



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2017 – 10:17 PM EDT

PDB ID : 5LSE  
Title : PHOTOSYNTHETIC REACTION CENTER MUTANT WITH Glu L212 replaced with Ala (CHAIN L, EL212W), Asp L213 replaced with ALA (Chain L, DL213A) AND LEU M215 REPLACED WITH ALA (CHAIN M, LM215A)  
Authors : Fyfe, P.K.; Jones, M.R.  
Deposited on : unknown  
Resolution : 2.50 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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-20029824

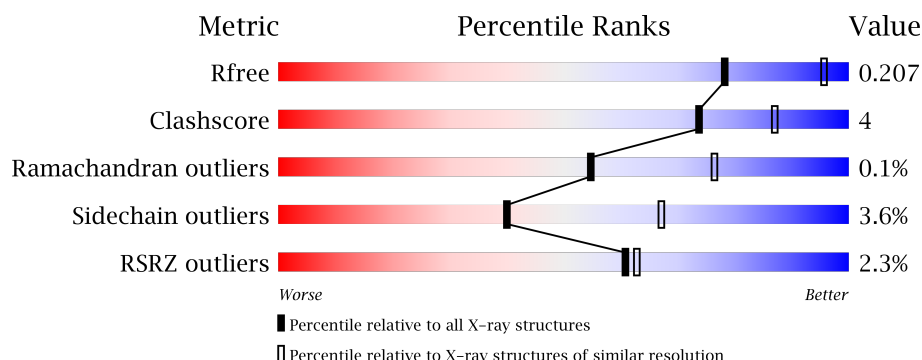
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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  $\geq 3$ , 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>2%</div> <div> <div></div> <div>93%</div> <div>6%</div> </div> </div>
2	M	307	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>9%</div> <div>..</div> </div> </div>
3	H	260	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>8%</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
10	LDA	M	406	-	-	-	X
12	CDL	M	409	-	-	-	X
4	BCL	M	401	-	-	-	X
6	U10	L	304	-	-	-	X
9	SPN	M	405	-	-	-	X

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 7439 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	0	0
			2225	1504	355	358	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	212	ALA	GLU	engineered mutation	UNP P0C0Y8
L	213	ALA	ASP	engineered mutation	UNP P0C0Y8

- 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
			2397	1599	395	393	10			

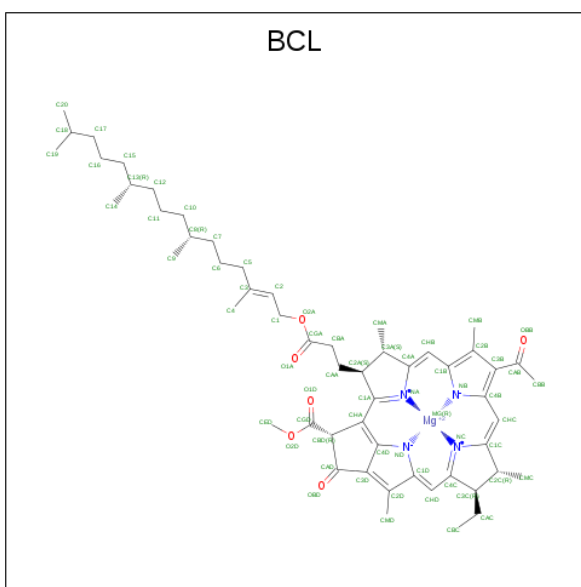
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	215	ALA	LEU	engineered mutation	UNP P0C0Y9

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

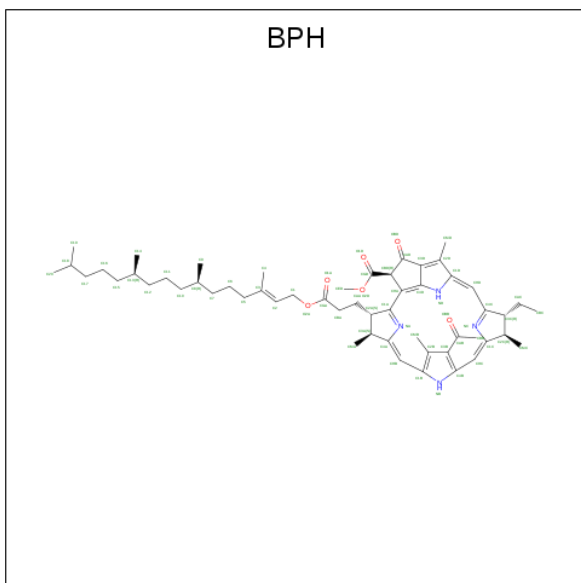
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	240	Total	C	N	O	S	0	1	0
			1837	1173	316	339	9			

- Molecule 4 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C<sub>55</sub>H<sub>74</sub>MgN<sub>4</sub>O<sub>6</sub>).



