



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:32 PM GMT

PDB ID : 4IN7
Title : (M)L214N mutant of the Rhodobacter sphaeroides Reaction Center
Authors : Saer, R.G.; Hardjasa, A.; Murphy, M.E.P.; Beatty, J.T.
Deposited on : 2013-01-04
Resolution : 2.85 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

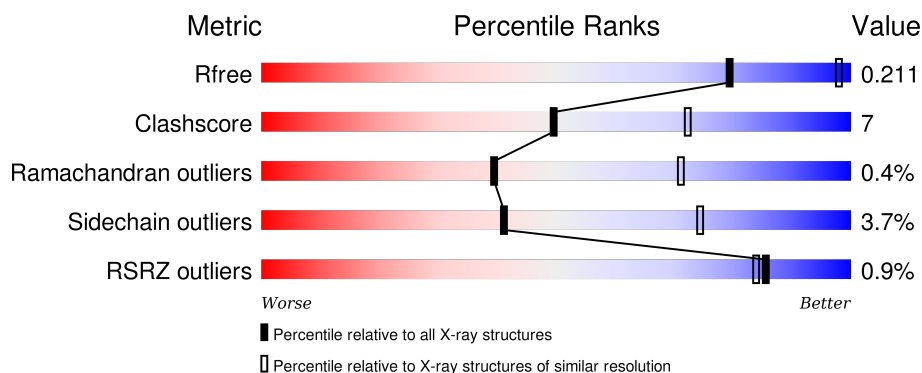
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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 $\leq 5\%$. 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	H	266	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>11%</div> <div>•</div> <div>10%</div> </div> </div>
2	L	282	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>10%</div> <div>•</div> </div> </div>
3	M	307	<div> <div></div> <div> <div></div> <div>84%</div> <div>14%</div> <div>••</div> </div> </div>

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
11	HTO	L	308	-	-	-	X
15	CDL	M	409	-	-	-	X
16	PC1	M	410	-	-	-	X
4	GOL	H	304	-	-	-	X
4	GOL	H	306	-	-	-	X
4	GOL	L	310	-	-	-	X
6	GGD	H	307	-	-	-	X
8	LDA	L	302	-	-	-	X
8	LDA	L	303	-	-	-	X
8	LDA	L	304	-	-	-	X
8	LDA	M	403	-	-	-	X
8	LDA	M	404	-	-	-	X

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 7359 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 Reaction center protein H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	240	Total	C	N	O	S	0	5	0
			1849	1183	320	337	9			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-5	HIS	-	EXPRESSION TAG	UNP P0C0Y7
H	-4	HIS	-	EXPRESSION TAG	UNP P0C0Y7
H	-3	HIS	-	EXPRESSION TAG	UNP P0C0Y7
H	-2	HIS	-	EXPRESSION TAG	UNP P0C0Y7
H	-1	HIS	-	EXPRESSION TAG	UNP P0C0Y7
H	0	HIS	-	EXPRESSION TAG	UNP P0C0Y7
H	251	VAL	-	EXPRESSION TAG	UNP P0C0Y7
H	252	VAL	-	EXPRESSION TAG	UNP P0C0Y7
H	253	ALA	-	EXPRESSION TAG	UNP P0C0Y7
H	254	ALA	-	EXPRESSION TAG	UNP P0C0Y7
H	255	MET	-	EXPRESSION TAG	UNP P0C0Y7
H	256	LEU	-	EXPRESSION TAG	UNP P0C0Y7
H	257	ALA	-	EXPRESSION TAG	UNP P0C0Y7
H	258	GLU	-	EXPRESSION TAG	UNP P0C0Y7
H	259	TYR	-	EXPRESSION TAG	UNP P0C0Y7
H	260	ALA	-	EXPRESSION TAG	UNP P0C0Y7

- Molecule 2 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	281	Total	C	N	O	S	0	2	0
			2239	1513	355	363	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	0	MET	-	EXPRESSION TAG	UNP P0C0Y8

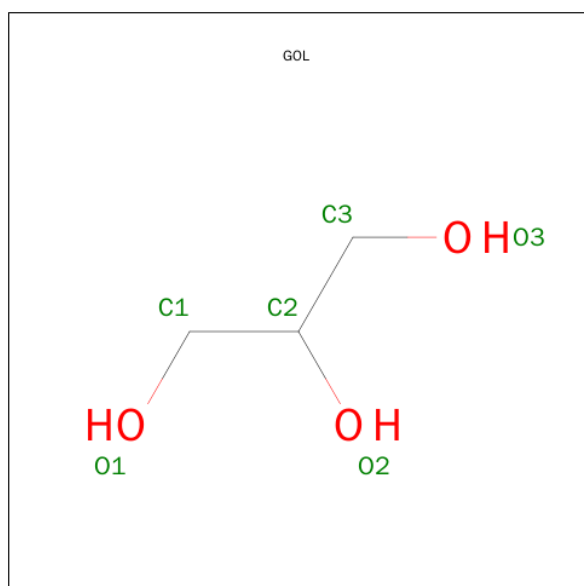
- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	302	Total	C	N	O	S	0	1	0
			2410	1605	396	399	10			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	0	MET	-	EXPRESSION TAG	UNP P0C0Y9
M	214	ASN	LEU	ENGINEERED MUTATION	UNP P0C0Y9
M	303	MET	-	EXPRESSION TAG	UNP P0C0Y9
M	304	ALA	-	EXPRESSION TAG	UNP P0C0Y9
M	305	PRO	-	EXPRESSION TAG	UNP P0C0Y9
M	306	LEU	-	EXPRESSION TAG	UNP P0C0Y9

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



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

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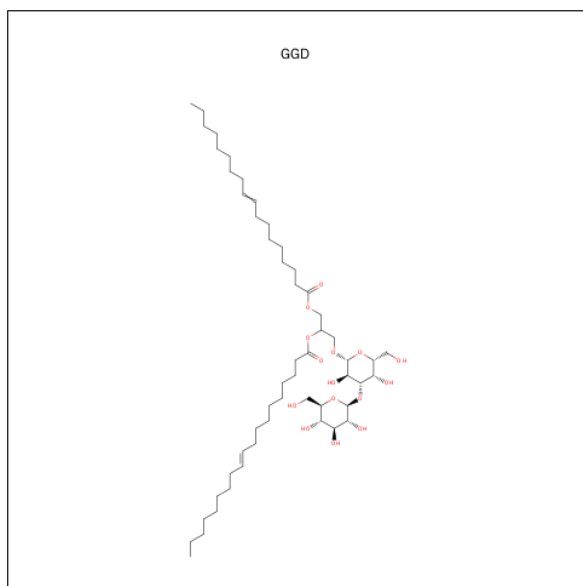
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

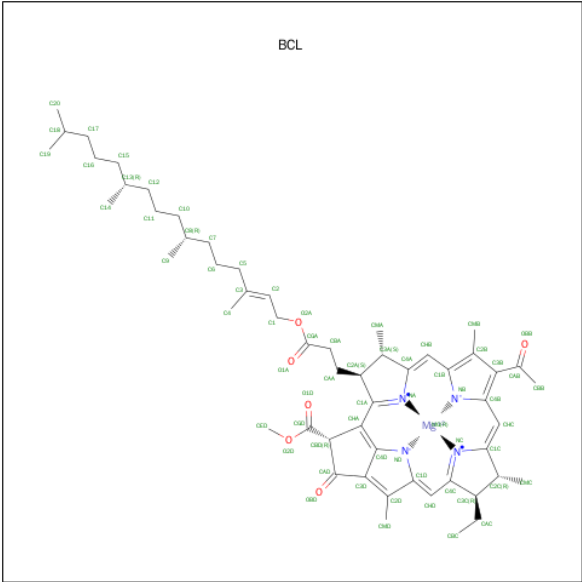
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total	K	0	0
			1	1		

- Molecule 6 is NONADEC-10-ENOIC ACID 2-[3,4-DIHYDROXY-6-HYDROXYMETHYL-5-(3,4,5-TRIHYDROXY-6-HYDROXYMETHYL-TETRAHYDRO-PYRAN-2-YLOXY)-TETRAHYDRO-PYRAN-2-YLOXY]-1-OCTADEC-9-ENOYLOXYMETHYL-ETHYL ESTER (three-letter code: GGD) (formula: C₅₂H₉₄O₁₅).



