



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 06:13 am GMT

PDB ID : 3DTS  
Title : E(L212)A, D(L213)A, R(M233)L triple mutant structure of photosynthetic reaction center from Rhodobacter sphaeroides  
Authors : Pokkuluri, P.R.; Schiffer, M.  
Deposited on : 2008-07-15  
Resolution : 3.10 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 : trunk28620  
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) : recalc28949

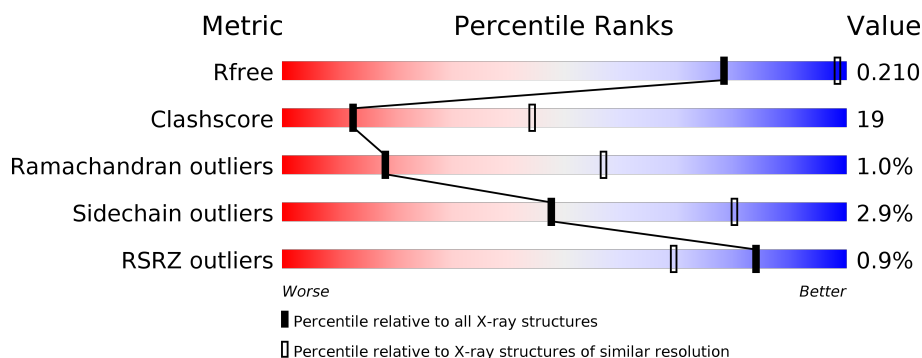
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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 style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 64%, yellow 35%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> <span>%</span> <span>64%</span> <span>35%</span> <span>•</span> </div> </div>
2	M	314	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 63%, yellow 31%, orange 3%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> <span>%</span> <span>63%</span> <span>31%</span> <span>• •</span> </div> </div>
3	H	260	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 60%, yellow 30%, orange 8%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> <span>%</span> <span>60%</span> <span>30%</span> <span>• 8%</span> </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	CDL	M	800	-	-	-	X
4	BCL	L	501	X	-	-	-
4	BCL	M	501	X	-	-	X
5	U10	L	504	-	-	-	X
5	U10	M	505	-	-	-	X
6	LDA	H	703	-	-	-	X
6	LDA	L	709	-	-	-	X
6	LDA	M	701	-	-	-	X
6	LDA	M	704	-	-	-	X
7	BPH	M	504	X	-	-	-
9	SPN	M	600	-	-	-	X

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7226 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	UNP P0C0Y8
L	213	ALA	ASP	ENGINEERED	UNP P0C0Y8

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	302	Total	C	N	O	S	0	0	0
			2405	1607	391	397	10			

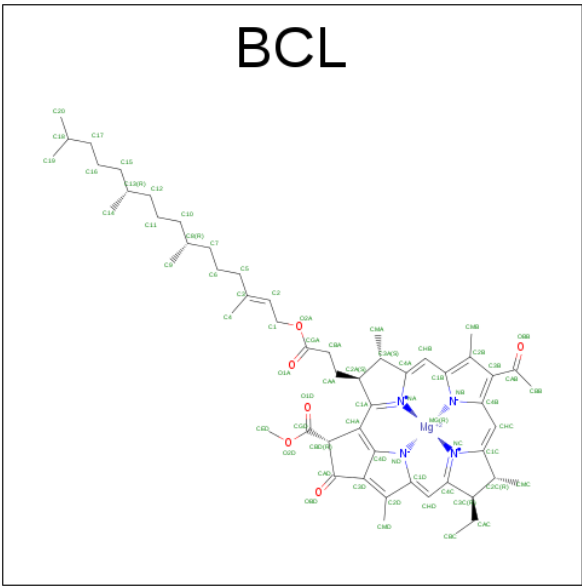
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	233	LEU	ARG	ENGINEERED	UNP P0C0Y9
M	308	HIS	-	EXPRESSION TAG	UNP P0C0Y9
M	309	HIS	-	EXPRESSION TAG	UNP P0C0Y9
M	310	HIS	-	EXPRESSION TAG	UNP P0C0Y9
M	311	HIS	-	EXPRESSION TAG	UNP P0C0Y9
M	312	HIS	-	EXPRESSION TAG	UNP P0C0Y9
M	313	HIS	-	EXPRESSION TAG	UNP P0C0Y9
M	314	HIS	-	EXPRESSION TAG	UNP P0C0Y9

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

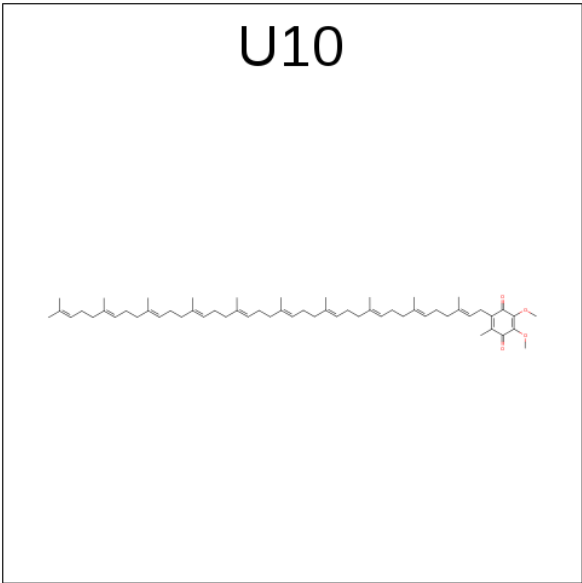
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	240	Total	C	N	O	S	0	0	0
			1829	1169	314	337	9			

- Molecule 4 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula:  $C_{55}H_{74}MgN_4O_6$ ).



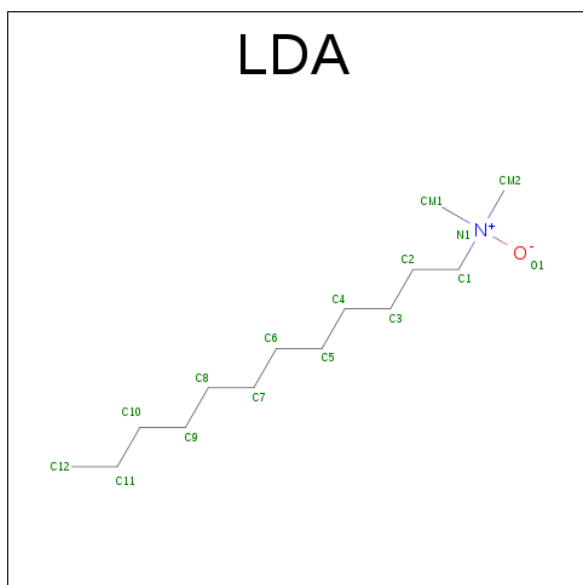
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 5 is UBIQUINONE-10 (three-letter code: U10) (formula:  $C_{59}H_{90}O_4$ ).



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

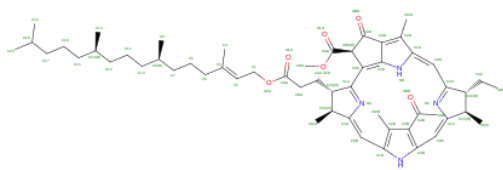
- Molecule 6 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:  $C_{14}H_{31}NO$ ).



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

- Molecule 7 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula:  $C_{55}H_{76}N_4O_6$ ).

## BPH



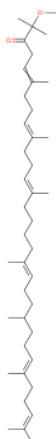
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	M	1	Total	C	N	O	0	0
			65	55	4	6		
7	M	1	Total	C	N	O	10	0
			65	55	4	6		

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

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

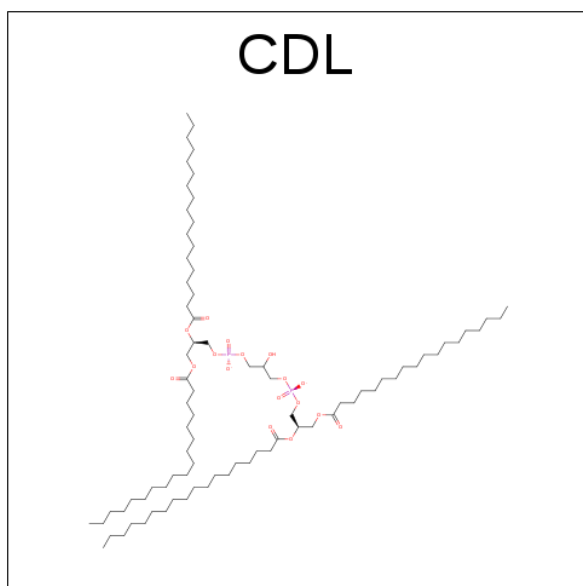
- Molecule 9 is SPEROIDENONE (three-letter code: SPN) (formula: C<sub>41</sub>H<sub>70</sub>O<sub>2</sub>).

