1:D:96:GLY:CA	2:D:139:GOL:H31	2.04	0.88
1:A:133:GLN:NE2	1:B:134:ILE:H	1.76	0.84
1:C:109:THR:HG22	1:C:110:LEU:H	1.44	0.81
1:D:41:ASN:HD21	1:D:52:ARG:HH11	1.24	0.81
1:D:109:THR:HG22	1:D:110:LEU:N	1.97	0.80
1:D:52:ARG:HE	1:D:54:ASN:HD21	1.32	0.77
1:C:109:THR:CG2	1:C:110:LEU:H	1.97	0.77
1:D:96:GLY:HA3	2:D:139:GOL:H31	1.66	0.76
1:A:52:ARG:HE	1:A:54:ASN:HD21	1.34	0.76
1:B:52:ARG:HE	1:B:54:ASN:HD21	1.34	0.75
2:A:140:GOL:H12	1:C:52:ARG:HH12	1.54	0.73
1:B:41:ASN:HD21	1:B:52:ARG:HH11	1.33	0.73
1:D:96:GLY:HA2	2:D:139:GOL:H31	1.72	0.72
1:A:11:ILE:HB	1:A:133:GLN:HB2	1.72	0.72
1:B:77:MET:HA	1:B:77:MET:HE2	1.71	0.71
1:A:26:LYS:HG2	1:A:66:MET:HE2	1.75	0.69
1:D:109:THR:CG2	1:D:110:LEU:H	1.92	0.69
1:C:109:THR:HG22	1:C:110:LEU:N	2.08	0.68
1:C:35:SER:HB2	1:C:90:ILE:CD1	2.24	0.67
1:D:109:THR:OG1	1:D:120:ASN:ND2	2.27	0.67
1:B:16:LYS:HE3	3:B:183:HOH:O	1.94	0.67
1:D:50:VAL:HG22	1:D:77:MET:HE2	1.76	0.66
1:C:117:LEU:O	1:C:118:MET:HG2	1.95	0.66
1:C:26:LYS:HG2	1:C:66:MET:HG2	1.79	0.65
1:A:41:ASN:HD21	1:A:52:ARG:HH11	1.44	0.64
1:C:41:ASN:HD21	1:C:52:ARG:HH11	1.45	0.62
1:A:20:ASP:OD2	1:A:22:LYS:HE3	2.00	0.61
1:B:52:ARG:HE	1:B:54:ASN:ND2	2.01	0.59
1:A:52:ARG:HE	1:A:54:ASN:ND2	2.02	0.58
1:A:135:ILE:H	1:B:30:ASN:HD21	1.52	0.57
1:D:117:LEU:O	1:D:118:MET:HG2	2.05	0.57
1:B:26:LYS:HG2	1:B:66:MET:HG2	1.87	0.56
1:D:117:LEU:C	1:D:118:MET:HG2	2.29	0.56
1:C:77:MET:HA	1:C:77:MET:HE2	1.89	0.55
1:C:35:SER:HB2	1:C:90:ILE:HD11	1.89	0.54
1:A:133:GLN:HE22	1:B:134:ILE:H	1.50	0.54
1:C:133:GLN:O	1:C:134:ILE:C	2.51	0.53
2:A:140:GOL:H12	1:C:52:ARG:NH1	2.23	0.52
1:B:20:ASP:OD1	1:B:22:LYS:HG2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50:VAL:CG2	1:D:77:MET:HE2	2.41	0.51
1:D:41:ASN:HD21	1:D:52:ARG:NH1	2.01	0.51
1:A:133:GLN:NE2	1:B:134:ILE:N	2.53	0.51
1:B:41:ASN:HD21	1:B:52:ARG:NH1	2.06	0.50
1:B:99:THR:HB	1:B:101:LEU:HD13	1.93	0.50
1:A:98:GLN:OE1	2:A:141:GOL:H32	2.13	0.49
1:D:7:GLY:HA2	1:D:104:ASN:HD21	1.78	0.49
1:A:54:ASN:HB2	2:A:138:GOL:H11	1.95	0.48
1:C:11:ILE:HG22	1:C:133:GLN:HG3	1.96	0.47
1:A:30:ASN:ND2	1:A:100:TYR:OH	2.47	0.47
1:A:77:MET:HE1	3:A:164:HOH:O	2.14	0.47
1:D:52:ARG:HE	1:D:54:ASN:ND2	2.06	0.46
1:A:51:ASN:ND2	2:A:139:GOL:H31	2.12	0.46
1:A:133:GLN:HE21	1:B:134:ILE:H	1.56	0.46
1:D:11:ILE:HG22	1:D:100:TYR:HB3	1.98	0.46
1:B:5:LEU:O	1:B:8:ARG:HB2	2.16	0.45
1:D:109:THR:CG2	1:D:110:LEU:N	2.62	0.44
1:B:133:GLN:O	1:B:134:ILE:C	2.60	0.44