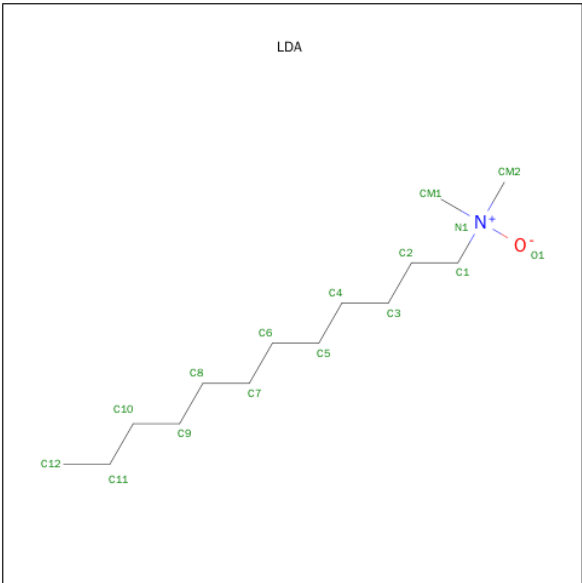
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	H	1	Total	C	O	0	0
			57	42	15		

- Molecule 7 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



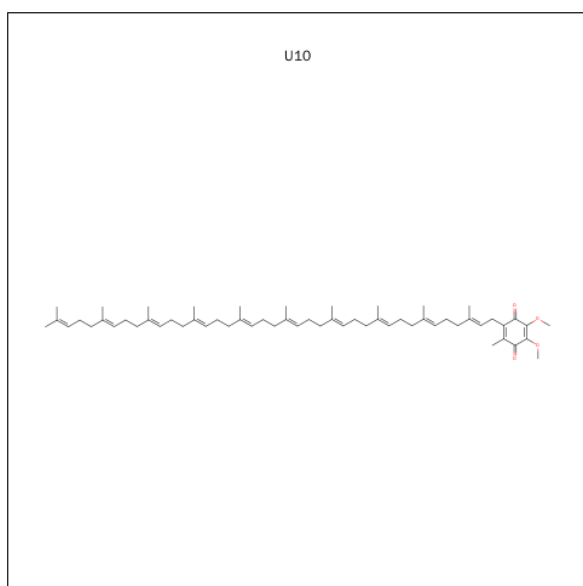
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 8 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: C₁₄H₃₁NO).



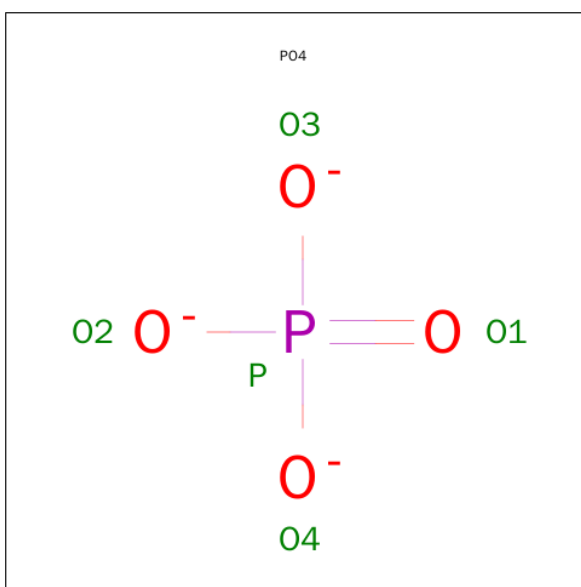
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	L	1	Total	C	N	O	0	0
			16	14	1	1		
8	L	1	Total	C	N	O	0	0
			16	14	1	1		
8	L	1	Total	C	N	O	0	0
			16	14	1	1		
8	M	1	Total	C	N	O	0	0
			16	14	1	1		
8	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 9 is UBIQUINONE-10 (three-letter code: U10) (formula: C₅₉H₉₀O₄).



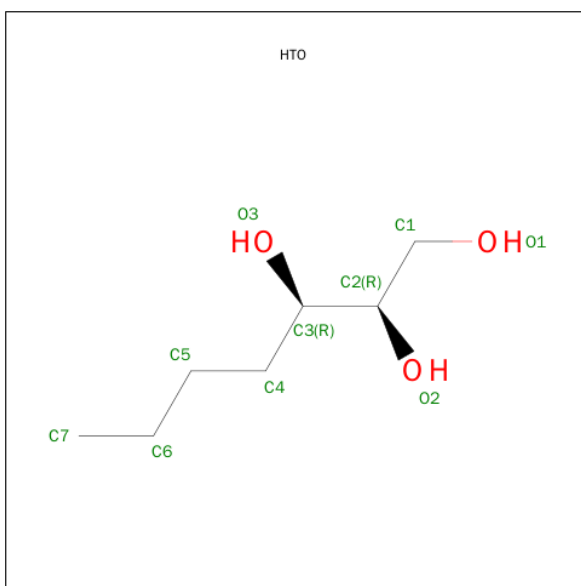
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	L	1	Total	C	O	0	1
			46	38	8		
9	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 10 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	L	1	Total	O	P	0	0
			5	4	1		

- Molecule 11 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: $C_7H_{16}O_3$).

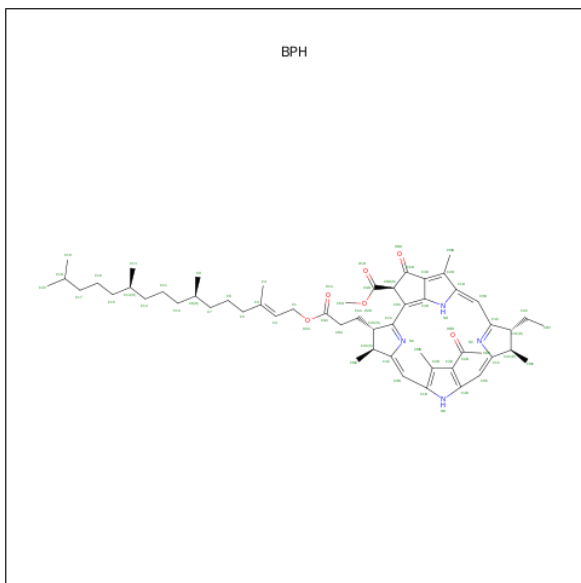


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	L	1	Total	C	O	0	0
			10	7	3		
11	L	1	Total	C	O	0	0
			10	7	3		

- Molecule 12 is FE (III) ION (three-letter code: FE) (formula: Fe).