## SPN



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

- Molecule 10 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



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

- Molecule 11 is water.

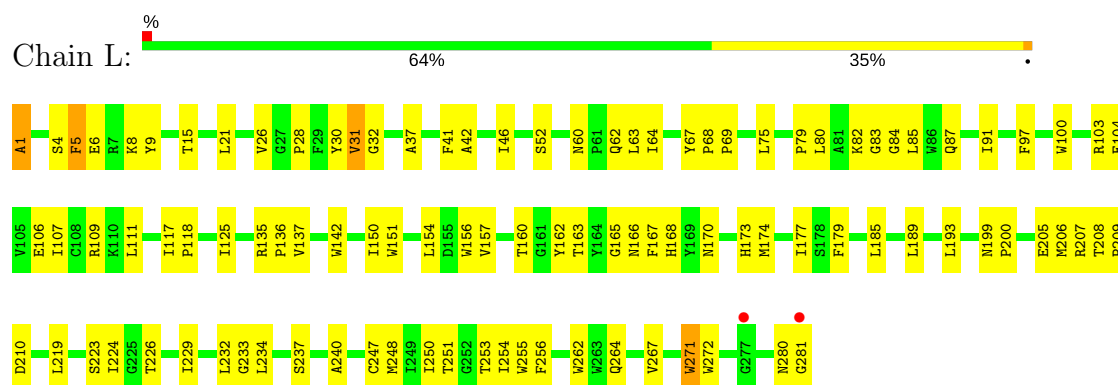
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	L	28	Total	O	0	0
			28	28		
11	M	27	Total	O	0	0
			27	27		
11	H	33	Total	O	0	0
			33	33		



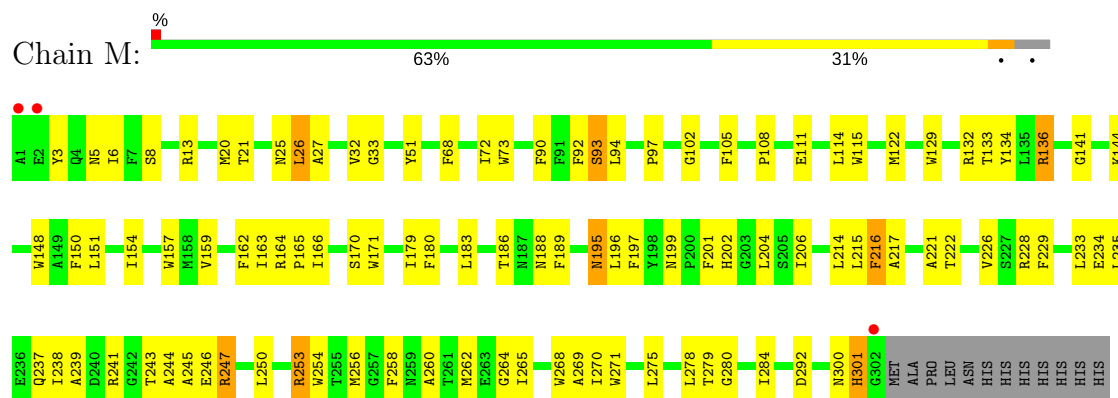
### 3 Residue-property plots [i](#)

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.

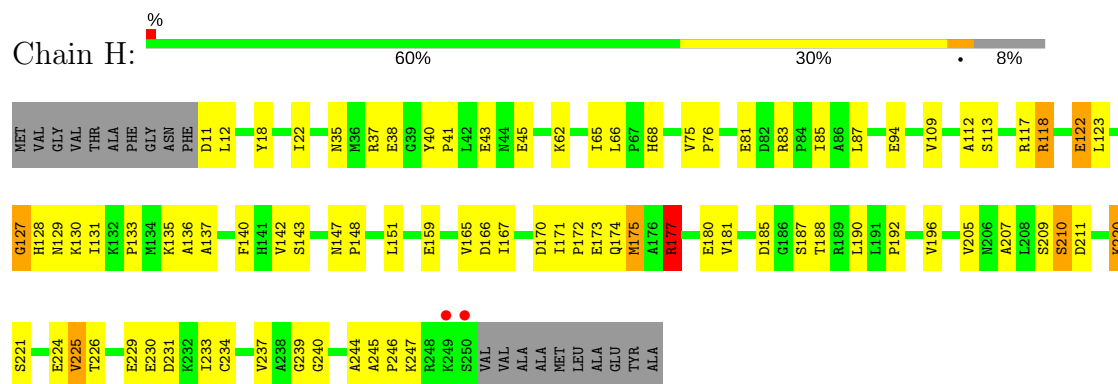
#### • Molecule 1: Reaction center protein L chain



#### • 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, $\alpha$ , $\beta$ , $\gamma$	141.30Å 141.30Å 187.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.10 26.89 – 3.10	Depositor EDS
% Data completeness (in resolution range)	81.0 (30.00-3.10) 80.8 (26.89-3.10)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.80 (at 3.11Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.209 , 0.224 0.197 , 0.210	Depositor DCC
$R_{free}$ test set	2253 reflections (7.53%)	DCC
Wilson B-factor (Å <sup>2</sup> )	60.3	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 58.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7226	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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, CDL, BPH, 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	0.95	5/2313 (0.2%)	0.92	7/3166 (0.2%)
2	M	0.92	5/2497 (0.2%)	0.86	5/3410 (0.1%)
3	H	0.85	2/1877 (0.1%)	0.94	5/2553 (0.2%)
All	All	0.91	12/6687 (0.2%)	0.91	17/9129 (0.2%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	1	ALA	N-CA	11.39	1.69	1.46
1	L	280	ASN	C-N	-7.25	1.20	1.33
2	M	105	PHE	CE2-CZ	6.80	1.50	1.37
3	H	122	GLU	CB-CG	6.55	1.64	1.52
2	M	68	PHE	CE2-CZ	6.36	1.49	1.37
2	M	189	PHE	CE1-CZ	5.81	1.48	1.37
2	M	105	PHE	CE1-CZ	5.68	1.48	1.37
3	H	127	GLY	N-CA	5.66	1.54	1.46
1	L	281	GLY	C-OXT	-5.15	1.13	1.23
1	L	5	PHE	CE2-CZ	5.13	1.47	1.37
1	L	256	PHE	CE2-CZ	5.12	1.47	1.37
2	M	68	PHE	CE1-CZ	5.06	1.47	1.37

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	280	ASN	C-N-CA	10.11	143.54	122.30
1	L	280	ASN	O-C-N	-9.73	106.66	123.20
3	H	122	GLU	CB-CG-CD	-9.54	88.46	114.20
1	L	280	ASN	CA-C-N	8.30	132.79	116.20
2	M	247	ARG	NE-CZ-NH2	8.11	124.36	120.30
3	H	177	ARG	NE-CZ-NH2	7.42	124.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	118	ARG	NE-CZ-NH2	7.31	123.95	120.30
2	M	247	ARG	NE-CZ-NH1	-7.04	116.78	120.30
1	L	109	ARG	NE-CZ-NH2	6.78	123.69	120.30
3	H	117	ARG	NE-CZ-NH2	6.76	123.68	120.30
2	M	241	ARG	NE-CZ-NH2	6.59	123.59	120.30
2	M	253	ARG	NE-CZ-NH2	6.09	123.35	120.30
1	L	174	MET	CG-SD-CE	5.97	109.76	100.20
1	L	206	MET	CG-SD-CE	5.79	109.47	100.20
2	M	20	MET	CG-SD-CE	5.76	109.42	100.20
3	H	175	MET	CG-SD-CE	5.76	109.41	100.20
1	L	210	ASP	CB-CG-OD1	5.00	122.80	118.30

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	2225	0	2186	91	0
2	M	2405	0	2319	99	0
3	H	1829	0	1836	80	0
4	L	132	0	148	15	0
4	M	132	0	148	17	0
5	L	48	0	62	6	0
5	M	48	0	63	7	0
6	H	16	0	31	4	0
6	L	16	0	31	4	0
6	M	32	0	62	3	0
7	M	130	0	152	4	0
8	M	1	0	0	0	0
9	M	43	0	69	2	0
10	M	81	0	106	2	0
11	H	33	0	0	8	0
11	L	28	0	0	2	0
11	M	27	0	0	5	0
All	All	7226	0	7213	267	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 19.

