



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2016 – 12:15 PM EDT

PDB ID : 5LRI
Title : PHOTOSYNTHETIC REACTION CENTER MUTANT WITH GLUL212
REPLACED WITH TRP (CHAIN L, EL212W)
Authors : Fyfe, P.K.; Jones, M.R.
Deposited on : 2016-08-19
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028320
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-20028320

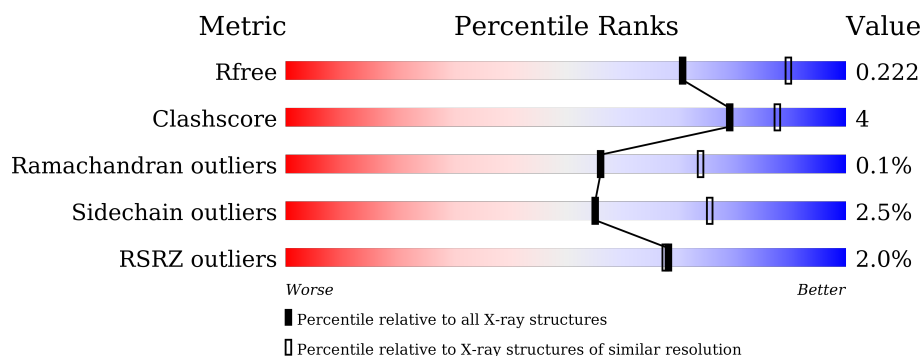
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	L	281	<div> <div>3%</div> <div> <div></div> <div>93%</div> <div>6%</div> <div>.</div> </div> </div>
2	M	307	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>8%</div> <div>.</div> </div> </div>
3	H	260	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>8%</div> <div>.</div> <div>8%</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
5	BPH	M	707	-	-	-	X
6	U10	L	303	-	-	-	X
7	DD9	L	304	-	-	-	X
9	LDA	M	701	-	-	-	X
9	LDA	M	702	-	-	-	X
9	LDA	M	711	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 7494 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 L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	281	Total	C	N	O	S	0	1	0
			2249	1522	357	362	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	212	TRP	GLU	engineered mutation	UNP Q3J1A5

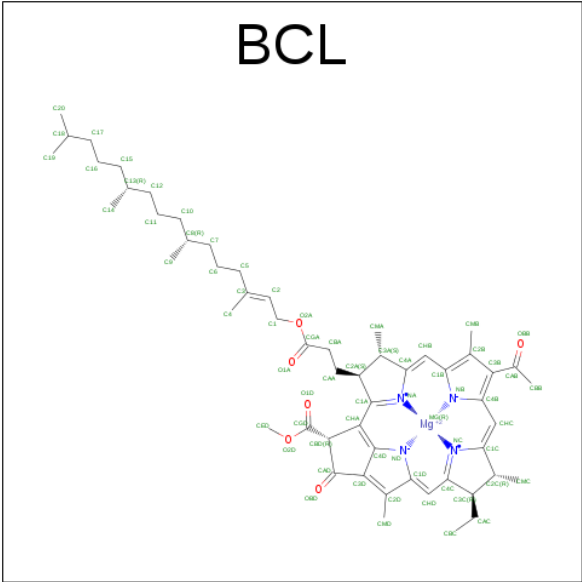
- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	300	Total	C	N	O	S	0	1	0
			2400	1602	395	393	10			

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

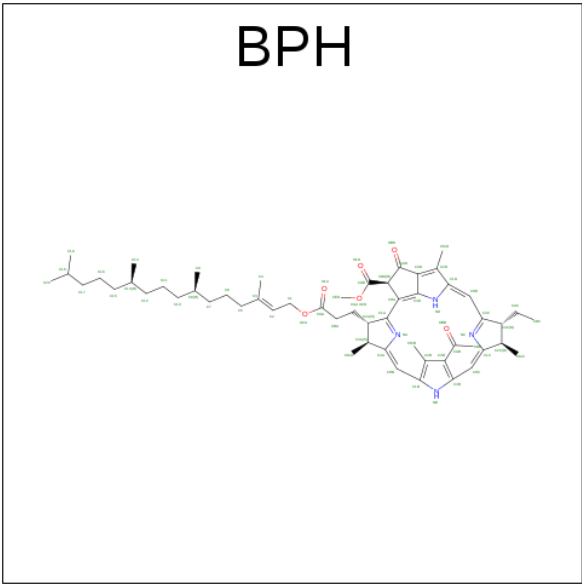
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	239	Total	C	N	O	S	0	2	0
			1837	1174	314	340	9			

- Molecule 4 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



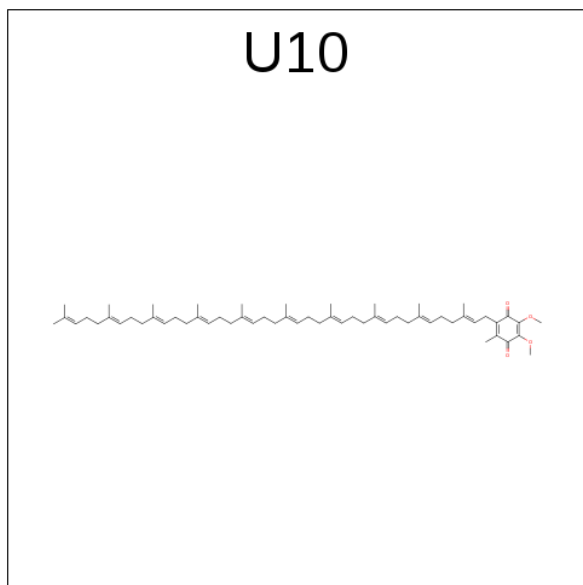
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 5 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: C₅₅H₇₆N₄O₆).



