wwPDB X-ray Structure Validation Summary Report (i)

May 25, 2020 – 07:27 am BST

PDB ID	:	4GN3
Title	:	OBody AM1L10 bound to hen egg-white lysozyme
Authors	:	Steemson, J.D.; Liddament, M.T.
Deposited on	:	2012-08-16
Resolution	:	1.95 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

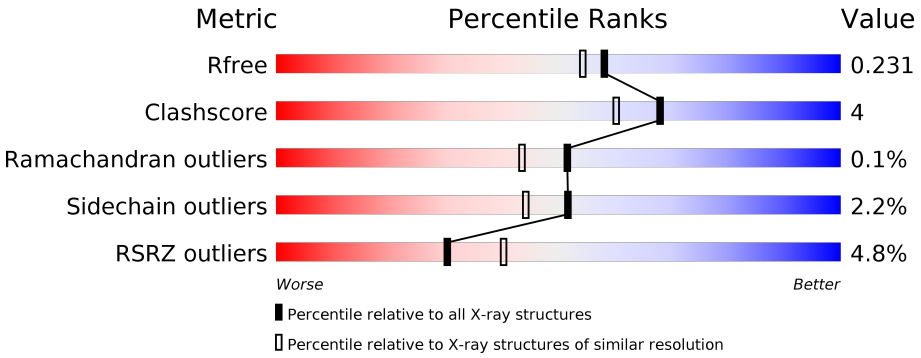
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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.



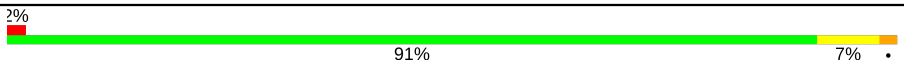
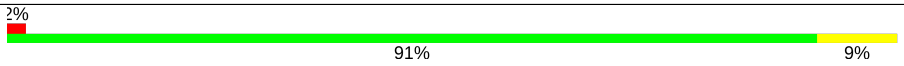
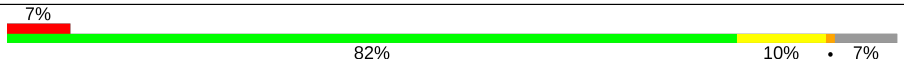
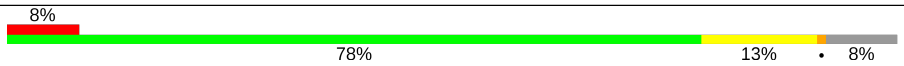
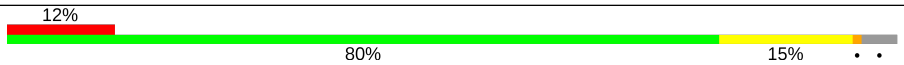
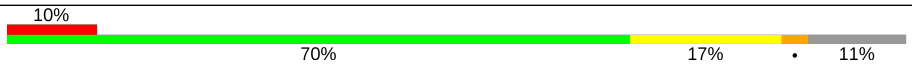
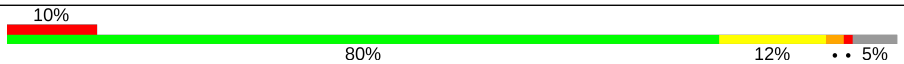
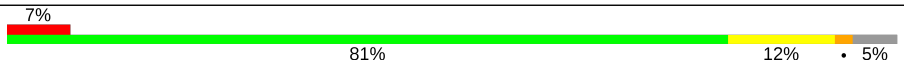
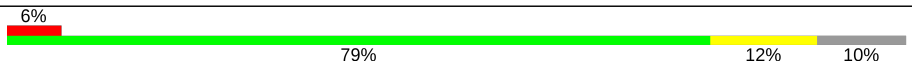
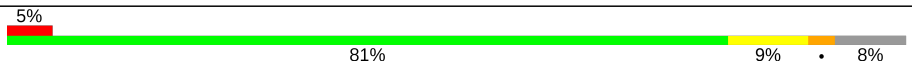
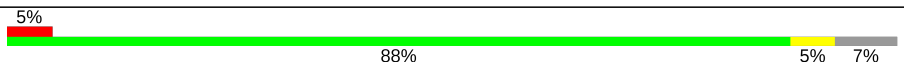
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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 <=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	129	92% 7%
1	C	129	2% 91% 9%
1	E	129	2% 95%
1	G	129	2% 94% 5%
1	I	129	3% 91% 9%
1	K	129	3% 95% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	M	129	
1	O	129	
1	Q	129	
2	B	113	
2	D	113	
2	F	113	
2	H	113	
2	J	113	
2	L	113	
2	N	113	
2	P	113	
2	R	113	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 19197 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 Lysozyme C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	129	Total	C	N	O	S	0	0	0
			1001	613	193	185	10			
1	C	129	Total	C	N	O	S	3	0	0
			1001	613	193	185	10			
1	E	129	Total	C	N	O	S	3	0	0
			1001	613	193	185	10			
1	G	129	Total	C	N	O	S	3	1	0
			1006	618	193	185	10			
1	I	129	Total	C	N	O	S	3	0	0
			1001	613	193	185	10			
1	K	129	Total	C	N	O	S	0	0	0
			1001	613	193	185	10			
1	M	129	Total	C	N	O	S	4	0	0
			1001	613	193	185	10			
1	O	129	Total	C	N	O	S	3	0	0
			1001	613	193	185	10			
1	Q	129	Total	C	N	O	S	0	1	0
			1009	618	196	185	10			

- Molecule 2 is a protein called OBody AM1L10.

