Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:22 AM GMT

PDB ID	:	2GUF
Title	:	In meso crystal structure of the cobalamin transporter, BtuB
Authors	:	Caffrey, M.; Cherezov, V.; Yamashita, E.; Cramer, W.A.
Deposited on	:	2006-04-29
Resolution	:	1.95 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:

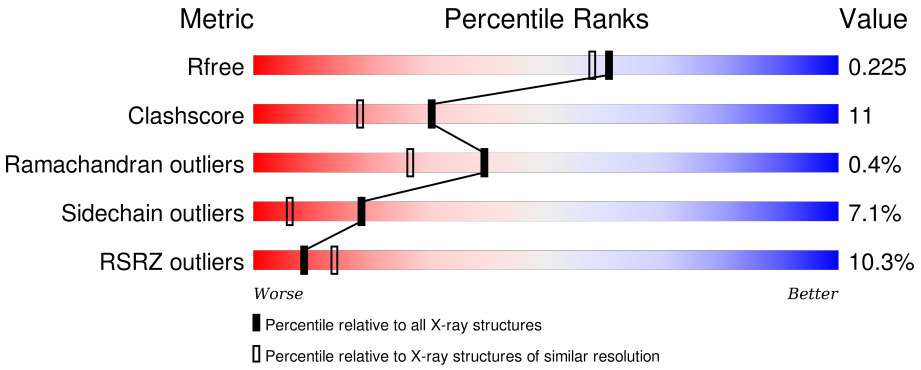
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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}	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (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. 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	594	10% 71% 19% • 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MPG	A	702	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MPG	A	706	-	-	-	X
2	MPG	A	707	-	-	-	X
2	MPG	A	708	-	-	-	X
2	MPG	A	710	-	-	-	X
2	MPG	A	711	-	-	-	X
4	MPD	A	902	-	-	-	X
4	MPD	A	903	-	-	-	X
4	MPD	A	904	-	-	-	X

2 Entry composition

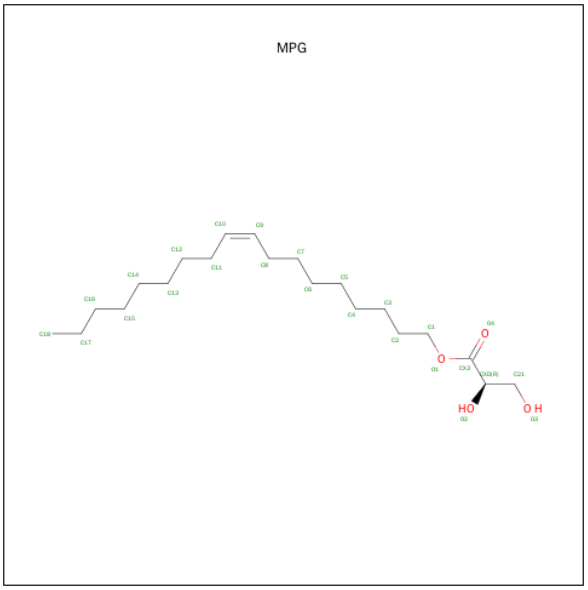
There are 5 unique types of molecules in this entry. The entry contains 5054 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Vitamin B12 transporter btuB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	0	14	0
			4458	2814	771	871	2			

- Molecule 2 is 1-MONOOLEOYL-RAC-GLYCEROL (three-letter code: MPG) (formula: $C_{21}H_{40}O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O		0	0
			24	21	3			
2	A	1	Total	C	O		0	0
			24	21	3			
2	A	1	Total	C	O		0	0
			24	21	3			
2	A	1	Total	C	O		0	0
			24	21	3			
2	A	1	Total	C	O		0	0
			24	21	3			