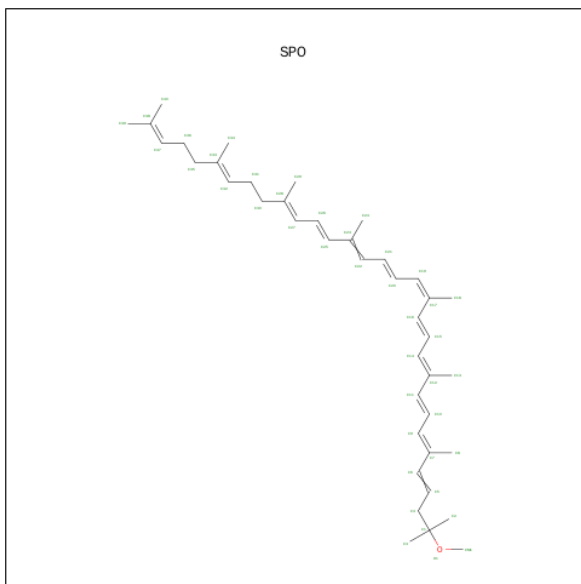
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	M	1	Total	Fe	0	0
			1	1		

- Molecule 13 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



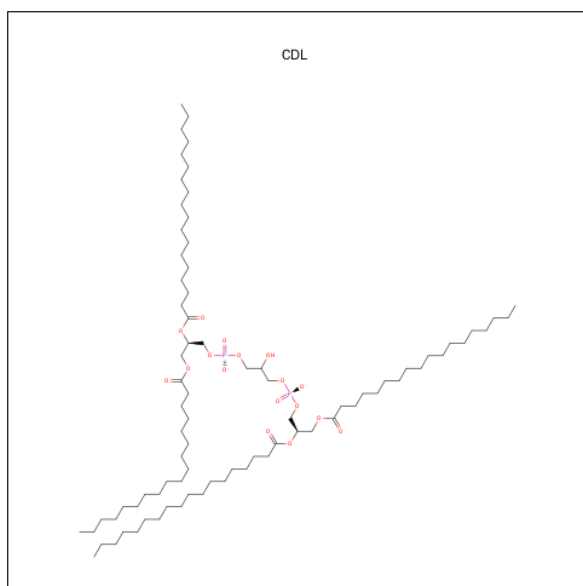
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	M	1	Total	C	N	O	0	0
			65	55	4	6		
13	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 14 is SPHEROIDENE (three-letter code: SPO) (formula: $C_{41}H_{60}O$).



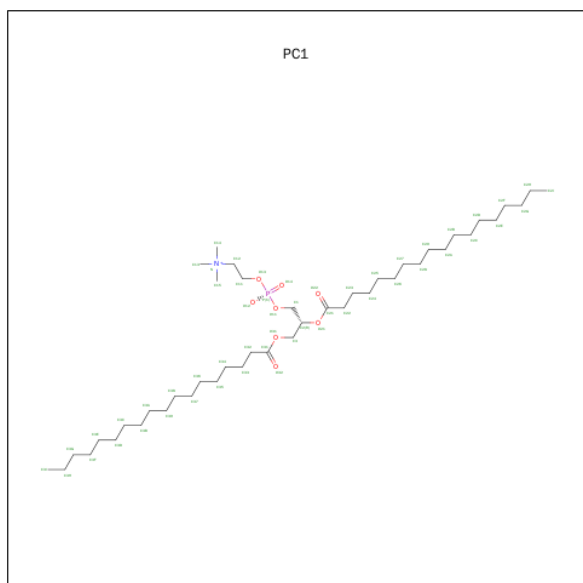
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	M	1	Total	C	O	0	0
			42	41	1		

- Molecule 15 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	M	1	Total	C	O	P	0	0
			81	62	17	2		

- Molecule 16 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	M	1	Total	C	N	O	P	0	0
			43	33	1	8	1		

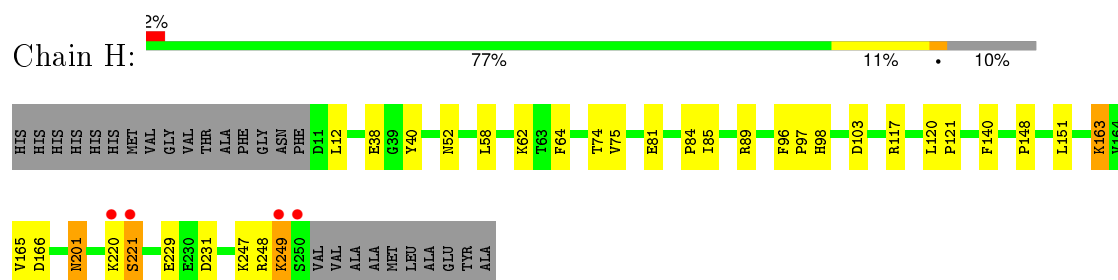
- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	M	1	Total	Mg	0	0
			1	1		

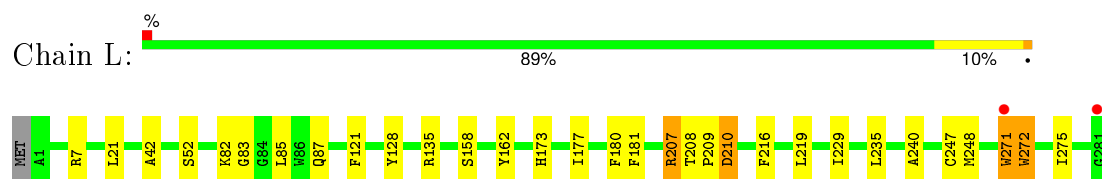
3 Residue-property plots

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.

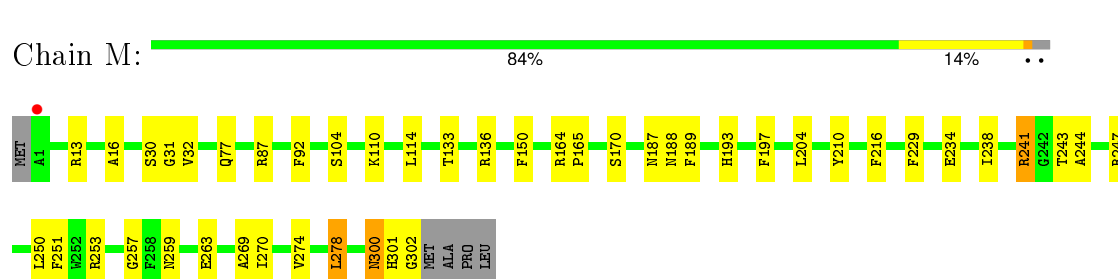
• Molecule 1: Reaction center protein H chain



• Molecule 2: Reaction center protein L chain



• Molecule 3: Reaction center protein M chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	139.14Å 139.14Å 185.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.57 – 2.85 38.54 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.57-2.85) 99.9 (38.54-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.96 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.174 , 0.213 0.179 , 0.211	Depositor DCC
R_{free} test set	2474 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	50.8	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.1	EDS
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 48860 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7359	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 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: BCL, GOL, LDA, CDL, BPH, K, PC1, MG, PO4, GGD, FE, SPO, U10, HTO

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	H	0.89	0/1929	1.05	5/2619 (0.2%)
2	L	0.85	0/2339	0.90	5/3203 (0.2%)
3	M	0.86	1/2507 (0.0%)	0.90	3/3422 (0.1%)
All	All	0.86	1/6775 (0.0%)	0.95	13/9244 (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
3	M	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	263	GLU	CD-OE1	5.51	1.31	1.25

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	210	ASP	CB-CG-OD1	7.19	124.77	118.30
2	L	207	ARG	NE-CZ-NH1	7.03	123.82	120.30
1	H	89	ARG	NE-CZ-NH2	-6.90	116.85	120.30
3	M	241	ARG	NE-CZ-NH2	6.70	123.65	120.30
3	M	253	ARG	NE-CZ-NH1	-6.66	116.97	120.30
3	M	136	ARG	NE-CZ-NH1	-6.34	117.13	120.30
2	L	207	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	H	117	ARG	NE-CZ-NH1	-6.08	117.26	120.30
1	H	89	ARG	NE-CZ-NH1	5.72	123.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	166	ASP	CB-CG-OD1	5.52	123.27	118.30
1	H	103	ASP	CB-CG-OD2	-5.46	113.38	118.30
2	L	271[A]	TRP	N-CA-CB	5.43	120.37	110.60
2	L	271[B]	TRP	N-CA-CB	5.43	120.37	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	M	300	ASN	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	H	1849	0	1873	25	0
2	L	2239	0	2185	24	0
3	M	2410	0	2314	27	0
4	H	30	0	40	0	0
4	L	12	0	16	1	0
5	H	1	0	0	0	0
6	H	57	0	68	3	0
7	L	132	0	148	13	0
7	M	132	0	148	14	0
8	L	48	0	93	2	0
8	M	32	0	62	4	0
9	L	46	0	46	6	0
9	M	48	0	63	1	0
10	L	5	0	0	1	0
11	L	20	0	32	0	0
12	M	1	0	0	0	0
13	M	130	0	150	18	0
14	M	42	0	60	3	0
15	M	81	0	102	1	0
16	M	43	0	60	1	0
17	M	1	0	0	0	0
All	All	7359	0	7460	105	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 7.

