



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:03 PM UTC

PDB ID : 4V3Q / pdb_00004v3q
Title : Designed armadillo repeat protein with 4 internal repeats, 2nd generation C-cap and 3rd generation N-cap.
Authors : Reichen, C.; Madhurantakam, C.; Pluckthun, A.; Mittl, P.
Deposited on : 2014-10-20
Resolution : 1.80 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

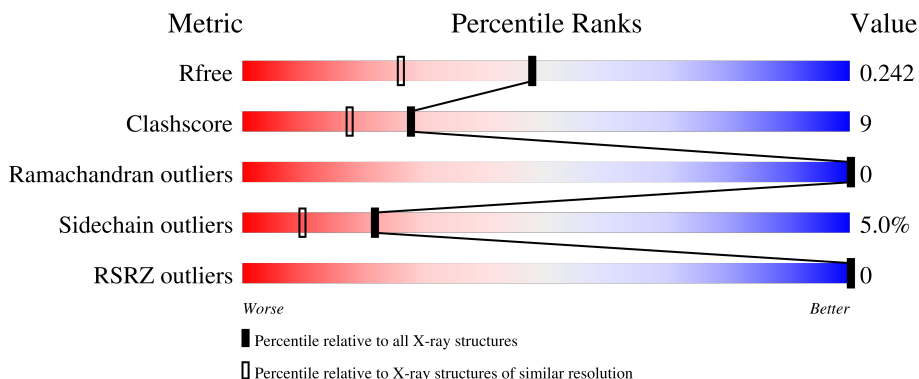
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	247	81% 17% .
1	B	247	82% 17% .
1	C	247	81% 17% ..
1	D	247	79% 17% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8169 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 YIII_M4_AII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	247	Total	C	N	O	S	0	7	0
			1908	1180	332	395	1			
1	B	247	Total	C	N	O	S	0	5	0
			1881	1164	327	389	1			
1	C	245	Total	C	N	O	S	0	3	0
			1851	1150	320	380	1			
1	D	244	Total	C	N	O	S	0	3	0
			1847	1145	320	381	1			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	8	Total 8	Ca 8	0	0
3	B	2	Total 2	Ca 2	0	0
3	C	4	Total 4	Ca 4	0	0
3	D	2	Total 2	Ca 2	0	0

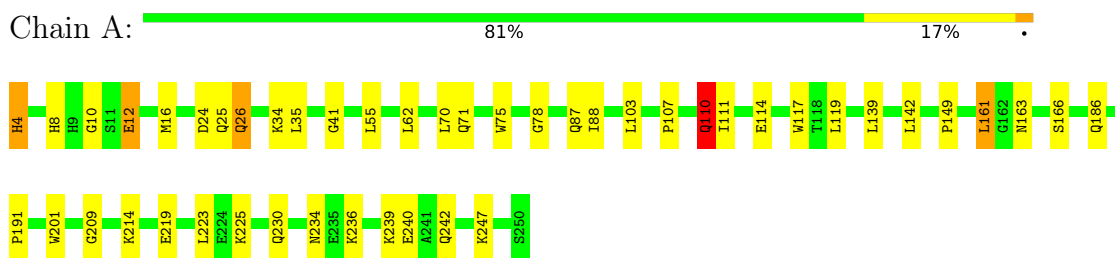
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	219	Total 219	O 219	0	0
4	B	185	Total 185	O 185	0	0
4	C	143	Total 143	O 143	0	0
4	D	107	Total 107	O 107	0	0

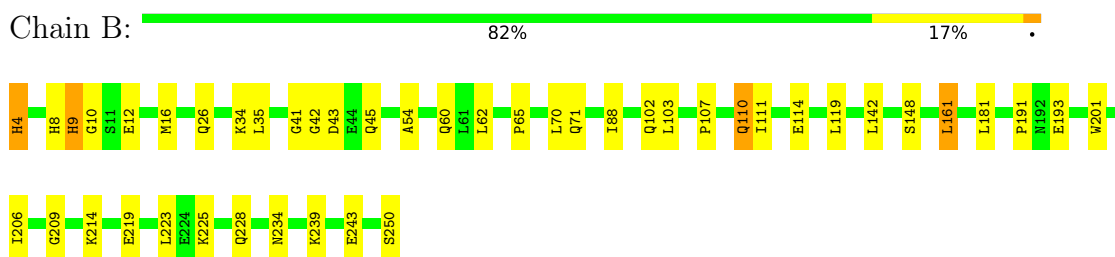
3 Residue-property plots

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.