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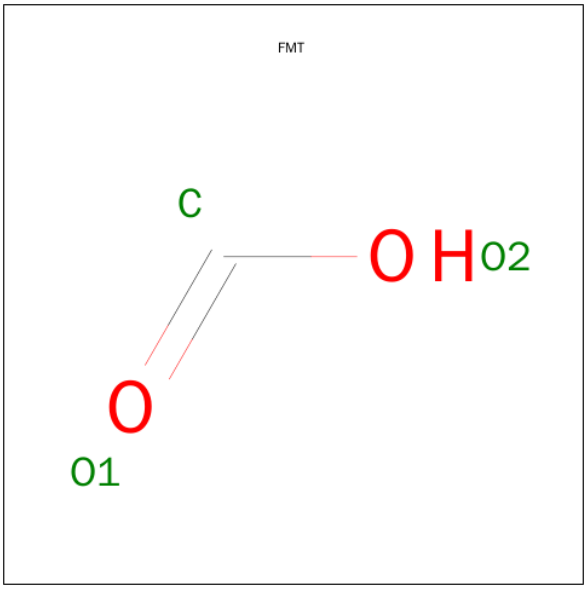
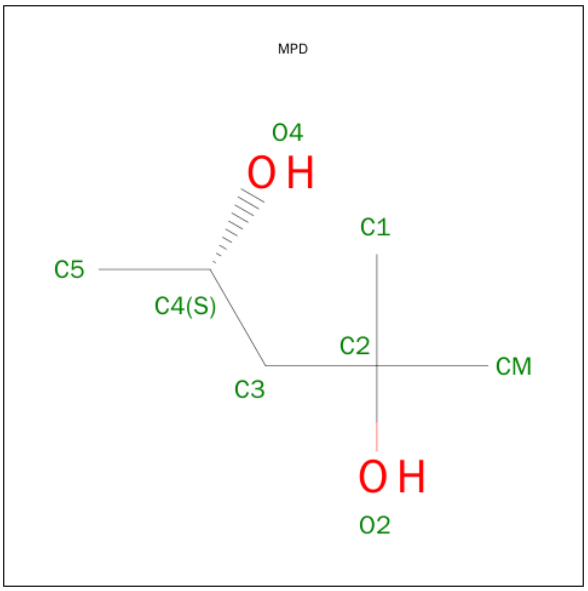
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 24 21 3	0	0
2	A	1	Total C O 24 21 3	0	0
2	A	1	Total C O 24 21 3	0	0
2	A	1	Total C O 24 21 3	0	0
2	A	1	Total C O 24 21 3	0	0
2	A	1	Total C O 24 21 3	0	0

- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



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

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 8 6 2	0	0
4	A	1	Total C O 8 6 2	0	0
4	A	1	Total C O 8 6 2	0	0
4	A	1	Total C O 8 6 2	0	0

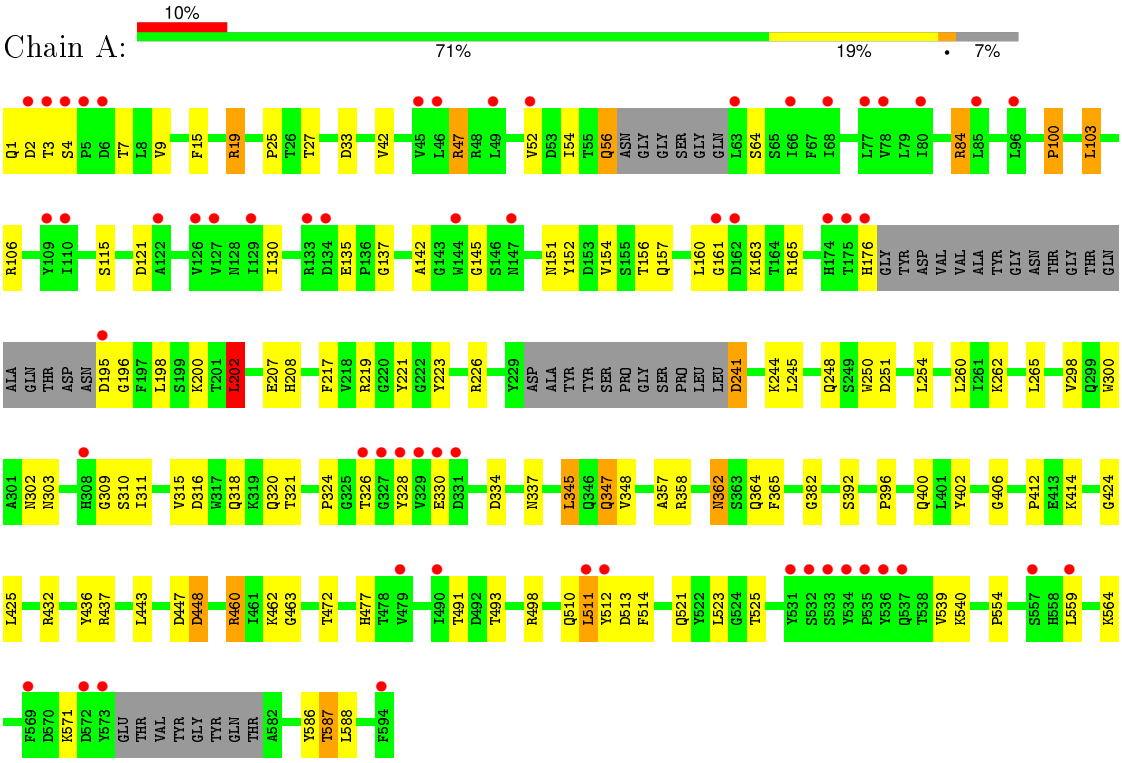
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	297	Total O 297 297	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: Vitamin B12 transporter btuB