1:A:5:LEU:HD22	1:B:32:PRO:HA	2.00	0.43
1:B:16:LYS:CE	3:B:183:HOH:O	2.60	0.43
1:A:29:LEU:HD13	1:A:97:LEU:HD13	2.01	0.43
1:B:33:VAL:HG12	1:B:34:SER:N	2.34	0.42
1:D:11:ILE:CG2	1:D:100:TYR:HB3	2.49	0.42
2:A:140:GOL:C1	1:C:52:ARG:HH22	2.31	0.42
1:B:6:VAL:HG22	1:B:107:SER:HA	2.01	0.41
1:B:88:THR:HB	1:B:97:LEU:HD11	2.02	0.41
1:D:85:GLU:HG3	2:D:139:GOL:H2	2.02	0.41
1:A:133:GLN:HE21	1:B:134:ILE:N	2.16	0.41
1:A:62:SER:OG	1:B:134:ILE:HG23	2.21	0.41
1:A:72:SER:OG	2:A:140:GOL:H31	2.21	0.41
1:A:7:GLY:HA2	1:A:104:ASN:HD21	1.86	0.41
1:D:5:LEU:O	1:D:6:VAL:C	2.63	0.41
1:A:75:ASN:HD21	1:D:57:GLN:H	1.68	0.40
1:D:12:VAL:HG22	1:D:14:THR:HB	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	127/138 (92%)	123 (97%)	2 (2%)	2 (2%)	7	6
1	B	127/138 (92%)	123 (97%)	3 (2%)	1 (1%)	16	17
1	C	128/138 (93%)	124 (97%)	4 (3%)	0	100	100
1	D	125/138 (91%)	118 (94%)	7 (6%)	0	100	100
All	All	507/552 (92%)	488 (96%)	16 (3%)	3 (1%)	21	24

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	134	ILE
1	A	5	LEU
1	A	134	ILE

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	109/114 (96%)	100 (92%)	9 (8%)	10	11
1	B	107/114 (94%)	100 (94%)	7 (6%)	15	18
1	C	108/114 (95%)	100 (93%)	8 (7%)	13	14
1	D	108/114 (95%)	99 (92%)	9 (8%)	10	11
All	All	432/456 (95%)	399 (92%)	33 (8%)	12	13

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	5	LEU
1	A	9	LYS
1	A	57	GLN
1	A	93	LYS
1	A	109	THR
1	A	116	GLU
1	A	129	LEU
1	A	133	GLN
1	B	9	LYS
1	B	30	ASN
1	B	49	VAL
1	B	101	LEU
1	B	105	VAL
1	B	120	ASN
1	B	129	LEU
1	C	12	VAL
1	C	33	VAL
1	C	46	LYS
1	C	108	VAL
1	C	109	THR
1	C	110	LEU
1	C	126	SER
1	C	129	LEU
1	D	8	ARG
1	D	12	VAL
1	D	46	LYS
1	D	52	ARG
1	D	57	GLN
1	D	64	SER
1	D	108	VAL
1	D	129	LEU
1	D	133	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	54	ASN
1	A	98	GLN
1	A	104	ASN
1	A	133	GLN
1	B	30	ASN

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Mol	Chain	Res	Type
1	B	41	ASN
1	B	54	ASN
1	B	120	ASN
1	C	30	ASN
1	C	41	ASN
1	C	104	ASN
1	D	41	ASN
1	D	54	ASN
1	D	104	ASN
1	D	120	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GOL	A	139	-	5,5,5	0.51	0	5,5,5	0.90	0
2	GOL	A	138	-	5,5,5	0.19	0	5,5,5	0.83	0
2	GOL	A	141	-	5,5,5	0.50	0	5,5,5	0.69	0
2	GOL	B	138	-	5,5,5	0.51	0	5,5,5	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	B	140	-	5,5,5	0.51	0	5,5,5	1.10	0
2	GOL	A	140	-	5,5,5	0.35	0	5,5,5	0.54	0
2	GOL	B	139	-	5,5,5	0.58	0	5,5,5	0.20	0
2	GOL	C	138	-	5,5,5	0.38	0	5,5,5	1.24	0