All (105) 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)
13:M:412:BPH:HBB3	13:M:412:BPH:HHC	1.50	0.91
13:M:406:BPH:HHC	13:M:406:BPH:HBB3	1.66	0.78
3:M:16:ALA:HB1	3:M:32:VAL:HG11	1.63	0.78
1:H:248:ARG:HA	1:H:249[A]:LYS:HB2	1.68	0.75
1:H:220[B]:LYS:HE2	1:H:221:SER:OG	1.91	0.71
2:L:229:ILE:HD13	9:L:305[B]:U10:H3M2	1.73	0.71
1:H:248:ARG:HA	1:H:249[B]:LYS:HB2	1.73	0.70
7:L:306:BCL:HBB3	7:L:306:BCL:HMB1	1.76	0.68
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.75	0.67
3:M:210:TYR:HB3	13:M:412:BPH:HBB2	1.77	0.67
7:L:306:BCL:HMB1	7:L:306:BCL:CBB	2.24	0.67
1:H:84:PRO:O	1:H:85[A]:ILE:HD13	1.95	0.67
7:M:402:BCL:CBB	7:M:402:BCL:HHC	2.24	0.67
1:H:120:LEU:HB3	1:H:121:PRO:HD2	1.76	0.67
7:L:301:BCL:HHC	7:L:301:BCL:HBB2	1.80	0.63
1:H:201:ASN:HD22	1:H:201:ASN:H	1.45	0.63
7:M:402:BCL:HHC	7:M:402:BCL:HBB2	1.80	0.63
7:M:401:BCL:HBB2	14:M:408:SPO:H243	1.82	0.61
1:H:120:LEU:HB3	1:H:121:PRO:CD	2.30	0.60
3:M:189:PHE:O	3:M:193:HIS:HD2	1.84	0.60
1:H:148:PRO:HA	1:H:151:LEU:HD12	1.84	0.59
1:H:163[A]:LYS:HE2	1:H:165:VAL:HG12	1.83	0.59
13:M:412:BPH:C2	13:M:412:BPH:O1A	2.50	0.59
3:M:31:GLY:N	16:M:410:PC1:O12	2.31	0.57
1:H:220[B]:LYS:HD3	1:H:229:GLU:OE2	2.05	0.57
3:M:270:ILE:O	3:M:274:VAL:HG13	2.03	0.57
2:L:128:TYR:HD1	7:L:301:BCL:HBB1	1.69	0.57
7:M:401:BCL:HHC	7:M:401:BCL:CBB	2.34	0.57
13:M:412:BPH:CBB	13:M:412:BPH:HHC	2.29	0.57
7:M:401:BCL:HHC	7:M:401:BCL:HBB2	1.88	0.55
7:M:401:BCL:H72	7:M:402:BCL:H192	1.89	0.55
2:L:180:PHE:CE2	2:L:240:ALA:HB1	2.42	0.55
7:L:306:BCL:C1C	7:M:402:BCL:HBB3	2.38	0.54
2:L:181:PHE:CD2	13:M:406:BPH:HBB1	2.43	0.53
1:H:81:GLU:HG3	1:H:85[B]:ILE:HD11	1.91	0.53
2:L:181:PHE:HB3	13:M:406:BPH:HBB2	1.90	0.53
13:M:412:BPH:HBB3	13:M:412:BPH:CHC	2.31	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:234:GLU:O	3:M:238:ILE:HG13	2.09	0.52
7:M:401:BCL:C7	7:M:402:BCL:H192	2.40	0.52
7:M:401:BCL:CBB	14:M:408:SPO:H243	2.40	0.52
3:M:300:ASN:O	3:M:302:GLY:N	2.44	0.51
2:L:82:LYS:NZ	10:L:307:PO4:O4	2.40	0.51
9:L:305[B]:U10:H103	8:M:404:LDA:H121	1.93	0.50
2:L:121:PHE:CZ	13:M:412:BPH:HBA2	2.46	0.50
2:L:162:TYR:OH	3:M:187:ASN:ND2	2.45	0.49
1:H:98:HIS:HD2	2:L:7:ARG:HH21	1.60	0.49
1:H:38:GLU:OE1	3:M:241:ARG:NH2	2.46	0.49
7:M:401:BCL:OBB	7:M:401:BCL:HMB1	2.11	0.49
2:L:272:TRP:HA	2:L:275:ILE:HD12	1.95	0.49
1:H:52:ASN:ND2	6:H:307:GGD:HA41	2.27	0.49
1:H:62:LYS:HE3	1:H:64:PHE:CZ	2.47	0.49
1:H:96:PHE:HB3	1:H:97:PRO:CD	2.42	0.48
8:L:304:LDA:C12	9:L:305[B]:U10:H1M1	2.43	0.48
1:H:140:PHE:HA	3:M:13:ARG:O	2.14	0.48
7:L:301:BCL:HHC	7:L:301:BCL:CBB	2.43	0.48
2:L:181:PHE:HB3	13:M:406:BPH:CBB	2.44	0.48
2:L:42:ALA:HA	13:M:412:BPH:H9C3	1.95	0.47
3:M:197:PHE:CZ	7:M:402:BCL:HBB2	2.49	0.47
2:L:128:TYR:CD1	7:L:301:BCL:HBB1	2.48	0.47
2:L:272:TRP:CD1	3:M:87:ARG:HG3	2.50	0.47
4:L:311:GOL:H12	8:M:403:LDA:O1	2.15	0.47
1:H:98:HIS:CD2	2:L:7:ARG:HE	2.32	0.46
3:M:77:GLN:NE2	3:M:92:PHE:HB3	2.31	0.46
3:M:300:ASN:C	3:M:302:GLY:N	2.69	0.46
13:M:412:BPH:CBB	13:M:412:BPH:CHC	2.91	0.46
1:H:62:LYS:O	1:H:74:THR:HA	2.16	0.45
13:M:406:BPH:HHO	13:M:406:BPH:HBC2	1.99	0.45
3:M:197:PHE:HZ	7:M:402:BCL:HBB2	1.82	0.45
3:M:269:ALA:O	3:M:270:ILE:C	2.55	0.44
1:H:52:ASN:HD21	6:H:307:GGD:HA41	1.83	0.44
7:L:306:BCL:H193	9:M:407:U10:H252	2.00	0.44
3:M:204:LEU:HG	8:M:403:LDA:HM13	1.99	0.44
9:L:305[B]:U10:C10	8:M:404:LDA:H121	2.47	0.44
3:M:251:PHE:CD1	3:M:251:PHE:C	2.90	0.44
7:L:301:BCL:H193	13:M:412:BPH:H7C1	2.00	0.44
2:L:229:ILE:HD13	9:L:305[B]:U10:C3M	2.43	0.44
1:H:40:TYR:HB3	1:H:58:LEU:HD21	1.98	0.44
7:M:402:BCL:HBD	7:M:402:BCL:HAA2	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:243:THR:O	3:M:247:ARG:HG3	2.19	0.43
3:M:16:ALA:CB	3:M:32:VAL:HG11	2.40	0.43
2:L:83:GLY:O	2:L:87:GLN:HG3	2.19	0.43
7:L:306:BCL:H161	7:L:306:BCL:H203	1.91	0.43
2:L:180:PHE:CD2	2:L:240:ALA:HB1	2.54	0.43
1:H:98:HIS:CD2	2:L:7:ARG:HH21	2.37	0.43
2:L:52:SER:HB2	2:L:85:LEU:HD13	2.02	0.42
2:L:135:ARG:HD2	2:L:248:MET:O	2.19	0.42
13:M:412:BPH:H4C1	13:M:412:BPH:H6C2	1.81	0.42
3:M:274:VAL:O	3:M:278:LEU:HB2	2.19	0.42
2:L:208:THR:HB	2:L:209:PRO:HD2	2.00	0.42
13:M:412:BPH:H1C1	13:M:412:BPH:H5C2	1.82	0.42
3:M:150:PHE:N	13:M:406:BPH:HMD3	2.35	0.42
3:M:164:ARG:HB3	3:M:165:PRO:HD3	2.00	0.42
15:M:409:CDL:C34	15:M:409:CDL:C36	2.97	0.42
2:L:173:HIS:CE1	2:L:177:ILE:HD11	2.55	0.41
8:L:304:LDA:H122	9:L:305[B]:U10:H1M1	2.02	0.41
2:L:219:LEU:HD11	3:M:133:THR:HG22	2.03	0.41
1:H:248:ARG:HA	1:H:249[B]:LYS:HB3	1.96	0.41
7:L:301:BCL:HBC1	7:L:306:BCL:CGA	2.51	0.41
3:M:250:LEU:HA	3:M:250:LEU:HD23	1.90	0.41
7:L:301:BCL:C2B	13:M:412:BPH:H202	2.51	0.41
7:L:306:BCL:NC	7:M:402:BCL:HBB3	2.35	0.41
14:M:408:SPO:H20	14:M:408:SPO:H181	1.86	0.40
6:H:307:GGD:HC62	3:M:257:GLY:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	H	244/266 (92%)	231 (95%)	11 (4%)	2 (1%)	24 56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	281/282 (100%)	265 (94%)	16 (6%)	0	100	100
3	M	301/307 (98%)	288 (96%)	11 (4%)	2 (1%)	26	59
All	All	826/855 (97%)	784 (95%)	38 (5%)	4 (0%)	39	67