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.61Å 80.88Å 118.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.44 – 1.95 40.44 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.7 (40.44-1.95) 98.8 (40.44-1.95)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.80 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.189 , 0.225 0.190 , 0.225	Depositor DCC
R_{free} test set	2592 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	25.4	Xtriage
Anisotropy	0.909	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 51.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 51039 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5054	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MPG, FMT, MPD

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	3/4623 (0.1%)	0.96	7/6285 (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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	414	LYS	CD-CE	5.85	1.65	1.51
1	A	42	VAL	CB-CG1	-5.22	1.41	1.52
1	A	262	LYS	CE-NZ	5.03	1.61	1.49

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	47	ARG	NE-CZ-NH2	-9.19	115.70	120.30
1	A	47	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	A	202	LEU	CB-CG-CD1	5.64	120.59	111.00
1	A	202	LEU	CA-CB-CG	5.27	127.42	115.30
1	A	84	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	A	498	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	A	447	ASP	CB-CG-OD1	5.04	122.83	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	241	ASP	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	4458	0	4220	99	0
2	A	264	0	440	26	0
3	A	3	0	1	0	0
4	A	32	0	56	5	0
5	A	297	0	0	13	0
All	All	5054	0	4717	104	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 11.

All (104) 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:432[A]:ARG:NH2	5:A:957:HOH:O	1.78	1.15
1:A:84:ARG:HE	1:A:318:GLN:HE22	1.11	0.96
1:A:311:ILE:HD12	2:A:705:MPG:H182	1.51	0.91
1:A:248:GLN:HE22	2:A:708:MPG:H181	1.40	0.86
1:A:56:GLN:HG3	1:A:64:SER:HB3	1.60	0.82
1:A:154[B]:VAL:HG23	2:A:702:MPG:H61	1.63	0.81
1:A:248:GLN:HE22	2:A:708:MPG:C18	1.95	0.79
1:A:248:GLN:NE2	2:A:708:MPG:H183	1.98	0.78
