



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 02:05 am BST

PDB ID : 4DBA  
Title : Designed Armadillo repeat protein (YIIM3AII)  
Authors : Madhurantakam, C.; Varadamsetty, G.; Grutter, M.G.; Pluckthun, A.; Mittl, P.R.E.  
Deposited on : 2012-01-13  
Resolution : 2.40 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

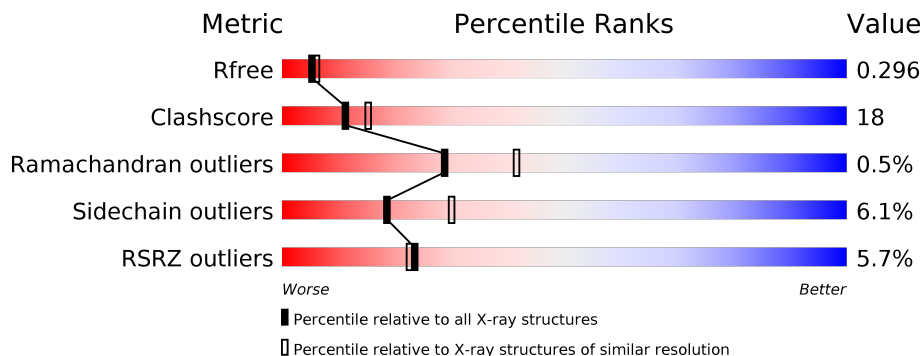
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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  $\geq 3$ , 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	210	
1	B	210	
1	C	210	
1	D	210	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	B	302	-	-	X	-

## 2 Entry composition [i](#)

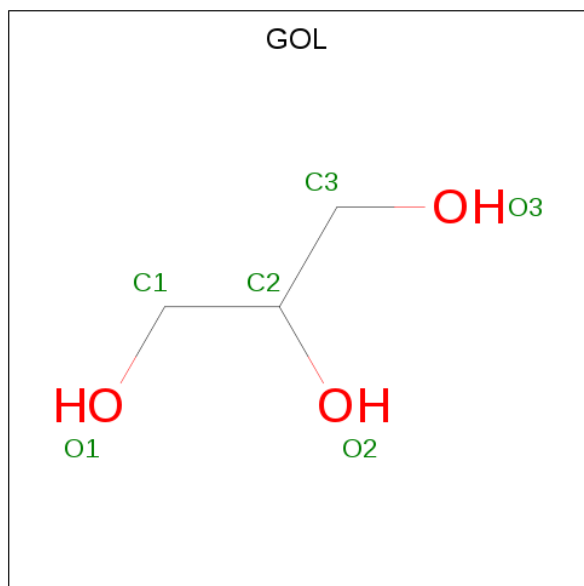
There are 3 unique types of molecules in this entry. The entry contains 5976 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Designed Armadillo repeat protein, YIIM3AII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	196	Total 1470	C 912	N 251	O 305	S 2	0	0	0
1	B	196	Total 1466	C 910	N 251	O 303	S 2	0	0	0
1	C	196	Total 1470	C 912	N 251	O 305	S 2	0	0	0
1	D	196	Total 1470	C 912	N 251	O 305	S 2	0	0	0

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

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

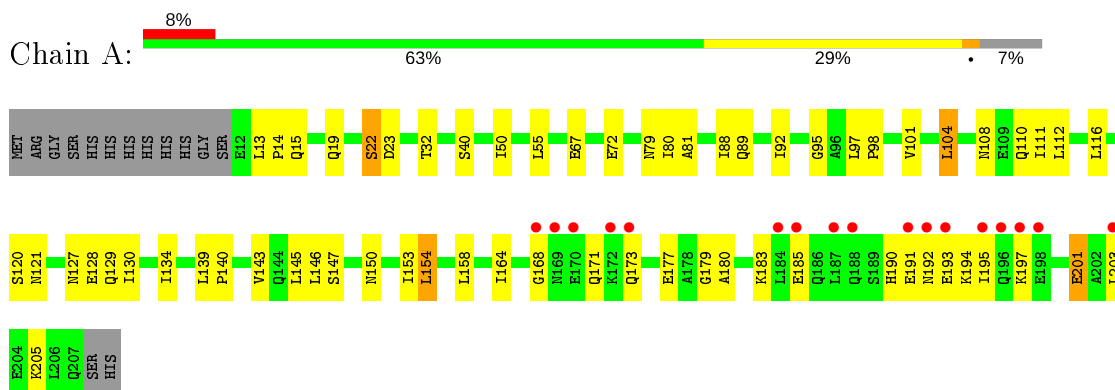
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	13	Total	O	0	0
			13	13		
3	B	22	Total	O	0	0
			22	22		
3	C	21	Total	O	0	0
			21	21		
3	D	14	Total	O	0	0
			14	14		