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	249[A]	LYS
1	H	249[B]	LYS
3	M	30	SER
3	M	301	HIS

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	H	200/214 (94%)	192 (96%)	8 (4%)	38	72
2	L	221/221 (100%)	211 (96%)	10 (4%)	34	67
3	M	237/240 (99%)	229 (97%)	8 (3%)	44	77
All	All	658/675 (98%)	632 (96%)	26 (4%)	41	72

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	12	LEU
1	H	75	VAL
1	H	163[A]	LYS
1	H	163[B]	LYS
1	H	201	ASN
1	H	221	SER
1	H	231	ASP
1	H	247	LYS
2	L	21	LEU
2	L	158	SER

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Mol	Chain	Res	Type
2	L	207	ARG
2	L	210	ASP
2	L	216	PHE
2	L	235	LEU
2	L	247	CYS
2	L	271[A]	TRP
2	L	271[B]	TRP
2	L	272	TRP
3	M	104	SER
3	M	110	LYS
3	M	114	LEU
3	M	170	SER
3	M	188	ASN
3	M	216	PHE
3	M	259	ASN
3	M	278	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	32	GLN
1	H	98	HIS
1	H	201	ASN
3	M	77	GLN
3	M	187	ASN
3	M	193	HIS

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

Of 31 ligands modelled in this entry, 3 are monoatomic - leaving 28 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	GOL	H	301	-	5,5,5	0.74	0	5,5,5	1.10	0
4	GOL	H	302	-	5,5,5	0.45	0	5,5,5	0.65	0
4	GOL	H	303	-	5,5,5	0.53	0	5,5,5	0.63	0
4	GOL	H	304	-	5,5,5	0.76	0	5,5,5	0.76	0
4	GOL	H	306	-	5,5,5	1.10	0	5,5,5	1.03	0
6	GGD	H	307	-	58,58,68	1.12	3 (5%)	72,72,82	1.72	14 (19%)
7	BCL	L	301	-	53,74,74	1.40	7 (13%)	57,115,115	2.45	20 (35%)
8	LDA	L	302	-	15,15,15	3.80	1 (6%)	16,17,17	1.37	1 (6%)
8	LDA	L	303	-	15,15,15	4.08	1 (6%)	16,17,17	1.72	2 (12%)
8	LDA	L	304	-	15,15,15	3.97	1 (6%)	16,17,17	0.95	1 (6%)
9	U10	L	305[A]	-	23,23,63	1.48	2 (8%)	28,31,79	1.52	7 (25%)
9	U10	L	305[B]	-	23,23,63	1.72	2 (8%)	28,31,79	1.42	5 (17%)
7	BCL	L	306	-	53,74,74	1.39	7 (13%)	57,115,115	1.48	9 (15%)
10	PO4	L	307	-	4,4,4	0.79	0	6,6,6	0.29	0
11	HTO	L	308	-	9,9,9	1.24	1 (11%)	8,10,10	1.06	0
11	HTO	L	309	-	9,9,9	1.43	1 (11%)	8,10,10	1.66	2 (25%)
4	GOL	L	310	-	5,5,5	0.42	0	5,5,5	0.50	0
4	GOL	L	311	-	5,5,5	0.32	0	5,5,5	0.34	0
7	BCL	M	401	-	53,74,74	1.60	7 (13%)	57,115,115	1.84	10 (17%)
7	BCL	M	402	-	53,74,74	1.32	7 (13%)	57,115,115	1.65	10 (17%)
8	LDA	M	403	-	15,15,15	3.95	2 (13%)	16,17,17	1.99	2 (12%)
8	LDA	M	404	-	15,15,15	3.81	1 (6%)	16,17,17	1.21	3 (18%)
13	BPH	M	406	-	64,70,70	1.92	14 (21%)	73,101,101	1.96	18 (24%)
9	U10	M	407	-	48,48,63	1.30	5 (10%)	58,61,79	2.45	19 (32%)
14	SPO	M	408	-	40,41,41	0.79	1 (2%)	45,50,50	1.93	10 (22%)
15	CDL	M	409	-	79,79,99	1.47	5 (6%)	80,90,111	1.45	8 (10%)
16	PC1	M	410	-	42,42,53	1.47	4 (9%)	46,50,61	1.61	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	BPH	M	412	-	64,70,70	1.93	15 (23%)	73,101,101	2.47	19 (26%)

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
4	GOL	H	301	-	-	0/4/4/4	0/0/0/0
4	GOL	H	302	-	-	0/4/4/4	0/0/0/0
4	GOL	H	303	-	-	0/4/4/4	0/0/0/0
4	GOL	H	304	-	-	0/4/4/4	0/0/0/0
4	GOL	H	306	-	-	0/4/4/4	0/0/0/0
6	GGD	H	307	-	-	0/47/87/97	0/2/2/2
7	BCL	L	301	-	-	0/37/137/137	0/0/9/9
8	LDA	L	302	-	-	0/13/13/13	0/0/0/0
8	LDA	L	303	-	-	0/13/13/13	0/0/0/0
8	LDA	L	304	-	-	0/13/13/13	0/0/0/0
9	U10	L	305[A]	-	-	0/15/39/87	0/1/1/1
9	U10	L	305[B]	-	-	0/15/39/87	0/1/1/1
7	BCL	L	306	-	-	0/37/137/137	0/0/9/9
10	PO4	L	307	-	-	0/0/0/0	0/0/0/0
11	HTO	L	308	-	-	0/10/10/10	0/0/0/0
11	HTO	L	309	-	-	0/10/10/10	0/0/0/0
4	GOL	L	310	-	-	0/4/4/4	0/0/0/0
4	GOL	L	311	-	-	0/4/4/4	0/0/0/0
7	BCL	M	401	-	-	0/37/137/137	0/0/9/9
7	BCL	M	402	-	-	0/37/137/137	0/0/9/9
8	LDA	M	403	-	-	0/13/13/13	0/0/0/0
8	LDA	M	404	-	-	0/13/13/13	0/0/0/0
13	BPH	M	406	-	-	0/54/105/105	0/1/6/6
9	U10	M	407	-	-	0/45/69/87	0/1/1/1
14	SPO	M	408	-	-	0/47/47/47	0/0/0/0
15	CDL	M	409	-	-	0/88/88/110	0/0/0/0
16	PC1	M	410	-	-	0/46/46/57	0/0/0/0
13	BPH	M	412	-	-	0/54/105/105	0/1/6/6