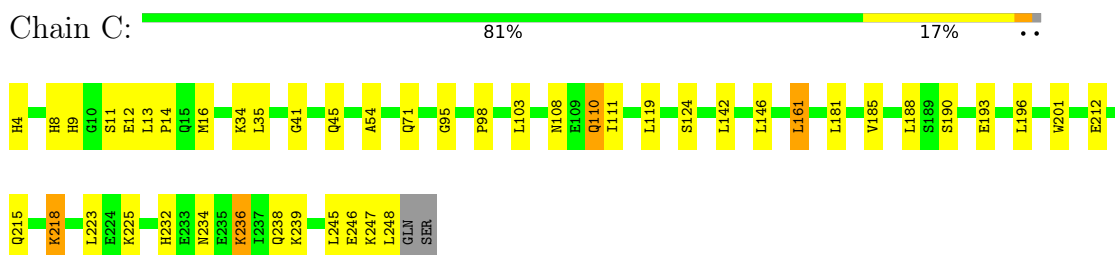
• Molecule 1: YIII_M4_AII



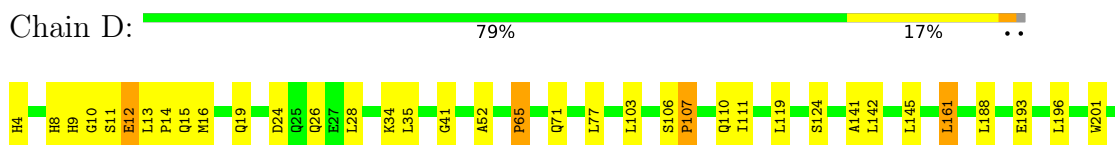
• Molecule 1: YIII_M4_AII



• Molecule 1: YIII_M4_AII



• Molecule 1: YIII_M4_AII



N211	E212	K218	A222	L223	E224	K225	L226	E233	K236	K239	L245	E246	K247	LEU	GLN	SER
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4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	96.50Å 96.50Å 96.34Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	96.34 – 1.80 83.57 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (96.34-1.80) 99.9 (83.57-1.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.189 , 0.236 0.195 , 0.242	Depositor DCC
R_{free} test set	4660 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	26.5	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 29.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l 0.487 for h,-h-k,-l 0.025 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8169	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% 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: CA, 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	1.20	3/1932 (0.2%)	1.11	8/2627 (0.3%)
1	B	1.21	4/1905 (0.2%)	1.12	5/2591 (0.2%)
1	C	1.18	1/1875 (0.1%)	1.19	8/2551 (0.3%)
1	D	1.24	5/1871 (0.3%)	1.19	14/2545 (0.6%)
All	All	1.21	13/7583 (0.2%)	1.15	35/10314 (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	1
1	B	0	1
All	All	0	2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	107	PRO	C-O	11.53	1.38	1.24
1	D	65	PRO	C-O	10.77	1.35	1.23
1	B	107	PRO	C-O	7.04	1.32	1.24
1	A	107	PRO	C-O	6.95	1.32	1.24
1	B	60	GLN	N-CA	6.27	1.54	1.46
1	B	65	PRO	C-O	6.04	1.31	1.24
1	C	13	LEU	N-CA	-5.55	1.43	1.46
1	D	13	LEU	N-CA	-5.41	1.42	1.46
1	A	149	PRO	C-O	5.39	1.30	1.24
1	B	191	PRO	CA-C	5.34	1.59	1.52
1	D	218	LYS	N-CA	5.29	1.52	1.46
1	A	191	PRO	CA-C	5.12	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	77	LEU	C-O	-5.00	1.18	1.24