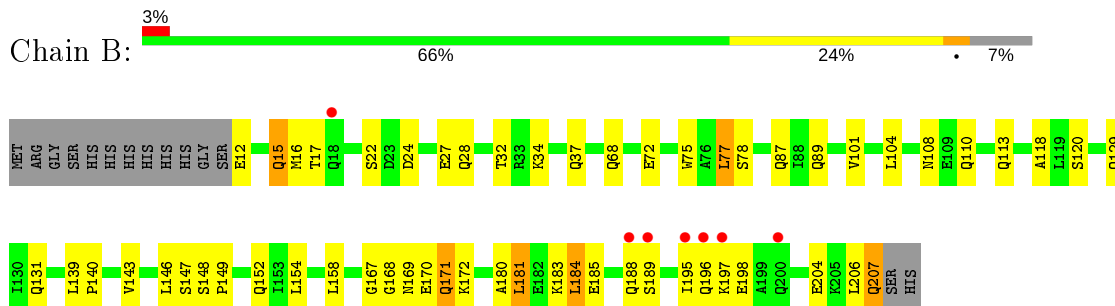
### 3 Residue-property plots i

These plots are drawn for all protein, RNA and DNA 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.

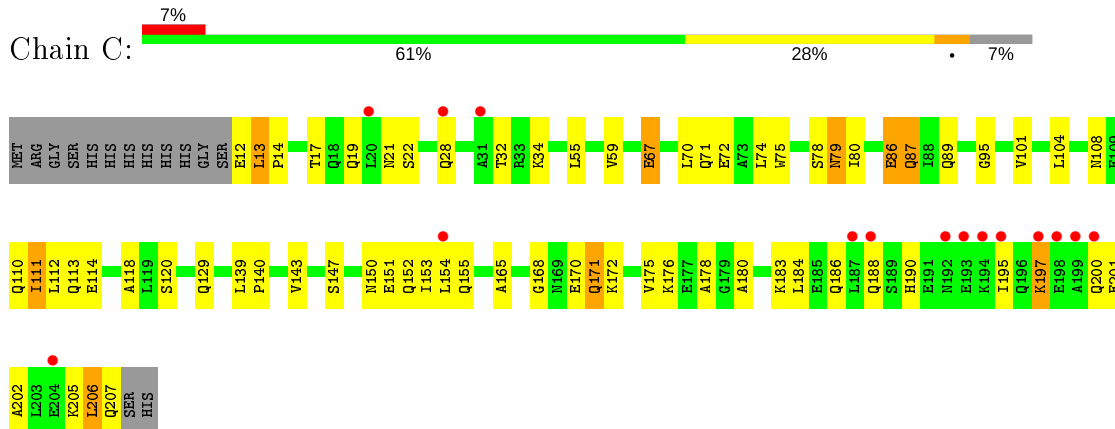
- Molecule 1: Designed Armadillo repeat protein, YIIM3AII



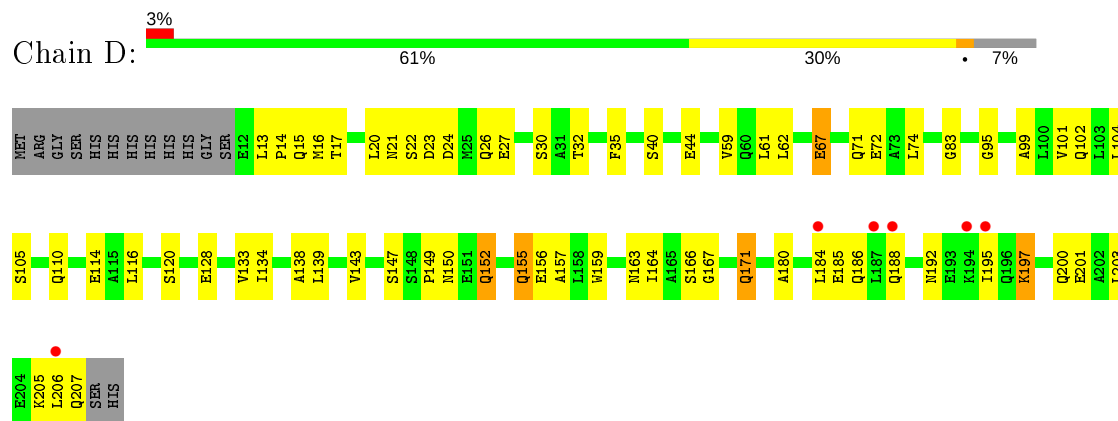
- Molecule 1: Designed Armadillo repeat protein, YIIM3AII



