Full wwPDB X-ray Structure Validation Report (i)

Feb 21, 2017 – 11:47 AM EST

PDB ID	:	5M2Q
Title	:	Structure of cobinamide-bound BtuF mutant W66F, the periplasmic vitamin B12 binding protein in E.coli
Authors	:	Mireku, S.A.; Ruetz, M.; Zhou, T.; Korkhov, V.M.; Kraeutler, B.; Locher, K.P.
Deposited on	:	2016-10-13
Resolution	:	1.70 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
http://wwpdb.org/validation/2016/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:

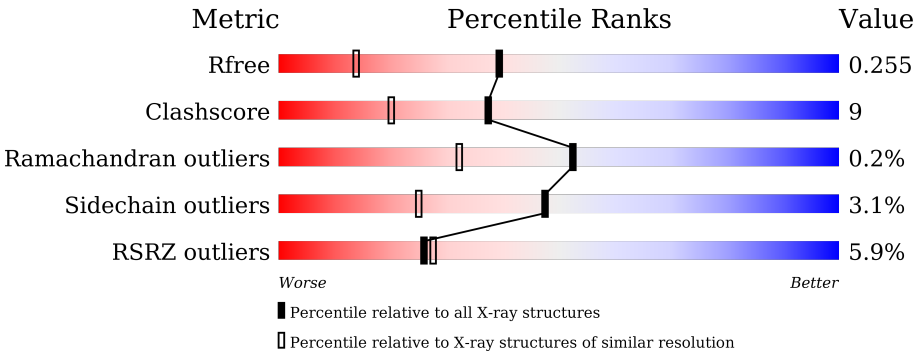
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 1.70 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}	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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. 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	289	4% 69% 9% · 21%
1	B	289	5% 66% 11% ·· 21%

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
3	CYN	A	302	-	-	X	-
4	GOL	A	303	-	-	-	X
4	GOL	B	303	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4085 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 Outer membrane protein A,Vitamin B12-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	0	0
			1765	1123	308	330	4			
1	B	228	Total	C	N	O	S	0	1	0
			1772	1129	309	329	5			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	SER	-	linker	UNP P0A910
A	21	MET	-	linker	UNP P0A910
A	66	PHE	TRP	engineered mutation	UNP P37028
A	267	SER	-	expression tag	UNP P37028
A	268	GLY	-	expression tag	UNP P37028
A	269	SER	-	expression tag	UNP P37028
A	270	LEU	-	expression tag	UNP P37028
A	271	GLU	-	expression tag	UNP P37028
A	272	VAL	-	expression tag	UNP P37028
A	273	LEU	-	expression tag	UNP P37028
A	274	PHE	-	expression tag	UNP P37028
A	275	GLN	-	expression tag	UNP P37028
A	276	GLY	-	expression tag	UNP P37028
A	277	PRO	-	expression tag	UNP P37028
A	278	GLY	-	expression tag	UNP P37028
A	279	GLY	-	expression tag	UNP P37028
A	280	SER	-	expression tag	UNP P37028
A	281	HIS	-	expression tag	UNP P37028
A	282	HIS	-	expression tag	UNP P37028
A	283	HIS	-	expression tag	UNP P37028
A	284	HIS	-	expression tag	UNP P37028
A	285	HIS	-	expression tag	UNP P37028
A	286	HIS	-	expression tag	UNP P37028
B	20	SER	-	linker	UNP P0A910
B	21	MET	-	linker	UNP P0A910