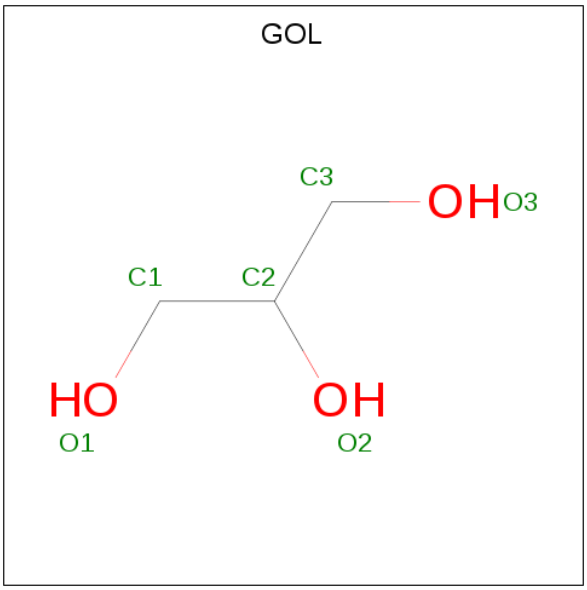
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	105	Total	C	N	O		3	1	0
			819	533	135	151				
2	D	104	Total	C	N	O		0	1	0
			811	529	133	149				
2	F	108	Total	C	N	O	S	0	1	0
			837	544	138	154	1			
2	H	101	Total	C	N	O		13	1	0
			795	520	130	145				
2	J	107	Total	C	N	O	S	4	1	0
			829	540	136	152	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	L	107	Total 847	C 554	N 138	O 155	6	3	0
2	N	102	Total 805	C 525	N 132	O 148	6	1	0
2	P	104	Total 802	C 521	N 133	O 148	6	0	0
2	R	105	Total 811	C 527	N 135	O 149	0	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



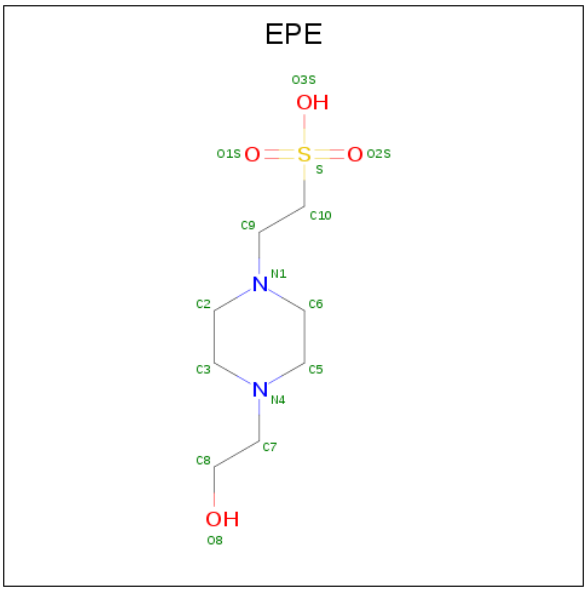
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 6	C 3	O 3		0	0
3	A	1	Total 6	C 3	O 3		0	0
3	C	1	Total 6	C 3	O 3		0	0
3	C	1	Total 6	C 3	O 3		0	0
3	D	1	Total 6	C 3	O 3		0	0
3	D	1	Total 6	C 3	O 3		0	0
3	E	1	Total 6	C 3	O 3		0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total C O 6 3 3	0	0
3	G	1	Total C O 6 3 3	0	0
3	G	1	Total C O 6 3 3	0	0
3	I	1	Total C O 6 3 3	0	0
3	I	1	Total C O 6 3 3	0	0
3	K	1	Total C O 6 3 3	0	0
3	L	1	Total C O 6 3 3	0	0
3	M	1	Total C O 6 3 3	0	0
3	M	1	Total C O 6 3 3	0	0
3	O	1	Total C O 6 3 3	0	0
3	Q	1	Total C O 6 3 3	0	0

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	F	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	H	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	J	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	L	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	N	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	P	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	R	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	174	Total	O	0	0
			174	174		
5	B	163	Total	O	0	0
			163	163		
5	C	175	Total	O	0	0
			175	175		
5	D	137	Total	O	0	0
			137	137		
5	E	155	Total	O	0	0
			155	155		
5	F	140	Total	O	0	0
			140	140		
5	G	143	Total	O	0	0
			143	143		
5	H	105	Total	O	0	0
			105	105		
5	I	153	Total	O	0	0
			153	153		
5	J	129	Total	O	0	0
			129	129		
5	K	150	Total	O	0	0
			150	150		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	156	Total O 156 156	0	0
5	M	140	Total O 140 140	0	0
5	N	118	Total O 118 118	0	0
5	O	141	Total O 141 141	0	0
5	P	134	Total O 134 134	0	0
5	Q	135	Total O 135 135	0	0
5	R	128	Total O 128 128	0	0