- Molecule 1: Designed Armadillo repeat protein, YIIM3AII



- Molecule 1: Designed Armadillo repeat protein, YIIM3AII



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.15Å 60.60Å 61.86Å 74.82° 89.55° 75.53°	Depositor
Resolution (Å)	25.29 – 2.40 36.42 – 2.40	Depositor EDS
% Data completeness (in resolution range)	89.7 (25.29-2.40) 89.7 (36.42-2.40)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.07 (at 2.39Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.234 , 0.301 0.231 , 0.296	Depositor DCC
$R_{free}$ test set	1434 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.5	Xtrriage
Anisotropy	0.256	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 56.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5976	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.18% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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	0.46	0/1484	0.56	0/2015
1	B	0.47	0/1480	0.60	0/2010
1	C	0.43	0/1484	0.57	0/2015
1	D	0.42	0/1484	0.59	0/2015
All	All	0.44	0/5932	0.58	0/8055

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	1470	0	1466	50	0
1	B	1466	0	1462	50	0
1	C	1470	0	1466	60	0
1	D	1470	0	1466	61	0
2	B	18	0	24	4	0
2	D	12	0	16	0	0
3	A	13	0	0	7	0
3	B	22	0	0	7	0
3	C	21	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	14	0	0	14	0
All	All	5976	0	5900	211	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 18.