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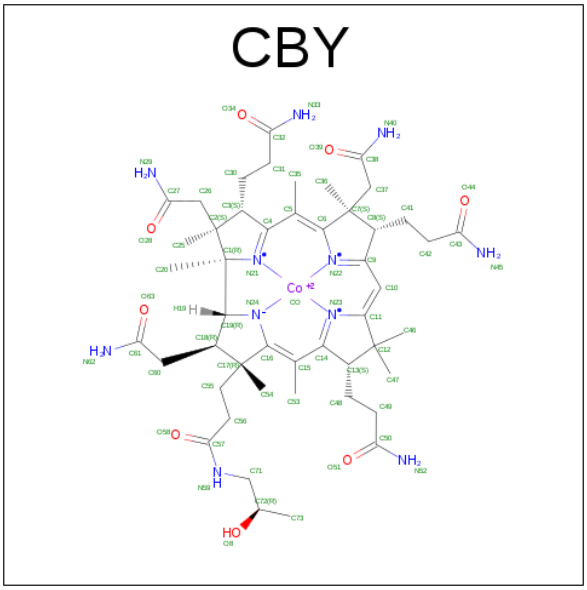
Chain	Residue	Modelled	Actual	Comment	Reference
B	66	PHE	TRP	engineered mutation	UNP P37028
B	267	SER	-	expression tag	UNP P37028
B	268	GLY	-	expression tag	UNP P37028
B	269	SER	-	expression tag	UNP P37028
B	270	LEU	-	expression tag	UNP P37028
B	271	GLU	-	expression tag	UNP P37028
B	272	VAL	-	expression tag	UNP P37028
B	273	LEU	-	expression tag	UNP P37028
B	274	PHE	-	expression tag	UNP P37028
B	275	GLN	-	expression tag	UNP P37028
B	276	GLY	-	expression tag	UNP P37028
B	277	PRO	-	expression tag	UNP P37028
B	278	GLY	-	expression tag	UNP P37028
B	279	GLY	-	expression tag	UNP P37028
B	280	SER	-	expression tag	UNP P37028
B	281	HIS	-	expression tag	UNP P37028
B	282	HIS	-	expression tag	UNP P37028
B	283	HIS	-	expression tag	UNP P37028
B	284	HIS	-	expression tag	UNP P37028
B	285	HIS	-	expression tag	UNP P37028
B	286	HIS	-	expression tag	UNP P37028

- Molecule 2 is COB(II)INAMIDE (three-letter code: CBY) (formula: $C_{48}H_{72}CoN_{11}O_8$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Co	N	O	0	0
			68	48	1	11	8		

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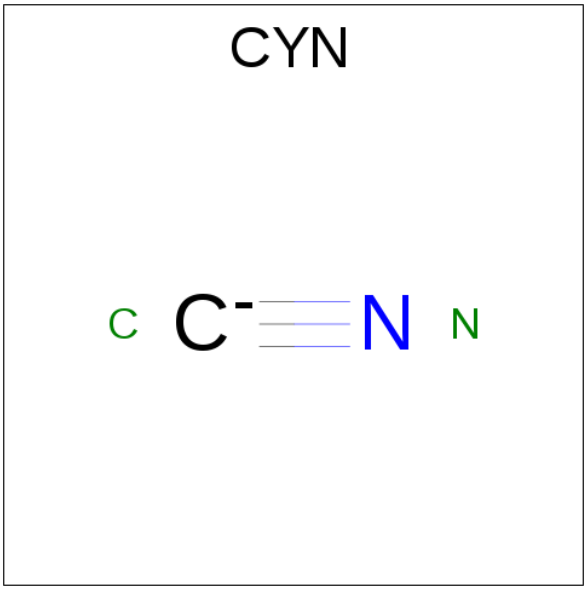
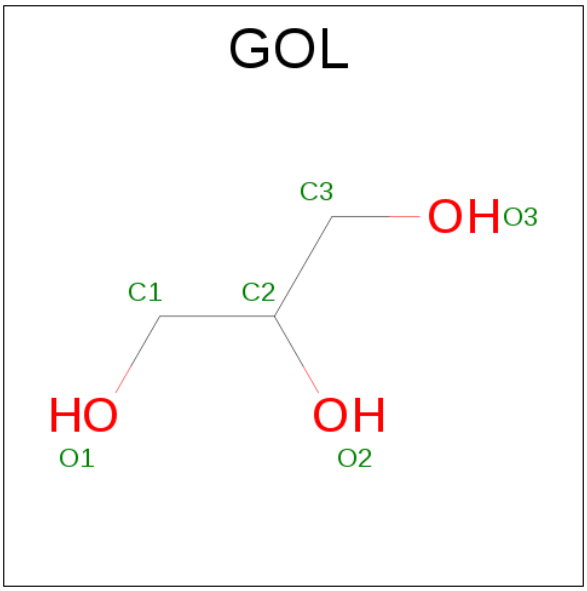
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Co	N	O	0	0
			68	48	1	11	8		

- Molecule 3 is CYANIDE ION (three-letter code: CYN) (formula: CN).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is water.