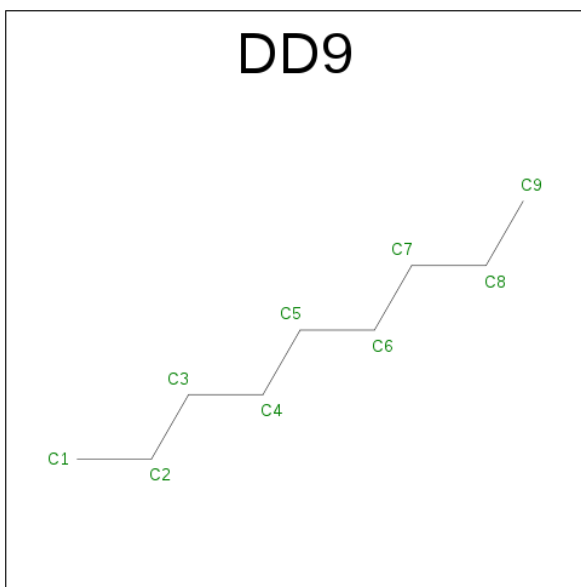
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 6 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	0
			48	44	4		
6	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 7 is nonane (three-letter code: DD9) (formula: C_9H_{20}).

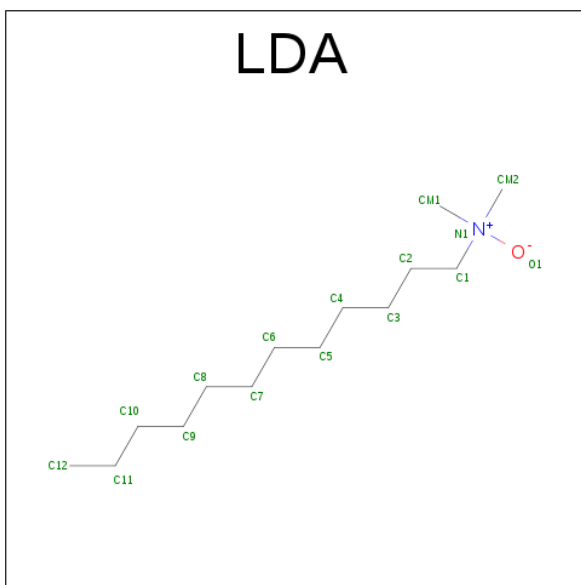


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	1	Total C 8 8	0	0
7	H	1	Total C 9 9	0	0
7	H	1	Total C 7 7	0	0

- Molecule 8 is FE (III) ION (three-letter code: FE) (formula: Fe).

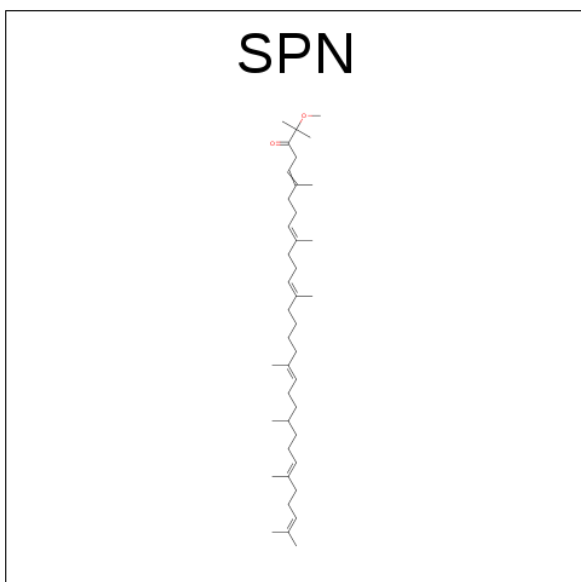
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	L	1	Total Fe 1 1	0	0

- Molecule 9 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: C₁₄H₃₁NO).



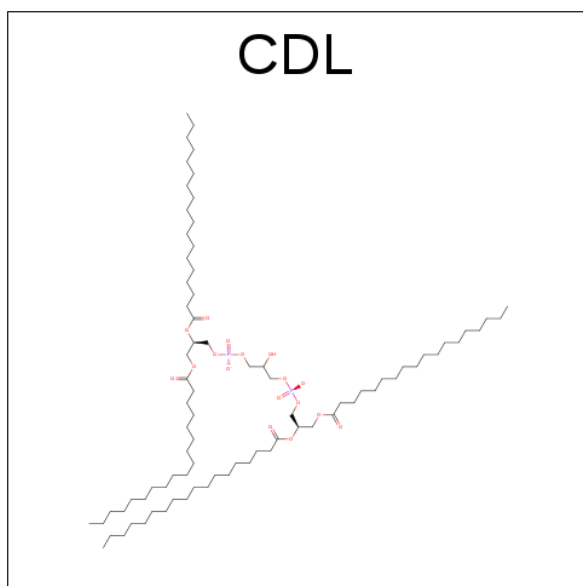
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	M	1	Total	C	N	O	0	0
			16	14	1	1		
9	M	1	Total	C	N	O	0	0
			16	14	1	1		
9	M	1	Total	C	N	O	0	0
			16	14	1	1		
9	M	1	Total	C	N	O	0	0
			16	14	1	1		
9	H	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 10 is SPEROIDENONE (three-letter code: SPN) (formula: $C_{41}H_{70}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	M	1	Total	C	O	0	0
			43	41	2		