All (87) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	303	LDA	O1-N1	-15.55	1.24	1.39
8	L	304	LDA	O1-N1	-15.26	1.25	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	403	LDA	O1-N1	-14.77	1.25	1.39
8	M	404	LDA	O1-N1	-14.61	1.25	1.39
8	L	302	LDA	O1-N1	-14.42	1.25	1.39
13	M	406	BPH	C3D-C4D	-5.88	1.33	1.41
13	M	406	BPH	C4C-NC	-5.53	1.25	1.37
13	M	412	BPH	C1A-NA	-5.26	1.25	1.37
13	M	412	BPH	C3D-C4D	-4.41	1.35	1.41
13	M	406	BPH	C1A-NA	-3.95	1.28	1.37
7	L	306	BCL	C3C-C4C	-3.88	1.46	1.51
13	M	412	BPH	C4C-NC	-3.79	1.29	1.37
13	M	406	BPH	CHB-C4A	-2.71	1.35	1.40
7	M	402	BCL	C2C-C3C	-2.26	1.47	1.54
13	M	412	BPH	C1B-NB	-2.23	1.33	1.38
7	M	401	BCL	CMB-C2B	-2.21	1.47	1.51
8	M	403	LDA	CM1-N1	-2.20	1.46	1.49
7	L	301	BCL	C2C-C3C	-2.10	1.48	1.54
7	M	402	BCL	CMB-C2B	-2.06	1.47	1.51
13	M	412	BPH	CHB-C4A	-2.02	1.36	1.40
16	M	410	PC1	C1-C2	2.18	1.56	1.50
13	M	412	BPH	C3B-C2B	2.21	1.44	1.38
7	L	306	BCL	C1B-CHB	2.23	1.46	1.39
13	M	412	BPH	O1D-CGD	2.24	1.26	1.21
13	M	406	BPH	C1D-CHD	2.25	1.48	1.40
7	L	306	BCL	C4B-CHC	2.25	1.46	1.39
7	M	402	BCL	C4B-CHC	2.26	1.46	1.39
13	M	412	BPH	O2D-CGD	2.30	1.39	1.33
13	M	406	BPH	CHD-C4C	2.30	1.44	1.38
13	M	406	BPH	OBD-CAD	2.32	1.25	1.22
7	M	402	BCL	C3B-C2B	2.33	1.45	1.40
14	M	408	SPO	C25-C23	2.37	1.51	1.45
7	L	306	BCL	C3B-C2B	2.37	1.45	1.40
11	L	308	HTO	C4-C3	2.42	1.57	1.52
9	M	407	U10	C33-C34	2.49	1.37	1.33
15	M	409	CDL	CA3-CA4	2.57	1.58	1.50
13	M	406	BPH	C3B-C2B	2.61	1.45	1.38
7	L	301	BCL	C3B-C2B	2.64	1.46	1.40
11	L	309	HTO	C4-C3	2.65	1.57	1.52
9	L	305[A]	U10	C4-C3	2.66	1.47	1.35
6	H	307	GGD	OA1-CA1	2.67	1.44	1.40
7	M	401	BCL	C3B-C2B	2.75	1.46	1.40
9	M	407	U10	C31-C29	2.80	1.57	1.51
13	M	412	BPH	C3D-C2D	2.80	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	301	BCL	C1B-CHB	2.83	1.47	1.39
9	M	407	U10	C18-C19	2.86	1.38	1.33
7	L	301	BCL	OBD-CAD	2.87	1.26	1.22
7	L	301	BCL	C3D-C2D	2.87	1.47	1.40
9	M	407	U10	C4-C3	2.88	1.48	1.35
16	M	410	PC1	C3-C2	2.89	1.58	1.50
13	M	406	BPH	O2D-CGD	2.99	1.40	1.33
13	M	406	BPH	CHC-C4B	3.02	1.47	1.40
13	M	412	BPH	CHD-C4C	3.14	1.46	1.38
9	L	305[B]	U10	C4-C3	3.22	1.49	1.35
7	M	401	BCL	C1B-CHB	3.24	1.48	1.39
13	M	412	BPH	O2A-CGA	3.27	1.43	1.33
13	M	412	BPH	CHC-C4B	3.30	1.48	1.40
13	M	406	BPH	C3D-C2D	3.32	1.48	1.40
7	M	401	BCL	O2D-CGD	3.35	1.41	1.33
7	L	306	BCL	O2A-CGA	3.38	1.43	1.33
7	M	401	BCL	C3D-C2D	3.39	1.48	1.40
7	M	402	BCL	O2A-CGA	3.55	1.44	1.33
6	H	307	GGD	OC8-CC7	3.85	1.44	1.33
7	M	402	BCL	O2D-CGD	3.85	1.43	1.33
7	L	306	BCL	OBD-CAD	3.88	1.28	1.22
6	H	307	GGD	OC6-CC5	3.92	1.46	1.34
9	M	407	U10	C6-C1	4.11	1.44	1.35
7	L	306	BCL	O2D-CGD	4.12	1.43	1.33
7	M	402	BCL	OBD-CAD	4.14	1.28	1.22
13	M	406	BPH	CHB-C1B	4.23	1.47	1.38
13	M	406	BPH	O2A-CGA	4.30	1.46	1.33
13	M	406	BPH	CHA-C1A	4.35	1.47	1.37
7	L	301	BCL	O2D-CGD	4.45	1.44	1.33
15	M	409	CDL	OB8-CB7	4.53	1.47	1.33
7	L	301	BCL	O2A-CGA	4.56	1.47	1.33
13	M	412	BPH	CHA-C1A	4.67	1.48	1.37
16	M	410	PC1	O21-C21	4.93	1.49	1.34
7	M	401	BCL	O2A-CGA	4.93	1.48	1.33
15	M	409	CDL	OA8-CA7	5.17	1.48	1.33
15	M	409	CDL	OA6-CA5	5.20	1.49	1.34
15	M	409	CDL	OB6-CB5	5.28	1.50	1.34
13	M	412	BPH	CHB-C1B	5.42	1.49	1.38
13	M	412	BPH	OBD-CAD	5.47	1.30	1.22
7	M	401	BCL	OBD-CAD	5.58	1.30	1.22
16	M	410	PC1	O31-C31	5.77	1.50	1.33
9	L	305[A]	U10	C6-C1	5.91	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	L	305[B]	U10	C6-C1	6.53	1.50	1.35