All (267) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:1:ALA:CA	1:L:1:ALA:N	1.69	1.51
1:L:219:LEU:HA	2:M:132:ARG:HH12	1.23	1.00
1:L:154:LEU:HD11	4:L:501:BCL:HED3	1.52	0.89
2:M:21:THR:HG23	2:M:26:LEU:HD21	1.52	0.89
5:M:505:U10:H202	6:H:703:LDA:H112	1.54	0.88
1:L:219:LEU:HD12	2:M:132:ARG:NH1	1.88	0.87
2:M:195:ASN:ND2	2:M:197:PHE:HB2	1.92	0.85
1:L:142:TRP:CH2	6:L:709:LDA:H71	2.13	0.83
2:M:196:LEU:HD23	2:M:202:HIS:CD2	2.14	0.83
1:L:80:LEU:HA	1:L:84:GLY:HA3	1.60	0.82
2:M:233:LEU:HD11	3:H:177:ARG:CZ	2.09	0.81
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.17	0.80
2:M:233:LEU:CD1	3:H:177:ARG:CZ	2.60	0.80
2:M:108:PRO:HG2	2:M:111:GLU:HB2	1.63	0.80
4:L:502:BCL:HHC	4:L:502:BCL:OBB	1.81	0.79
2:M:300:ASN:O	2:M:301:HIS:HB2	1.81	0.78
3:H:122:GLU:OE2	3:H:130:LYS:CD	2.32	0.77
1:L:219:LEU:HD12	2:M:132:ARG:HH11	1.49	0.74
3:H:190:LEU:HB2	3:H:233:ILE:HD13	1.68	0.74
3:H:38:GLU:OE2	11:H:1060:HOH:O	2.04	0.74
3:H:137:ALA:O	11:H:1072:HOH:O	2.06	0.73
3:H:196:VAL:HG12	3:H:205:VAL:HG22	1.70	0.73
4:M:502:BCL:HHC	4:M:502:BCL:CBB	2.19	0.73
1:L:8:LYS:HA	3:H:87:LEU:HD11	1.70	0.73
2:M:264:GLY:HA3	3:H:35:ASN:OD1	1.89	0.73
3:H:37:ARG:HA	3:H:76:PRO:HG3	1.72	0.72
1:L:142:TRP:CZ2	6:L:709:LDA:H51	2.24	0.72
3:H:45:GLU:OE2	11:H:1062:HOH:O	2.06	0.72
3:H:226:THR:OG1	3:H:229:GLU:HG3	1.89	0.71
1:L:60:ASN:O	1:L:64:ILE:HG13	1.91	0.71
2:M:8:SER:OG	11:M:1041:HOH:O	2.08	0.71
2:M:245:ALA:O	11:M:1032:HOH:O	2.08	0.71
2:M:300:ASN:O	2:M:301:HIS:CB	2.38	0.71
3:H:122:GLU:OE2	3:H:130:LYS:HD2	1.90	0.71
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.75	0.69
3:H:122:GLU:OE2	3:H:130:LYS:HD3	1.93	0.69
3:H:142:VAL:HG21	3:H:147:ASN:ND2	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:233:LEU:CD1	3:H:177:ARG:NH2	2.57	0.68
1:L:170:ASN:HB3	1:L:173:HIS:HB3	1.76	0.68
2:M:150:PHE:O	2:M:154:ILE:HG13	1.94	0.68
3:H:207:ALA:CB	11:H:1081:HOH:O	2.42	0.68
4:M:502:BCL:HHC	4:M:502:BCL:HBB3	1.77	0.67
3:H:246:PRO:HG2	3:H:247:LYS:HD2	1.75	0.67
1:L:117:ILE:HB	1:L:118:PRO:HD3	1.74	0.67
2:M:222:THR:O	2:M:226:VAL:HG22	1.94	0.67
3:H:181:VAL:O	3:H:188:THR:HA	1.95	0.67
3:H:112:ALA:HB2	3:H:239:GLY:HA3	1.76	0.67
1:L:1:ALA:CB	1:L:1:ALA:N	2.54	0.67
2:M:90:PHE:HD1	2:M:179:ILE:HG13	1.60	0.67
2:M:243:THR:O	2:M:247:ARG:HG3	1.93	0.66
3:H:131:ILE:HD11	3:H:177:ARG:NH1	2.11	0.66
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.75	0.66
4:M:501:BCL:C11	4:M:502:BCL:H203	2.26	0.66
3:H:207:ALA:HB2	11:H:1081:HOH:O	1.95	0.66
1:L:103:ARG:O	1:L:107:ILE:HG13	1.96	0.66
1:L:264:GLN:HA	1:L:267:VAL:HG12	1.77	0.65
3:H:131:ILE:HD11	3:H:177:ARG:CZ	2.27	0.65
4:L:501:BCL:HBB2	4:L:501:BCL:HMB1	1.79	0.65
2:M:204:LEU:HB3	2:M:279:THR:HG21	1.78	0.65
5:M:505:U10:H202	6:H:703:LDA:C11	2.27	0.64
2:M:164:ARG:HB3	2:M:165:PRO:HD3	1.80	0.64
3:H:171:ILE:HB	3:H:172:PRO:HD3	1.80	0.63
3:H:123:LEU:HD22	3:H:127:GLY:O	1.99	0.62
3:H:122:GLU:CD	3:H:130:LYS:HD3	2.19	0.62
4:M:501:BCL:H111	4:M:502:BCL:H203	1.80	0.62
1:L:173:HIS:HE1	1:L:177:ILE:HD11	1.64	0.62
3:H:118:ARG:NH1	11:H:1074:HOH:O	2.27	0.61
1:L:208:THR:HB	1:L:209:PRO:HD2	1.81	0.61
3:H:233:ILE:O	3:H:237:VAL:HG23	2.00	0.61
1:L:60:ASN:HD22	1:L:63:LEU:HG	1.65	0.61
2:M:13:ARG:O	3:H:140:PHE:HA	1.99	0.61
2:M:157:TRP:HB2	4:M:502:BCL:H62	1.81	0.61
4:L:501:BCL:H192	7:M:503:BPH:H7C2	1.83	0.60
1:L:208:THR:HB	11:L:1017:HOH:O	2.01	0.60
5:M:505:U10:H201	6:M:704:LDA:HM13	1.83	0.60
4:M:501:BCL:HMB1	4:M:501:BCL:CBB	2.32	0.60
2:M:195:ASN:HD21	2:M:197:PHE:HB2	1.65	0.59
2:M:270:ILE:HG23	2:M:271:TRP:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:45:GLU:HG3	3:H:94:GLU:OE1	2.03	0.58
3:H:220:LYS:HB3	3:H:220:LYS:NZ	2.18	0.58
2:M:260:ALA:HA	3:H:35:ASN:HB3	1.84	0.58
1:L:52:SER:HB2	1:L:85:LEU:HD13	1.85	0.58
3:H:81:GLU:O	3:H:83:ARG:HG2	2.04	0.58
2:M:197:PHE:CZ	4:M:502:BCL:HBB2	2.40	0.57
2:M:262:MET:SD	5:M:505:U10:H3M1	2.44	0.57
1:L:199:ASN:N	1:L:200:PRO:HD3	2.20	0.57
4:M:501:BCL:HMB1	4:M:501:BCL:HBB2	1.85	0.57
3:H:123:LEU:HA	3:H:128:HIS:O	2.05	0.57
2:M:21:THR:HG23	2:M:26:LEU:CD2	2.30	0.57