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	218	LYS	N-CA-C	7.25	119.27	111.36
1	C	41	GLY	CA-C-N	-7.25	111.96	121.96
1	C	41	GLY	C-N-CA	-7.25	111.96	121.96
1	D	65	PRO	CA-C-O	7.09	126.77	118.68
1	C	218	LYS	N-CA-C	6.85	118.75	111.28
1	C	13	LEU	CA-C-O	6.41	125.02	119.13
1	D	41	GLY	CA-C-N	-6.27	113.31	121.96
1	D	41	GLY	C-N-CA	-6.27	113.31	121.96
1	C	13	LEU	CA-C-N	-6.06	113.44	119.56
1	C	13	LEU	C-N-CA	-6.06	113.44	119.56
1	D	106	SER	CA-C-N	5.86	126.95	120.45
1	D	106	SER	C-N-CA	5.86	126.95	120.45
1	D	13	LEU	CA-C-O	5.78	124.34	118.79
1	B	148	SER	CA-C-N	5.73	126.81	120.45
1	B	148	SER	C-N-CA	5.73	126.81	120.45
1	D	107	PRO	CA-C-O	5.50	125.70	118.98
1	D	211	ASN	N-CA-C	5.48	117.25	111.28
1	B	43	ASP	N-CA-C	-5.45	105.45	111.71
1	D	218	LYS	CB-CA-C	-5.44	101.61	110.85
1	B	88	ILE	CB-CA-C	-5.42	105.03	111.97
1	A	88	ILE	CB-CA-C	-5.42	104.82	112.14
1	A	55	LEU	CA-C-N	-5.37	113.37	119.28
1	A	55	LEU	C-N-CA	-5.37	113.37	119.28
1	A	139	LEU	CA-C-N	-5.29	113.47	118.97
1	A	139	LEU	C-N-CA	-5.29	113.47	118.97
1	C	54	ALA	N-CA-C	5.21	117.70	111.71
1	A	87	GLN	N-CA-C	-5.18	105.32	111.69
1	B	54	ALA	N-CA-C	5.11	117.75	111.82
1	C	124	SER	N-CA-C	-5.07	107.09	113.28
1	D	41	GLY	O-C-N	-5.07	118.31	122.92
1	A	110	GLN	CB-CG-CD	-5.07	103.99	112.60
1	A	75	TRP	N-CA-C	-5.04	105.87	111.36
1	D	124	SER	N-CA-C	-5.03	107.20	113.38
1	D	13	LEU	CA-C-N	-5.02	113.76	119.28
1	D	13	LEU	C-N-CA	-5.02	113.76	119.28

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4	HIS	Peptide
1	B	4	HIS	Peptide

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	1908	0	1870	38	0
1	B	1881	0	1851	35	0
1	C	1851	0	1832	35	0
1	D	1847	0	1819	37	0
2	A	6	0	8	2	0
2	B	6	0	8	2	0
3	A	8	0	0	0	0
3	B	2	0	0	0	0
3	C	4	0	0	0	0
3	D	2	0	0	0	0
4	A	219	0	0	7	0
4	B	185	0	0	11	0
4	C	143	0	0	6	0
4	D	107	0	0	6	0
All	All	8169	0	7388	134	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 9.