- Molecule 11 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	M	1	Total	C	O	P	0	0
			78	59	17	2		

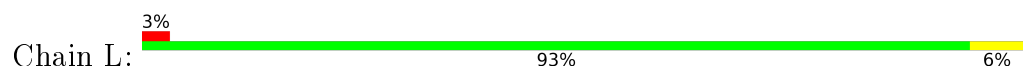
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	L	60	Total	O	0	0
			60	60		
12	M	75	Total	O	0	0
			75	75		
12	H	157	Total	O	0	0
			157	157		

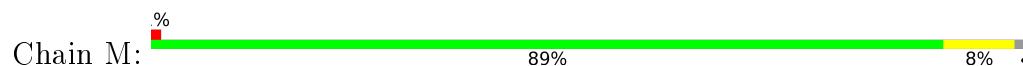
3 Residue-property plots [i](#)

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: Reaction center protein L chain

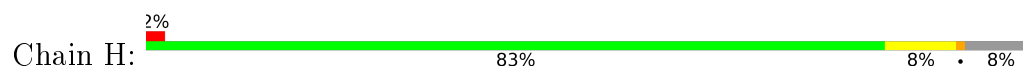


- Molecule 2: Reaction center protein M chain



LEU
ASN

- Molecule 3: Reaction center protein H chain



SER
VAL
VAL
ALA
ALA
MET
MET
LEU
ALA
GLU
TYR
ALA

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	139.82Å 139.82Å 185.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	17.91 – 2.40 17.89 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.6 (17.91-2.40) 94.9 (17.89-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.189 , 0.217 0.195 , 0.222	Depositor DCC
R_{free} test set	3863 reflections (5.23%)	DCC
Wilson B-factor (Å ²)	46.3	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7494	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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, 0.333 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: BCL, DD9, CDL, BPH, LDA, FE, SPN, U10

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	L	0.75	0/2340	0.77	3/3205 (0.1%)
2	M	0.74	0/2497	0.83	8/3408 (0.2%)
3	H	0.75	0/1889	0.97	11/2569 (0.4%)
All	All	0.75	0/6726	0.85	22/9182 (0.2%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	37	ARG	NE-CZ-NH2	-12.78	113.91	120.30
3	H	37	ARG	NE-CZ-NH1	11.50	126.05	120.30
2	M	241	ARG	NE-CZ-NH2	-9.98	115.31	120.30
3	H	83	ARG	NE-CZ-NH2	-9.37	115.61	120.30
2	M	241	ARG	NE-CZ-NH1	8.45	124.52	120.30
3	H	83	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	L	135	ARG	NE-CZ-NH1	8.05	124.32	120.30
1	L	135	ARG	NE-CZ-NH2	-7.57	116.52	120.30
3	H	248	ARG	NE-CZ-NH1	7.34	123.97	120.30
3	H	117	ARG	NE-CZ-NH2	-6.97	116.81	120.30
1	L	210	ASP	CB-CG-OD1	6.73	124.35	118.30
3	H	117	ARG	NE-CZ-NH1	6.65	123.62	120.30
2	M	29	ARG	NE-CZ-NH2	-6.35	117.13	120.30
2	M	136	ARG	NE-CZ-NH2	-6.29	117.15	120.30
2	M	29	ARG	NE-CZ-NH1	5.96	123.28	120.30
3	H	248	ARG	NE-CZ-NH2	-5.83	117.38	120.30
3	H	37	ARG	CG-CD-NE	-5.83	99.55	111.80
3	H	124	ASP	CB-CG-OD1	5.81	123.53	118.30
2	M	136	ARG	NE-CZ-NH1	5.76	123.18	120.30
2	M	267	ARG	NE-CZ-NH2	-5.54	117.53	120.30
2	M	164	ARG	NE-CZ-NH1	5.12	122.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	37	ARG	CD-NE-CZ	5.09	130.72	123.60

There are no chirality outliers.

There are no planarity outliers.

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	L	2249	0	2200	9	0
2	M	2400	0	2316	18	0
3	H	1837	0	1838	10	0
4	L	66	0	74	3	0
4	M	198	0	222	10	0
5	L	65	0	76	3	0
5	M	65	0	76	3	0
6	L	48	0	63	0	0
6	M	48	0	63	0	0
7	H	16	0	33	0	0
7	L	8	0	15	0	0
8	L	1	0	0	0	0
9	H	16	0	31	1	0
9	M	64	0	124	3	0
10	M	43	0	69	5	0
11	M	78	0	100	0	0
12	H	157	0	0	0	0
12	L	60	0	0	1	0
12	M	75	0	0	2	0
All	All	7494	0	7300	51	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.