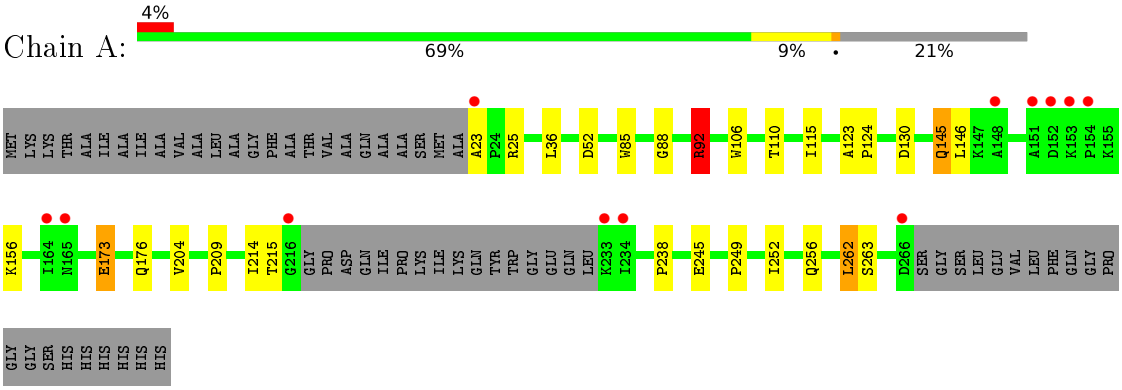
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	205	Total O 205 205	0	0
5	B	185	Total O 185 185	0	0

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 errors 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.

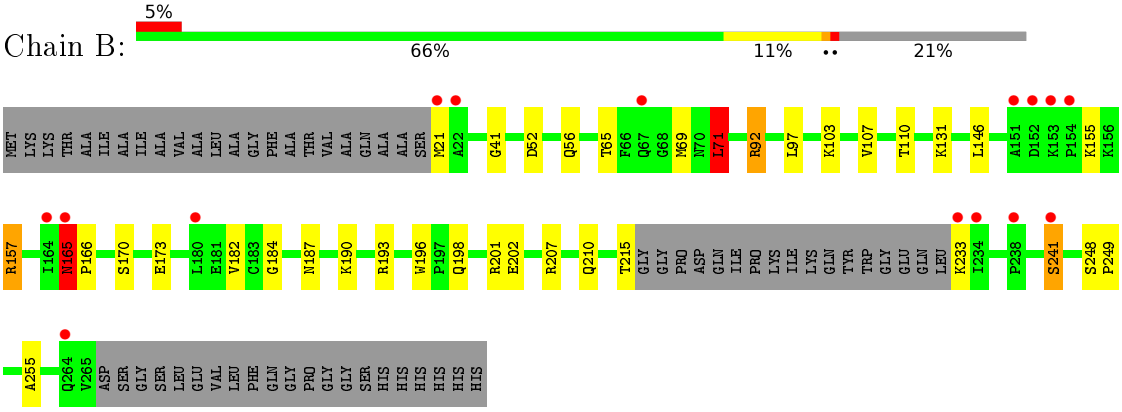
- Molecule 1: Outer membrane protein A,Vitamin B12-binding protein

Chain A:



- Molecule 1: Outer membrane protein A,Vitamin B12-binding protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	136.56Å 90.67Å 50.81Å 90.00° 110.87° 90.00°	Depositor
Resolution (Å)	19.71 – 1.70 19.71 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.3 (19.71-1.70) 96.3 (19.71-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.77 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.209 , 0.249 0.217 , 0.255	Depositor DCC
R_{free} test set	3060 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	24.8	Xtriage
Anisotropy	0.532	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 40.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.029 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4085	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.36% of the height of the origin peak. No significant pseudotranslation is detected.*