2:M:234:GLU:O	2:M:238:ILE:HG13	2.05	0.56
2:M:233:LEU:HD12	3:H:177:ARG:NH2	2.20	0.56
2:M:233:LEU:HD13	3:H:177:ARG:NH1	2.20	0.56
2:M:239:ALA:HB1	3:H:66:LEU:HD22	1.87	0.56
1:L:75:LEU:HD21	1:L:137:VAL:HA	1.87	0.56
11:M:1041:HOH:O	3:H:175:MET:HE1	2.06	0.55
2:M:3:TYR:CZ	2:M:5:ASN:HA	2.42	0.55
3:H:165:VAL:CG2	3:H:180:GLU:HB3	2.37	0.55
1:L:103:ARG:HG2	1:L:103:ARG:HH11	1.72	0.54
1:L:15:THR:HA	1:L:106:GLU:OE2	2.07	0.54
2:M:25:ASN:O	2:M:27:ALA:N	2.40	0.54
3:H:40:TYR:HA	3:H:41:PRO:C	2.28	0.54
1:L:185:LEU:C	1:L:185:LEU:HD23	2.29	0.54
3:H:122:GLU:OE1	3:H:130:LYS:HD3	2.09	0.54
1:L:168:HIS:HE1	2:M:186:THR:HB	1.73	0.54
3:H:68:HIS:CD2	3:H:123:LEU:HB2	2.44	0.53
2:M:94:LEU:HD21	2:M:115:TRP:HA	1.91	0.53
3:H:130:LYS:HG3	3:H:172:PRO:HG2	1.90	0.53
1:L:205:GLU:HA	3:H:65:ILE:HB	1.92	0.52
4:L:502:BCL:H203	4:L:501:BCL:H102	1.91	0.52
1:L:219:LEU:HD11	2:M:133:THR:HG22	1.90	0.52
6:M:701:LDA:H101	6:H:703:LDA:C12	2.39	0.52
1:L:103:ARG:HG2	1:L:103:ARG:NH1	2.24	0.52
1:L:271:TRP:CD1	1:L:271:TRP:N	2.77	0.52
2:M:32:VAL:HG12	2:M:33:GLY:O	2.10	0.52
3:H:209:SER:O	3:H:210:SER:C	2.48	0.52
2:M:197:PHE:HZ	4:M:502:BCL:HBB2	1.74	0.52
2:M:233:LEU:CD1	3:H:177:ARG:NH1	2.72	0.51
2:M:268:TRP:CD1	5:M:505:U10:H111	2.45	0.51
2:M:73:TRP:HB2	2:M:114:LEU:HD23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:190:LEU:CD1	3:H:225:VAL:HG11	2.41	0.51
3:H:37:ARG:NH1	3:H:76:PRO:HD3	2.26	0.51
3:H:165:VAL:HG22	3:H:180:GLU:HB3	1.92	0.51
1:L:31:VAL:HG12	1:L:32:GLY:N	2.25	0.50
1:L:42:ALA:O	1:L:46:ILE:HG13	2.12	0.50
3:H:75:VAL:HA	3:H:76:PRO:C	2.30	0.50
2:M:202:HIS:CE1	2:M:206:ILE:HD11	2.47	0.50
1:L:233:GLY:HA3	2:M:216:PHE:CE1	2.47	0.50
2:M:132:ARG:O	2:M:136:ARG:HB2	2.12	0.49
2:M:148:TRP:O	2:M:151:LEU:HB3	2.12	0.49
3:H:133:PRO:HD2	3:H:136:ALA:HB3	1.95	0.49
3:H:229:GLU:O	3:H:233:ILE:HG13	2.13	0.49
1:L:91:ILE:CG1	6:L:709:LDA:H91	2.42	0.49
2:M:199:ASN:HB3	2:M:202:HIS:HB3	1.94	0.49
3:H:129:ASN:HD22	3:H:224:GLU:HG2	1.78	0.49
4:L:502:BCL:HAA2	4:L:501:BCL:HAC1	1.93	0.49
3:H:109:VAL:HA	3:H:113:SER:HB3	1.94	0.49
3:H:190:LEU:HD12	3:H:233:ILE:CD1	2.43	0.49
2:M:154:ILE:HG23	2:M:157:TRP:CE3	2.47	0.49
2:M:270:ILE:CG2	2:M:271:TRP:N	2.76	0.49
3:H:240:GLY:O	3:H:244:ALA:HB3	2.13	0.48
3:H:62:LYS:O	3:H:62:LYS:HG3	2.12	0.48
3:H:166:ASP:OD1	3:H:167:ILE:N	2.40	0.48
1:L:157:VAL:HG11	4:M:502:BCL:HBB1	1.94	0.48
1:L:6:GLU:HG3	2:M:250:LEU:CD2	2.44	0.48
3:H:190:LEU:CD1	3:H:225:VAL:CG1	2.91	0.48
1:L:69:PRO:HG2	1:L:142:TRP:HB2	1.94	0.48
1:L:250:ILE:HB	1:L:254:ILE:HD11	1.95	0.48
2:M:215:LEU:CD2	2:M:269:ALA:HA	2.44	0.48
3:H:130:LYS:HE3	3:H:170:ASP:OD2	2.13	0.48
1:L:226:THR:O	1:L:229:ILE:HG22	2.14	0.48
1:L:262:TRP:C	1:L:264:GLN:H	2.18	0.47
4:L:502:BCL:CHC	4:L:502:BCL:OBB	2.55	0.47
1:L:5:PHE:CE1	2:M:246:GLU:HB3	2.49	0.47
2:M:256:MET:HE3	2:M:258:PHE:CE1	2.49	0.47
1:L:179:PHE:HB3	1:L:240:ALA:HB2	1.96	0.47
2:M:148:TRP:CD1	10:M:800:CDL:H511	2.50	0.47
1:L:37:ALA:O	1:L:41:PHE:CD2	2.68	0.47
1:L:248:MET:HE2	4:L:502:BCL:HMD1	1.95	0.47
1:L:83:GLY:O	1:L:87:GLN:HG3	2.15	0.47
6:M:701:LDA:H101	6:H:703:LDA:H121	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:180:PHE:O	2:M:183:LEU:HB2	2.14	0.47
3:H:37:ARG:HH11	3:H:76:PRO:HD3	1.79	0.47
1:L:248:MET:HE2	4:L:502:BCL:OBD	2.15	0.47
1:L:189:LEU:HD23	7:M:504:BPH:HMD2	1.97	0.47
3:H:173:GLU:O	3:H:175:MET:HG3	2.15	0.46
2:M:144:LYS:N	2:M:144:LYS:HD2	2.30	0.46
1:L:5:PHE:O	1:L:5:PHE:HD1	1.99	0.46
2:M:201:PHE:HD1	2:M:279:THR:HG23	1.81	0.46
3:H:129:ASN:ND2	3:H:224:GLU:HG2	2.31	0.46
3:H:226:THR:O	3:H:230:GLU:HG3	2.16	0.46
1:L:8:LYS:HE2	1:L:9:TYR:CE2	2.51	0.46
2:M:129:TRP:O	2:M:133:THR:HG23	2.15	0.46
2:M:214:LEU:HD13	7:M:503:BPH:ND	2.31	0.46
1:L:162:TYR:HA	1:L:165:GLY:O	2.16	0.46
2:M:73:TRP:CG	2:M:94:LEU:HD13	2.50	0.45
1:L:232:LEU:HD21	5:L:504:U10:H13	1.98	0.45
3:H:118:ARG:NH2	11:H:1074:HOH:O	2.48	0.45
1:L:26:VAL:HG23	1:L:31:VAL:CG2	2.46	0.45
1:L:97:PHE:HB3	1:L:125:ILE:HG12	1.98	0.45
3:H:245:ALA:N	3:H:246:PRO:HD2	2.32	0.45
2:M:25:ASN:C	2:M:27:ALA:H	2.20	0.45
1:L:28:PRO:O	2:M:254:TRP:HA	2.17	0.45