All (51) 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)
2:M:242:GLY:HA2	3:H:117:ARG:HD3	1.72	0.72
5:L:302:BPH:HHC	5:L:302:BPH:HBB3	1.72	0.71
2:M:157:TRP:CD1	10:M:709:SPN:H202	2.35	0.62
2:M:242:GLY:CA	3:H:117:ARG:HD3	2.29	0.62
1:L:177:ILE:HG12	4:L:301:BCL:HMB3	1.81	0.61
3:H:118:ARG:HD2	3:H:120:LEU:HD12	1.82	0.60
4:M:705:BCL:HBB3	4:M:706:BCL:HMD2	1.82	0.60
5:L:302:BPH:HBB2	2:M:210:TYR:HB3	1.88	0.56
4:M:706:BCL:HMB1	4:M:706:BCL:HBB2	1.88	0.56
1:L:181:PHE:CD2	5:M:707:BPH:HBB1	2.41	0.55
4:M:704:BCL:C3B	10:M:709:SPN:H152	2.37	0.55
4:M:704:BCL:H141	10:M:709:SPN:H101	1.87	0.55
4:M:704:BCL:CAB	10:M:709:SPN:H162	2.36	0.55
4:M:704:BCL:H71	4:M:705:BCL:H202	1.89	0.54
1:L:217:ARG:NH1	12:L:401:HOH:O	2.41	0.53
1:L:250:ILE:HG22	1:L:254:ILE:HD12	1.91	0.53
1:L:116:HIS:HE1	2:M:4:GLN:O	1.92	0.52
2:M:253[B]:ARG:NH2	9:M:702:LDA:HM23	2.25	0.52
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.94	0.50
2:M:133:THR:HG22	2:M:147:ALA:HB2	1.94	0.50
1:L:207:ARG:HG3	2:M:142:MET:HG2	1.94	0.50
2:M:157:TRP:NE1	10:M:709:SPN:H202	2.26	0.49
4:L:301:BCL:CBB	4:L:301:BCL:HMB1	2.43	0.48
5:M:707:BPH:HHC	5:M:707:BPH:HBB3	1.95	0.48
2:M:13:ARG:O	3:H:140:PHE:HA	2.14	0.47
3:H:40:TYR:HB3	3:H:58:LEU:HD21	1.97	0.47
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.97	0.46
5:M:707:BPH:HBC3	5:M:707:BPH:HHD	1.97	0.46
4:M:706:BCL:HMB1	4:M:706:BCL:CBB	2.46	0.46
1:L:52:SER:HB2	1:L:85:LEU:HD13	1.98	0.45
2:M:136:ARG:HA	2:M:136:ARG:NE	2.31	0.45
9:M:703:LDA:HM13	9:M:703:LDA:H21	1.87	0.45
1:L:51:TRP:CH2	1:L:80:LEU:HD23	2.52	0.45
2:M:241:ARG:HD3	2:M:246:GLU:HG2	1.99	0.44
9:H:301:LDA:H21	9:H:301:LDA:HM13	1.85	0.44
2:M:253[A]:ARG:NH2	12:M:803:HOH:O	2.49	0.44
3:H:206:ASN:HD21	3:H:248:ARG:HD2	1.82	0.43
5:L:302:BPH:CBB	5:L:302:BPH:HHC	2.45	0.43
2:M:129:TRP:CH2	2:M:132:ARG:NH1	2.85	0.43
4:M:704:BCL:HBB2	4:M:704:BCL:HMB1	2.00	0.43
3:H:169:VAL:HG23	3:H:171:ILE:HD12	2.00	0.43
2:M:189:PHE:O	2:M:193:HIS:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:704:BCL:CBB	4:M:704:BCL:HMB1	2.50	0.42
2:M:202:HIS:CE1	2:M:206:ILE:HD11	2.55	0.41
2:M:44:ASN:ND2	12:M:806:HOH:O	2.53	0.41
9:M:702:LDA:HM22	9:M:702:LDA:H22	1.84	0.41
3:H:37:ARG:NH2	3:H:60:LYS:O	2.47	0.41
3:H:241:LEU:O	3:H:248:ARG:NH2	2.54	0.40
4:L:301:BCL:OBB	4:L:301:BCL:HHC	2.21	0.40
4:M:705:BCL:HBD	4:M:705:BCL:HAA2	2.03	0.40
3:H:122:GLU:HB2	3:H:227:LEU:HD21	2.02	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	L	280/281 (100%)	273 (98%)	7 (2%)	0	100	100
2	M	299/307 (97%)	285 (95%)	13 (4%)	1 (0%)	46	63
3	H	239/260 (92%)	237 (99%)	2 (1%)	0	100	100
All	All	818/848 (96%)	795 (97%)	22 (3%)	1 (0%)	56	74

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	301	HIS

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	L	221/220 (100%)	214 (97%)	7 (3%)	46	68
2	M	236/240 (98%)	233 (99%)	3 (1%)	76	89
3	H	196/208 (94%)	190 (97%)	6 (3%)	47	69
All	All	653/668 (98%)	637 (98%)	16 (2%)	55	76