3 Residue-property plots (i)

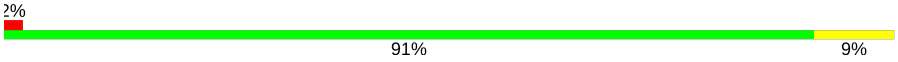
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Lysozyme C

Chain A:

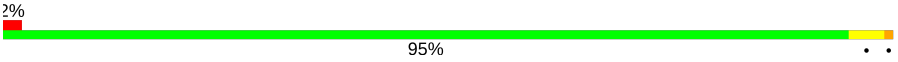
- Molecule 1: Lysozyme C

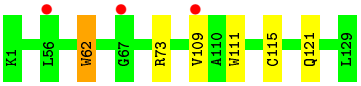
Chain C:



- Molecule 1: Lysozyme C

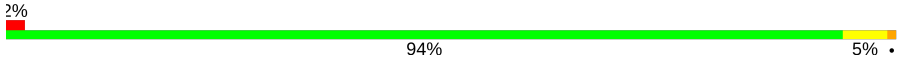
Chain E:

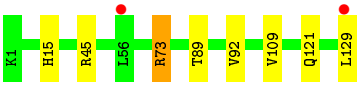




- Molecule 1: Lysozyme C

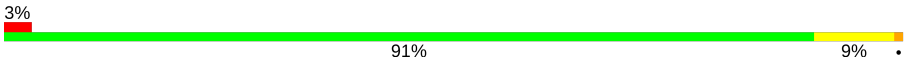
Chain G:

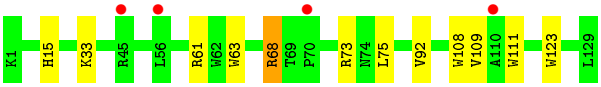




- Molecule 1: Lysozyme C

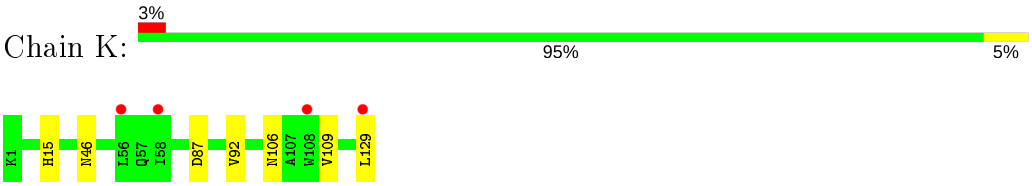
Chain I:





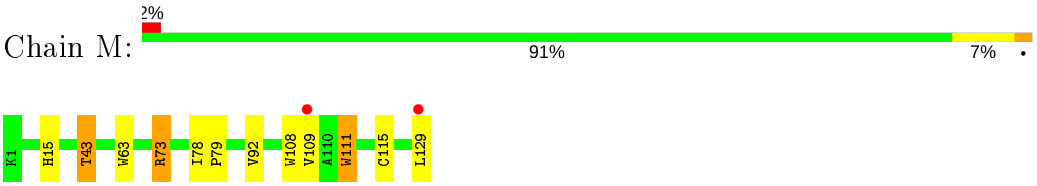
- Molecule 1: Lysozyme C

Chain K:



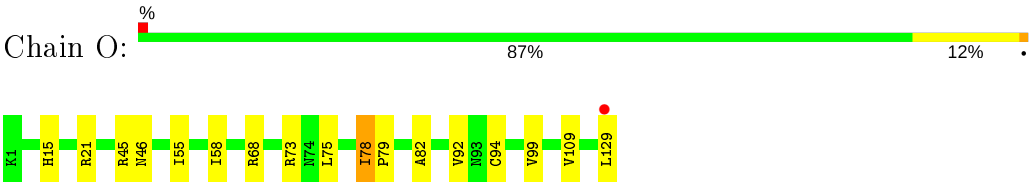
• Molecule 1: Lysozyme C

Chain M:



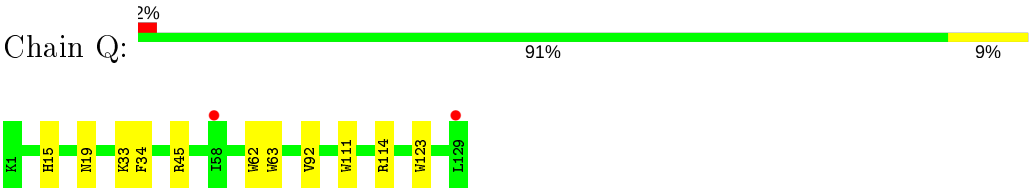
• Molecule 1: Lysozyme C

Chain O:



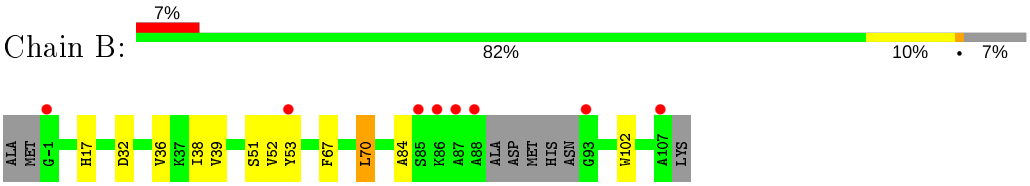
• Molecule 1: Lysozyme C

Chain Q:



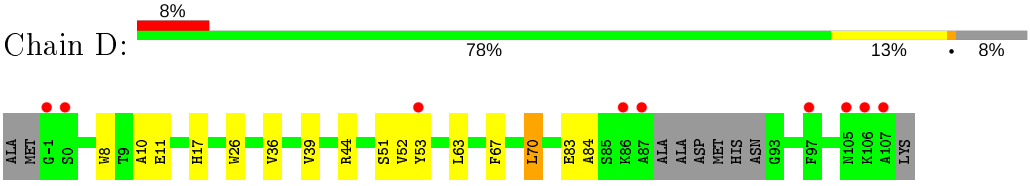
• Molecule 2: OBody AM1L10

Chain B:



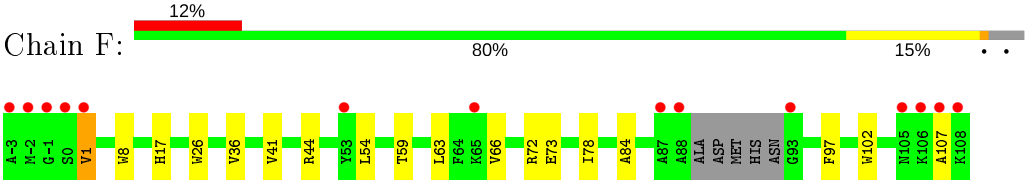
• Molecule 2: OBody AM1L10

Chain D:



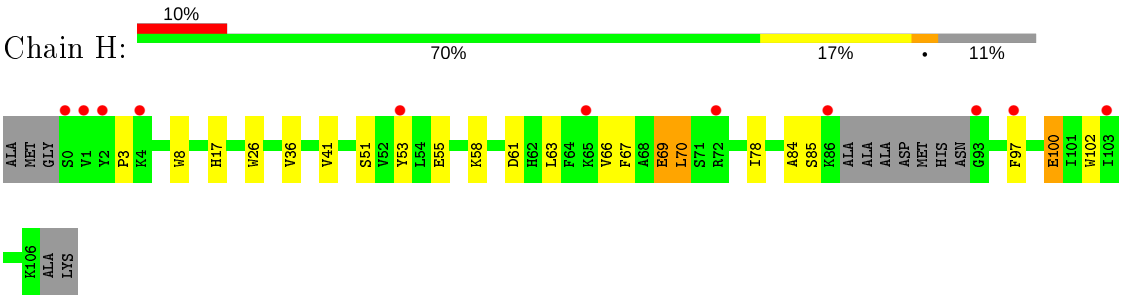
• Molecule 2: OBody AM1L10

Chain F:



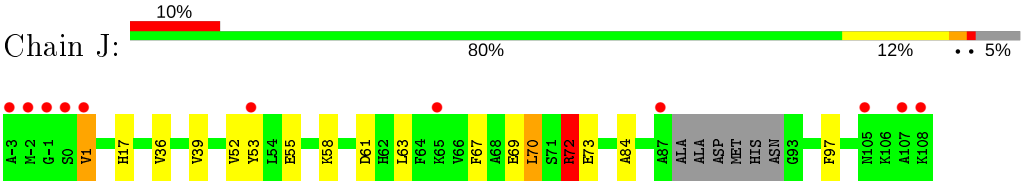
• Molecule 2: OBody AM1L10

Chain H:



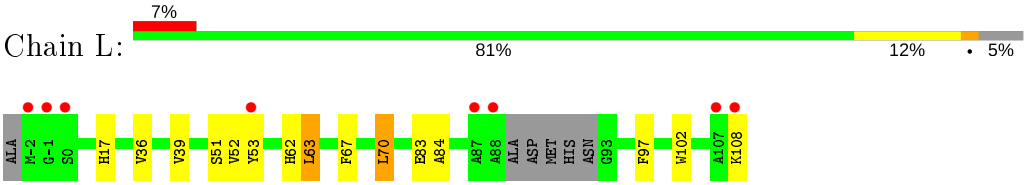
• Molecule 2: OBody AM1L10

Chain J:



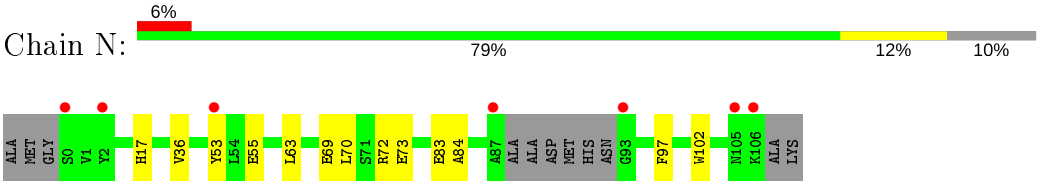
• Molecule 2: OBody AM1L10

Chain L:



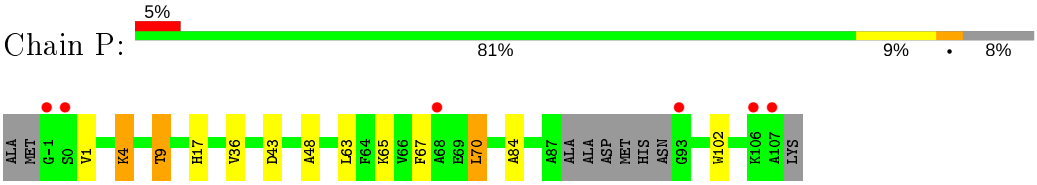
• Molecule 2: OBody AM1L10

Chain N:



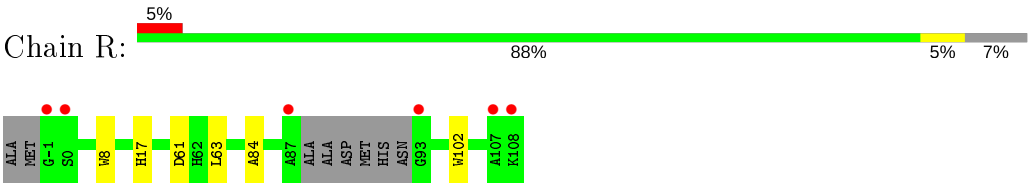
• Molecule 2: OBody AM1L10

Chain P:



• Molecule 2: OBody AM1L10

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	60.54Å 186.25Å 245.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.77 – 1.95 29.76 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.8 (29.77-1.95) 98.9 (29.76-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.28 (at 1.95Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.199 , 0.228 0.201 , 0.231	Depositor DCC
R_{free} test set	10150 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	28.3	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 46.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	19197	wwPDB-VP
Average B, all atoms (Å^2)	34.0	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 50.87 % 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 6.0788e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, EPE

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	0.59	1/1021 (0.1%)	0.55	0/1379
1	C	0.61	4/1021 (0.4%)	0.58	0/1379
1	E	0.61	1/1021 (0.1%)	0.61	1/1379 (0.1%)
1	G	0.61	1/1029 (0.1%)	0.60	1/1391 (0.1%)
1	I	1.82	7/1021 (0.7%)	1.22	6/1379 (0.4%)
1	K	0.58	0/1021	0.57	0/1379
1	M	0.59	3/1021 (0.3%)	0.54	0/1379
1	O	0.58	0/1021	0.56	0/1379
1	Q	0.59	3/1032 (0.3%)	0.55	0/1393
2	B	0.55	1/838 (0.1%)	0.58	0/1138
2	D	0.54	2/833 (0.2%)	0.58	0/1131
2	F	0.54	3/856 (0.4%)	0.56	0/1162
2	H	8.24	7/817 (0.9%)	2.77	3/1109 (0.3%)
2	J	2.08	3/851 (0.4%)	3.04	4/1155 (0.3%)
2	L	0.61	2/873 (0.2%)	0.62	2/1185 (0.2%)
2	N	0.92	2/824 (0.2%)	0.60	1/1119 (0.1%)
2	P	1.10	2/820 (0.2%)	0.85	2/1113 (0.2%)
2	R	0.53	2/829 (0.2%)	0.56	0/1124
All	All	2.02	44/16749 (0.3%)	1.11	20/22673 (0.1%)

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	I	0	1
2	H	0	1
2	J	0	1
All	All	0	3

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	69	GLU	CD-OE1	207.08	3.53	1.25
2	H	69	GLU	CD-OE2	110.14	2.46	1.25
2	J	72	ARG	CZ-NH1	54.02	2.03	1.33
1	I	68	ARG	CZ-NH2	34.42	1.77	1.33
1	I	68	ARG	NE-CZ	33.74	1.76	1.33

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	72	ARG	NE-CZ-NH2	-75.52	82.54	120.30
2	H	69	GLU	OE1-CD-OE2	-71.16	37.91	123.30
2	J	72	ARG	NE-CZ-NH1	-55.76	92.42	120.30
2	H	69	GLU	CG-CD-OE1	-47.22	23.87	118.30
2	J	72	ARG	NH1-CZ-NH2	-37.88	77.73	119.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	69	GLU	Sidechain
1	I	68	ARG	Sidechain
2	J	72	ARG	Sidechain