All (211) 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:15:GLN:HB2	3:D:405:HOH:O	1.60	1.00
1:B:75:TRP:HZ3	2:B:302:GOL:HO2	1.00	0.95
1:C:152:GLN:HG3	3:C:310:HOH:O	1.73	0.88
1:D:185:GLU:O	1:D:188:GLN:HG2	1.79	0.83
1:A:32:THR:CG2	1:B:72:GLU:HB2	2.10	0.80
1:C:86:GLU:OE1	1:C:86:GLU:HA	1.83	0.78
1:C:168:GLY:O	1:C:172:LYS:HG3	1.85	0.76
1:B:169:ASN:HA	1:B:172:LYS:HE3	1.68	0.75
1:C:147:SER:HB3	1:C:183:LYS:NZ	2.01	0.75
1:B:101:VAL:O	1:B:104:LEU:HB2	1.88	0.74
1:A:101:VAL:O	1:A:104:LEU:HB2	1.88	0.73
1:C:72:GLU:HB3	3:D:413:HOH:O	1.88	0.73
1:C:72:GLU:HB3	1:D:32:THR:HG22	1.71	0.73
1:C:28:GLN:NE2	1:D:61:LEU:HD21	2.04	0.72
1:C:183:LYS:HD2	1:C:186:GLN:NE2	2.06	0.71
1:B:183:LYS:HE3	3:B:415:HOH:O	1.91	0.70
1:B:131:GLN:NE2	1:B:171:GLN:OE1	2.26	0.69
1:D:59:VAL:HG13	3:D:411:HOH:O	1.93	0.68
1:A:89:GLN:HG2	1:A:129:GLN:HE21	1.58	0.68
1:A:32:THR:HG22	1:B:72:GLU:HB2	1.75	0.67
1:D:139:LEU:O	1:D:143:VAL:HG23	1.93	0.67
1:C:201:GLU:O	1:C:205:LYS:HG3	1.94	0.67
1:A:23:ASP:HB2	3:A:306:HOH:O	1.94	0.67
1:A:32:THR:HG21	1:B:72:GLU:HB2	1.77	0.67
1:B:185:GLU:O	1:B:188:GLN:HG2	1.94	0.66
1:A:89:GLN:HG2	1:A:129:GLN:NE2	2.10	0.66
1:B:204:GLU:O	1:B:207:GLN:HG3	1.96	0.66
1:C:13:LEU:N	1:C:14:PRO:HD2	2.10	0.66
1:D:105:SER:HA	3:D:408:HOH:O	1.96	0.65
1:C:12:GLU:C	1:C:14:PRO:HD2	2.17	0.65
1:D:134:ILE:HG12	1:D:139:LEU:HD11	1.78	0.64
1:A:95:GLY:HA2	3:A:301:HOH:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:GLN:O	1:C:175:VAL:HG23	1.98	0.64
1:B:87:GLN:HG3	3:B:410:HOH:O	1.98	0.63
1:A:108:ASN:OD1	1:A:110:GLN:HB2	1.99	0.63
1:A:14:PRO:HA	3:A:313:HOH:O	1.98	0.63
1:B:78:SER:HB2	1:B:118:ALA:HB2	1.78	0.63
1:C:28:GLN:HE21	1:D:61:LEU:HD21	1.63	0.63
1:D:67:GLU:H	1:D:67:GLU:CD	2.03	0.61
1:C:151:GLU:O	1:C:155:GLN:HG3	2.00	0.61
1:B:12:GLU:N	3:B:413:HOH:O	2.33	0.60
1:D:150:ASN:OD1	1:D:152:GLN:HG2	2.01	0.60
1:C:176:LYS:HA	3:C:317:HOH:O	2.01	0.60
1:D:197:LYS:O	1:D:200:GLN:HB2	2.02	0.60
1:A:140:PRO:HA	3:A:309:HOH:O	2.01	0.59
1:A:143:VAL:HB	3:A:309:HOH:O	2.01	0.59
1:C:89:GLN:HG2	1:C:129:GLN:HE21	1.67	0.59
1:C:180:ALA:O	1:C:184:LEU:HB2	2.03	0.59
2:B:301:GOL:H2	2:B:302:GOL:O3	2.03	0.58
1:C:104:LEU:HB2	3:C:316:HOH:O	2.03	0.58
1:C:72:GLU:HB3	1:D:32:THR:CG2	2.32	0.58
1:B:68:GLN:O	1:B:72:GLU:HG2	2.03	0.58
1:D:101:VAL:O	1:D:104:LEU:HB2	2.03	0.58
1:B:37:GLN:HA	1:B:37:GLN:NE2	2.19	0.57
1:A:72:GLU:HG2	3:A:312:HOH:O	2.03	0.57
1:D:32:THR:HG22	3:D:413:HOH:O	2.05	0.57
1:D:99:ALA:CB	3:D:411:HOH:O	2.52	0.57
1:A:134:ILE:HG12	1:A:139:LEU:HD11	1.87	0.57
1:C:147:SER:HB3	1:C:183:LYS:CE	2.35	0.57
1:C:188:GLN:OE1	1:C:200:GLN:HG3	2.04	0.57
1:D:167:GLY:HA3	1:D:171:GLN:HG3	1.86	0.56
1:B:206:LEU:O	1:B:207:GLN:HB2	2.03	0.56
1:B:139:LEU:O	1:B:143:VAL:HG23	2.05	0.56
1:C:13:LEU:N	1:C:14:PRO:CD	2.68	0.56
1:A:72:GLU:HB3	1:B:32:THR:HG22	1.87	0.56
1:B:37:GLN:HA	1:B:37:GLN:HE21	1.70	0.56
1:B:75:TRP:HZ3	2:B:302:GOL:O2	1.78	0.56
1:C:101:VAL:HG13	3:C:316:HOH:O	2.06	0.55
1:C:55:LEU:HD11	1:C:80:ILE:HD13	1.89	0.55
1:D:14:PRO:HD2	3:D:404:HOH:O	2.07	0.55
1:D:185:GLU:HA	1:D:203:LEU:HD11	1.89	0.55
1:C:150:ASN:HB3	1:C:153:ILE:HD12	1.88	0.55