1:A:248:GLN:NE2	2:A:708:MPG:C18	2.47	0.77
1:A:135:GLU:H	1:A:157:GLN:NE2	1.83	0.77
1:A:221:TYR:OH	5:A:1032:HOH:O	1.98	0.75
1:A:84:ARG:NE	1:A:318:GLN:HE22	1.82	0.75
1:A:326:THR:HB	1:A:328:TYR:HD1	1.53	0.73
1:A:135:GLU:H	1:A:157:GLN:HE22	1.35	0.72
1:A:200:LYS:HB3	2:A:702:MPG:H142	1.71	0.72
1:A:25:PRO:HG3	1:A:432[A]:ARG:NH2	2.05	0.72
1:A:347:GLN:HG2	5:A:1052:HOH:O	1.90	0.71
1:A:337:ASN:HB3	4:A:902:MPD:HM3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:GLN:NE2	1:A:27:THR:HG23	2.10	0.67
1:A:564[A]:LYS:HE2	1:A:587:THR:HG23	1.76	0.66
1:A:3:THR:HA	1:A:19[B]:ARG:HH12	1.62	0.64
1:A:302:ASN:ND2	2:A:704:MPG:H181	2.13	0.63
1:A:7:THR:O	1:A:19[B]:ARG:HG3	1.99	0.62
1:A:326:THR:HB	1:A:328:TYR:CD1	2.33	0.61
1:A:472:THR:OG1	1:A:477:HIS:HE1	1.84	0.60
1:A:226:ARG:HD3	1:A:244:LYS:HE2	1.83	0.60
1:A:1:GLN:HA	1:A:33:ASP:OD1	2.01	0.59
1:A:221:TYR:HA	2:A:708:MPG:H171	1.86	0.58
1:A:302:ASN:HD22	2:A:704:MPG:H181	1.68	0.57
1:A:364[A]:GLN:NE2	1:A:402:TYR:OH	2.30	0.56
1:A:357:ALA:HB1	2:A:704:MPG:H32	1.87	0.56
1:A:460:ARG:HD2	1:A:462:LYS:HE3	1.87	0.55
1:A:362:ASN:HD22	1:A:365:PHE:H	1.55	0.55
1:A:564[B]:LYS:HE3	5:A:1132:HOH:O	2.07	0.54
1:A:163:LYS:NZ	2:A:709:MPG:H12	2.23	0.53
1:A:47:ARG:NH2	5:A:941:HOH:O	2.40	0.53
1:A:2:ASP:O	1:A:19[B]:ARG:NH1	2.43	0.52
1:A:491:THR:OG1	1:A:493:THR:HG23	2.08	0.52
1:A:154[A]:VAL:HG13	2:A:708:MPG:H71	1.92	0.52
2:A:705:MPG:H122	2:A:711:MPG:H162	1.93	0.51
1:A:200:LYS:O	1:A:223:TYR:HA	2.12	0.50
1:A:303:ASN:HD21	1:A:310:SER:HB2	1.76	0.50
1:A:437:ARG:CZ	1:A:460:ARG:HH11	2.24	0.50
1:A:250:TRP:HB3	2:A:706:MPG:H112	1.93	0.50
1:A:25:PRO:HG3	1:A:432[A]:ARG:CZ	2.42	0.49
1:A:115:SER:HB2	1:A:392:SER:HA	1.95	0.49
1:A:52:VAL:HG12	1:A:54:ILE:HG13	1.94	0.48
1:A:510:GLN:HA	1:A:514:PHE:O	2.14	0.48
1:A:396:PRO:HD3	1:A:412:PRO:HA	1.95	0.48
1:A:165[A]:ARG:NH2	1:A:207:GLU:OE1	2.47	0.48
1:A:84:ARG:HE	1:A:318:GLN:NE2	1.95	0.48
1:A:337:ASN:CB	4:A:902:MPD:HM3	2.42	0.47
1:A:248:GLN:HE21	2:A:708:MPG:H183	1.73	0.47
1:A:300:TRP:CE2	2:A:703:MPG:H131	2.49	0.47
1:A:202:LEU:HD13	2:A:702:MPG:H122	1.96	0.47
1:A:382:GLY:O	1:A:424:GLY:HA2	2.14	0.47
1:A:254:LEU:HG	2:A:709:MPG:H162	1.96	0.47