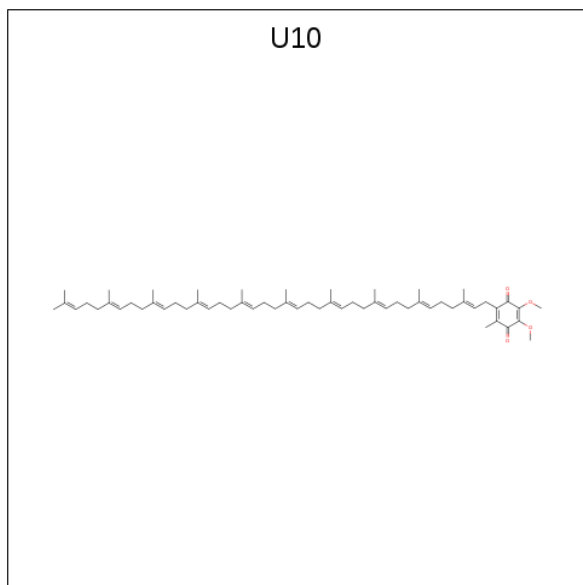
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 5 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula:  $\text{C}_{55}\text{H}_{76}\text{N}_4\text{O}_6$ ).



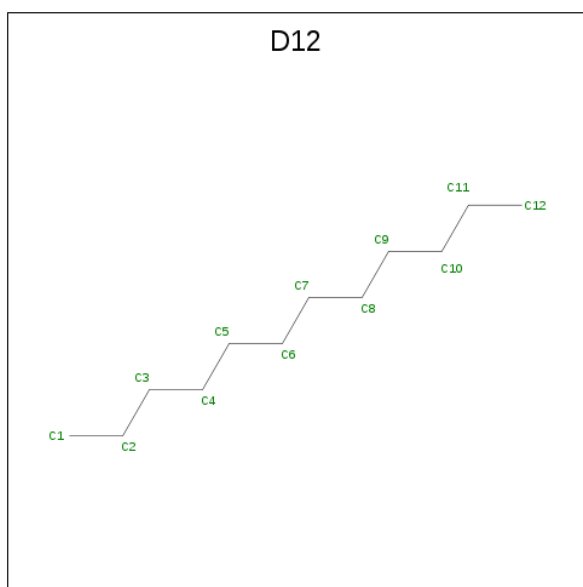
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	M	1	Total	C	N	O	0	0
			65	55	4	6		

- 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 DODECANE (three-letter code: D12) (formula:  $C_{12}H_{26}$ ).

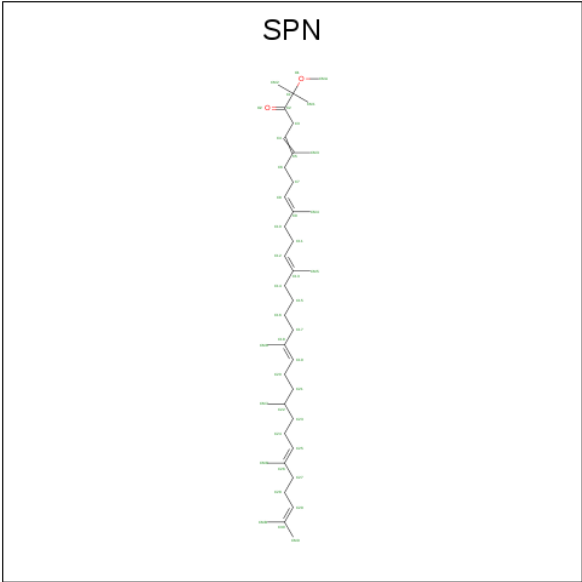


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	1	Total C 8 8	0	0
7	H	1	Total C 12 12	0	0
7	H	1	Total C 9 9	0	0
7	H	1	Total C 8 8	0	0
7	H	1	Total C 8 8	0	0

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

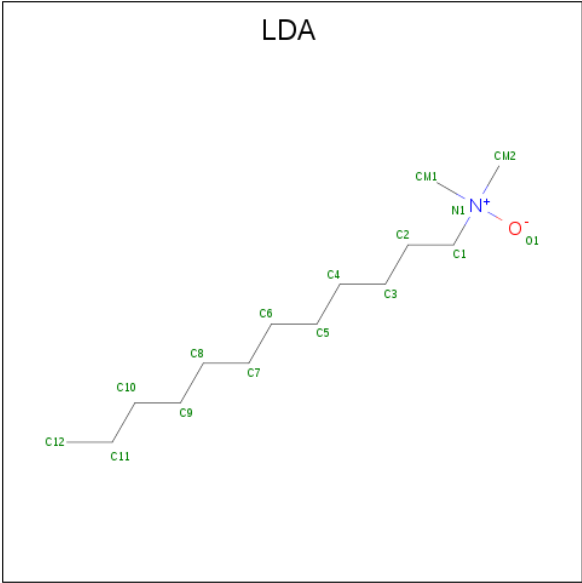
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	L	1	Total Fe 1 1	0	0

- Molecule 9 is SPEROIDENONE (three-letter code: SPN) (formula: C<sub>41</sub>H<sub>70</sub>O<sub>2</sub>).



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

- Molecule 10 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: C<sub>14</sub>H<sub>31</sub>NO).