All (134) 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:114:GLU:HG2	4:A:2122:HOH:O	1.26	1.30
1:B:114:GLU:HG2	4:B:2113:HOH:O	1.22	1.28
1:C:45:GLN:HG2	4:C:2039:HOH:O	1.40	1.18
1:D:19:GLN:HG2	4:D:2014:HOH:O	1.53	1.06
1:A:186:GLN:HG3	4:A:2186:HOH:O	1.63	0.98
1:B:45:GLN:HG2	4:B:2045:HOH:O	1.65	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246:GLU:O	1:D:247:LYS:O	1.91	0.89
1:D:16:MET:HE2	1:D:35:LEU:HG	1.58	0.85
1:A:25[B]:GLN:HE21	1:A:25[B]:GLN:H	1.24	0.83
1:A:25[B]:GLN:HE21	1:A:25[B]:GLN:N	1.76	0.83
1:C:146:LEU:O	4:C:2110:HOH:O	1.98	0.82
1:B:10:GLY:N	4:B:2016:HOH:O	2.02	0.81
1:C:16:MET:HE3	1:C:34:LYS:HB2	1.63	0.80
1:A:110:GLN:OE1	1:B:110:GLN:OE1	1.99	0.80
1:B:16:MET:CE	1:B:35:LEU:HG	2.14	0.78
1:B:16:MET:HE2	1:B:35:LEU:HG	1.66	0.78
1:B:12:GLU:HG3	4:B:2016:HOH:O	1.85	0.76
1:C:110:GLN:OE1	1:D:110:GLN:OE1	2.04	0.75
1:C:16:MET:HE2	1:C:35:LEU:HG	1.71	0.72
1:C:190:SER:OG	4:C:2128:HOH:O	2.09	0.70
1:C:9:HIS:HA	1:C:12:GLU:OE2	1.92	0.70
1:C:223:LEU:HD12	1:C:245:LEU:HD11	1.76	0.67
1:D:16:MET:HE3	1:D:34:LYS:HB2	1.77	0.66
1:A:16:MET:CE	1:A:35:LEU:HG	2.25	0.66
1:C:111[B]:ILE:CD1	1:C:111[B]:ILE:N	2.59	0.66
1:B:102:GLN:HG2	4:B:2106:HOH:O	1.97	0.65
1:C:16:MET:CE	1:C:34:LYS:HB2	2.26	0.65
1:A:16:MET:HE2	1:A:35:LEU:HG	1.79	0.63
1:D:71:GLN:OE1	1:D:110:GLN:HG2	1.99	0.62
2:B:1251:GOL:H12	4:B:2142:HOH:O	2.01	0.61
1:D:223:LEU:HD12	1:D:245:LEU:HD11	1.83	0.60
1:C:188:LEU:O	1:C:196:LEU:HD21	2.02	0.60
1:B:71:GLN:HG3	1:B:111:ILE:CD1	2.32	0.59
1:B:42:GLY:N	4:B:2045:HOH:O	2.35	0.58
1:C:111[B]:ILE:H	1:C:111[B]:ILE:HD13	1.69	0.58
1:B:201:TRP:CE2	1:D:8:HIS:HB3	2.38	0.58
1:A:71:GLN:OE1	1:A:110:GLN:HG2	2.04	0.58
1:D:188:LEU:O	1:D:196:LEU:HD21	2.04	0.58
1:A:71:GLN:HG3	1:A:111:ILE:HD11	1.86	0.57
1:A:247:LYS:NZ	4:A:2193:HOH:O	2.37	0.57
1:A:41:GLY:O	4:A:2048:HOH:O	2.17	0.57
1:A:10:GLY:H	1:A:12:GLU:HG3	1.70	0.56
1:A:10:GLY:N	1:A:12:GLU:HG3	2.20	0.56
1:A:201:TRP:CE2	1:C:8:HIS:HB3	2.40	0.56
1:B:71:GLN:HG3	1:B:111:ILE:HD11	1.86	0.56
1:C:111[B]:ILE:N	1:C:111[B]:ILE:HD13	2.21	0.56
1:D:9:HIS:ND1	4:D:2006:HOH:O	2.33	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:MET:HE2	1:D:35:LEU:CG	2.36	0.54
2:A:1251:GOL:H12	4:A:2162:HOH:O	2.07	0.53
1:C:108:ASN:OD1	1:C:111[B]:ILE:HD13	2.08	0.53
1:C:246:GLU:O	1:C:247:LYS:C	2.51	0.53
1:B:16:MET:HE2	1:B:35:LEU:CG	2.38	0.53
1:C:71:GLN:CD	1:C:110:GLN:HG2	2.33	0.53
1:B:12:GLU:CG	4:B:2016:HOH:O	2.50	0.52
4:C:2095:HOH:O	1:D:107:PRO:O	2.19	0.52
1:B:71:GLN:HG2	1:B:114:GLU:OE2	2.10	0.52
1:C:11:SER:O	1:C:14:PRO:HD2	2.09	0.52
1:A:234:ASN:HD21	1:B:26[A]:GLN:CG	2.23	0.52
1:D:11:SER:C	1:D:14:PRO:HD2	2.36	0.51
1:D:16:MET:CE	1:D:35:LEU:HG	2.36	0.51
1:A:142:LEU:HB3	1:A:161:LEU:HD22	1.91	0.51
1:C:71:GLN:OE1	1:C:110:GLN:HG2	2.11	0.51
1:A:230:GLN:NE2	1:A:242:GLN:HA	2.26	0.50
1:B:9:HIS:HA	4:B:2016:HOH:O	2.12	0.50
1:C:45:GLN:NE2	4:C:2039:HOH:O	2.30	0.50
1:C:234:ASN:HD21	1:D:26:GLN:CG	2.25	0.50
1:A:16:MET:HE3	1:A:34:LYS:HB2	1.92	0.50
1:B:41:GLY:O	4:B:2044:HOH:O	2.20	0.49
1:D:71:GLN:CD	1:D:110:GLN:HG2	2.38	0.49
1:D:246:GLU:O	1:D:247:LYS:C	2.55	0.49
1:A:24:ASP:HA	1:B:193:GLU:OE1	2.13	0.49
1:B:8:HIS:HB3	1:D:201:TRP:CE2	2.48	0.49
1:C:11:SER:C	1:C:14:PRO:HD2	2.37	0.49