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	1001	0	959	7	0
1	C	1001	0	959	4	0
1	E	1001	0	959	3	0
1	G	1006	0	970	6	0
1	I	1001	0	959	7	0
1	K	1001	0	959	4	0
1	M	1001	0	959	9	0
1	O	1001	0	959	10	0
1	Q	1009	0	972	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	819	0	826	9	0
2	D	811	0	822	11	0
2	F	837	0	842	10	0
2	H	795	0	805	12	0
2	J	829	0	837	13	0
2	L	847	0	856	11	0
2	N	805	0	813	7	0
2	P	802	0	813	10	0
2	R	811	0	826	2	0
3	A	12	0	16	2	0
3	C	12	0	16	1	0
3	D	12	0	16	3	0
3	E	12	0	16	0	0
3	G	12	0	16	0	0
3	I	12	0	16	1	0
3	K	6	0	8	0	0
3	L	6	0	8	0	0
3	M	12	0	16	1	0
3	O	6	0	8	0	0
3	Q	6	0	8	0	0
4	B	15	0	18	1	0
4	D	15	0	17	0	0
4	F	15	0	17	0	0
4	H	15	0	17	0	0
4	J	15	0	18	0	0
4	L	15	0	18	0	0
4	N	15	0	17	0	0
4	P	15	0	18	0	0
4	R	15	0	17	0	0
5	A	174	0	0	0	0
5	B	163	0	0	0	0
5	C	175	0	0	0	0
5	D	137	0	0	0	0
5	E	155	0	0	0	0
5	F	140	0	0	0	0
5	G	143	0	0	1	0
5	H	105	0	0	2	0
5	I	153	0	0	1	0
5	J	129	0	0	2	0
5	K	150	0	0	0	0
5	L	156	0	0	0	0
5	M	140	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	N	118	0	0	0	0
5	O	141	0	0	0	0
5	P	134	0	0	0	0
5	Q	135	0	0	0	0
5	R	128	0	0	0	0
All	All	19197	0	16396	126	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 4.

The worst 5 of 126 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:M:73:ARG:HG2	1:M:73:ARG:HH11	1.38	0.88
2:J:17:HIS:HD2	2:J:84:ALA:H	1.20	0.87
2:L:17:HIS:HD2	2:L:84:ALA:H	1.24	0.83
2:B:51:SER:HB3	2:B:53[B]:TYR:CE1	2.14	0.83
2:B:38:ILE:HG12	2:B:53[B]:TYR:CD1	2.15	0.82

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	127/129 (98%)	126 (99%)	1 (1%)	0	100	100
1	C	127/129 (98%)	127 (100%)	0	0	100	100
1	E	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
1	G	128/129 (99%)	127 (99%)	1 (1%)	0	100	100
1	I	127/129 (98%)	126 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	K	127/129 (98%)	127 (100%)	0	0	100 100
1	M	127/129 (98%)	127 (100%)	0	0	100 100
1	O	127/129 (98%)	127 (100%)	0	0	100 100
1	Q	128/129 (99%)	128 (100%)	0	0	100 100
2	B	102/113 (90%)	101 (99%)	1 (1%)	0	100 100
2	D	101/113 (89%)	99 (98%)	2 (2%)	0	100 100
2	F	105/113 (93%)	102 (97%)	1 (1%)	2 (2%)	8 2
2	H	98/113 (87%)	95 (97%)	3 (3%)	0	100 100
2	J	104/113 (92%)	100 (96%)	3 (3%)	1 (1%)	15 6
2	L	106/113 (94%)	102 (96%)	4 (4%)	0	100 100
2	N	99/113 (88%)	97 (98%)	2 (2%)	0	100 100
2	P	100/113 (88%)	99 (99%)	1 (1%)	0	100 100
2	R	101/113 (89%)	98 (97%)	3 (3%)	0	100 100
All	All	2061/2178 (95%)	2033 (99%)	25 (1%)	3 (0%)	51 43

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	107	ALA
2	J	1	VAL
2	F	1	VAL

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	105/105 (100%)	104 (99%)	1 (1%)	76 74
1	C	105/105 (100%)	104 (99%)	1 (1%)	76 74
1	E	105/105 (100%)	105 (100%)	0	100 100
1	G	106/105 (101%)	104 (98%)	2 (2%)	57 50

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	105/105 (100%)	105 (100%)	0	100	100
1	K	105/105 (100%)	103 (98%)	2 (2%)	57	50
1	M	105/105 (100%)	102 (97%)	3 (3%)	42	31
1	O	105/105 (100%)	102 (97%)	3 (3%)	42	31
1	Q	106/105 (101%)	104 (98%)	2 (2%)	57	50
2	B	86/91 (94%)	85 (99%)	1 (1%)	71	68
2	D	86/91 (94%)	83 (96%)	3 (4%)	36	24
2	F	87/91 (96%)	85 (98%)	2 (2%)	50	42
2	H	85/91 (93%)	81 (95%)	4 (5%)	26	13
2	J	87/91 (96%)	84 (97%)	3 (3%)	37	25
2	L	89/91 (98%)	87 (98%)	2 (2%)	52	44
2	N	86/91 (94%)	84 (98%)	2 (2%)	50	42
2	P	85/91 (93%)	80 (94%)	5 (6%)	19	8
2	R	86/91 (94%)	84 (98%)	2 (2%)	50	42
All	All	1724/1764 (98%)	1686 (98%)	38 (2%)	52	44

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	87	ASP
1	M	43	THR
1	Q	45	ARG
2	L	63	LEU
1	M	73	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	41	GLN
2	J	17	HIS
1	Q	44	ASN
1	I	44	ASN
1	I	46	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 carbohydrates in this entry.