1:A:364[B]:GLN:HG2	1:A:365:PHE:CE1	2.49	0.47
1:A:448:ASP:N	1:A:448:ASP:OD1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:GLN:NE2	5:A:919:HOH:O	2.48	0.46
1:A:315:VAL:HG13	2:A:703:MPG:H61	1.97	0.46
1:A:84:ARG:NE	1:A:318:GLN:NE2	2.59	0.46
1:A:436:TYR:CZ	1:A:463:GLY:HA3	2.51	0.46
1:A:100:PRO:HG2	1:A:103:LEU:HD22	1.98	0.46
1:A:219[A]:ARG:NH2	5:A:1149:HOH:O	2.48	0.46
1:A:298:VAL:HG12	2:A:703:MPG:H71	1.97	0.45
1:A:142:ALA:HA	1:A:151:ASN:O	2.17	0.45
1:A:511:LEU:HB3	5:A:1178:HOH:O	2.16	0.45
4:A:902:MPD:HM1	5:A:1167:HOH:O	2.17	0.45
1:A:437:ARG:NH2	1:A:460:ARG:NH1	2.65	0.45
1:A:165[A]:ARG:CZ	1:A:207:GLU:OE1	2.64	0.45
1:A:165[A]:ARG:NE	1:A:207:GLU:OE1	2.49	0.44
1:A:512:TYR:O	1:A:513:ASP:HB2	2.15	0.44
1:A:163:LYS:HE2	1:A:208:HIS:CE1	2.53	0.44
2:A:706:MPG:H121	2:A:706:MPG:H151	1.77	0.44
1:A:163:LYS:HZ2	2:A:709:MPG:H12	1.82	0.44
1:A:154[B]:VAL:CG2	2:A:702:MPG:H61	2.41	0.43
1:A:176:HIS:HA	1:A:196:GLY:HA3	2.00	0.43
1:A:9:VAL:HG13	1:A:19[B]:ARG:HG2	1.99	0.43
1:A:226:ARG:HG2	1:A:226:ARG:HH21	1.83	0.43
1:A:217:PHE:CD1	1:A:217:PHE:C	2.92	0.42
1:A:400:GLN:O	1:A:406:GLY:HA3	2.19	0.42
1:A:152:TYR:HB3	2:A:702:MPG:H52	2.02	0.42
4:A:901:MPD:H4	4:A:901:MPD:HM1	1.84	0.42
1:A:137:GLY:O	1:A:156:THR:HA	2.18	0.42
1:A:432[A]:ARG:HD3	5:A:1009:HOH:O	2.19	0.42
1:A:521:GLN:NE2	5:A:996:HOH:O	2.48	0.42
1:A:564[B]:LYS:CE	5:A:1132:HOH:O	2.65	0.42
1:A:321:THR:HG22	1:A:334:ASP:HB2	2.00	0.42
1:A:309:GLY:HA3	1:A:345:LEU:O	2.19	0.42
4:A:904:MPD:O4	4:A:904:MPD:O2	2.26	0.42
1:A:1:GLN:HE22	1:A:27:THR:HG23	1.81	0.42
1:A:161:GLY:HA3	2:A:709:MPG:H211	2.01	0.42
1:A:15:PHE:CD1	1:A:303:ASN:HB2	2.55	0.41
1:A:145:GLY:HA2	1:A:586[A]:TYR:CE2	2.56	0.41
1:A:19[A]:ARG:NH2	5:A:1023:HOH:O	2.49	0.40
1:A:115:SER:O	1:A:358:ARG:HD3	2.20	0.40
1:A:56:GLN:HB2	1:A:56:GLN:HE21	1.51	0.40
1:A:106:ARG:HB3	1:A:130:ILE:HB	2.03	0.40
1:A:437:ARG:CZ	1:A:460:ARG:NH1	2.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:PRO:HG2	1:A:554:PRO:O	2.21	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	555/594 (93%)	544 (98%)	9 (2%)	2 (0%)	39 27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	324	PRO
1	A	121	ASP