1:A:55:LEU:HD11	1:A:80:ILE:HD13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:LYS:HB2	1:D:197:LYS:NZ	2.22	0.54
1:A:67:GLU:H	1:A:67:GLU:CD	2.10	0.54
1:A:201:GLU:O	1:A:205:LYS:HG3	2.08	0.53
1:D:197:LYS:HA	1:D:200:GLN:OE1	2.09	0.53
1:D:67:GLU:O	1:D:71:GLN:HG3	2.09	0.53
1:C:67:GLU:O	1:C:71:GLN:HG3	2.09	0.53
1:B:89:GLN:HG2	1:B:129:GLN:HE21	1.74	0.52
1:C:74:LEU:HG	1:C:114:GLU:HG3	1.90	0.52
1:C:172:LYS:HB3	1:C:206:LEU:HD12	1.90	0.52
1:D:152:GLN:O	1:D:155:GLN:HB2	2.10	0.52
1:D:207:GLN:HB2	3:D:403:HOH:O	2.09	0.52
1:A:139:LEU:O	1:A:143:VAL:HG23	2.10	0.52
1:D:197:LYS:HZ3	1:D:197:LYS:HB2	1.75	0.52
1:B:22:SER:O	1:B:28:GLN:NE2	2.43	0.51
1:D:186:GLN:C	1:D:188:GLN:H	2.14	0.51
1:B:158:LEU:HG	1:B:198:GLU:HG2	1.92	0.51
1:C:202:ALA:O	1:C:206:LEU:HD22	2.10	0.51
1:C:75:TRP:CH2	1:C:79:ASN:ND2	2.78	0.51
1:D:62:LEU:HD12	3:D:411:HOH:O	2.09	0.51
1:A:50:ILE:HG23	1:A:55:LEU:HD22	1.93	0.51
1:A:128:GLU:CD	1:A:128:GLU:H	2.15	0.50
1:B:181:LEU:HD22	3:B:417:HOH:O	2.11	0.50
1:C:70:LEU:HD22	1:C:111:ILE:HG12	1.93	0.50
1:C:104:LEU:HD12	3:C:316:HOH:O	2.12	0.50
1:C:113:GLN:NE2	1:C:152:GLN:HB3	2.26	0.50
1:D:95:GLY:HA2	3:D:407:HOH:O	2.11	0.50
1:C:139:LEU:HB2	3:C:303:HOH:O	2.11	0.49
1:C:147:SER:HB3	1:C:183:LYS:HZ3	1.74	0.49
1:A:173:GLN:O	1:A:177:GLU:HB2	2.12	0.49
1:B:16:MET:CE	1:B:34:LYS:HD3	2.42	0.49
1:D:101:VAL:HG22	1:D:138:ALA:HA	1.93	0.49
1:C:78:SER:HB3	1:C:118:ALA:HB2	1.95	0.49
1:B:72:GLU:HB3	3:B:406:HOH:O	2.13	0.49
1:D:163:ASN:O	1:D:166:SER:HB2	2.12	0.49
1:B:139:LEU:HB2	1:B:140:PRO:HD3	1.95	0.49
1:D:22:SER:OG	1:D:23:ASP:N	2.46	0.49
1:D:192:ASN:HB3	1:D:195:ILE:HD12	1.94	0.48
1:C:89:GLN:HG2	1:C:129:GLN:NE2	2.28	0.48
1:C:19:GLN:O	1:C:22:SER:HB3	2.13	0.48
1:C:32:THR:HG22	1:D:72:GLU:HB3	1.96	0.48
1:C:176:LYS:C	1:C:178:ALA:H	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:MET:HG3	3:D:410:HOH:O	2.14	0.47
1:C:59:VAL:HG11	1:C:95:GLY:O	2.13	0.47
1:B:168:GLY:H	1:B:171:GLN:CG	2.26	0.47
1:D:116:LEU:HD13	1:D:156:GLU:HB3	1.95	0.47
1:C:17:THR:O	1:C:21:ASN:ND2	2.48	0.47
1:A:116:LEU:HD11	1:A:145:LEU:HD13	1.97	0.47
2:B:301:GOL:H2	2:B:302:GOL:C3	2.45	0.47
1:A:192:ASN:HD21	1:A:194:LYS:HB2	1.81	0.46
1:C:206:LEU:O	1:C:207:GLN:CB	2.64	0.46
1:A:112:LEU:C	1:A:112:LEU:HD23	2.36	0.46
1:D:13:LEU:N	1:D:14:PRO:CD	2.79	0.46
1:A:134:ILE:HD11	1:A:164:ILE:CG2	2.46	0.46
1:D:17:THR:O	1:D:21:ASN:ND2	2.48	0.46
1:D:20:LEU:HD11	1:D:35:PHE:CE2	2.50	0.46
1:A:193:GLU:HG2	1:A:194:LYS:N	2.30	0.46
1:B:77:LEU:HA	1:B:77:LEU:HD12	1.76	0.46
1:B:167:GLY:HA3	1:B:171:GLN:HG3	1.96	0.46
1:C:34:LYS:HE3	3:C:302:HOH:O	2.14	0.46
1:D:67:GLU:N	1:D:67:GLU:CD	2.69	0.46
1:B:195:ILE:O	1:B:196:GLN:C	2.53	0.46
1:A:22:SER:OG	1:A:23:ASP:N	2.49	0.46
1:B:198:GLU:HG3	3:B:412:HOH:O	2.15	0.46
1:A:143:VAL:O	1:A:146:LEU:HB2	2.16	0.45
1:B:168:GLY:H	1:B:171:GLN:HG3	1.82	0.45
1:B:16:MET:HG2	3:B:402:HOH:O	2.16	0.45
1:D:156:GLU:O	1:D:159:TRP:N	2.50	0.45
1:A:15:GLN:HB3	3:A:302:HOH:O	2.17	0.45
1:B:168:GLY:N	1:B:171:GLN:CG	2.80	0.45
1:A:190:HIS:O	1:A:191:GLU:C	2.55	0.45
1:B:17:THR:O	1:B:17:THR:HG22	2.16	0.45
1:C:139:LEU:O	1:C:143:VAL:HG23	2.17	0.45
1:A:19:GLN:O	1:A:22:SER:HB3	2.17	0.45
1:C:190:HIS:CE1	1:C:195:ILE:HD12	2.52	0.45