2:M:280:GLY:O	2:M:284:ILE:HG12	2.16	0.45
3:H:142:VAL:CG2	3:H:147:ASN:ND2	2.79	0.44
3:H:190:LEU:HD11	3:H:225:VAL:HG13	2.00	0.44
1:L:166:ASN:OD1	1:L:168:HIS:HB2	2.16	0.44
1:L:237:SER:HB3	2:M:217:ALA:HB2	1.98	0.44
2:M:102:GLY:HA2	2:M:170:SER:HB3	1.99	0.44
2:M:215:LEU:HD21	2:M:269:ALA:HA	1.99	0.44
2:M:21:THR:HG21	2:M:26:LEU:HD11	2.00	0.44
1:L:117:ILE:HB	1:L:118:PRO:CD	2.44	0.44
1:L:209:PRO:HD2	11:L:1017:HOH:O	2.16	0.44
1:L:179:PHE:CE1	5:L:504:U10:H23	2.52	0.44
3:H:192:PRO:HD2	3:H:237:VAL:HG21	2.00	0.44
1:L:173:HIS:O	1:L:177:ILE:HG13	2.17	0.44
2:M:157:TRP:NE1	9:M:600:SPN:H202	2.33	0.44
2:M:216:PHE:HD1	2:M:216:PHE:O	2.01	0.44
1:L:253:THR:OG1	1:L:254:ILE:N	2.51	0.44
2:M:265:ILE:HG21	5:M:505:U10:H3M3	1.99	0.44
3:H:18:TYR:O	3:H:22:ILE:HG13	2.18	0.44
1:L:193:LEU:HD23	5:L:504:U10:C3M	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:73:TRP:HB2	2:M:114:LEU:CD2	2.47	0.44
1:L:234:LEU:HD13	2:M:221:ALA:HB2	2.00	0.43
2:M:134:TYR:CE1	2:M:144:LYS:HG2	2.53	0.43
1:L:233:GLY:HA3	2:M:216:PHE:CD1	2.53	0.43
1:L:30:TYR:HB2	2:M:254:TRP:HB3	2.01	0.43
1:L:179:PHE:CZ	5:L:504:U10:H23	2.53	0.43
2:M:235:LEU:O	2:M:238:ILE:HB	2.18	0.43
5:M:505:U10:H28	5:M:505:U10:H322	1.47	0.43
1:L:156:TRP:O	1:L:160:THR:OG1	2.29	0.43
4:L:502:BCL:HBB3	4:L:502:BCL:HMB1	2.00	0.43
4:M:502:BCL:HHC	4:M:502:BCL:HBB2	1.98	0.43
1:L:255:TRP:CZ2	1:L:262:TRP:HB2	2.53	0.43
1:L:67:TYR:HA	1:L:68:PRO:HD3	1.79	0.43
2:M:228:ARG:O	3:H:234:CYS:HB3	2.18	0.43
3:H:221:SER:HB2	11:H:1085:HOH:O	2.17	0.43
2:M:51:TYR:CD1	2:M:51:TYR:C	2.92	0.43
2:M:97:PRO:HG2	2:M:171:TRP:HB2	2.00	0.43
2:M:122:MET:O	2:M:122:MET:HG2	2.19	0.42
3:H:185:ASP:OD1	3:H:187:SER:OG	2.29	0.42
4:M:502:BCL:H121	4:M:502:BCL:H162	1.85	0.42
1:L:163:THR:O	1:L:163:THR:HG22	2.19	0.42
3:H:85:ILE:HG22	3:H:87:LEU:HG	2.00	0.42
1:L:251:THR:O	1:L:251:THR:HG22	2.19	0.42
2:M:275:LEU:HD23	2:M:278:LEU:HD23	2.00	0.42
2:M:6:ILE:N	11:M:1042:HOH:O	2.12	0.42
4:L:502:BCL:H141	4:L:502:BCL:H162	1.90	0.42
1:L:91:ILE:HG12	6:L:709:LDA:H91	2.02	0.42
2:M:92:PHE:O	2:M:93:SER:HB2	2.20	0.42
1:L:150:ILE:HG22	1:L:151:TRP:CD1	2.55	0.41
1:L:111:LEU:HD21	2:M:254:TRP:CH2	2.55	0.41
1:L:200:PRO:HB3	2:M:141:GLY:O	2.20	0.41
2:M:90:PHE:CD1	2:M:179:ILE:HG21	2.55	0.41
1:L:79:PRO:HG2	1:L:82:LYS:HB2	2.02	0.41
1:L:107:ILE:HG23	2:M:254:TRP:HE3	1.84	0.41
2:M:25:ASN:C	2:M:27:ALA:N	2.73	0.41
2:M:6:ILE:HB	11:M:1042:HOH:O	2.20	0.41
3:H:135:LYS:HG2	3:H:166:ASP:OD2	2.21	0.41
1:L:168:HIS:CD2	4:L:502:BCL:HMC2	2.55	0.41
1:L:224:ILE:HG22	5:L:504:U10:C5	2.51	0.41
1:L:6:GLU:OE1	2:M:253:ARG:NH1	2.54	0.41
2:M:134:TYR:CD2	2:M:134:TYR:C	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:157:VAL:CG1	4:M:502:BCL:HBB1	2.50	0.41
4:L:501:BCL:H122	4:L:501:BCL:H161	1.80	0.41
1:L:226:THR:HG23	3:H:173:GLU:OE2	2.20	0.41
2:M:159:VAL:HA	2:M:163:ILE:HB	2.02	0.41
3:H:220:LYS:HG3	3:H:221:SER:N	2.36	0.41
3:H:173:GLU:O	3:H:174:GLN:C	2.58	0.41
1:L:135:ARG:HD2	1:L:248:MET:O	2.21	0.41
4:L:501:BCL:H202	4:L:501:BCL:H162	1.84	0.41
3:H:66:LEU:HD13	3:H:118:ARG:NH2	2.36	0.41
4:M:501:BCL:C4A	4:M:501:BCL:HBA1	2.50	0.41
1:L:5:PHE:CD1	1:L:5:PHE:C	2.94	0.41
2:M:157:TRP:CE2	9:M:600:SPN:HM73	2.56	0.41
1:L:97:PHE:N	1:L:97:PHE:CD1	2.88	0.40
2:M:237:GLN:OE1	2:M:245:ALA:HB2	2.20	0.40
3:H:148:PRO:HA	3:H:151:LEU:HD12	2.03	0.40
2:M:148:TRP:CE2	10:M:800:CDL:H511	2.56	0.40
2:M:162:PHE:O	2:M:166:ILE:HG13	2.21	0.40
1:L:5:PHE:O	1:L:5:PHE:CD1	2.73	0.40
7:M:504:BPH:H8	4:M:502:BCL:H191	2.04	0.40
1:L:167:PHE:HB3	4:L:502:BCL:HMC3	2.04	0.40
1:L:223:SER:OG	5:L:504:U10:C4M	2.69	0.40
4:M:501:BCL:OBB	4:M:501:BCL:HHC	2.21	0.40
4:M:502:BCL:CBB	4:M:502:BCL:CHC	2.92	0.40
2:M:72:ILE:HG13	2:M:73:TRP:N	2.36	0.40
1:L:100:TRP:O	1:L:104:GLU:HG3	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	L	279/281 (99%)	249 (89%)	28 (10%)	2 (1%)	25 64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	M	300/314 (96%)	275 (92%)	21 (7%)	4 (1%)	14	48
3	H	238/260 (92%)	220 (92%)	16 (7%)	2 (1%)	22	62
All	All	817/855 (96%)	744 (91%)	65 (8%)	8 (1%)	18	57