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

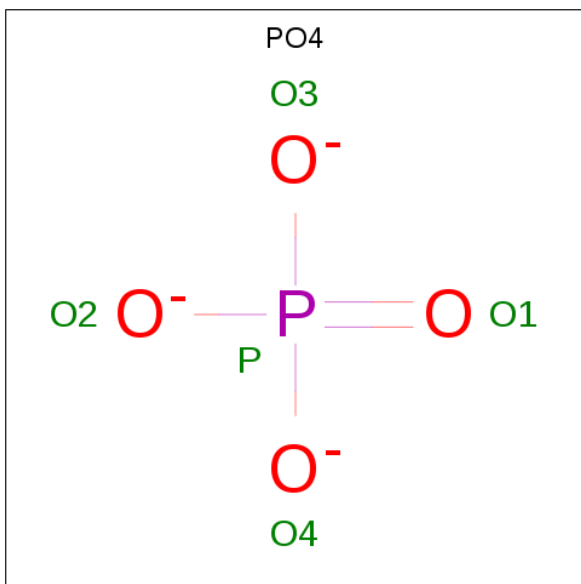
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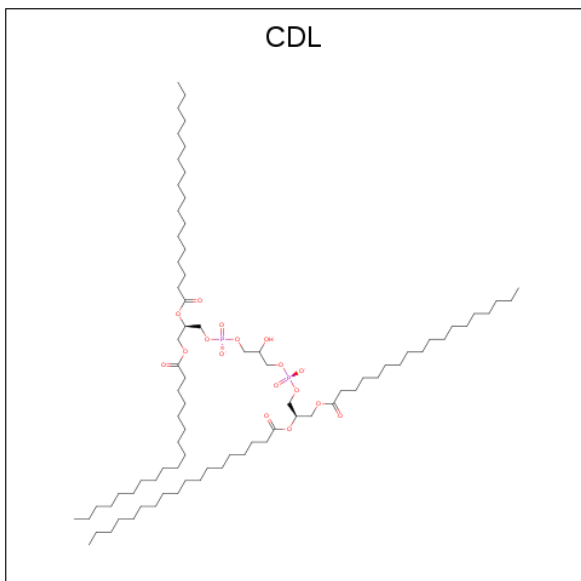
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	H	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 11 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	M	1	Total	O	P	0	0
			5	4	1		

- Molecule 12 is CARDIOLIPIN (three-letter code: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>).



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

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	L	72	Total	O	0	0
			72	72		
13	M	83	Total	O	0	0
			83	83		
13	H	115	Total	O	0	0
			115	115		

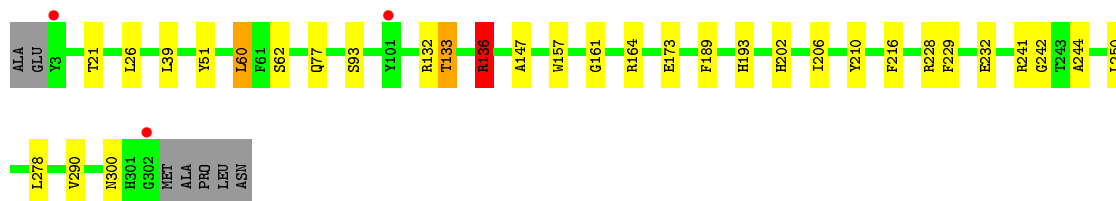
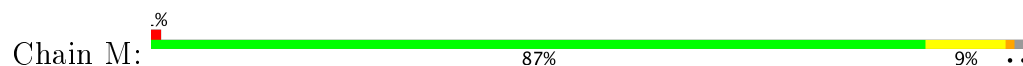
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

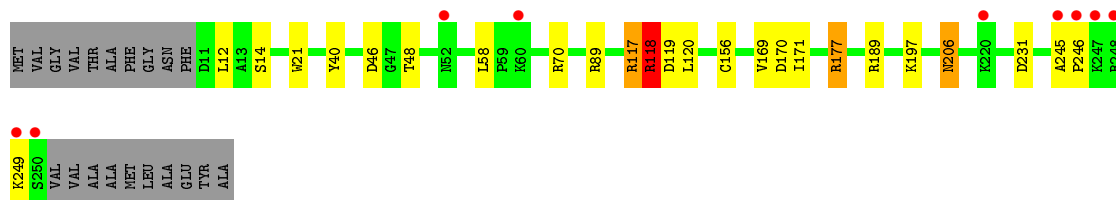
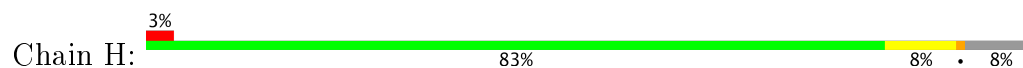
- Molecule 1: Reaction center protein L chain



- Molecule 2: Reaction center protein M chain



- Molecule 3: Reaction center protein H chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	138.99Å 138.99Å 184.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	23.90 – 2.50 27.05 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.8 (23.90-2.50) 98.9 (27.05-2.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.17 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, $R_{free}$	0.168 , 0.201 0.175 , 0.207	Depositor DCC
$R_{free}$ test set	3515 reflections (5.21%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.5	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 59.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7439	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, LDA, D12, CDL, BPH, PO4, 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	0.77	0/2313	0.77	3/3166 (0.1%)
2	M	0.76	0/2494	0.82	5/3404 (0.1%)
3	H	0.79	0/1885	0.94	9/2564 (0.4%)
All	All	0.77	0/6692	0.84	17/9134 (0.2%)