1:C:87:GLN:OE1	1:C:87:GLN:N	2.50	0.45
1:D:152:GLN:HG2	1:D:152:GLN:H	1.50	0.45
1:D:99:ALA:HB3	3:D:411:HOH:O	2.17	0.45
1:B:180:ALA:O	1:B:184:LEU:HB2	2.18	0.44
1:C:147:SER:HA	3:C:306:HOH:O	2.16	0.44
1:A:81:ALA:O	1:A:121:ASN:HB3	2.16	0.44
1:A:185:GLU:HA	1:A:203:LEU:HD11	1.99	0.44
1:B:16:MET:HE2	1:B:34:LYS:HD3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:LEU:O	1:B:185:GLU:HB2	2.18	0.44
1:D:206:LEU:O	1:D:207:GLN:HB3	2.17	0.44
1:B:154:LEU:HD23	1:B:154:LEU:O	2.17	0.44
1:A:130:ILE:CG2	1:A:164:ILE:HG23	2.48	0.44
1:A:150:ASN:HB3	1:A:153:ILE:HD12	1.99	0.44
1:D:134:ILE:HG12	1:D:139:LEU:CD1	2.47	0.44
1:D:201:GLU:O	1:D:205:LYS:HG3	2.17	0.44
1:A:134:ILE:HG23	1:A:139:LEU:HD12	2.00	0.44
1:A:192:ASN:ND2	1:A:194:LYS:HB2	2.33	0.44
1:C:197:LYS:O	1:C:200:GLN:HB2	2.17	0.44
1:D:150:ASN:OD1	1:D:150:ASN:C	2.56	0.43
1:C:72:GLU:CB	1:D:32:THR:CG2	2.96	0.43
1:A:179:GLY:O	1:A:180:ALA:C	2.56	0.43
1:C:207:GLN:HB2	3:C:315:HOH:O	2.17	0.43
1:D:180:ALA:O	1:D:184:LEU:HB2	2.19	0.43
1:D:184:LEU:HD23	1:D:203:LEU:HD23	2.00	0.43
1:C:72:GLU:HG2	3:C:319:HOH:O	2.18	0.43
1:A:116:LEU:HD23	1:A:116:LEU:HA	1.87	0.43
1:A:13:LEU:N	1:A:14:PRO:CD	2.81	0.43
1:A:154:LEU:HD13	1:A:195:ILE:HD13	2.00	0.43
1:A:127:ASN:O	1:A:171:GLN:NE2	2.52	0.43
1:D:133:VAL:HG11	1:D:164:ILE:HD11	2.00	0.43
1:A:134:ILE:HG12	1:A:139:LEU:CD1	2.47	0.43
1:B:12:GLU:O	1:B:16:MET:HG3	2.19	0.43
1:B:113:GLN:NE2	1:B:152:GLN:HB3	2.34	0.43
1:C:139:LEU:HB2	1:C:140:PRO:HD3	2.00	0.43
1:C:70:LEU:C	1:C:70:LEU:HD23	2.40	0.43
1:D:150:ASN:OD1	1:D:152:GLN:CG	2.67	0.42
1:D:83:GLY:HA3	3:D:406:HOH:O	2.19	0.42
1:A:147:SER:HB3	1:A:183:LYS:CE	2.48	0.42
1:B:24:ASP:HB3	1:B:27:GLU:HG3	2.01	0.42
1:D:74:LEU:HD21	1:D:114:GLU:HB3	2.01	0.42
1:A:197:LYS:HE2	1:A:201:GLU:OE1	2.20	0.42
1:B:148:SER:OG	1:B:149:PRO:HD2	2.19	0.42
1:B:168:GLY:N	1:B:171:GLN:HG2	2.34	0.42
1:D:203:LEU:HA	1:D:203:LEU:HD23	1.79	0.42
1:C:72:GLU:CB	1:D:32:THR:HG21	2.50	0.42
1:A:108:ASN:HB3	1:A:111:ILE:HD12	2.01	0.42
1:B:104:LEU:HA	1:B:104:LEU:HD23	1.65	0.42
1:C:165:ALA:HB1	1:C:206:LEU:HD13	2.02	0.42
1:B:207:GLN:HE21	1:B:207:GLN:HB2	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:LEU:C	1:C:112:LEU:HD23	2.40	0.42
1:C:32:THR:HG21	1:D:72:GLU:HB2	2.02	0.41
1:D:24:ASP:HB3	1:D:27:GLU:HG2	2.02	0.41
1:D:156:GLU:O	1:D:157:ALA:C	2.58	0.41
1:A:88:ILE:O	1:A:92:ILE:HG13	2.20	0.41
1:B:146:LEU:HB2	1:B:183:LYS:HG2	2.02	0.41
1:B:15:GLN:HG2	1:B:16:MET:N	2.30	0.41
1:D:26:GLN:O	1:D:30:SER:HB2	2.20	0.41
1:D:147:SER:HA	3:D:412:HOH:O	2.20	0.41
1:C:108:ASN:OD1	1:C:110:GLN:HB2	2.20	0.41
1:D:99:ALA:O	1:D:102:GLN:HB3	2.21	0.41
1:A:154:LEU:O	1:A:158:LEU:HB2	2.21	0.41
1:C:17:THR:HG22	1:C:17:THR:O	2.20	0.40
1:A:97:LEU:O	1:A:98:PRO:C	2.58	0.40
1:B:108:ASN:OD1	1:B:110:GLN:HB2	2.22	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	194/210 (92%)	179 (92%)	13 (7%)	2 (1%)	15	23
1	B	194/210 (92%)	185 (95%)	8 (4%)	1 (0%)	29	41
1	C	194/210 (92%)	183 (94%)	11 (6%)	0	100	100
1	D	194/210 (92%)	173 (89%)	20 (10%)	1 (0%)	29	41
All	All	776/840 (92%)	720 (93%)	52 (7%)	4 (0%)	29	41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	168	GLY
1	B	189	SER
1	A	22	SER
1	D	149	PRO