All (165) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	M	408	SPO	C4-C5-C6	-7.08	114.60	124.67
9	M	407	U10	C31-C29-C28	-6.54	108.64	121.05
8	M	403	LDA	O1-N1-CM2	-6.54	100.31	109.05
13	M	412	BPH	CED-O2D-CGD	-6.13	101.60	115.99
8	L	303	LDA	O1-N1-CM2	-5.92	101.14	109.05
9	M	407	U10	C26-C27-C28	-5.34	97.71	111.69
7	L	301	BCL	OBD-CAD-C3D	-4.98	118.19	128.35
6	H	307	GGD	CA4-CA3-CA2	-4.65	104.76	110.89
8	L	302	LDA	O1-N1-C1	-4.63	105.06	110.27
6	H	307	GGD	CC4-OC6-CC5	-4.60	106.84	117.89
7	L	301	BCL	C1D-CHD-C4C	-4.42	119.32	126.07
13	M	412	BPH	CAA-CBA-CGA	-4.39	100.48	113.32
7	L	306	BCL	C3C-C4C-CHD	-4.35	113.62	123.33
7	M	402	BCL	C3C-C4C-CHD	-4.30	113.73	123.33
13	M	406	BPH	OBD-CAD-CBD	-4.24	119.53	125.94
7	M	402	BCL	C1D-CHD-C4C	-4.21	119.65	126.07
7	M	401	BCL	C3C-C4C-CHD	-4.19	113.97	123.33
7	L	301	BCL	C3C-C4C-CHD	-4.10	114.17	123.33
13	M	406	BPH	C4-C3-C2	-4.10	115.44	123.50
7	M	401	BCL	C1D-CHD-C4C	-4.10	119.81	126.07
7	L	301	BCL	O2D-CGD-O1D	-4.10	115.32	123.79
13	M	412	BPH	O2D-CGD-O1D	-4.04	115.45	123.79
13	M	412	BPH	CBB-CAB-C3B	-4.00	111.63	120.52
14	M	408	SPO	C15-C14-C12	-3.82	121.67	127.20
13	M	412	BPH	C4-C3-C2	-3.80	116.03	123.50
7	L	306	BCL	C1D-CHD-C4C	-3.72	120.40	126.07
13	M	412	BPH	O2D-CGD-CBD	-3.65	106.28	111.30
9	M	407	U10	C7-C8-C9	-3.61	120.58	126.70
13	M	406	BPH	O2D-CGD-O1D	-3.55	116.47	123.79
7	M	402	BCL	OBD-CAD-C3D	-3.52	121.18	128.35
13	M	412	BPH	CAC-C3C-C4C	-3.49	103.70	112.67
7	L	301	BCL	C5-C3-C2	-3.47	114.48	121.05
7	M	401	BCL	O2D-CGD-O1D	-3.46	116.65	123.79
13	M	406	BPH	CAC-C3C-C2C	-3.43	105.50	114.13
7	L	301	BCL	O1D-CGD-CBD	-3.38	119.78	124.62
8	M	404	LDA	O1-N1-C1	-3.38	106.47	110.27
7	M	402	BCL	O2D-CGD-O1D	-3.27	117.03	123.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	301	BCL	C2A-C1A-CHA	-2.89	118.56	123.89
7	L	306	BCL	O2A-CGA-O1A	-2.86	116.11	123.49
9	M	407	U10	C32-C33-C34	-2.83	121.60	127.76
15	M	409	CDL	OA8-CA7-OA9	-2.78	116.31	123.49
6	H	307	GGD	OC8-CC7-OC9	-2.77	116.33	123.49
9	M	407	U10	C17-C18-C19	-2.77	121.73	127.76
14	M	408	SPO	C27-C26-C25	-2.77	114.67	123.13
14	M	408	SPO	C20-C19-C17	-2.75	123.22	127.20
13	M	406	BPH	C3A-C4A-NA	-2.70	108.84	113.57
9	L	305[B]	U10	O5-C5-C4	-2.67	115.00	120.79
15	M	409	CDL	OA6-CA5-OA7	-2.67	116.50	123.67
9	L	305[A]	U10	C16-C14-C13	-2.64	114.12	122.61
15	M	409	CDL	OB8-CB7-OB9	-2.57	116.86	123.49
14	M	408	SPO	C6-C7-C9	-2.54	114.89	118.98
13	M	412	BPH	O2A-CGA-O1A	-2.53	116.95	123.49
9	L	305[B]	U10	C1-C6-C5	-2.53	117.24	120.12
9	M	407	U10	C35-C34-C33	-2.52	118.55	123.50
7	M	401	BCL	CED-O2D-CGD	-2.50	110.13	115.99
9	L	305[A]	U10	C7-C6-C5	-2.48	115.65	118.56
7	L	306	BCL	C2A-C1A-CHA	-2.47	119.33	123.89
9	L	305[A]	U10	O2-C2-C3	-2.42	115.55	120.79
13	M	406	BPH	C3B-C2B-C1B	-2.40	101.92	105.77
14	M	408	SPO	C21-C22-C23	-2.39	123.74	127.20
13	M	406	BPH	CMA-C3A-C4A	-2.39	105.23	113.01
9	L	305[A]	U10	C7-C8-C9	-2.30	122.80	126.70
15	M	409	CDL	OB6-CB5-OB7	-2.30	117.50	123.67
7	L	306	BCL	OBD-CAD-C3D	-2.30	123.67	128.35
14	M	408	SPO	C13-C12-C14	-2.27	119.55	122.90
9	M	407	U10	C30-C29-C28	-2.26	119.07	123.50
14	M	408	SPO	C40-C38-C37	-2.25	115.38	122.61
8	L	304	LDA	O1-N1-C1	-2.22	107.77	110.27
9	M	407	U10	C26-C24-C23	-2.21	116.85	121.05
7	M	401	BCL	C3A-C2A-C1A	-2.20	97.77	101.50
7	L	301	BCL	C6-C5-C3	-2.14	107.79	112.48
7	L	301	BCL	O2A-CGA-O1A	-2.13	117.99	123.49
7	L	301	BCL	C16-C15-C13	-2.12	108.47	115.49
9	L	305[B]	U10	C15-C14-C13	-2.10	115.87	122.61
8	M	404	LDA	CM2-N1-CM1	-2.07	106.49	108.83
9	M	407	U10	C20-C19-C21	-2.07	112.25	115.41
13	M	406	BPH	C3A-C2A-C1A	-2.03	99.26	101.84
9	L	305[A]	U10	C6-C1-C2	-2.02	118.30	120.42
6	H	307	GGD	OC6-CC5-OC7	-2.00	118.29	123.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	M	408	SPO	C13-C12-C11	2.02	121.46	118.10
7	L	301	BCL	CED-O2D-CGD	2.05	120.80	115.99
6	H	307	GGD	CB1-OB1-CA3	2.05	123.36	118.01
7	M	402	BCL	O1D-CGD-CBD	2.06	127.58	124.62
9	M	407	U10	C31-C32-C33	2.09	117.17	111.69
8	L	303	LDA	CM2-N1-CM1	2.13	111.23	108.83
9	M	407	U10	C41-C39-C40	2.17	119.97	114.64
13	M	412	BPH	C7-C6-C5	2.24	119.69	113.06
13	M	406	BPH	C2B-C1B-NB	2.29	113.17	109.73
13	M	406	BPH	CHB-C4A-NA	2.31	128.27	124.40
9	M	407	U10	C16-C17-C18	2.32	117.78	111.69
11	L	309	HTO	C5-C4-C3	2.35	118.41	114.20
6	H	307	GGD	OB1-CA3-CA4	2.36	113.25	107.17
7	M	402	BCL	CMB-C2B-C3B	2.37	129.73	125.09
9	M	407	U10	C10-C9-C11	2.39	119.06	115.41
13	M	412	BPH	C3A-C2A-C1A	2.41	104.90	101.84
8	M	404	LDA	O1-N1-CM2	2.41	112.27	109.05
6	H	307	GGD	OC8-CC6-CC4	2.45	115.28	108.69
9	M	407	U10	C15-C14-C16	2.45	119.15	115.41
7	M	401	BCL	CHB-C4A-NA	2.46	127.91	124.51
6	H	307	GGD	OB5-CB5-CB6	2.51	112.70	106.36
13	M	412	BPH	OBB-CAB-C3B	2.51	125.16	120.31
16	M	410	PC1	O21-C2-C3	2.56	117.38	108.36
9	M	407	U10	C25-C24-C26	2.57	119.33	115.41
9	L	305[B]	U10	C16-C14-C15	2.59	121.01	114.64
7	M	402	BCL	OBB-CAB-C3B	2.60	124.13	120.00
13	M	412	BPH	CBA-CAA-C2A	2.62	121.14	113.73
6	H	307	GGD	OA5-CA1-CA2	2.63	115.67	110.28
6	H	307	GGD	OA2-CA2-CA3	2.65	116.15	109.87
13	M	406	BPH	CMB-C2B-C1B	2.66	129.39	125.06
6	H	307	GGD	OC8-CC7-C31	2.66	120.01	111.90
7	L	301	BCL	C3D-CAD-CBD	2.66	111.36	107.60
13	M	412	BPH	O2A-CGA-CBA	2.67	120.04	111.90
9	M	407	U10	C35-C34-C36	2.68	119.50	115.41
13	M	412	BPH	CMB-C2B-C1B	2.72	129.48	125.06
7	M	401	BCL	CHC-C1C-NC	2.80	128.39	124.51
7	L	306	BCL	CHC-C1C-NC	2.82	128.41	124.51
9	L	305[A]	U10	C16-C14-C15	2.86	121.66	114.64
13	M	406	BPH	C5-C3-C2	2.87	126.50	121.05
7	L	301	BCL	OBD-CAD-CBD	2.94	130.38	125.94
7	M	402	BCL	O2D-CGD-CBD	2.95	115.34	111.30
7	L	306	BCL	O2A-CGA-CBA	2.98	120.97	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	306	BCL	CHB-C4A-NA	3.01	128.67	124.51
7	L	301	BCL	O2A-CGA-CBA	3.02	121.11	111.90
9	L	305[A]	U10	C8-C7-C6	3.05	120.79	111.64
7	L	301	BCL	CHC-C1C-NC	3.17	128.89	124.51
7	L	301	BCL	C4-C3-C5	3.18	120.26	115.41
15	M	409	CDL	OA8-CA7-C31	3.20	121.64	111.90
7	M	401	BCL	O2A-CGA-CBA	3.22	121.72	111.90
7	M	402	BCL	CHB-C4A-NA	3.26	129.01	124.51
16	M	410	PC1	O31-C31-C32	3.27	121.85	111.90
7	L	301	BCL	CHB-C4A-NA	3.31	129.09	124.51
9	M	407	U10	C4M-O4-C4	3.31	128.39	116.61
9	L	305[B]	U10	C10-C9-C11	3.34	120.51	115.41
7	L	301	BCL	OBB-CAB-C3B	3.40	125.39	120.00
15	M	409	CDL	CA6-OA8-CA7	3.41	126.38	116.85
7	L	306	BCL	CHD-C4C-NC	3.53	129.16	125.06
16	M	410	PC1	O31-C3-C2	3.55	118.25	108.69
8	M	403	LDA	O1-N1-C1	3.56	114.28	110.27
7	M	402	BCL	CHD-C4C-NC	3.66	129.31	125.06
11	L	309	HTO	O1-C1-C2	3.70	119.14	111.10
13	M	406	BPH	C4A-NA-C1A	3.73	111.54	108.21
13	M	406	BPH	C6-C5-C3	3.93	121.12	112.48
7	L	301	BCL	CHD-C4C-NC	4.13	129.85	125.06
13	M	412	BPH	C4-C3-C5	4.17	121.78	115.41
13	M	406	BPH	C3D-CAD-CBD	4.27	113.62	107.60
13	M	406	BPH	O2D-CGD-CBD	4.32	117.22	111.30
13	M	412	BPH	CAA-C2A-C1A	4.40	124.45	112.86
9	M	407	U10	C32-C31-C29	4.43	127.13	112.71
14	M	408	SPO	O1-C1-C4	4.45	116.75	105.87
13	M	412	BPH	C4A-NA-C1A	4.59	112.31	108.21
7	M	401	BCL	CHD-C4C-NC	4.87	130.71	125.06
6	H	307	GGD	CA1-OA5-CA5	4.93	123.32	113.75
6	H	307	GGD	OC6-CC5-C14	4.95	122.30	111.53
13	M	406	BPH	CAC-C3C-C4C	5.07	125.69	112.67
6	H	307	GGD	OB1-CA3-CA2	5.09	120.30	107.17
15	M	409	CDL	OA6-CA5-C11	5.18	122.78	111.53
16	M	410	PC1	O21-C21-C22	5.27	122.99	111.53
16	M	410	PC1	C3-O31-C31	5.49	132.21	116.85
13	M	406	BPH	C3C-C4C-NC	5.71	113.65	107.93
15	M	409	CDL	OB6-CB5-C51	6.30	125.23	111.53
7	M	401	BCL	O2D-CGD-CBD	6.34	119.99	111.30
13	M	412	BPH	C3C-C4C-NC	8.53	116.48	107.93
13	M	412	BPH	O1D-CGD-CBD	9.49	138.23	124.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	301	BCL	O2D-CGD-CBD	9.89	124.87	111.30
9	M	407	U10	C30-C29-C31	10.99	132.20	115.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