[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, CBY, CYN

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	0.93	0/1802	0.93	3/2455 (0.1%)
1	B	0.97	1/1812 (0.1%)	0.96	4/2468 (0.2%)
All	All	0.95	1/3614 (0.0%)	0.95	7/4923 (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	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	241	SER	C-O	5.03	1.32	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	165	ASN	C-N-CD	9.56	148.47	128.40
1	B	52	ASP	CB-CG-OD1	8.93	126.33	118.30
1	A	92	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	A	92	ARG	NE-CZ-NH2	-7.03	116.78	120.30
1	A	52	ASP	CB-CG-OD1	5.95	123.65	118.30
1	B	165	ASN	C-N-CA	-5.91	97.18	122.00
1	B	71	LEU	CB-CG-CD2	5.46	120.28	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	215	THR	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	1765	0	1785	27	0
1	B	1772	0	1800	28	0
2	A	68	0	72	6	0
2	B	68	0	72	7	0
3	A	2	0	0	3	0
3	B	2	0	0	0	0
4	A	12	0	16	5	0
4	B	6	0	8	3	0
5	A	205	0	0	11	0
5	B	185	0	0	9	0
All	All	4085	0	3753	69	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 (69) 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:173:GLU:OE1	5:A:401:HOH:O	1.61	1.17
1:A:92:ARG:NH2	5:A:402:HOH:O	2.02	0.90
1:B:107:VAL:HA	4:B:303:GOL:H32	1.62	0.81
1:B:193:ARG:NH2	5:B:402:HOH:O	2.13	0.80
1:B:173:GLU:OE1	5:B:401:HOH:O	2.00	0.78
1:A:106:TRP:O	4:A:303:GOL:H12	1.87	0.73
1:B:215:THR:HB	1:B:241:SER:HA	1.70	0.73
1:B:165:ASN:HB3	1:B:166:PRO:CD	2.18	0.72
1:A:256:GLN:HG2	5:A:528:HOH:O	1.91	0.70
1:B:41:GLY:HA2	1:B:131:LYS:HE3	1.74	0.68
1:B:21:MET:N	5:B:404:HOH:O	2.27	0.67
2:A:301:CBY:H36	2:A:301:CBY:H35A	1.80	0.62
1:A:106:TRP:O	4:A:303:GOL:C1	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:THR:HB	1:B:173:GLU:O	2.03	0.58
1:A:23:ALA:N	5:A:406:HOH:O	2.34	0.58
1:A:156:LYS:HE2	1:A:262:LEU:HD22	1.86	0.58
2:A:301:CBY:C35	2:A:301:CBY:H36	2.34	0.57
2:B:301:CBY:H35A	2:B:301:CBY:H36	1.86	0.56
1:A:25:ARG:NH2	4:A:304:GOL:O1	2.34	0.55
1:B:157:ARG:NH2	1:B:207:ARG:O	2.36	0.54
1:B:21:MET:N	5:B:410:HOH:O	2.41	0.54
1:B:65:THR:HG23	5:B:505:HOH:O	2.08	0.53
4:B:303:GOL:H2	5:B:501:HOH:O	2.08	0.53
2:B:301:CBY:C35	2:B:301:CBY:H36	2.39	0.52
1:B:56:GLN:HB2	5:B:516:HOH:O	2.09	0.52
1:A:173:GLU:HB3	5:A:569:HOH:O	2.09	0.52
1:B:71:LEU:HD13	1:B:97:LEU:HD21	1.93	0.50
1:A:25:ARG:HH22	4:A:304:GOL:C1	2.25	0.48
1:B:165:ASN:HB3	1:B:166:PRO:HD3	1.94	0.48
1:A:256:GLN:CG	5:A:528:HOH:O	2.54	0.48
1:B:146:LEU:HD21	1:B:255:ALA:HB1	1.95	0.48
1:A:36:LEU:HD21	1:A:115:ILE:HG23	1.96	0.47
2:A:301:CBY:H31A	2:A:301:CBY:H25B	1.97	0.47
1:A:85:TRP:CZ3	1:A:88:GLY:HA3	2.49	0.47
1:B:170:SER:HB2	1:B:196:TRP:CZ3	2.50	0.46
2:A:301:CBY:H35B	2:A:301:CBY:H37A	1.98	0.45
2:B:301:CBY:H25	2:B:301:CBY:H60	1.97	0.45
1:B:173:GLU:CD	1:B:173:GLU:H	2.20	0.45
1:B:92:ARG:HB2	5:B:503:HOH:O	2.17	0.45
4:A:303:GOL:O1	4:B:303:GOL:C1	2.64	0.45
1:B:187:ASN:O	1:B:190:LYS:HB2	2.17	0.44
1:B:248:SER:HB2	1:B:249:PRO:HD2	1.98	0.44
1:B:69:MET:HG3	1:B:71:LEU:HD23	1.98	0.44
1:A:145:GLN:HG3	5:A:518:HOH:O	2.17	0.44
1:A:110:THR:HB	1:A:173:GLU:O	2.17	0.44
1:A:146:LEU:HD13	1:A:256:GLN:HG2	1.98	0.44
1:A:214:ILE:HG13	1:A:238:PRO:HA	2.00	0.43
1:B:157:ARG:HG3	1:B:210:GLN:OE1	2.18	0.43
2:B:301:CBY:C53	2:B:301:CBY:H55	2.48	0.43
1:A:249:PRO:O	1:A:252:ILE:HG22	2.19	0.42
1:A:245:GLU:OE1	3:A:302:CYN:N	2.52	0.42
1:B:155:LYS:HA	1:B:184:GLY:O	2.18	0.42
1:A:156:LYS:HE3	5:A:432:HOH:O	2.19	0.42
1:A:156:LYS:CE	5:A:432:HOH:O	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:ARG:NH2	5:B:425:HOH:O	2.53	0.42
1:A:204:VAL:O	1:A:209:PRO:HD3	2.18	0.42
1:A:245:GLU:OE1	3:A:302:CYN:C	2.69	0.41
2:B:301:CBY:H30	2:B:301:CBY:H20	2.02	0.41
1:B:71:LEU:HD13	1:B:97:LEU:CD2	2.49	0.41
2:B:301:CBY:H55	2:B:301:CBY:H53A	2.03	0.41
1:A:256:GLN:HB3	5:A:443:HOH:O	2.19	0.41
2:A:301:CBY:C9	3:A:302:CYN:C	2.93	0.41
1:A:123:ALA:N	1:A:124:PRO:CD	2.84	0.41
2:B:301:CBY:H35	2:B:301:CBY:H3	1.98	0.41
1:B:166:PRO:HB2	1:B:198:GLN:HG3	2.03	0.41
1:B:201:ARG:NH1	1:B:202:GLU:OE2	2.52	0.41
1:A:245:GLU:OE1	2:A:301:CBY:H37	2.21	0.41
1:A:92:ARG:HD3	1:A:92:ARG:HA	1.80	0.40
5:A:487:HOH:O	1:B:103:LYS:HE3	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	224/289 (78%)	221 (99%)	3 (1%)	0	100	100
1	B	225/289 (78%)	218 (97%)	6 (3%)	1 (0%)	39	20
All	All	449/578 (78%)	439 (98%)	9 (2%)	1 (0%)	52	32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	165	ASN