1:A:209:GLY:O	1:A:214:LYS:HE2	2.13	0.49
1:C:71:GLN:NE2	1:C:111[B]:ILE:HD11	2.27	0.48
1:C:16:MET:CE	1:C:34:LYS:CB	2.91	0.48
1:C:181:LEU:O	1:C:185:VAL:HG23	2.13	0.48
1:D:28:LEU:C	1:D:28:LEU:HD23	2.38	0.48
1:D:71:GLN:HG3	1:D:111:ILE:HD11	1.97	0.47
1:C:193:GLU:OE1	1:D:24:ASP:HA	2.15	0.47
2:B:1251:GOL:C1	4:B:2142:HOH:O	2.61	0.47
1:A:142:LEU:HB3	1:A:161:LEU:CD2	2.45	0.47
1:A:71:GLN:HG3	1:A:111:ILE:CD1	2.44	0.46
1:A:230:GLN:HE22	1:A:242:GLN:HA	1.79	0.46
1:C:232:HIS:O	1:C:238:GLN:NE2	2.44	0.46
1:C:218:LYS:NZ	4:C:2138:HOH:O	2.45	0.46
1:D:52:ALA:HB2	4:D:2038:HOH:O	2.16	0.46
1:A:26:GLN:HE21	1:B:234:ASN:HD21	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:LEU:HA	1:A:70:LEU:CD1	2.46	0.45
1:B:71:GLN:OE1	1:B:110:GLN:HG2	2.16	0.45
1:D:193:GLU:HA	1:D:196:LEU:HB2	1.97	0.45
1:A:201:TRP:NE1	1:A:240[B]:GLU:OE2	2.42	0.45
1:A:236:LYS:O	1:A:240[B]:GLU:HG2	2.17	0.45
1:D:222:ALA:O	1:D:226:LEU:HG	2.17	0.44
1:D:65:PRO:HA	4:D:2017:HOH:O	2.18	0.44
1:A:26:GLN:CG	1:B:234:ASN:HD21	2.30	0.44
1:D:142:LEU:HB3	1:D:161:LEU:HD22	2.00	0.44
1:A:186:GLN:CG	4:A:2186:HOH:O	2.43	0.44
1:B:71:GLN:CD	1:B:110:GLN:HG2	2.43	0.44
1:A:163:ASN:O	1:A:166:SER:HB2	2.18	0.43
1:A:236:LYS:HA	1:A:236:LYS:HD3	1.84	0.43
1:C:212:GLU:O	1:C:215:GLN:HB3	2.18	0.43
1:D:11:SER:O	1:D:14:PRO:HD2	2.18	0.43
1:D:141:ALA:O	1:D:145:LEU:HG	2.18	0.43
1:B:239:LYS:NZ	1:B:243:GLU:OE1	2.51	0.43
1:C:71:GLN:HE21	1:C:111[B]:ILE:HD11	1.82	0.43
1:C:95:GLY:O	1:C:98:PRO:HD2	2.18	0.43
1:D:233[B]:GLU:CD	1:D:233[B]:GLU:H	2.24	0.43
1:D:218:LYS:NZ	4:D:2102:HOH:O	2.50	0.43
1:A:234:ASN:HD21	1:B:26[A]:GLN:HE21	1.67	0.43
1:B:142:LEU:HB3	1:B:161:LEU:HD22	1.99	0.43
1:D:19:GLN:CG	4:D:2014:HOH:O	2.35	0.43
1:D:71:GLN:HG2	1:D:111:ILE:HD13	2.00	0.43
1:D:26:GLN:C	1:D:26:GLN:CD	2.87	0.42
1:B:16:MET:HE1	1:B:35:LEU:HG	2.00	0.42
1:B:239:LYS:NZ	1:D:10:GLY:HA3	2.34	0.42
1:D:9:HIS:HA	1:D:12:GLU:OE1	2.19	0.42
1:A:10:GLY:H	1:A:12:GLU:CG	2.33	0.42
1:A:16:MET:CE	1:A:34:LYS:HB2	2.50	0.42
2:A:1251:GOL:C1	4:A:2162:HOH:O	2.65	0.41
1:A:8:HIS:HB3	1:C:201:TRP:CE2	2.55	0.41
1:D:225:LYS:HD3	1:D:225:LYS:HA	1.80	0.41
1:C:142:LEU:HD13	1:C:161:LEU:HD13	2.02	0.41
1:A:78:GLY:HA3	1:A:117:TRP:CZ3	2.55	0.41
1:A:16:MET:HE2	1:A:16:MET:HB3	1.65	0.41
1:B:16:MET:HE3	1:B:34:LYS:HB2	2.02	0.41
1:B:62:LEU:HA	1:B:70:LEU:CD1	2.51	0.41
1:A:234:ASN:ND2	1:B:26[A]:GLN:CG	2.84	0.41
1:B:181:LEU:HD21	1:B:206:ILE:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:GLY:O	1:B:214:LYS:HE2	2.21	0.40
1:C:234:ASN:O	1:C:238:GLN:HG3	2.20	0.40
1:C:234:ASN:OD1	1:C:236:LYS:HB2	2.21	0.40
1:D:15:GLN:O	1:D:19:GLN:HG3	2.21	0.40
1:B:228:GLN:HE21	1:B:228:GLN:HB2	1.69	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	252/247 (102%)	249 (99%)	3 (1%)	0	100	100
1	B	250/247 (101%)	249 (100%)	1 (0%)	0	100	100
1	C	246/247 (100%)	241 (98%)	5 (2%)	0	100	100
1	D	245/247 (99%)	241 (98%)	4 (2%)	0	100	100
All	All	993/988 (100%)	980 (99%)	13 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	203/196 (104%)	192 (95%)	11 (5%)	20	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	201/196 (103%)	191 (95%)	10 (5%)	22	10
1	C	197/196 (100%)	188 (95%)	9 (5%)	24	12
1	D	196/196 (100%)	186 (95%)	10 (5%)	21	9
All	All	797/784 (102%)	757 (95%)	40 (5%)	22	10