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	211	ASP
2	M	26	LEU
2	M	301	HIS
3	H	210	SER
1	L	4	SER
2	M	195	ASN
1	L	31	VAL
2	M	93	SER

### 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%)	212 (97%)	6 (3%)	49	81
2	M	236/247 (96%)	232 (98%)	4 (2%)	66	88
3	H	195/208 (94%)	186 (95%)	9 (5%)	31	68
All	All	649/673 (96%)	630 (97%)	19 (3%)	48	80

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	21	LEU
1	L	62	GLN
1	L	207	ARG
1	L	247	CYS
1	L	271	TRP
1	L	272	TRP

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Mol	Chain	Res	Type
2	M	136	ARG
2	M	188	ASN
2	M	216	PHE
2	M	292	ASP
3	H	11	ASP
3	H	12	LEU
3	H	43	GLU
3	H	143	SER
3	H	159	GLU
3	H	177	ARG
3	H	220	LYS
3	H	225	VAL
3	H	231	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	60	ASN
2	M	4	GLN
2	M	5	ASN
2	M	28	ASN
2	M	44	ASN
2	M	188	ASN
2	M	195	ASN
2	M	300	ASN
3	H	68	HIS
3	H	206	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

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 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$
6	LDA	H	703	-	13,15,15	2.84	2 (15%)	14,17,17	0.84	1 (7%)
4	BCL	L	501	-	55,74,74	1.48	7 (12%)	65,115,115	1.93	11 (16%)
4	BCL	L	502	1	55,74,74	1.62	8 (14%)	65,115,115	1.90	11 (16%)
5	U10	L	504	-	48,48,63	1.88	12 (25%)	58,61,79	2.77	14 (24%)
6	LDA	L	709	-	13,15,15	2.74	1 (7%)	14,17,17	0.68	0
4	BCL	M	501	2	55,74,74	1.74	9 (16%)	65,115,115	2.38	23 (35%)
4	BCL	M	502	2	55,74,74	1.24	5 (9%)	65,115,115	1.59	11 (16%)
7	BPH	M	503	-	65,70,70	1.29	8 (12%)	75,101,101	1.92	20 (26%)
7	BPH	M	504	-	65,70,70	1.30	7 (10%)	75,101,101	2.29	26 (34%)
5	U10	M	505	-	48,48,63	2.38	20 (41%)	58,61,79	1.25	6 (10%)
9	SPN	M	600	-	40,42,42	3.61	18 (45%)	48,52,52	2.60	16 (33%)
6	LDA	M	701	-	13,15,15	2.92	1 (7%)	14,17,17	0.49	0
6	LDA	M	704	-	13,15,15	2.34	1 (7%)	14,17,17	0.69	0
10	CDL	M	800	-	80,80,99	0.48	0	82,92,111	0.96	5 (6%)

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
6	LDA	H	703	-	-	0/13/13/13	0/0/0/0
4	BCL	L	501	-	1/1/21/25	0/37/137/137	0/0/9/9
4	BCL	L	502	1	-	0/37/137/137	0/0/9/9
5	U10	L	504	-	-	0/45/69/87	0/1/1/1
6	LDA	L	709	-	-	0/13/13/13	0/0/0/0
4	BCL	M	501	2	2/2/21/25	1/37/137/137	0/0/9/9
4	BCL	M	502	2	-	0/37/137/137	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BPH	M	503	-	-	0/54/105/105	0/1/6/6
7	BPH	M	504	-	1/1/18/22	0/54/105/105	0/1/6/6
5	U10	M	505	-	-	0/45/69/87	0/1/1/1
9	SPN	M	600	-	-	0/50/51/51	0/0/0/0
6	LDA	M	701	-	-	0/13/13/13	0/0/0/0
6	LDA	M	704	-	-	0/13/13/13	0/0/0/0
10	CDL	M	800	-	-	0/91/91/110	0/0/0/0

All (99) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	701	LDA	O1-N1	-10.41	1.21	1.42
6	H	703	LDA	O1-N1	-9.89	1.22	1.42
6	L	709	LDA	O1-N1	-9.79	1.22	1.42
6	M	704	LDA	O1-N1	-8.30	1.25	1.42
5	M	505	U10	C27-C28	-6.98	1.26	1.50
9	M	600	SPN	C3-C4	-6.26	1.41	1.50
9	M	600	SPN	C17-C18	-5.58	1.39	1.51
9	M	600	SPN	C10-C9	-5.48	1.39	1.51
9	M	600	SPN	C14-C13	-5.08	1.40	1.51
4	L	502	BCL	O2D-CED	-5.00	1.33	1.45
9	M	600	SPN	C6-C5	-4.91	1.40	1.51
4	L	502	BCL	C1-C2	-4.09	1.36	1.49
5	L	504	U10	C7-C8	-3.67	1.45	1.50
5	M	505	U10	C17-C18	-3.63	1.38	1.50
9	M	600	SPN	C20-C19	-3.37	1.39	1.50
5	M	505	U10	C37-C38	-3.14	1.39	1.50
5	M	505	U10	C22-C23	-3.12	1.39	1.50
9	M	600	SPN	C7-C8	-2.95	1.40	1.50
5	L	504	U10	O3-C3M	-2.94	1.38	1.45
9	M	600	SPN	C11-C12	-2.93	1.40	1.50
7	M	504	BPH	O2D-CED	-2.78	1.38	1.45
5	L	504	U10	C32-C33	-2.62	1.41	1.50
6	H	703	LDA	C1-N1	-2.60	1.45	1.51
4	L	501	BCL	CMB-C2B	-2.53	1.46	1.51
9	M	600	SPN	C21-C22	-2.48	1.39	1.52
5	M	505	U10	O4-C4M	-2.45	1.39	1.45
7	M	503	BPH	O2D-CED	-2.41	1.39	1.45
4	M	501	BCL	C2C-C3C	-2.35	1.47	1.54
7	M	504	BPH	C2C-C3C	-2.34	1.47	1.54
4	M	502	BCL	O2D-CED	-2.26	1.39	1.45
5	M	505	U10	O3-C3M	-2.21	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	505	U10	C7-C8	-2.15	1.47	1.50
9	M	600	SPN	C16-C15	-2.14	1.39	1.51
4	L	502	BCL	CMC-C2C	-2.08	1.48	1.53
4	M	501	BCL	C3B-C2B	-2.02	1.35	1.39
4	L	501	BCL	C3D-C2D	-2.00	1.35	1.39
5	L	504	U10	C15-C14	2.01	1.55	1.50
7	M	504	BPH	CAA-C2A	2.04	1.58	1.54
4	L	502	BCL	O2D-CGD	2.04	1.38	1.33
9	M	600	SPN	O1-C1	2.08	1.52	1.41
7	M	503	BPH	C4A-NA	2.08	1.40	1.35
4	M	502	BCL	O2A-CGA	2.12	1.39	1.33
5	M	505	U10	O2-C2	2.25	1.28	1.23
7	M	504	BPH	C2-C3	2.25	1.38	1.33
5	M	505	U10	C18-C19	2.26	1.38	1.33
4	M	501	BCL	C2-C3	2.26	1.38	1.33
4	L	502	BCL	C4-C3	2.28	1.56	1.50
4	M	501	BCL	CMA-C3A	2.33	1.58	1.53
7	M	504	BPH	C15-C13	2.33	1.65	1.52
5	M	505	U10	C13-C14	2.35	1.38	1.33
7	M	503	BPH	CAA-C2A	2.39	1.58	1.54
7	M	503	BPH	O1D-CGD	2.39	1.27	1.21
5	M	505	U10	C15-C14	2.40	1.56	1.50
7	M	503	BPH	C3D-C4D	2.40	1.44	1.41
5	M	505	U10	C30-C29	2.42	1.56	1.50
7	M	503	BPH	C2-C3	2.44	1.39	1.33
4	L	501	BCL	O2A-CGA	2.49	1.40	1.33
4	M	501	BCL	CAA-C2A	2.52	1.59	1.54
5	L	504	U10	C18-C19	2.53	1.39	1.33
4	L	501	BCL	C2-C3	2.54	1.39	1.33
5	L	504	U10	C38-C39	2.62	1.40	1.32
4	M	502	BCL	C2-C3	2.65	1.39	1.33
5	M	505	U10	C38-C39	2.67	1.40	1.32
5	L	504	U10	C8-C9	2.68	1.39	1.33
5	M	505	U10	C23-C24	2.71	1.39	1.33
5	M	505	U10	C8-C9	2.74	1.39	1.33
9	M	600	SPN	O1-CMA	2.93	1.52	1.43
5	L	504	U10	C23-C24	2.99	1.40	1.33
9	M	600	SPN	C29-C30	3.01	1.41	1.32
5	M	505	U10	C33-C34	3.05	1.40	1.33
5	L	504	U10	O3-C3	3.14	1.44	1.36
9	M	600	SPN	C25-C26	3.18	1.40	1.33
5	M	505	U10	C35-C34	3.24	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	502	BCL	CHB-C4A	3.25	1.37	1.33
5	L	504	U10	C13-C14	3.25	1.41	1.33
5	M	505	U10	C36-C34	3.28	1.58	1.51
7	M	503	BPH	O2A-CGA	3.43	1.43	1.33
5	M	505	U10	O4-C4	3.58	1.45	1.36
7	M	503	BPH	O2D-CGD	3.71	1.42	1.33
7	M	504	BPH	O2D-CGD	3.73	1.42	1.33
4	M	501	BCL	O2A-CGA	3.74	1.44	1.33
7	M	504	BPH	O2A-CGA	3.84	1.44	1.33
4	M	502	BCL	CHB-C4A	3.96	1.38	1.33
4	L	502	BCL	O2A-CGA	4.16	1.45	1.33
5	L	504	U10	O4-C4	4.35	1.47	1.36
4	L	501	BCL	O2D-CGD	4.43	1.44	1.33
4	M	501	BCL	O2D-CGD	4.65	1.45	1.33
4	M	502	BCL	CHC-C1C	4.81	1.39	1.33
4	L	501	BCL	CHC-C1C	4.81	1.39	1.33
4	L	501	BCL	CHB-C4A	4.82	1.39	1.33
5	L	504	U10	C31-C29	5.04	1.62	1.51
4	M	501	BCL	CHB-C4A	5.39	1.40	1.33
4	L	502	BCL	CHC-C1C	5.81	1.40	1.33
4	M	501	BCL	CHC-C1C	6.89	1.42	1.33
5	M	505	U10	O3-C3	7.08	1.54	1.36
9	M	600	SPN	C12-C13	7.85	1.52	1.33
9	M	600	SPN	C8-C9	8.11	1.53	1.33
9	M	600	SPN	C19-C18	8.46	1.54	1.33
9	M	600	SPN	C4-C5	8.55	1.54	1.33