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	54	VAL
1	L	72	GLU
1	L	202	LYS
1	L	210	ASP
1	L	212	TRP
1	L	247	CYS
1	L	272	TRP
2	M	18	LEU
2	M	136	ARG
2	M	216	PHE
3	H	70	ARG
3	H	133	PRO
3	H	135	LYS
3	H	221	SER
3	H	231	ASP
3	H	237	VAL

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

Mol	Chain	Res	Type
1	L	116	HIS
1	L	183	ASN
2	M	4	GLN
2	M	44	ASN
2	M	193	HIS
3	H	206	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 ⓘ

Of 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 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	$\# Z > 2$
9	LDA	H	301	-	15,15,15	4.42	1 (6%)	16,17,17	4.78	6 (37%)
7	DD9	H	302	-	8,8,8	0.33	0	7,7,7	0.38	0
7	DD9	H	303	-	6,6,8	0.38	0	5,5,7	0.25	0
4	BCL	L	301	-	55,74,74	1.17	2 (3%)	55,115,115	1.32	10 (18%)
5	BPH	L	302	-	64,70,70	0.71	1 (1%)	73,101,101	1.44	11 (15%)
6	U10	L	303	-	48,48,63	1.59	3 (6%)	60,61,79	1.60	11 (18%)
7	DD9	L	304	-	7,7,8	0.35	0	6,6,7	0.32	0
9	LDA	M	701	-	15,15,15	3.75	1 (6%)	16,17,17	1.55	2 (12%)
9	LDA	M	702	-	15,15,15	4.38	1 (6%)	16,17,17	4.49	6 (37%)
9	LDA	M	703	-	15,15,15	4.07	1 (6%)	16,17,17	4.86	6 (37%)
4	BCL	M	704	-	55,74,74	1.20	2 (3%)	55,115,115	1.43	10 (18%)
4	BCL	M	705	-	55,74,74	1.18	2 (3%)	55,115,115	1.35	9 (16%)
4	BCL	M	706	-	55,74,74	1.19	3 (5%)	55,115,115	1.68	15 (27%)
5	BPH	M	707	-	64,70,70	0.70	2 (3%)	73,101,101	1.28	10 (13%)
6	U10	M	708	-	48,48,63	1.51	3 (6%)	60,61,79	1.44	9 (15%)
10	SPN	M	709	-	40,42,42	3.35	15 (37%)	41,52,52	2.85	21 (51%)
11	CDL	M	710	-	77,77,99	1.15	4 (5%)	79,89,111	1.16	5 (6%)
9	LDA	M	711	-	15,15,15	3.88	1 (6%)	16,17,17	0.52	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
9	LDA	H	301	-	-	0/13/13/13	0/0/0/0
7	DD9	H	302	-	-	0/6/6/6	0/0/0/0
7	DD9	H	303	-	-	0/4/4/6	0/0/0/0
4	BCL	L	301	-	-	0/37/137/137	0/0/9/9
5	BPH	L	302	-	-	0/54/105/105	0/1/6/6
6	U10	L	303	-	-	0/45/69/87	0/1/1/1
7	DD9	L	304	-	-	0/5/5/6	0/0/0/0
9	LDA	M	701	-	-	0/13/13/13	0/0/0/0
9	LDA	M	702	-	-	0/13/13/13	0/0/0/0
9	LDA	M	703	-	-	0/13/13/13	0/0/0/0
4	BCL	M	704	-	-	0/37/137/137	0/0/9/9
4	BCL	M	705	-	-	0/37/137/137	0/0/9/9
4	BCL	M	706	-	-	0/37/137/137	0/0/9/9
5	BPH	M	707	-	-	0/54/105/105	0/1/6/6
6	U10	M	708	-	-	0/45/69/87	0/1/1/1
10	SPN	M	709	-	-	0/50/51/51	0/0/0/0
11	CDL	M	710	-	-	0/88/88/110	0/0/0/0
9	LDA	M	711	-	-	0/13/13/13	0/0/0/0