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	HIS
1	A	12	GLU
1	A	26	GLN
1	A	103	LEU
1	A	110	GLN
1	A	119	LEU
1	A	161	LEU
1	A	219	GLU
1	A	223	LEU
1	A	225	LYS
1	A	239	LYS
1	B	4	HIS
1	B	9	HIS
1	B	103	LEU
1	B	110	GLN
1	B	119	LEU
1	B	161	LEU
1	B	219	GLU
1	B	223	LEU
1	B	225	LYS
1	B	250	SER
1	C	4	HIS
1	C	103	LEU
1	C	110	GLN
1	C	119	LEU
1	C	161	LEU
1	C	225	LYS
1	C	236	LYS
1	C	239	LYS
1	C	248	LEU
1	D	4	HIS
1	D	12	GLU
1	D	103	LEU

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Mol	Chain	Res	Type
1	D	119	LEU
1	D	161	LEU
1	D	212	GLU
1	D	233[A]	GLU
1	D	233[B]	GLU
1	D	236	LYS
1	D	239	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	26	GLN
1	A	45	GLN
1	A	110	GLN
1	A	230	GLN
1	B	9	HIS
1	B	113	GLN
1	B	152	GLN
1	B	228	GLN
1	B	249	GLN
1	C	205	ASN
1	D	110	GLN