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	L	0	1
2	M	0	1
All	All	0	2

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	241	ARG	NE-CZ-NH1	9.11	124.86	120.30
2	M	241	ARG	NE-CZ-NH2	-8.28	116.16	120.30
3	H	117	ARG	NE-CZ-NH2	-8.12	116.24	120.30
3	H	117	ARG	NE-CZ-NH1	7.65	124.13	120.30
3	H	177	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	L	210	ASP	CB-CG-OD1	6.54	124.19	118.30
3	H	189	ARG	NE-CZ-NH2	-6.47	117.07	120.30
2	M	136	ARG	NE-CZ-NH2	-6.40	117.10	120.30
3	H	89	ARG	NE-CZ-NH2	-6.24	117.18	120.30
2	M	136	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	L	207	ARG	NE-CZ-NH2	-6.14	117.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	177	ARG	NE-CZ-NH2	-5.95	117.33	120.30
3	H	119	ASP	CB-CG-OD1	5.51	123.26	118.30
3	H	170	ASP	CB-CG-OD1	5.31	123.08	118.30
3	H	118	ARG	NE-CZ-NH2	5.29	122.94	120.30
2	M	228	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	L	207	ARG	NE-CZ-NH1	5.09	122.85	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	203	GLY	Peptide
2	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	L	2225	0	2187	6	0
2	M	2397	0	2310	20	0
3	H	1837	0	1841	12	0
4	L	132	0	148	6	0
4	M	132	0	148	7	0
5	L	65	0	75	4	0
5	M	65	0	76	9	0
6	L	48	0	63	1	0
6	M	48	0	63	0	0
7	H	37	0	73	0	0
7	L	8	0	15	0	0
8	L	1	0	0	0	0
9	M	43	0	69	5	0
10	H	16	0	31	1	0
10	M	32	0	62	3	0
11	M	5	0	0	0	0
12	M	78	0	100	0	0
13	H	115	0	0	0	0
13	L	72	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	M	83	0	0	0	0
All	All	7439	0	7261	55	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 (55) 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)
5:L:303:BPH:HBB3	5:L:303:BPH:HHC	1.60	0.84
2:M:21:THR:HG23	2:M:26:LEU:HD11	1.73	0.71
3:H:46:ASP:OD1	3:H:48:THR:HB	1.94	0.67
4:M:401:BCL:HBB2	4:M:401:BCL:HMB1	1.78	0.65
4:L:302:BCL:HBB2	4:L:302:BCL:HMB1	1.80	0.63
5:L:303:BPH:HBB2	2:M:210:TYR:HB3	1.83	0.60
4:M:401:BCL:CBB	4:M:401:BCL:HMB1	2.32	0.59
1:L:181:PHE:CD2	5:M:403:BPH:HBB1	2.37	0.59
5:L:303:BPH:CBB	5:L:303:BPH:HHC	2.31	0.59
5:M:403:BPH:HBB3	5:M:403:BPH:HHC	1.83	0.59
4:L:302:BCL:O1D	10:M:406:LDA:HM22	2.04	0.58
2:M:232:GLU:OE2	3:H:177:ARG:NH2	2.37	0.57
4:M:401:BCL:CAB	9:M:405:SPN:H162	2.36	0.56
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.88	0.55
6:L:304:U10:H251	6:L:304:U10:H28	1.89	0.54
3:H:118:ARG:HD3	3:H:120:LEU:HD12	1.90	0.53
4:L:301:BCL:CBB	4:L:301:BCL:HMB1	2.39	0.53
2:M:77:GLN:HE22	2:M:93:SER:H	1.57	0.53
2:M:242:GLY:CA	3:H:117:ARG:HD3	2.38	0.53
2:M:161:GLY:HA3	9:M:405:SPN:H201	1.90	0.52
2:M:189:PHE:O	2:M:193:HIS:HD2	1.94	0.51
4:M:402:BCL:CBB	4:M:402:BCL:HMB1	2.41	0.51
2:M:157:TRP:CD1	9:M:405:SPN:H202	2.45	0.51
1:L:181:PHE:HB3	5:M:403:BPH:CBB	2.40	0.50
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.94	0.50
2:M:202:HIS:CE1	2:M:206:ILE:HD11	2.48	0.49
4:L:302:BCL:HMB1	4:L:302:BCL:CBB	2.43	0.49
3:H:169:VAL:HG23	3:H:171:ILE:HD13	1.95	0.48
2:M:51:TYR:O	2:M:132:ARG:NH2	2.39	0.47
2:M:21:THR:CG2	2:M:26:LEU:HD11	2.44	0.46
3:H:70:ARG:O	3:H:118:ARG:NH1	2.48	0.46
5:M:403:BPH:H142	5:M:403:BPH:H7C2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:242:GLY:HA2	3:H:117:ARG:HD3	1.99	0.45
2:M:136:ARG:HA	2:M:136:ARG:NE	2.31	0.45
4:M:401:BCL:H92	5:M:403:BPH:HMB1	1.97	0.45
2:M:164:ARG:HH12	2:M:173:GLU:HG3	1.82	0.45
5:M:403:BPH:HHH	5:M:403:BPH:HBC3	1.97	0.45
1:L:181:PHE:HB3	5:M:403:BPH:HBB2	1.99	0.45
2:M:157:TRP:NE1	9:M:405:SPN:H202	2.32	0.45
3:H:40:TYR:HB3	3:H:58:LEU:HD21	2.00	0.44
4:M:401:BCL:H93	4:M:402:BCL:H172	2.00	0.44
5:M:403:BPH:H6C1	5:M:403:BPH:H4C1	1.70	0.44
4:M:401:BCL:C3B	9:M:405:SPN:H152	2.47	0.44
10:M:406:LDA:H92	10:H:301:LDA:H122	1.99	0.44
5:L:303:BPH:HBB1	2:M:210:TYR:CD2	2.52	0.44
2:M:60:LEU:HD21	5:M:403:BPH:H192	1.98	0.44
4:L:301:BCL:HBB3	4:L:301:BCL:HMB1	1.99	0.44
2:M:133:THR:CG2	2:M:147:ALA:HA	2.48	0.44
4:L:301:BCL:CGA	4:L:302:BCL:HBC1	2.48	0.43
1:L:38:THR:HG21	1:L:100:TRP:HE3	1.83	0.43
1:L:50:ALA:O	1:L:53:ALA:HB3	2.19	0.43
3:H:156:CYS:HB3	3:H:206:ASN:O	2.19	0.42
3:H:245:ALA:N	3:H:246:PRO:CD	2.83	0.42
2:M:290:VAL:HG21	3:H:12:LEU:HD23	2.02	0.42
10:M:406:LDA:HM13	3:H:21:TRP:HZ2	1.85	0.41