### 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	157/170 (92%)	151 (96%)	6 (4%)	33	51
1	B	156/170 (92%)	146 (94%)	10 (6%)	17	28
1	C	157/170 (92%)	145 (92%)	12 (8%)	13	20
1	D	157/170 (92%)	147 (94%)	10 (6%)	17	28
All	All	627/680 (92%)	589 (94%)	38 (6%)	18	30

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	SER
1	A	79	ASN
1	A	104	LEU
1	A	120	SER
1	A	154	LEU
1	A	201	GLU
1	B	15	GLN
1	B	77	LEU
1	B	120	SER
1	B	147	SER
1	B	170	GLU
1	B	171	GLN
1	B	181	LEU
1	B	184	LEU
1	B	197	LYS
1	B	207	GLN
1	C	13	LEU
1	C	67	GLU

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Mol	Chain	Res	Type
1	C	79	ASN
1	C	86	GLU
1	C	87	GLN
1	C	111	ILE
1	C	120	SER
1	C	154	LEU
1	C	170	GLU
1	C	171	GLN
1	C	197	LYS
1	C	206	LEU
1	D	40	SER
1	D	44	GLU
1	D	67	GLU
1	D	110	GLN
1	D	120	SER
1	D	128	GLU
1	D	152	GLN
1	D	155	GLN
1	D	171	GLN
1	D	197	LYS