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 ⓘ

Of 18 ligands modelled in this entry, 16 are monoatomic - leaving 2 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	B	1251	-	5,5,5	0.34	0	5,5,5	1.29	0
2	GOL	A	1251	-	5,5,5	0.28	0	5,5,5	1.73	2 (40%)

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	B	1251	-	-	2/4/4/4	-
2	GOL	A	1251	-	-	1/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1251	GOL	O3-C3-C2	2.37	121.05	110.38
2	A	1251	GOL	C3-C2-C1	-2.06	104.22	111.80

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1251	GOL	C1-C2-C3-O3
2	B	1251	GOL	O2-C2-C3-O3
2	A	1251	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1251	GOL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1251	GOL	2	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(Å ²)	Q<0.9
1	A	247/247 (100%)	-1.32	0 100 100	13, 29, 48, 60	7 (2%)
1	B	247/247 (100%)	-1.32	0 100 100	12, 30, 48, 58	5 (2%)
1	C	245/247 (99%)	-1.03	0 100 100	11, 38, 62, 84	3 (1%)
1	D	244/247 (98%)	-1.05	0 100 100	10, 37, 62, 81	3 (1%)
All	All	983/988 (99%)	-1.18	0 100 100	10, 33, 56, 84	18 (1%)

There are no RSRZ outliers to report.

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	1251	6/6	0.99	0.04	30,45,50,51	0
2	GOL	B	1251	6/6	0.99	0.04	30,42,46,47	0
3	CA	C	1250	1/1	0.99	0.03	37,37,37,37	0
3	CA	C	1251	1/1	0.99	0.07	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	D	1248	1/1	0.99	0.09	37,37,37,37	0
3	CA	A	1255	1/1	1.00	0.03	31,31,31,31	0
3	CA	A	1256	1/1	1.00	0.04	32,32,32,32	0
3	CA	A	1257	1/1	1.00	0.02	27,27,27,27	0
3	CA	A	1258	1/1	1.00	0.04	30,30,30,30	0
3	CA	A	1300	1/1	1.00	0.02	49,49,49,49	0
3	CA	B	1252	1/1	1.00	0.02	27,27,27,27	0
3	CA	B	1253	1/1	1.00	0.04	31,31,31,31	0
3	CA	C	1249	1/1	1.00	0.02	40,40,40,40	0
3	CA	A	1252	1/1	1.00	0.05	34,34,34,34	0
3	CA	A	1253	1/1	1.00	0.03	32,32,32,32	0
3	CA	C	1300	1/1	1.00	0.03	49,49,49,49	0
3	CA	A	1254	1/1	1.00	0.02	32,32,32,32	0
3	CA	D	1249	1/1	1.00	0.04	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.