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	191/235 (81%)	184 (96%)	7 (4%)	41 18
1	B	192/235 (82%)	187 (97%)	5 (3%)	54 32
All	All	383/470 (82%)	371 (97%)	12 (3%)	47 25

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	ARG
1	A	130	ASP
1	A	145	GLN
1	A	173	GLU
1	A	176	GLN
1	A	262	LEU
1	A	263	SER
1	B	71	LEU
1	B	92	ARG
1	B	157	ARG
1	B	182	VAL
1	B	233	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	176	GLN
1	B	58	GLN

5.3.3 RNA

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)

7 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	CBY	A	301	3	51,75,75	1.08	2 (3%)	80,125,125	1.87	17 (21%)
3	CYN	A	302	2	0,1,1	0.00	-	0,0,0	0.00	-
4	GOL	A	303	-	5,5,5	0.81	0	5,5,5	1.52	1 (20%)
4	GOL	A	304	-	5,5,5	0.34	0	5,5,5	1.04	0
2	CBY	B	301	3	51,75,75	0.99	1 (1%)	80,125,125	1.78	13 (16%)
3	CYN	B	302	2	0,1,1	0.00	-	0,0,0	0.00	-
4	GOL	B	303	-	5,5,5	1.19	0	5,5,5	1.59	1 (20%)

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	CBY	A	301	3	-	0/39/191/191	0/0/8/8
3	CYN	A	302	2	-	0/0/0/0	0/0/0/0
4	GOL	A	303	-	-	0/4/4/4	0/0/0/0
4	GOL	A	304	-	-	0/4/4/4	0/0/0/0
2	CBY	B	301	3	-	0/39/191/191	0/0/8/8
3	CYN	B	302	2	-	0/0/0/0	0/0/0/0
4	GOL	B	303	-	-	0/4/4/4	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	CBY	C11-C10	-5.26	1.31	1.41
2	B	301	CBY	C11-C10	-4.45	1.33	1.41
2	A	301	CBY	C53-C15	2.28	1.57	1.51