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	279/281 (99%)	271 (97%)	7 (2%)	1 (0%)	38	59
2	M	299/307 (97%)	285 (95%)	14 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	H	239/260 (92%)	236 (99%)	3 (1%)	0	100	100
All	All	817/848 (96%)	792 (97%)	24 (3%)	1 (0%)	55	76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	58	THR

### 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	L	218/218 (100%)	209 (96%)	9 (4%)	35	61
2	M	235/239 (98%)	227 (97%)	8 (3%)	42	69
3	H	196/208 (94%)	190 (97%)	6 (3%)	45	73
All	All	649/665 (98%)	626 (96%)	23 (4%)	40	68

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	59	TRP
1	L	206	MET
1	L	210	ASP
1	L	216	PHE
1	L	235	LEU
1	L	247	CYS
1	L	264	GLN
1	L	267	VAL
1	L	272	TRP
2	M	39	LEU
2	M	60	LEU
2	M	62	SER
2	M	133	THR
2	M	136	ARG

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Mol	Chain	Res	Type
2	M	216	PHE
2	M	250	LEU
2	M	278	LEU
3	H	14	SER
3	H	118	ARG
3	H	197	LYS
3	H	206	ASN
3	H	231	ASP
3	H	249	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	M	44	ASN
2	M	77	GLN
2	M	193	HIS
3	H	44	ASN

### 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](#)

Of 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 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	$\# Z  > 2$
10	LDA	H	301	-	13,15,15	2.54	1 (7%)	14,17,17	2.98	4 (28%)
7	D12	H	302	-	11,11,11	0.37	0	10,10,10	0.27	0
7	D12	H	303	-	8,8,11	0.43	0	7,7,10	0.25	0
7	D12	H	304	-	7,7,11	0.45	0	6,6,10	0.43	0
7	D12	H	305	-	7,7,11	0.50	0	6,6,10	0.17	0
4	BCL	L	301	-	55,74,74	1.24	2 (3%)	65,115,115	1.19	7 (10%)
4	BCL	L	302	-	55,74,74	1.25	3 (5%)	65,115,115	1.52	12 (18%)
5	BPH	L	303	-	65,70,70	0.72	2 (3%)	75,101,101	1.48	10 (13%)
6	U10	L	304	-	48,48,63	1.67	4 (8%)	58,61,79	1.64	12 (20%)
7	D12	L	305	-	7,7,11	0.47	0	6,6,10	0.29	0
4	BCL	M	401	-	55,74,74	1.28	2 (3%)	65,115,115	1.61	12 (18%)
4	BCL	M	402	-	55,74,74	1.26	3 (5%)	65,115,115	1.23	8 (12%)
5	BPH	M	403	-	65,70,70	0.77	0	75,101,101	1.56	15 (20%)
6	U10	M	404	-	48,48,63	1.56	3 (6%)	58,61,79	1.38	6 (10%)
9	SPN	M	405	-	40,42,42	3.44	15 (37%)	48,52,52	2.45	20 (41%)
10	LDA	M	406	-	13,15,15	2.81	1 (7%)	14,17,17	1.86	4 (28%)
10	LDA	M	407	-	13,15,15	2.77	1 (7%)	14,17,17	2.40	4 (28%)
11	PO4	M	408	-	4,4,4	0.78	0	6,6,6	0.49	0
12	CDL	M	409	-	77,77,99	1.19	4 (5%)	79,89,111	1.14	7 (8%)

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
10	LDA	H	301	-	-	0/13/13/13	0/0/0/0
7	D12	H	302	-	-	0/9/9/9	0/0/0/0
7	D12	H	303	-	-	0/6/6/9	0/0/0/0
7	D12	H	304	-	-	0/5/5/9	0/0/0/0
7	D12	H	305	-	-	0/5/5/9	0/0/0/0
4	BCL	L	301	-	-	0/37/137/137	0/0/9/9
4	BCL	L	302	-	-	0/37/137/137	0/0/9/9
5	BPH	L	303	-	-	0/54/105/105	0/1/6/6
6	U10	L	304	-	-	0/45/69/87	0/1/1/1
7	D12	L	305	-	-	0/5/5/9	0/0/0/0
4	BCL	M	401	-	-	0/37/137/137	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BCL	M	402	-	-	0/37/137/137	0/0/9/9
5	BPH	M	403	-	-	0/54/105/105	0/1/6/6
6	U10	M	404	-	-	0/45/69/87	0/1/1/1
9	SPN	M	405	-	-	0/50/51/51	0/0/0/0
10	LDA	M	406	-	-	0/13/13/13	0/0/0/0
10	LDA	M	407	-	-	0/13/13/13	0/0/0/0
11	PO4	M	408	-	-	0/0/0/0	0/0/0/0
12	CDL	M	409	-	-	0/88/88/110	0/0/0/0