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	H	301	LDA	O1-N1	-16.98	1.23	1.39
9	M	702	LDA	O1-N1	-16.88	1.23	1.39
9	M	703	LDA	O1-N1	-15.61	1.24	1.39
9	M	711	LDA	O1-N1	-14.92	1.25	1.39
9	M	701	LDA	O1-N1	-14.31	1.25	1.39
10	M	709	SPN	C3-C4	-8.85	1.37	1.50
6	L	303	U10	C36-C34	-6.53	1.36	1.51
10	M	709	SPN	C17-C18	-6.47	1.36	1.51
10	M	709	SPN	C10-C9	-6.39	1.36	1.51
10	M	709	SPN	C6-C5	-6.10	1.37	1.51
10	M	709	SPN	C14-C13	-6.08	1.37	1.51
6	M	708	U10	C36-C34	-6.08	1.37	1.51
10	M	709	SPN	C20-C19	-4.20	1.35	1.50
10	M	709	SPN	C7-C8	-3.86	1.36	1.50
10	M	709	SPN	C11-C12	-3.86	1.36	1.50
10	M	709	SPN	C21-C22	-3.33	1.35	1.52
10	M	709	SPN	C16-C15	-2.77	1.35	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	706	BCL	C3C-C4C	-2.19	1.48	1.51
5	M	707	BPH	C1C-NC	-2.14	1.32	1.37
10	M	709	SPN	C21-C20	-2.06	1.46	1.53
5	L	302	BPH	CHC-C1C	2.06	1.40	1.36
5	M	707	BPH	CHC-C1C	2.27	1.41	1.36
6	L	303	U10	C4-C3	3.05	1.48	1.35
6	M	708	U10	C4-C3	3.34	1.50	1.35
4	M	706	BCL	CHC-C1C	3.95	1.38	1.33
11	M	710	CDL	OB8-CB7	4.37	1.46	1.33
11	M	710	CDL	OA6-CA5	4.44	1.47	1.34
11	M	710	CDL	OA8-CA7	4.51	1.46	1.33
11	M	710	CDL	OB6-CB5	4.56	1.47	1.34
4	M	705	BCL	CHB-C4A	4.68	1.39	1.33
4	L	301	BCL	CHB-C4A	4.83	1.40	1.33
4	M	704	BCL	CHB-C4A	4.83	1.40	1.33
4	M	706	BCL	CHB-C4A	4.83	1.40	1.33
4	L	301	BCL	CHC-C1C	5.05	1.40	1.33
4	M	704	BCL	CHC-C1C	5.23	1.40	1.33
10	M	709	SPN	C19-C18	5.43	1.46	1.32
4	M	705	BCL	CHC-C1C	5.53	1.40	1.33
10	M	709	SPN	C8-C9	5.60	1.47	1.32
10	M	709	SPN	C12-C13	5.66	1.47	1.32
6	M	708	U10	C6-C1	5.66	1.48	1.35
10	M	709	SPN	C4-C5	5.71	1.47	1.32
6	L	303	U10	C6-C1	6.40	1.50	1.35