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

Mol	Chain	Res	Type
1	A	37	GLN
1	A	68	GLN
1	A	186	GLN
1	B	37	GLN
1	B	45	GLN
1	B	47	GLN
1	B	87	GLN
1	B	89	GLN
1	B	131	GLN
1	B	171	GLN
1	B	207	GLN
1	C	21	ASN
1	C	28	GLN
1	C	131	GLN
1	C	186	GLN
1	D	45	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

5 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	D	301	-	5,5,5	0.35	0	5,5,5	0.25	0
2	GOL	D	302	-	5,5,5	0.33	0	5,5,5	0.28	0
2	GOL	B	301	-	5,5,5	0.36	0	5,5,5	0.44	0
2	GOL	B	303	-	5,5,5	0.40	0	5,5,5	0.18	0
2	GOL	B	302	-	5,5,5	0.35	0	5,5,5	0.18	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	D	301	-	-	1/4/4/4	-
2	GOL	D	302	-	-	4/4/4/4	-
2	GOL	B	301	-	-	3/4/4/4	-
2	GOL	B	303	-	-	3/4/4/4	-
2	GOL	B	302	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	302	GOL	O1-C1-C2-C3
2	B	301	GOL	C1-C2-C3-O3
2	B	303	GOL	O1-C1-C2-C3
2	B	301	GOL	O2-C2-C3-O3
2	D	302	GOL	C1-C2-C3-O3
2	B	303	GOL	O1-C1-C2-O2
2	D	302	GOL	O1-C1-C2-O2
2	B	303	GOL	C1-C2-C3-O3
2	D	302	GOL	O2-C2-C3-O3
2	D	301	GOL	O1-C1-C2-C3
2	B	301	GOL	O1-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	GOL	2	0
2	B	302	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	196/210 (93%)	0.44	17 (8%) 10 9	37, 63, 118, 129	0
1	B	196/210 (93%)	0.26	7 (3%) 42 42	36, 64, 98, 111	0
1	C	196/210 (93%)	0.40	15 (7%) 13 12	38, 68, 113, 122	0
1	D	196/210 (93%)	0.12	6 (3%) 49 47	47, 72, 114, 124	0
All	All	784/840 (93%)	0.30	45 (5%) 23 22	36, 67, 113, 129	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	195	ILE	9.3
1	A	187	LEU	5.9
1	D	206	LEU	4.8
1	B	189	SER	4.7
1	C	195	ILE	4.5
1	D	184	LEU	4.4
1	D	194	LYS	4.2
1	A	203	LEU	4.1
1	A	170	GLU	4.1
1	C	188	GLN	3.7
1	C	200	GLN	3.6
1	A	184	LEU	3.5
1	A	188	GLN	3.5
1	A	169	ASN	3.4
1	B	197	LYS	3.2
1	A	193	GLU	3.1
1	C	193	GLU	3.1
1	C	187	LEU	3.0
1	D	195	ILE	3.0
1	C	197	LYS	2.9
1	D	188	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	187	LEU	2.8
1	A	168	GLY	2.8
1	A	192	ASN	2.8
1	C	31	ALA	2.8
1	A	173	GLN	2.6
1	A	172	LYS	2.6
1	C	192	ASN	2.6
1	A	196	GLN	2.5
1	C	194	LYS	2.5
1	A	191	GLU	2.5
1	B	195	ILE	2.3
1	B	188	GLN	2.2
1	C	28	GLN	2.2
1	C	199	ALA	2.2
1	A	197	LYS	2.2
1	B	200	GLN	2.2
1	B	18	GLN	2.2
1	B	196	GLN	2.2
1	C	198	GLU	2.1
1	A	185	GLU	2.1
1	A	198	GLU	2.1
1	C	20	LEU	2.1
1	C	154	LEU	2.1
1	C	204	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 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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	B	301	6/6	0.62	0.31	79,86,92,94	0
2	GOL	B	303	6/6	0.67	0.25	87,90,93,96	0
2	GOL	D	302	6/6	0.83	0.18	89,90,94,97	0
2	GOL	B	302	6/6	0.83	0.23	76,77,81,83	0
2	GOL	D	301	6/6	0.90	0.29	84,87,91,92	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.