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	477/495 (96%)	443 (93%)	34 (7%)	18 6

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER

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Mol	Chain	Res	Type
1	A	19[A]	ARG
1	A	19[B]	ARG
1	A	56	GLN
1	A	100	PRO
1	A	103	LEU
1	A	160	LEU
1	A	195	ASP
1	A	198	LEU
1	A	202	LEU
1	A	241	ASP
1	A	245	LEU
1	A	251	ASP
1	A	260	LEU
1	A	265	LEU
1	A	316	ASP
1	A	330	GLU
1	A	345	LEU
1	A	347	GLN
1	A	348	VAL
1	A	362	ASN
1	A	425	LEU
1	A	443	LEU
1	A	448	ASP
1	A	460	ARG
1	A	511	LEU
1	A	523	LEU
1	A	525	THR
1	A	539	VAL
1	A	540	LYS
1	A	559	LEU
1	A	571	LYS
1	A	587	THR
1	A	588	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	157	GLN
1	A	158	GLN
1	A	176	HIS
1	A	225	ASN

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Mol	Chain	Res	Type
1	A	248	GLN
1	A	295	GLN
1	A	303	ASN
1	A	318	GLN
1	A	320	GLN
1	A	335	GLN
1	A	362	ASN
1	A	477	HIS
1	A	558	HIS

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)

16 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	MPG	A	701	-	23,23,24	0.29	0	23,23,25	0.91	1 (4%)
2	MPG	A	702	-	23,23,24	0.40	0	23,23,25	0.58	0
2	MPG	A	703	-	23,23,24	0.51	0	23,23,25	0.54	0
2	MPG	A	704	-	23,23,24	0.44	0	23,23,25	1.46	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MPG	A	705	-	23,23,24	0.33	0	23,23,25	0.94	1 (4%)
2	MPG	A	706	-	23,23,24	0.46	0	23,23,25	0.51	0
2	MPG	A	707	-	23,23,24	0.53	0	23,23,25	0.56	0
2	MPG	A	708	-	23,23,24	0.51	0	23,23,25	0.39	0
2	MPG	A	709	-	23,23,24	0.39	0	23,23,25	0.56	0
2	MPG	A	710	-	23,23,24	0.43	0	23,23,25	0.52	0
2	MPG	A	711	-	23,23,24	0.47	0	23,23,25	0.48	0
3	FMT	A	801	-	0,2,2	0.00	-	0,1,1	0.00	-
4	MPD	A	901	-	6,7,7	0.33	0	7,10,10	0.85	0
4	MPD	A	902	-	6,7,7	0.52	0	7,10,10	0.76	0
4	MPD	A	903	-	6,7,7	0.40	0	7,10,10	0.57	0
4	MPD	A	904	-	6,7,7	0.46	0	7,10,10	0.67	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	MPG	A	701	-	-	0/22/22/25	0/0/0/0
2	MPG	A	702	-	-	0/22/22/25	0/0/0/0
2	MPG	A	703	-	-	0/22/22/25	0/0/0/0
2	MPG	A	704	-	-	0/22/22/25	0/0/0/0
2	MPG	A	705	-	-	0/22/22/25	0/0/0/0
2	MPG	A	706	-	-	0/22/22/25	0/0/0/0
2	MPG	A	707	-	-	0/22/22/25	0/0/0/0
2	MPG	A	708	-	-	0/22/22/25	0/0/0/0
2	MPG	A	709	-	-	0/22/22/25	0/0/0/0
2	MPG	A	710	-	-	0/22/22/25	0/0/0/0
2	MPG	A	711	-	-	0/22/22/25	0/0/0/0
3	FMT	A	801	-	-	0/0/0/0	0/0/0/0
4	MPD	A	901	-	-	0/5/5/5	0/0/0/0
4	MPD	A	902	-	-	0/5/5/5	0/0/0/0
4	MPD	A	903	-	-	0/5/5/5	0/0/0/0
4	MPD	A	904	-	-	0/5/5/5	0/0/0/0