All (131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	703	LDA	O1-N1-C1	-14.41	94.06	110.27
9	H	301	LDA	O1-N1-C1	-14.11	94.40	110.27
9	M	702	LDA	O1-N1-C1	-11.69	97.12	110.27
9	M	702	LDA	CM1-N1-C1	-4.64	94.82	109.77
5	L	302	BPH	C4-C3-C5	-4.61	108.35	115.37
9	M	701	LDA	O1-N1-CM2	-4.50	103.03	109.05
4	M	706	BCL	CMB-C2B-C1B	-4.14	121.27	128.31
4	M	704	BCL	CMB-C2B-C1B	-4.12	121.31	128.31
6	L	303	U10	C30-C29-C28	-4.05	115.75	123.58
4	M	705	BCL	CMB-C2B-C1B	-3.92	121.64	128.31
4	M	706	BCL	O1D-CGD-CBD	-3.61	119.03	124.64
9	M	701	LDA	O1-N1-C1	-3.42	106.42	110.27
5	M	707	BPH	C4-C3-C5	-3.33	110.29	115.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	706	BCL	CAC-C3C-C2C	-3.30	105.92	114.17
6	M	708	U10	C30-C29-C28	-3.17	117.45	123.58
4	L	301	BCL	CMB-C2B-C1B	-3.11	123.02	128.31
4	M	705	BCL	OBB-CAB-CBB	-3.07	112.81	120.14
6	L	303	U10	C32-C33-C34	-3.02	121.09	127.75
9	H	301	LDA	CM2-N1-C1	-3.00	100.09	109.77
4	M	704	BCL	CHA-C1A-NA	-2.97	118.78	126.21
9	M	703	LDA	CM2-N1-C1	-2.94	100.30	109.77
9	M	703	LDA	CM1-N1-C1	-2.89	100.47	109.77
4	M	705	BCL	CHA-C1A-NA	-2.88	119.02	126.21
4	L	301	BCL	CAA-C2A-C3A	-2.86	105.02	112.79
4	L	301	BCL	CHA-C1A-NA	-2.85	119.08	126.21
10	M	709	SPN	CM5-C13-C12	-2.84	118.08	123.58
4	M	706	BCL	C5-C3-C2	-2.82	115.73	120.98
10	M	709	SPN	C17-C18-C19	-2.76	115.83	120.98
6	M	708	U10	C17-C18-C19	-2.72	121.75	127.75
9	H	301	LDA	CM1-N1-C1	-2.70	101.06	109.77
4	M	704	BCL	C4-C3-C2	-2.64	118.48	123.58
5	M	707	BPH	C3B-C4B-NB	-2.63	104.33	109.85
4	M	704	BCL	C6-C5-C3	-2.63	108.05	112.76
6	L	303	U10	C7-C8-C9	-2.58	122.32	126.70
4	M	706	BCL	C6-C5-C3	-2.58	108.14	112.76
4	M	705	BCL	CAC-C3C-C4C	-2.57	106.88	112.58
4	M	706	BCL	CAA-C2A-C3A	-2.50	106.00	112.79
4	M	704	BCL	CAA-C2A-C3A	-2.49	106.03	112.79
6	L	303	U10	C35-C34-C33	-2.47	118.80	123.58
10	M	709	SPN	C10-C9-C8	-2.44	116.44	120.98
4	M	706	BCL	CAC-C3C-C4C	-2.43	107.20	112.58
4	M	706	BCL	OBD-CAD-CBD	-2.34	122.40	125.94
5	M	707	BPH	C2B-C1B-NB	-2.34	106.32	109.81
9	M	702	LDA	CM2-N1-C1	-2.29	102.41	109.77
5	M	707	BPH	O1D-CGD-CBD	-2.26	121.12	124.64
4	L	301	BCL	OBD-CAD-CBD	-2.21	122.60	125.94
4	M	705	BCL	CAC-C3C-C2C	-2.21	108.66	114.17
11	M	710	CDL	OA6-CA5-OA7	-2.18	117.73	123.67
10	M	709	SPN	CM3-C5-C4	-2.18	119.36	123.58
6	M	708	U10	C32-C33-C34	-2.18	122.95	127.75
6	M	708	U10	C16-C14-C13	-2.18	116.93	120.98
4	M	706	BCL	OBB-CAB-CBB	-2.17	114.95	120.14
10	M	709	SPN	C24-C25-C26	-2.16	122.98	127.75
5	L	302	BPH	C2B-C1B-NB	-2.14	106.61	109.81
4	L	301	BCL	C11-C12-C13	-2.11	108.93	115.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	301	BCL	OBB-CAB-CBB	-2.10	115.11	120.14
5	L	302	BPH	C3B-C4B-NB	-2.07	105.50	109.85
6	M	708	U10	C11-C9-C8	-2.06	117.15	120.98
4	M	705	BCL	OBD-CAD-CBD	-2.05	122.85	125.94
5	M	707	BPH	CAA-C2A-C3A	-2.05	107.23	112.79
4	M	704	BCL	OBD-CAD-CBD	-2.01	122.90	125.94
5	L	302	BPH	O2A-CGA-O1A	-2.00	118.26	123.51
6	M	708	U10	C31-C29-C28	2.03	124.76	120.98
10	M	709	SPN	CM7-C22-C23	2.05	118.77	111.10
5	L	302	BPH	CED-O2D-CGD	2.05	120.85	115.97
6	L	303	U10	C20-C19-C21	2.06	118.52	115.37
4	M	705	BCL	C2A-C1A-CHA	2.07	127.13	123.80
4	M	704	BCL	C5-C3-C2	2.08	124.85	120.98
5	L	302	BPH	C5-C3-C2	2.12	124.94	120.98
6	L	303	U10	C36-C34-C33	2.14	124.96	120.98
10	M	709	SPN	CMA-O1-C1	2.15	123.28	112.08
4	L	301	BCL	C2A-C1A-CHA	2.20	127.34	123.80
4	M	704	BCL	CAA-CBA-CGA	2.21	119.65	113.28
6	L	303	U10	C3M-O3-C3	2.24	124.62	116.64
4	M	706	BCL	CMB-C2B-C3B	2.26	129.51	125.09
4	L	301	BCL	CGD-CBD-CHA	2.27	118.67	110.88
4	L	301	BCL	CMB-C2B-C3B	2.28	129.54	125.09
4	M	705	BCL	CMB-C2B-C3B	2.29	129.57	125.09
5	L	302	BPH	CAC-C3C-C4C	2.31	118.61	112.67
5	M	707	BPH	O2D-CGD-CBD	2.33	114.58	111.22
4	L	301	BCL	CED-O2D-CGD	2.33	121.51	115.97
11	M	710	CDL	CB6-OB8-CB7	2.34	123.97	117.00
5	M	707	BPH	C5-C3-C2	2.40	125.45	120.98
4	M	706	BCL	C2A-C3A-C4A	2.48	104.38	101.84
10	M	709	SPN	CM8-C26-C27	2.50	119.19	115.37
4	M	706	BCL	CAA-CBA-CGA	2.61	120.81	113.28