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	407	LDA	O1-N1	-9.80	1.22	1.42
10	M	406	LDA	O1-N1	-9.79	1.22	1.42
10	H	301	LDA	O1-N1	-9.06	1.24	1.42
9	M	405	SPN	C3-C4	-8.76	1.37	1.50
9	M	405	SPN	C10-C9	-6.79	1.36	1.51
9	M	405	SPN	C17-C18	-6.57	1.36	1.51
9	M	405	SPN	C6-C5	-6.43	1.37	1.51
9	M	405	SPN	C14-C13	-6.30	1.37	1.51
6	L	304	U10	C36-C34	-5.92	1.38	1.51
6	M	404	U10	C36-C34	-5.81	1.38	1.51
9	M	405	SPN	C11-C12	-4.39	1.35	1.50
9	M	405	SPN	C20-C19	-4.25	1.36	1.50
9	M	405	SPN	C7-C8	-4.17	1.36	1.50
9	M	405	SPN	C21-C22	-3.28	1.34	1.52
9	M	405	SPN	C16-C15	-2.76	1.35	1.51
4	L	302	BCL	C3C-C4C	-2.29	1.48	1.51
9	M	405	SPN	C21-C20	-2.09	1.46	1.53
5	L	303	BPH	C1C-NC	-2.00	1.33	1.37
4	M	402	BCL	C3C-C4C	-2.00	1.49	1.51
6	L	304	U10	C38-C39	2.03	1.38	1.32
5	L	303	BPH	CHC-C1C	2.44	1.41	1.36
6	M	404	U10	C4-C3	3.25	1.49	1.35
6	L	304	U10	C4-C3	3.39	1.49	1.35
12	M	409	CDL	OB8-CB7	3.78	1.44	1.33
12	M	409	CDL	OA6-CA5	4.58	1.47	1.34
12	M	409	CDL	OB6-CB5	4.63	1.47	1.34
4	L	302	BCL	CHC-C1C	4.72	1.39	1.33
12	M	409	CDL	OA8-CA7	4.73	1.47	1.33
4	M	401	BCL	CHB-C4A	5.11	1.40	1.33
4	L	301	BCL	CHB-C4A	5.18	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	402	BCL	CHC-C1C	5.35	1.40	1.33
4	L	302	BCL	CHB-C4A	5.42	1.40	1.33
4	M	402	BCL	CHB-C4A	5.48	1.40	1.33
9	M	405	SPN	C12-C13	5.53	1.46	1.33
9	M	405	SPN	C8-C9	5.58	1.46	1.33
4	M	401	BCL	CHC-C1C	5.83	1.40	1.33
9	M	405	SPN	C19-C18	5.86	1.47	1.33
9	M	405	SPN	C4-C5	5.88	1.47	1.33
4	L	301	BCL	CHC-C1C	6.18	1.41	1.33
6	M	404	U10	C6-C1	6.23	1.49	1.35
6	L	304	U10	C6-C1	6.58	1.49	1.35