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	501	BCL	O1D-CGD-CBD	-6.35	113.20	124.60
4	M	501	BCL	C4-C3-C5	-5.75	105.31	115.29
7	M	503	BPH	O2A-CGA-O1A	-5.18	110.69	123.55
9	M	600	SPN	C6-C5-C4	-5.08	110.71	121.10
9	M	600	SPN	C17-C18-C19	-4.83	111.22	121.10
4	M	501	BCL	O2A-CGA-O1A	-4.75	111.75	123.55
5	L	504	U10	C31-C29-C28	-4.61	111.67	121.10
9	M	600	SPN	C3-C4-C5	-4.53	119.13	126.71
4	M	501	BCL	OBD-CAD-CBD	-4.46	119.20	125.94
7	M	503	BPH	O2D-CGD-O1D	-4.46	114.85	123.82
5	L	504	U10	O5-C5-C6	-4.40	113.71	121.82
4	L	501	BCL	OBB-CAB-CBB	-4.33	110.29	120.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	502	BCL	O1D-CGD-CBD	-4.32	116.83	124.60
4	L	502	BCL	OBB-CAB-CBB	-4.05	110.93	120.16
4	M	501	BCL	CAA-C2A-C3A	-3.94	102.00	112.81
7	M	504	BPH	O2D-CGD-O1D	-3.91	115.95	123.82
9	M	600	SPN	C20-C19-C18	-3.81	118.11	127.68
9	M	600	SPN	C10-C9-C8	-3.80	113.32	121.10
7	M	504	BPH	O1D-CGD-CBD	-3.67	118.02	124.60
9	M	600	SPN	C14-C13-C12	-3.66	113.61	121.10
9	M	600	SPN	C7-C8-C9	-3.64	118.53	127.68
9	M	600	SPN	C11-C12-C13	-3.60	118.63	127.68
4	M	501	BCL	CMB-C2B-C1B	-3.60	122.93	128.46
7	M	503	BPH	OBD-CAD-CBD	-3.49	120.67	125.94
5	L	504	U10	O2-C2-C3	-3.36	113.80	120.95
4	L	502	BCL	O1D-CGD-CBD	-3.33	118.61	124.60
7	M	504	BPH	CAA-C2A-C3A	-3.24	103.92	112.81
4	M	501	BCL	OBB-CAB-CBB	-3.17	112.94	120.16
4	M	501	BCL	O2D-CGD-O1D	-3.15	117.47	123.82
5	M	505	U10	C26-C27-C28	-3.13	101.23	111.97
4	M	501	BCL	C4B-CHC-C1C	-3.08	124.02	130.12
4	L	502	BCL	CBB-CAB-C3B	-3.08	111.44	120.39
7	M	503	BPH	CAA-C2A-C3A	-3.05	104.44	112.81
4	L	501	BCL	CMB-C2B-C1B	-3.01	123.83	128.46
4	L	502	BCL	OBD-CAD-CBD	-3.00	121.41	125.94
7	M	504	BPH	C11-C12-C13	-2.97	105.98	115.73
7	M	504	BPH	O2A-CGA-O1A	-2.94	116.25	123.55
7	M	504	BPH	CBB-CAB-C3B	-2.83	114.45	120.52
7	M	503	BPH	CMA-C3A-C4A	-2.81	103.93	112.37
7	M	504	BPH	C4D-CHA-C1A	-2.79	123.11	130.23
10	M	800	CDL	CB6-CB4-CB3	-2.76	105.62	111.86
4	M	501	BCL	CMA-C3A-C2A	-2.76	102.56	113.77
5	L	504	U10	C20-C19-C21	-2.71	110.57	115.29
4	L	502	BCL	CMB-C2B-C1B	-2.70	124.31	128.46
7	M	503	BPH	O1D-CGD-CBD	-2.69	119.77	124.60
7	M	504	BPH	C4B-C3B-CAB	-2.69	120.16	130.09
4	M	502	BCL	OBD-CAD-CBD	-2.69	121.88	125.94
7	M	503	BPH	C4B-C3B-CAB	-2.54	120.72	130.09
7	M	503	BPH	C4D-CHA-C1A	-2.53	123.77	130.23
4	L	501	BCL	O2A-CGA-O1A	-2.53	117.27	123.55
4	M	501	BCL	O1D-CGD-CBD	-2.45	120.21	124.60
7	M	503	BPH	C4-C3-C5	-2.43	111.08	115.29
7	M	504	BPH	C5-C3-C2	-2.40	116.18	121.10
4	L	501	BCL	CAC-C3C-C4C	-2.37	107.32	112.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	503	BPH	C3A-C4A-NA	-2.35	109.01	113.06
7	M	503	BPH	CAA-C2A-C1A	-2.35	106.22	112.28
5	M	505	U10	C25-C24-C26	-2.35	111.21	115.29
7	M	504	BPH	CAA-C2A-C1A	-2.32	106.30	112.28
4	M	502	BCL	CMB-C2B-C1B	-2.30	124.93	128.46
10	M	800	CDL	OA8-CA7-OA9	-2.25	117.96	123.55
4	M	501	BCL	C1B-CHB-C4A	-2.24	125.68	130.12
10	M	800	CDL	CA6-CA4-CA3	-2.21	106.88	111.86
7	M	504	BPH	OBD-CAD-CBD	-2.15	122.69	125.94
7	M	504	BPH	C2A-C1A-NA	-2.15	109.29	111.91
5	L	504	U10	C4-C3-C2	-2.12	116.25	120.67
4	M	502	BCL	O2A-CGA-O1A	-2.09	118.35	123.55
7	M	504	BPH	CMA-C3A-C4A	-2.08	106.12	112.37
6	H	703	LDA	CM2-N1-CM1	-2.07	107.03	110.99
4	M	501	BCL	CMA-C3A-C4A	-2.07	106.21	111.77
5	M	505	U10	C31-C29-C28	-2.05	116.91	121.10
10	M	800	CDL	OB6-CB5-OB7	-2.05	118.57	123.68
4	M	501	BCL	CHA-C1A-NA	-2.04	121.44	126.18
4	L	501	BCL	OBD-CAD-CBD	-2.03	122.87	125.94
5	L	504	U10	C7-C6-C5	-2.03	115.87	118.47
4	M	501	BCL	CMB-C2B-C3B	2.07	128.72	124.89
4	M	501	BCL	C3C-C2C-C1C	2.07	105.21	101.87
4	M	501	BCL	C6-C5-C3	2.11	117.44	112.66
5	L	504	U10	C17-C18-C19	2.12	133.00	127.68
9	M	600	SPN	C7-C6-C5	2.15	120.22	112.93
5	L	504	U10	C21-C19-C18	2.16	125.52	121.10
5	L	504	U10	O5-C5-C4	2.16	125.55	120.95
4	M	502	BCL	C3A-C2A-C1A	2.17	104.58	101.34
7	M	504	BPH	C11-C10-C8	2.18	122.90	115.73
5	M	505	U10	C3M-O3-C3	2.19	124.26	116.44
9	M	600	SPN	C15-C16-C17	2.19	121.27	113.24
7	M	503	BPH	C2A-C3A-C4A	2.22	105.76	101.33
4	L	502	BCL	CED-O2D-CGD	2.22	121.19	115.97
7	M	504	BPH	C14-C13-C12	2.27	119.64	111.36
7	M	503	BPH	C3A-C4A-CHB	2.29	125.62	121.75
7	M	504	BPH	CMD-C2D-C3D	2.29	129.15	124.89
4	L	502	BCL	C1-C2-C3	2.31	130.22	125.96
4	M	502	BCL	C1-C2-C3	2.34	130.26	125.96
7	M	503	BPH	C2C-C3C-C4C	2.34	104.84	101.34
9	M	600	SPN	CM3-C5-C6	2.38	119.41	115.29
7	M	503	BPH	C3C-C2C-C1C	2.38	105.72	101.87
5	M	505	U10	C7-C8-C9	2.46	130.82	126.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	501	BCL	CMD-C2D-C3D	2.47	129.47	124.89
7	M	503	BPH	CED-O2D-CGD	2.57	121.99	115.97
7	M	504	BPH	C3C-C2C-C1C	2.69	106.21	101.87
4	L	501	BCL	CMD-C2D-C3D	2.71	129.91	124.89
7	M	503	BPH	CAC-C3C-C2C	2.71	121.05	114.24
4	M	502	BCL	CED-O2D-CGD	2.80	122.54	115.97
7	M	503	BPH	C4A-NA-C1A	2.82	110.44	108.16
7	M	504	BPH	C2C-C3C-C4C	2.84	105.59	101.34
7	M	504	BPH	C17-C16-C15	2.88	127.16	113.25
4	M	501	BCL	C2C-C3C-C4C	3.01	105.85	101.34
4	L	501	BCL	O2A-CGA-CBA	3.02	120.70	111.90
4	M	502	BCL	C4A-NA-C1A	3.06	110.25	106.45
10	M	800	CDL	OB8-CB6-CB4	3.23	116.78	108.66
4	L	502	BCL	C4A-NA-C1A	3.24	110.48	106.45
5	L	504	U10	C16-C14-C13	3.25	127.77	121.10
4	L	501	BCL	C4A-NA-C1A	3.27	110.52	106.45
5	M	505	U10	C27-C28-C29	3.31	135.99	127.68
4	M	502	BCL	OBB-CAB-C3B	3.32	126.28	119.95
4	L	502	BCL	O2A-CGA-CBA	3.42	121.84	111.90
7	M	504	BPH	CED-O2D-CGD	3.60	124.41	115.97
7	M	504	BPH	CBC-CAC-C3C	3.64	121.76	113.51
4	M	502	BCL	O2A-CGA-CBA	3.67	122.59	111.90
7	M	503	BPH	O2A-CGA-CBA	3.69	122.64	111.90
9	M	600	SPN	CM4-C9-C10	3.77	121.82	115.29
4	M	501	BCL	C5-C3-C2	3.86	129.00	121.10
9	M	600	SPN	C16-C17-C18	3.87	121.43	112.66
7	M	504	BPH	C6-C5-C3	4.00	121.73	112.66
9	M	600	SPN	CM7-C22-C21	4.18	126.62	111.36
7	M	504	BPH	C16-C15-C13	4.34	129.98	115.73
4	M	501	BCL	O2D-CGD-CBD	4.56	119.45	111.30
5	L	504	U10	C30-C29-C31	4.64	123.34	115.29
7	M	504	BPH	C4A-NA-C1A	4.71	111.97	108.16
4	L	502	BCL	O2D-CGD-CBD	4.91	120.07	111.30
4	L	501	BCL	OBB-CAB-C3B	4.92	129.33	119.95
4	M	501	BCL	O2A-CGA-CBA	5.01	126.47	111.90
4	M	501	BCL	OBB-CAB-C3B	5.48	130.39	119.95
7	M	504	BPH	C1-C2-C3	5.60	136.28	125.96
4	M	502	BCL	O2D-CGD-CBD	5.62	121.34	111.30
5	L	504	U10	C27-C28-C29	6.15	143.13	127.68
9	M	600	SPN	CM5-C13-C14	6.23	126.10	115.29
5	L	504	U10	C3M-O3-C3	6.33	139.07	116.44
9	M	600	SPN	CM6-C18-C17	6.79	127.06	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	501	BCL	C1-C2-C3	7.38	139.54	125.96
4	L	501	BCL	O2D-CGD-CBD	7.84	125.31	111.30
7	M	503	BPH	O2D-CGD-CBD	7.86	125.34	111.30
7	M	504	BPH	O2D-CGD-CBD	8.23	126.00	111.30
4	L	502	BCL	OBB-CAB-C3B	8.67	136.48	119.95
5	L	504	U10	C32-C33-C34	14.05	162.97	127.68