17 monomers are involved in 56 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	307	GGD	3	0
7	L	301	BCL	7	0
8	L	304	LDA	2	0
9	L	305[B]	U10	6	0
7	L	306	BCL	7	0
10	L	307	PO4	1	0
4	L	311	GOL	1	0
7	M	401	BCL	7	0
7	M	402	BCL	9	0
8	M	403	LDA	2	0
8	M	404	LDA	2	0
13	M	406	BPH	6	0
9	M	407	U10	1	0
14	M	408	SPO	3	0
15	M	409	CDL	1	0
16	M	410	PC1	1	0
13	M	412	BPH	12	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	H	240/266 (90%)	-0.47	4 (1%) 73 70	33, 43, 61, 133	3 (1%)
2	L	281/282 (99%)	-0.63	2 (0%) 89 88	30, 41, 64, 89	0
3	M	302/307 (98%)	-0.46	1 (0%) 94 93	31, 45, 66, 99	6 (1%)
All	All	823/855 (96%)	-0.52	7 (0%) 85 84	30, 43, 64, 133	9 (1%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	250	SER	7.3
1	H	249[A]	LYS	3.3
3	M	1	ALA	3.2
2	L	281	GLY	2.5
2	L	271[A]	TRP	2.4
1	H	220[A]	LYS	2.4
1	H	221	SER	2.4

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
8	LDA	L	303	16/16	0.57	0.54	22.43	80,90,108,114	0
11	HTO	L	308	10/10	0.84	0.50	16.51	66,87,102,105	0
8	LDA	L	302	16/16	0.67	0.57	15.85	47,125,153,155	0
4	GOL	L	310	6/6	0.87	0.46	8.22	73,81,85,86	0
16	PC1	M	410	43/54	0.47	0.45	6.55	61,99,145,170	0
15	CDL	M	409	81/100	0.85	0.40	6.50	53,96,139,153	0
4	GOL	H	306	6/6	0.78	0.36	5.83	69,76,89,90	0
8	LDA	L	304	16/16	0.58	0.40	5.58	71,98,123,128	0
8	LDA	M	404	16/16	0.91	0.33	5.35	59,69,92,96	0
6	GGD	H	307	57/67	0.75	0.41	4.32	51,108,185,203	0
4	GOL	H	304	6/6	0.92	0.32	3.71	40,52,63,71	0
8	LDA	M	403	16/16	0.92	0.20	2.08	52,68,77,78	0
9	U10	L	305[A]	23/63	0.92	0.26	1.83	33,37,65,71	23
9	U10	L	305[B]	23/63	0.92	0.26	1.49	35,50,60,62	23
9	U10	M	407	48/63	0.94	0.24	1.46	33,46,91,110	0
14	SPO	M	408	42/42	0.94	0.21	1.43	33,47,80,92	0
13	BPH	M	406	65/65	0.93	0.23	1.27	35,47,119,134	0
7	BCL	M	402	66/66	0.98	0.20	1.16	33,40,51,75	0
7	BCL	M	401	66/66	0.97	0.21	1.08	28,38,95,105	0
7	BCL	L	306	66/66	0.97	0.15	0.55	28,39,49,65	0
13	BPH	M	412	65/65	0.98	0.15	0.18	30,39,48,57	0
5	K	H	305	1/1	0.96	0.12	-0.21	50,50,50,50	0
7	BCL	L	301	66/66	0.97	0.13	-0.45	26,34,56,61	0
10	PO4	L	307	5/5	0.96	0.11	-0.75	60,62,66,67	0
12	FE	M	405	1/1	0.99	0.16	-0.80	36,36,36,36	0
4	GOL	H	303	6/6	0.76	0.42	-	85,89,92,95	0
11	HTO	L	309	10/10	0.70	0.86	-	72,96,120,121	0
4	GOL	H	301	6/6	0.90	0.39	-	59,65,69,80	0
17	MG	M	411	1/1	0.96	0.15	-	39,39,39,39	0
4	GOL	H	302	6/6	0.85	0.34	-	81,82,85,90	0
4	GOL	L	311	6/6	0.83	0.33	-	83,88,91,94	0

6.5 Other polymers ⓘ

There are no such residues in this entry.