4	M	704	BCL	C2A-C1A-CHA	2.61	128.00	123.80
5	L	302	BPH	OBB-CAB-C3B	2.69	125.53	120.37
6	L	303	U10	C30-C29-C31	2.76	119.58	115.37
5	L	302	BPH	C1B-NB-C4B	2.81	111.85	106.50
5	M	707	BPH	C3C-C4C-NC	2.83	110.66	107.94
6	L	303	U10	C15-C14-C16	2.87	119.73	115.37
10	M	709	SPN	C10-C11-C12	2.88	119.17	111.61
11	M	710	CDL	OA8-CA7-C31	2.89	120.74	111.85
5	M	707	BPH	CED-O2D-CGD	2.91	122.89	115.97
10	M	709	SPN	C15-C16-C17	2.91	124.09	113.30
4	M	704	BCL	CMB-C2B-C3B	2.93	130.82	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	706	BCL	CMD-C2D-C3D	2.93	130.83	125.09
4	M	706	BCL	OBB-CAB-C3B	2.95	125.69	119.97
6	M	708	U10	C10-C9-C11	2.96	119.88	115.37
6	M	708	U10	C15-C14-C16	3.12	120.13	115.37
10	M	709	SPN	CM7-C22-C21	3.15	122.86	111.10
4	M	706	BCL	O2D-CGD-CBD	3.16	115.78	111.22
5	L	302	BPH	O2D-CGD-CBD	3.20	115.84	111.22
5	M	707	BPH	C1B-NB-C4B	3.21	112.60	106.50
10	M	709	SPN	C6-C7-C8	3.23	120.10	111.61
4	M	705	BCL	CED-O2D-CGD	3.25	123.69	115.97
10	M	709	SPN	C16-C15-C14	3.30	125.50	113.30
10	M	709	SPN	C11-C10-C9	3.49	124.16	112.61
6	L	303	U10	C37-C36-C34	3.60	124.53	112.61
10	M	709	SPN	C7-C6-C5	3.64	124.66	112.61
6	M	708	U10	C37-C36-C34	3.69	124.83	112.61
6	L	303	U10	C25-C24-C26	4.08	121.58	115.37
11	M	710	CDL	OB6-CB5-C51	4.39	120.79	111.53
10	M	709	SPN	CM4-C9-C10	4.40	122.07	115.37
5	L	302	BPH	C3C-C4C-NC	4.63	112.39	107.94
10	M	709	SPN	CM6-C18-C17	4.89	122.82	115.37
10	M	709	SPN	CM3-C5-C6	5.02	123.02	115.37
11	M	710	CDL	OA6-CA5-C11	5.02	122.11	111.53
10	M	709	SPN	CM5-C13-C14	5.85	124.28	115.37
9	H	301	LDA	O1-N1-CM2	5.95	117.00	109.05
10	M	709	SPN	C16-C17-C18	6.12	123.75	112.76
10	M	709	SPN	C15-C14-C13	6.26	123.99	112.76
9	M	703	LDA	O1-N1-CM2	6.33	117.51	109.05
9	M	703	LDA	CM2-N1-CM1	6.80	116.50	108.83
9	M	702	LDA	O1-N1-CM1	6.85	118.21	109.05
9	M	702	LDA	O1-N1-CM2	6.97	118.38	109.05
9	H	301	LDA	CM2-N1-CM1	7.49	117.28	108.83
9	H	301	LDA	O1-N1-CM1	7.63	119.25	109.05
9	M	702	LDA	CM2-N1-CM1	7.71	117.52	108.83
9	M	703	LDA	O1-N1-CM1	8.12	119.91	109.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	H	301	LDA	1	0
4	L	301	BCL	3	0
5	L	302	BPH	3	0
9	M	702	LDA	2	0
9	M	703	LDA	1	0
4	M	704	BCL	6	0
4	M	705	BCL	3	0
4	M	706	BCL	3	0
5	M	707	BPH	3	0
10	M	709	SPN	5	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	L	281/281 (100%)	-0.43	8 (2%) 56 55	34, 49, 82, 106	0
2	M	300/307 (97%)	-0.59	4 (1%) 79 79	32, 53, 81, 107	0
3	H	239/260 (91%)	-0.54	4 (1%) 73 72	35, 49, 68, 109	0
All	All	820/848 (96%)	-0.52	16 (1%) 68 68	32, 50, 80, 109	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	59	TRP	5.4
3	H	249	LYS	4.4
3	H	245	ALA	3.4
2	M	301	HIS	3.1
1	L	72	GLU	3.1
1	L	281	GLY	3.0
3	H	246	PRO	2.8
1	L	270	PRO	2.6
1	L	277	GLY	2.4
3	H	247	LYS	2.3
1	L	202	LYS	2.3
2	M	3	TYR	2.3
1	L	276	PRO	2.2
1	L	71	LEU	2.1
2	M	109	LEU	2.1
2	M	302	GLY	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, 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
9	LDA	M	701	16/16	0.80	0.23	6.76	56,69,79,81	0
7	DD9	L	304	8/9	0.46	0.36	6.39	62,80,90,91	0
9	LDA	M	711	16/16	0.69	0.28	5.39	77,83,106,107	0
6	U10	L	303	48/63	0.81	0.24	4.68	55,90,113,120	0
9	LDA	M	702	16/16	0.91	0.18	2.67	67,70,77,77	0
5	BPH	M	707	65/65	0.89	0.16	2.37	41,52,120,124	0
11	CDL	M	710	78/100	0.89	0.20	1.46	48,80,97,99	0
10	SPN	M	709	43/43	0.89	0.18	1.27	46,60,86,93	0
4	BCL	M	705	66/66	0.96	0.14	1.00	33,39,70,84	0
6	U10	M	708	48/63	0.92	0.13	0.61	30,41,74,81	0
4	BCL	L	301	66/66	0.97	0.13	0.51	36,40,55,61	0
4	BCL	M	704	66/66	0.95	0.12	0.46	38,45,90,91	0
5	BPH	L	302	65/65	0.97	0.11	0.13	28,39,50,52	0
4	BCL	M	706	66/66	0.96	0.10	-0.23	27,34,63,74	0
8	FE	L	305	1/1	0.99	0.07	-1.14	37,37,37,37	0
9	LDA	M	703	16/16	0.58	0.27	-	74,84,101,101	0
7	DD9	H	303	7/9	0.75	0.30	-	76,80,81,81	0
7	DD9	H	302	9/9	0.67	0.39	-	77,82,89,89	0
9	LDA	H	301	16/16	0.78	0.26	-	99,104,112,112	0

6.5 Other polymers [i](#)

There are no such residues in this entry.