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	M	501	BCL	C8
4	M	501	BCL	C13
4	L	501	BCL	C13
7	M	504	BPH	C8

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	501	BCL	C1-C2-C3-C4

There are no ring outliers.

14 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	703	LDA	4	0
4	L	501	BCL	7	0
4	L	502	BCL	10	0
5	L	504	U10	6	0
6	L	709	LDA	4	0
4	M	501	BCL	6	0
4	M	502	BCL	13	0
7	M	503	BPH	2	0
7	M	504	BPH	2	0
5	M	505	U10	7	0
9	M	600	SPN	2	0
6	M	701	LDA	2	0
6	M	704	LDA	1	0
10	M	800	CDL	2	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, 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%)	-0.67	2 (0%) 87 75	24, 43, 83, 99	0
2	M	302/314 (96%)	-0.62	3 (0%) 82 67	25, 51, 87, 109	0
3	H	240/260 (92%)	-0.53	2 (0%) 86 71	25, 48, 74, 109	0
All	All	823/855 (96%)	-0.61	7 (0%) 84 69	24, 47, 84, 109	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	250	SER	4.8
2	M	1	ALA	3.3
3	H	249	LYS	2.7
2	M	2	GLU	2.3
1	L	277	GLY	2.3
1	L	281	GLY	2.1
2	M	302	GLY	2.1

### 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
5	U10	L	504	48/63	0.78	0.50	9.84	76,89,95,96	0
6	LDA	M	704	16/16	0.79	0.33	7.71	90,97,121,122	0
6	LDA	M	701	16/16	0.90	0.24	6.60	57,75,79,82	0
10	CDL	M	800	81/100	0.84	0.37	5.17	25,68,82,85	81
6	LDA	L	709	16/16	0.79	0.59	4.29	104,109,119,120	0
4	BCL	M	501	66/66	0.93	0.21	2.81	31,41,88,91	0
9	SPN	M	600	43/43	0.86	0.28	2.61	44,64,91,94	0
5	U10	M	505	48/63	0.94	0.20	2.39	30,45,77,79	0
6	LDA	H	703	16/16	0.92	0.26	2.16	64,74,87,89	0
7	BPH	M	503	65/65	0.97	0.15	1.04	25,37,47,50	0
4	BCL	M	502	66/66	0.97	0.16	1.00	27,37,69,75	0
4	BCL	L	501	66/66	0.96	0.16	0.86	19,33,55,59	0
7	BPH	M	504	65/65	0.95	0.17	0.57	22,53,71,79	10
4	BCL	L	502	66/66	0.97	0.15	0.09	22,33,42,49	0
8	FE	M	500	1/1	0.97	0.10	-1.86	36,36,36,36	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.