2	GOL	D	139	-	5,5,5	0.71	0	5,5,5	0.60	0
2	GOL	D	138	-	5,5,5	0.53	0	5,5,5	0.78	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	139	-	-	0/4/4/4	-
2	GOL	A	138	-	-	0/4/4/4	-
2	GOL	A	141	-	-	0/4/4/4	-
2	GOL	B	138	-	-	2/4/4/4	-
2	GOL	B	140	-	-	1/4/4/4	-
2	GOL	A	140	-	-	4/4/4/4	-
2	GOL	B	139	-	-	4/4/4/4	-
2	GOL	C	138	-	-	4/4/4/4	-
2	GOL	D	139	-	-	2/4/4/4	-
2	GOL	D	138	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	140	GOL	O1-C1-C2-O2
2	A	140	GOL	O1-C1-C2-C3
2	A	140	GOL	C1-C2-C3-O3
2	A	140	GOL	O2-C2-C3-O3
2	B	139	GOL	O1-C1-C2-C3
2	B	139	GOL	C1-C2-C3-O3
2	C	138	GOL	O2-C2-C3-O3
2	D	138	GOL	C1-C2-C3-O3
2	D	139	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	B	138	GOL	C1-C2-C3-O3
2	C	138	GOL	O1-C1-C2-C3
2	C	138	GOL	C1-C2-C3-O3
2	D	139	GOL	C1-C2-C3-O3
2	B	138	GOL	O2-C2-C3-O3
2	B	139	GOL	O2-C2-C3-O3
2	D	138	GOL	O2-C2-C3-O3
2	B	139	GOL	O1-C1-C2-O2
2	C	138	GOL	O1-C1-C2-O2
2	B	140	GOL	O2-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	139	GOL	2	0
2	A	138	GOL	1	0
2	A	141	GOL	1	0
2	A	140	GOL	4	0
2	D	139	GOL	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	131/138 (94%)	-0.19	5 (3%)	44	50	22, 30, 54, 75	5 (3%)
1	B	131/138 (94%)	-0.17	6 (4%)	37	43	22, 31, 53, 63	4 (3%)
1	C	132/138 (95%)	-0.15	8 (6%)	27	31	21, 29, 52, 72	5 (3%)
1	D	129/138 (93%)	-0.25	5 (3%)	43	49	21, 29, 47, 71	5 (3%)
All	All	523/552 (94%)	-0.19	24 (4%)	37	43	21, 30, 52, 75	19 (3%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	ALA	5.3
1	B	110	LEU	5.1
1	D	110	LEU	4.2
1	C	2	ALA	4.2
1	A	110	LEU	4.0
1	C	111	GLY	3.9
1	A	3	SER	3.7
1	A	112	GLN	3.7
1	D	111	GLY	3.5
1	C	116	GLU	3.1
1	D	109	THR	2.9
1	C	115	GLY	2.8
1	D	3	SER	2.8
1	C	3	SER	2.7
1	C	110	LEU	2.6
1	B	116	GLU	2.6
1	C	109	THR	2.6
1	B	3	SER	2.5
1	A	136	GLY	2.3
1	B	4	SER	2.1
1	B	136	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	136	GLY	2.1
1	A	4	SER	2.0
1	D	116	GLU	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(Å ²)	Q<0.9
2	GOL	A	139	6/6	0.85	0.17	47,53,54,57	0
2	GOL	A	141	6/6	0.86	0.20	56,62,64,65	0
2	GOL	C	138	6/6	0.86	0.23	44,46,50,54	0
2	GOL	D	139	6/6	0.87	0.18	41,46,53,53	0
2	GOL	B	138	6/6	0.89	0.15	41,49,51,54	0
2	GOL	B	140	6/6	0.90	0.20	47,50,52,53	0
2	GOL	D	138	6/6	0.92	0.22	43,51,54,56	0
2	GOL	A	140	6/6	0.92	0.18	52,55,57,61	0
2	GOL	B	139	6/6	0.93	0.12	47,49,51,53	0
2	GOL	A	138	6/6	0.94	0.13	36,45,48,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.