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	H	301	LDA	O1-N1-C1	-6.58	93.13	109.27
10	M	407	LDA	O1-N1-C1	-5.70	95.29	109.27
10	H	301	LDA	CM1-N1-C1	-5.35	98.99	110.23
10	H	301	LDA	CM2-N1-C1	-5.27	99.15	110.23
4	M	401	BCL	CMB-C2B-C1B	-5.02	120.75	128.46
10	M	406	LDA	O1-N1-C1	-4.42	98.44	109.27
10	M	407	LDA	CM1-N1-C1	-4.36	101.07	110.23
4	L	302	BCL	CMB-C2B-C1B	-4.28	121.89	128.46
4	M	402	BCL	CMB-C2B-C1B	-3.74	122.72	128.46
5	L	303	BPH	C4-C3-C5	-3.60	109.03	115.29
5	M	403	BPH	OB8-CAD-CBD	-3.39	120.81	125.94
10	M	406	LDA	CM1-N1-C1	-3.39	103.11	110.23
10	M	407	LDA	CM2-N1-C1	-3.34	103.21	110.23
4	L	301	BCL	CMB-C2B-C1B	-3.34	123.33	128.46
4	M	401	BCL	CAA-C2A-C3A	-3.30	103.75	112.81
6	L	304	U10	C35-C34-C33	-3.23	115.07	123.69
6	L	304	U10	C32-C33-C34	-3.13	119.81	127.68
4	L	302	BCL	CAA-C2A-C3A	-3.12	104.27	112.81
4	M	402	BCL	CHA-C1A-NA	-3.09	119.01	126.18
6	L	304	U10	C7-C8-C9	-3.09	121.55	126.71
4	M	401	BCL	CHA-C1A-NA	-3.04	119.13	126.18
4	L	301	BCL	CAA-C2A-C3A	-2.97	104.68	112.81
5	M	403	BPH	C1-C2-C3	-2.93	120.55	125.96
4	L	302	BCL	CAC-C3C-C2C	-2.89	106.98	114.24
5	L	303	BPH	C2B-C1B-NB	-2.84	105.62	109.82
12	M	409	CDL	OB8-CB7-OB9	-2.75	116.73	123.55
4	M	402	BCL	CAC-C3C-C4C	-2.71	106.56	112.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	403	BPH	C4D-C3D-CAD	-2.68	106.25	107.78
5	M	403	BPH	C2B-C1B-NB	-2.65	105.90	109.82
4	M	402	BCL	CAC-C3C-C2C	-2.65	107.58	114.24
4	M	401	BCL	C4-C3-C2	-2.64	116.65	123.69
4	L	301	BCL	CHA-C1A-NA	-2.63	120.07	126.18
6	M	404	U10	C31-C29-C28	-2.58	115.82	121.10
5	L	303	BPH	C1-C2-C3	-2.56	121.23	125.96
4	M	401	BCL	CMA-C3A-C2A	-2.56	103.38	113.77
10	M	406	LDA	CM2-N1-C1	-2.54	104.89	110.23
4	L	302	BCL	O1D-CGD-CBD	-2.53	120.06	124.60
4	M	402	BCL	OB B-CAB-CBB	-2.53	114.40	120.16
5	M	403	BPH	CAA-C2A-C3A	-2.52	105.91	112.81
9	M	405	SPN	C17-C18-C19	-2.45	116.08	121.10
6	L	304	U10	C30-C29-C28	-2.42	117.24	123.69
5	L	303	BPH	CAA-C2A-C1A	-2.37	106.17	112.28
6	M	404	U10	C32-C33-C34	-2.36	121.75	127.68
4	L	301	BCL	OB B-CAB-CBB	-2.31	114.89	120.16
9	M	405	SPN	C6-C5-C4	-2.28	116.43	121.10
4	M	401	BCL	OB D-CAD-CBD	-2.23	122.57	125.94
6	M	404	U10	C17-C18-C19	-2.20	122.14	127.68
6	L	304	U10	C6-C1-C2	-2.16	118.03	120.29
5	M	403	BPH	CAC-C3C-C2C	-2.14	108.85	114.24
12	M	409	CDL	OA8-CA7-OA9	-2.14	118.24	123.55
9	M	405	SPN	CM5-C13-C12	-2.13	118.01	123.69
12	M	409	CDL	OB6-CB5-OB7	-2.11	118.41	123.68
4	L	302	BCL	CHA-C1A-NA	-2.09	121.33	126.18
4	L	302	BCL	C5-C3-C2	-2.06	116.88	121.10
4	L	301	BCL	CAA-C2A-C1A	-2.03	105.33	111.97
5	L	303	BPH	CAA-C2A-C3A	-2.02	107.26	112.81
9	M	405	SPN	C24-C23-C22	-2.01	110.25	116.23
5	M	403	BPH	C3C-C4C-NC	2.01	109.86	107.97
5	M	403	BPH	CAA-CBA-CGA	2.07	119.58	113.35
4	L	301	BCL	CED-O2D-CGD	2.08	120.84	115.97
6	L	304	U10	C20-C19-C21	2.08	118.90	115.29
4	L	301	BCL	CMB-C2B-C3B	2.10	128.78	124.89
4	M	401	BCL	CAA-CBA-CGA	2.17	119.90	113.35
9	M	405	SPN	CM7-C22-C23	2.19	119.35	111.36
4	M	402	BCL	C2A-C1A-CHA	2.19	127.81	123.92
9	M	405	SPN	CMA-O1-C1	2.23	123.79	112.50
5	M	403	BPH	C6-C7-C8	2.26	123.17	115.73
4	L	302	BCL	CMD-C2D-C3D	2.28	129.13	124.89
4	M	402	BCL	CED-O2D-CGD	2.28	121.32	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	304	U10	C3M-O3-C3	2.30	124.67	116.44
4	M	401	BCL	C5-C3-C2	2.32	125.85	121.10
9	M	405	SPN	CM8-C26-C27	2.39	119.44	115.29
9	M	405	SPN	C6-C7-C8	2.39	120.17	111.97
4	L	302	BCL	C1-O2A-CGA	2.40	122.53	116.77
4	L	302	BCL	CAA-CBA-CGA	2.42	120.63	113.35
5	L	303	BPH	C4A-NA-C1A	2.43	110.13	108.16
4	M	402	BCL	C1-O2A-CGA	2.50	122.76	116.77
4	M	401	BCL	OBB-CAB-C3B	2.55	124.81	119.95
12	M	409	CDL	OB8-CB7-C71	2.55	119.32	111.90
4	L	302	BCL	O2D-CGD-CBD	2.57	115.89	111.30
6	M	404	U10	C15-C14-C16	2.59	119.78	115.29