5.6 Ligand geometry

27 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	$\#\|Z\| > 2$
3	GOL	A	202	-	5,5,5	0.23	0	5,5,5	0.42	0
4	EPE	D	201	-	15,15,15	2.47	2 (13%)	18,20,20	6.49	8 (44%)
3	GOL	D	203	-	5,5,5	0.31	0	5,5,5	0.38	0
3	GOL	Q	201	-	5,5,5	0.38	0	5,5,5	0.09	0
3	GOL	I	202	-	5,5,5	0.21	0	5,5,5	0.28	0
3	GOL	G	201	-	5,5,5	0.25	0	5,5,5	0.41	0
3	GOL	C	202	-	5,5,5	0.27	0	5,5,5	0.27	0
4	EPE	J	201	-	15,15,15	2.17	2 (13%)	18,20,20	5.63	6 (33%)
4	EPE	L	201	-	15,15,15	2.17	2 (13%)	18,20,20	5.71	11 (61%)
4	EPE	P	201	-	15,15,15	2.10	2 (13%)	18,20,20	5.61	6 (33%)
4	EPE	R	201	-	15,15,15	2.41	2 (13%)	18,20,20	6.39	7 (38%)
3	GOL	M	201	-	5,5,5	0.22	0	5,5,5	0.32	0
3	GOL	E	201	-	5,5,5	0.25	0	5,5,5	0.40	0
3	GOL	G	202	-	5,5,5	0.32	0	5,5,5	0.25	0
4	EPE	F	201	-	15,15,15	2.40	2 (13%)	18,20,20	6.27	8 (44%)
4	EPE	N	201	-	15,15,15	2.47	2 (13%)	18,20,20	6.25	6 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	L	202	-	5,5,5	0.37	0	5,5,5	0.27	0
3	GOL	K	201	-	5,5,5	0.22	0	5,5,5	0.53	0
3	GOL	I	201	-	5,5,5	0.26	0	5,5,5	0.29	0
3	GOL	D	202	-	5,5,5	0.33	0	5,5,5	0.36	0
3	GOL	C	201	-	5,5,5	0.18	0	5,5,5	0.33	0
3	GOL	M	202	-	5,5,5	0.26	0	5,5,5	0.39	0
3	GOL	A	201	-	5,5,5	0.22	0	5,5,5	0.39	0
3	GOL	E	202	-	5,5,5	0.30	0	5,5,5	0.45	0
4	EPE	H	201	-	15,15,15	2.43	2 (13%)	18,20,20	6.39	7 (38%)
4	EPE	B	201	-	15,15,15	2.12	2 (13%)	18,20,20	5.72	5 (27%)
3	GOL	O	201	-	5,5,5	0.21	0	5,5,5	0.33	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
3	GOL	A	202	-	-	2/4/4/4	-
4	EPE	D	201	-	-	4/9/19/19	0/1/1/1
3	GOL	D	203	-	-	2/4/4/4	-
3	GOL	Q	201	-	-	2/4/4/4	-
3	GOL	I	202	-	-	2/4/4/4	-
3	GOL	G	201	-	-	0/4/4/4	-
3	GOL	C	202	-	-	2/4/4/4	-
4	EPE	J	201	-	-	3/9/19/19	0/1/1/1
4	EPE	L	201	-	-	3/9/19/19	0/1/1/1
4	EPE	P	201	-	-	3/9/19/19	0/1/1/1
4	EPE	R	201	-	-	7/9/19/19	0/1/1/1
3	GOL	M	201	-	-	4/4/4/4	-
3	GOL	E	201	-	-	2/4/4/4	-
3	GOL	G	202	-	-	0/4/4/4	-
4	EPE	F	201	-	-	5/9/19/19	0/1/1/1
4	EPE	N	201	-	-	8/9/19/19	0/1/1/1
3	GOL	L	202	-	-	3/4/4/4	-
3	GOL	K	201	-	-	2/4/4/4	-
3	GOL	I	201	-	-	4/4/4/4	-
3	GOL	D	202	-	-	0/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	C	201	-	-	2/4/4/4	-
3	GOL	M	202	-	-	2/4/4/4	-
3	GOL	A	201	-	-	4/4/4/4	-
3	GOL	E	202	-	-	0/4/4/4	-
4	EPE	H	201	-	-	1/9/19/19	0/1/1/1
4	EPE	B	201	-	-	6/9/19/19	0/1/1/1
3	GOL	O	201	-	-	4/4/4/4	-

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	201	EPE	C10-S	-6.97	1.67	1.77
4	J	201	EPE	C10-S	-6.89	1.67	1.77
4	D	201	EPE	C10-S	-6.85	1.67	1.77
4	L	201	EPE	C10-S	-6.78	1.67	1.77
4	H	201	EPE	C10-S	-6.69	1.68	1.77

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	201	EPE	O1S-S-C10	-18.63	84.49	106.92
4	D	201	EPE	O1S-S-C10	-18.53	84.60	106.92
4	R	201	EPE	O2S-S-C10	-18.27	84.91	106.92
4	N	201	EPE	O2S-S-C10	-17.97	85.28	106.92
4	F	201	EPE	O1S-S-C10	-17.79	85.49	106.92

There are no chirality outliers.