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	704	MPG	C1-O1-CX3	-4.57	98.53	113.44
2	A	701	MPG	C13-C12-C11	-2.68	103.39	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	705	MPG	C3-C2-C1	-2.40	102.75	113.47
2	A	704	MPG	C7-C6-C5	-2.26	102.88	114.53
2	A	704	MPG	C11-C10-C9	-2.10	110.70	125.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	702	MPG	5	0
2	A	703	MPG	3	0
2	A	704	MPG	3	0
2	A	705	MPG	2	0
2	A	706	MPG	2	0
2	A	708	MPG	7	0
2	A	709	MPG	4	0
2	A	711	MPG	1	0
4	A	901	MPD	1	0
4	A	902	MPD	3	0
4	A	904	MPD	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	551/594 (92%)	0.57	57 (10%) 9 14	21, 32, 52, 66	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	534	TYR	6.3
1	A	533	SER	5.3
1	A	6	ASP	5.3
1	A	536	TYR	5.2
1	A	3	THR	5.0
1	A	329	VAL	4.3
1	A	195	ASP	4.3
1	A	572	ASP	3.9
1	A	4	SER	3.9
1	A	144	TRP	3.8
1	A	512	TYR	3.8
1	A	162	ASP	3.8
1	A	535	PRO	3.8
1	A	532	SER	3.7
1	A	127	VAL	3.6
1	A	557	SER	3.6
1	A	330	GLU	3.6
1	A	52	VAL	3.4
1	A	134	ASP	3.4
1	A	126	VAL	3.3
1	A	326	THR	3.3
1	A	46	LEU	3.2
1	A	161	GLY	3.2
1	A	328	TYR	3.1
1	A	49	LEU	3.0
1	A	531	TYR	3.0
1	A	129	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	77	LEU	2.8
1	A	176	HIS	2.8
1	A	511	LEU	2.8
1	A	490	ILE	2.8
1	A	85	LEU	2.7
1	A	327	GLY	2.7
1	A	66	ILE	2.7
1	A	96	LEU	2.7
1	A	175	THR	2.6
1	A	110	ILE	2.6
1	A	45	VAL	2.5
1	A	63	LEU	2.5
1	A	594	PHE	2.5
1	A	78	VAL	2.5
1	A	147	ASN	2.4
1	A	308	HIS	2.4
1	A	479[A]	VAL	2.4
1	A	537	GLN	2.4
1	A	559	LEU	2.3
1	A	5	PRO	2.3
1	A	80	ILE	2.2
1	A	68	ILE	2.2
1	A	122	ALA	2.2
1	A	573	TYR	2.2
1	A	109	TYR	2.1
1	A	2	ASP	2.1
1	A	331	ASP	2.1
1	A	133	ARG	2.1
1	A	174	HIS	2.1
1	A	569	PHE	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

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
2	MPG	A	711	24/25	0.72	0.26	7.36	43,74,78,79	0
2	MPG	A	706	24/25	0.79	0.26	5.94	49,60,68,70	0
4	MPD	A	904	8/8	0.85	0.22	5.56	55,59,61,61	0
4	MPD	A	903	8/8	0.93	0.18	5.07	56,57,62,65	0
2	MPG	A	710	24/25	0.84	0.21	4.66	42,61,68,69	0
4	MPD	A	902	8/8	0.86	0.22	3.56	53,55,59,60	0
2	MPG	A	708	24/25	0.61	0.24	3.46	59,72,85,86	0
2	MPG	A	707	24/25	0.78	0.22	2.56	54,60,63,64	0
2	MPG	A	702	24/25	0.80	0.24	2.41	49,61,72,73	0
2	MPG	A	703	24/25	0.87	0.16	1.95	37,50,55,59	0
4	MPD	A	901	8/8	0.93	0.18	1.78	38,41,43,44	0
2	MPG	A	709	24/25	0.69	0.28	1.66	44,73,90,90	0
2	MPG	A	705	24/25	0.87	0.19	1.56	46,52,70,72	0
2	MPG	A	704	24/25	0.89	0.17	1.00	28,42,49,57	0
3	FMT	A	801	3/3	0.89	0.18	0.46	57,57,58,58	0
2	MPG	A	701	24/25	0.88	0.17	0.26	32,46,71,73	0

6.5 Other polymers

There are no such residues in this entry.