5	L	303	BPH	OBB-CAB-C3B	2.61	125.10	120.37
5	M	403	BPH	CED-O2D-CGD	2.69	122.28	115.97
9	M	405	SPN	C20-C21-C22	2.71	124.29	116.23
9	M	405	SPN	CM7-C22-C21	2.73	121.30	111.36
5	M	403	BPH	CAC-C3C-C4C	2.88	120.07	112.67
6	L	304	U10	C25-C24-C26	2.89	120.30	115.29
4	L	302	BCL	CMB-C2B-C3B	2.92	130.31	124.89
5	M	403	BPH	C1B-NB-C4B	3.02	112.49	106.52
10	M	406	LDA	CM2-N1-CM1	3.06	116.85	110.99
4	L	302	BCL	OBB-CAB-C3B	3.07	125.79	119.95
6	L	304	U10	C15-C14-C16	3.08	120.63	115.29
5	M	403	BPH	OBB-CAB-C3B	3.09	125.97	120.37
6	L	304	U10	C36-C34-C33	3.12	127.49	121.10
4	M	401	BCL	C7-C6-C5	3.18	121.96	113.11
5	M	403	BPH	O2D-CGD-CBD	3.20	117.02	111.30
9	M	405	SPN	C15-C16-C17	3.24	125.09	113.24
5	L	303	BPH	CAC-C3C-C2C	3.26	122.44	114.24
12	M	409	CDL	OA8-CA7-C31	3.38	121.73	111.90
6	L	304	U10	C30-C29-C31	3.43	121.24	115.29
9	M	405	SPN	C7-C6-C5	3.46	124.63	112.93
4	M	401	BCL	CMB-C2B-C3B	3.50	131.39	124.89
12	M	409	CDL	OA6-CA5-C11	3.52	118.87	111.55
5	L	303	BPH	C1B-NB-C4B	3.57	113.59	106.52
6	M	404	U10	C30-C29-C31	3.62	121.57	115.29
9	M	405	SPN	C16-C15-C14	3.68	126.72	113.24
9	M	405	SPN	C11-C10-C9	3.77	125.70	112.93
9	M	405	SPN	CM6-C18-C17	3.99	122.22	115.29
10	M	407	LDA	CM2-N1-CM1	4.11	118.86	110.99
9	M	405	SPN	CM4-C9-C10	4.13	122.46	115.29
5	M	403	BPH	C1-O2A-CGA	4.19	126.82	116.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	401	BCL	C1-O2A-CGA	4.20	126.85	116.77
6	L	304	U10	C37-C36-C34	4.21	127.19	112.93
6	M	404	U10	C37-C36-C34	4.45	127.99	112.93
9	M	405	SPN	C15-C14-C13	4.54	122.96	112.66
10	H	301	LDA	CM2-N1-CM1	4.63	119.86	110.99
5	L	303	BPH	C3C-C4C-NC	4.75	112.44	107.97
9	M	405	SPN	C16-C17-C18	4.76	123.44	112.66
12	M	409	CDL	OB6-CB5-C51	5.03	122.01	111.55
9	M	405	SPN	CM3-C5-C6	5.31	124.50	115.29
9	M	405	SPN	CM5-C13-C14	5.36	124.59	115.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	H	301	LDA	1	0
4	L	301	BCL	3	0
4	L	302	BCL	4	0
5	L	303	BPH	4	0
6	L	304	U10	1	0
4	M	401	BCL	6	0
4	M	402	BCL	2	0
5	M	403	BPH	9	0
9	M	405	SPN	5	0
10	M	406	LDA	3	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	L	281/281 (100%)	-0.50	7 (2%) 58 60	33, 43, 76, 118	0
2	M	300/307 (97%)	-0.46	3 (1%) 82 83	32, 47, 74, 108	0
3	H	240/260 (92%)	-0.39	9 (3%) 41 43	37, 46, 66, 146	0
All	All	821/848 (96%)	-0.45	19 (2%) 61 63	32, 46, 74, 146	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	250	SER	7.7
3	H	246	PRO	6.4
1	L	59	TRP	6.2
3	H	249	LYS	6.2
3	H	247	LYS	5.2
2	M	302	GLY	3.5
1	L	281	GLY	3.3
1	L	270	PRO	3.3
2	M	3	TYR	2.9
1	L	276	PRO	2.8
1	L	271	TRP	2.8
3	H	245	ALA	2.6
1	L	277	GLY	2.5
3	H	52[A]	ASN	2.3
2	M	101	TYR	2.3
1	L	74	GLY	2.2
3	H	248	ARG	2.2
3	H	60	LYS	2.0
3	H	220	LYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
6	U10	L	304	48/63	0.78	0.26	4.20	47,68,94,100	0
10	LDA	M	406	16/16	0.86	0.23	4.11	43,62,79,80	0
12	CDL	M	409	78/100	0.78	0.29	2.92	50,93,130,139	0
4	BCL	M	401	66/66	0.96	0.16	2.56	32,37,90,93	0
9	SPN	M	405	43/43	0.92	0.18	2.00	38,51,90,98	0
6	U10	M	404	48/63	0.91	0.23	1.88	34,49,91,103	0
5	BPH	M	403	65/65	0.91	0.16	1.66	38,45,97,103	0
5	BPH	L	303	65/65	0.97	0.14	1.46	30,37,46,48	0
4	BCL	M	402	66/66	0.98	0.16	1.45	34,40,60,71	0
4	BCL	L	301	66/66	0.97	0.17	1.31	33,40,50,64	0
4	BCL	L	302	66/66	0.97	0.15	0.69	28,34,60,72	0
11	PO4	M	408	5/5	0.97	0.20	0.59	70,71,78,79	0
10	LDA	H	301	16/16	0.95	0.12	-0.24	57,65,75,78	0
8	FE	L	306	1/1	0.99	0.12	-0.57	35,35,35,35	0
7	D12	H	304	8/12	0.84	0.20	-	74,76,86,87	0
7	D12	H	302	12/12	0.88	0.29	-	75,78,80,81	0
7	D12	H	305	8/12	0.53	0.51	-	81,85,87,88	0
10	LDA	M	407	16/16	0.72	0.30	-	79,92,108,111	0
7	D12	H	303	9/12	0.85	0.23	-	75,76,81,83	0
7	D12	L	305	8/12	0.68	0.23	-	83,90,93,94	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.