5 of 77 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	202	GOL	C1-C2-C3-O3
3	D	203	GOL	O1-C1-C2-C3
3	Q	201	GOL	C1-C2-C3-O3
3	I	202	GOL	O1-C1-C2-O2
4	J	201	EPE	S-C10-C9-N1

There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	202	GOL	1	0
3	D	203	GOL	3	0
3	M	201	GOL	1	0
3	I	201	GOL	1	0
3	C	201	GOL	1	0
3	A	201	GOL	1	0
4	B	201	EPE	1	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^{th} 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	129/129 (100%)	0.04	1 (0%) 86 90	20, 28, 39, 44	0
1	C	129/129 (100%)	0.03	2 (1%) 72 79	20, 27, 38, 39	1 (0%)
1	E	129/129 (100%)	0.18	3 (2%) 60 69	21, 29, 41, 46	1 (0%)
1	G	129/129 (100%)	0.14	2 (1%) 72 79	25, 34, 44, 48	1 (0%)
1	I	129/129 (100%)	0.24	4 (3%) 49 58	22, 31, 45, 51	1 (0%)
1	K	129/129 (100%)	0.22	4 (3%) 49 58	22, 31, 42, 44	0
1	M	129/129 (100%)	0.24	2 (1%) 72 79	26, 36, 45, 54	1 (0%)
1	O	129/129 (100%)	0.13	1 (0%) 86 90	22, 31, 43, 45	1 (0%)
1	Q	129/129 (100%)	0.29	2 (1%) 72 79	24, 34, 44, 52	0
2	B	105/113 (92%)	0.13	8 (7%) 13 21	20, 25, 50, 72	1 (0%)
2	D	104/113 (92%)	0.22	9 (8%) 10 16	22, 28, 52, 63	0
2	F	108/113 (95%)	0.53	14 (12%) 3 5	24, 31, 62, 77	0
2	H	101/113 (89%)	0.57	11 (10%) 5 9	28, 37, 58, 75	5 (4%)
2	J	107/113 (94%)	0.45	11 (10%) 6 10	23, 29, 57, 97	3 (2%)
2	L	107/113 (94%)	0.25	8 (7%) 14 22	21, 25, 60, 75	2 (1%)
2	N	102/113 (90%)	0.22	7 (6%) 16 25	25, 31, 47, 62	2 (1%)
2	P	104/113 (92%)	0.22	6 (5%) 23 31	23, 28, 52, 70	4 (3%)
2	R	105/113 (92%)	0.11	6 (5%) 23 32	23, 29, 55, 72	1 (0%)
All	All	2104/2178 (96%)	0.23	101 (4%) 30 40	20, 31, 46, 97	24 (1%)

The worst 5 of 101 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	0	SER	9.5
2	B	88	ALA	8.6
2	L	-2	MET	8.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	108	LYS	7.9
2	F	107	ALA	7.7

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^{th} 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
3	GOL	L	202	6/6	0.42	0.37	84,84,85,85	0
3	GOL	M	202	6/6	0.65	0.23	56,59,60,61	0
3	GOL	G	202	6/6	0.69	0.22	48,50,51,52	0
3	GOL	E	202	6/6	0.69	0.21	52,53,53,55	0
3	GOL	A	201	6/6	0.70	0.24	43,46,48,52	0
3	GOL	K	201	6/6	0.70	0.22	51,54,56,60	0
3	GOL	M	201	6/6	0.71	0.24	54,55,57,59	0
4	EPE	H	201	15/15	0.71	0.31	72,81,89,90	0
3	GOL	G	201	6/6	0.72	0.29	54,56,56,59	0
3	GOL	O	201	6/6	0.78	0.21	48,50,53,54	0
4	EPE	N	201	15/15	0.80	0.28	64,67,70,71	0
3	GOL	A	202	6/6	0.81	0.17	43,45,47,48	0
3	GOL	D	202	6/6	0.82	0.44	44,49,49,51	0
3	GOL	Q	201	6/6	0.82	0.23	60,63,65,67	0
3	GOL	E	201	6/6	0.82	0.14	48,50,50,53	0
4	EPE	L	201	15/15	0.83	0.23	51,54,61,62	0
3	GOL	C	202	6/6	0.84	0.18	43,45,47,50	0
4	EPE	F	201	15/15	0.85	0.20	56,59,65,66	0
3	GOL	D	203	6/6	0.85	0.23	49,49,50,52	0
4	EPE	P	201	15/15	0.86	0.21	50,52,61,61	0
4	EPE	D	201	15/15	0.86	0.20	58,59,62,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	I	201	6/6	0.86	0.17	50,51,53,56	0
4	EPE	B	201	15/15	0.87	0.21	49,53,61,62	0
4	EPE	J	201	15/15	0.87	0.24	47,51,59,59	0
3	GOL	C	201	6/6	0.88	0.20	44,47,51,52	0
3	GOL	I	202	6/6	0.89	0.16	46,47,49,51	0
4	EPE	R	201	15/15	0.89	0.21	52,54,56,56	0

6.5 Other polymers

There are no such residues in this entry.