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	CBY	C9-C10-C11	-5.18	119.77	132.31
2	B	301	CBY	C9-C10-C11	-3.88	122.91	132.31
2	B	301	CBY	C35-C5-C4	-3.35	113.20	117.81
2	A	301	CBY	C13-C14-C15	-3.34	121.57	132.12
2	B	301	CBY	C31-C30-C3	-3.26	105.12	114.76
2	A	301	CBY	C25-C2-C1	-3.16	108.95	113.84
2	B	301	CBY	O28-C27-N29	-3.05	113.87	122.52
2	A	301	CBY	C1-C19-N24	-2.99	102.42	106.12
2	B	301	CBY	C13-C14-C15	-2.98	122.71	132.12
2	A	301	CBY	C16-C15-C14	-2.93	119.12	124.08
2	A	301	CBY	C20-C1-N21	-2.80	100.09	108.03
2	B	301	CBY	C16-C15-C14	-2.58	119.72	124.08
2	A	301	CBY	C20-C1-C19	-2.50	106.89	109.36
2	A	301	CBY	O51-C50-N52	-2.33	115.92	122.52
2	A	301	CBY	C56-C57-N59	-2.25	112.53	116.46
4	A	303	GOL	O2-C2-C1	-2.24	97.69	108.47
2	B	301	CBY	C20-C1-N21	-2.24	101.67	108.03
2	A	301	CBY	C3-C4-C5	-2.19	125.19	132.12
2	A	301	CBY	C55-C17-C18	-2.17	107.13	111.03
2	B	301	CBY	C2-C1-C19	-2.12	116.62	118.62
2	B	301	CBY	C53-C15-C14	2.03	120.60	117.81
2	B	301	CBY	C26-C2-C1	2.04	113.32	110.00
2	A	301	CBY	C49-C48-C13	2.32	121.62	114.76
2	A	301	CBY	O58-C57-N59	2.33	127.58	122.96
4	B	303	GOL	O2-C2-C3	2.45	120.24	108.47
2	B	301	CBY	C18-C17-C16	2.46	103.71	100.57
2	A	301	CBY	C18-C17-C16	2.66	103.96	100.57
2	A	301	CBY	C2-C1-C19	3.82	122.23	118.62
2	A	301	CBY	C35-C5-C6	3.95	123.24	117.81
2	B	301	CBY	C35-C5-C6	5.22	124.99	117.81
2	A	301	CBY	C19-C1-N21	7.73	110.34	102.16
2	B	301	CBY	C19-C1-N21	8.63	111.29	102.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	CBY	6	0
3	A	302	CYN	3	0
4	A	303	GOL	3	0
4	A	304	GOL	2	0
2	B	301	CBY	7	0
4	B	303	GOL	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	228/289 (78%)	0.21	12 (5%)	30	32	18, 30, 55, 81	0
1	B	228/289 (78%)	0.20	15 (6%)	22	23	21, 32, 55, 85	0
All	All	456/578 (78%)	0.20	27 (5%)	26	27	18, 31, 57, 85	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	164	ILE	6.2
1	B	152	ASP	5.6
1	A	152	ASP	5.4
1	B	164	ILE	5.0
1	A	266	ASP	5.0
1	B	165	ASN	4.8
1	B	21	MET	4.5
1	B	233	LYS	4.4
1	A	151	ALA	4.0
1	B	234	ILE	4.0
1	A	233	LYS	3.8
1	A	165	ASN	3.6
1	B	153	LYS	3.5
1	A	216	GLY	3.0
1	A	154	PRO	2.9
1	B	154	PRO	2.8
1	B	241	SER	2.7
1	A	234	ILE	2.6
1	B	22	ALA	2.6
1	A	148	ALA	2.5
1	A	23	ALA	2.4
1	B	67	GLN	2.4
1	B	151	ALA	2.4
1	B	180	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	264	GLN	2.2
1	B	238	PRO	2.1
1	A	153	LYS	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
4	GOL	A	303	6/6	0.73	0.23	7.06	32,46,53,55	0
4	GOL	B	303	6/6	0.86	0.14	4.37	23,32,41,46	0
2	CBY	A	301	68/68	0.95	0.10	0.14	20,27,44,50	0
2	CBY	B	301	68/68	0.94	0.12	0.14	25,30,54,70	0
4	GOL	A	304	6/6	0.78	0.28	-	37,39,45,48	0
3	CYN	A	302	2/2	0.98	0.15	-	28,28,28,29	0
3	CYN	B	302	2/2	0.98	0.11	-	30,30,30,37	0

6.5 Other polymers (i)

There are no such residues in this entry.