



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 03:07 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 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/ValidationPDFNotes.html>

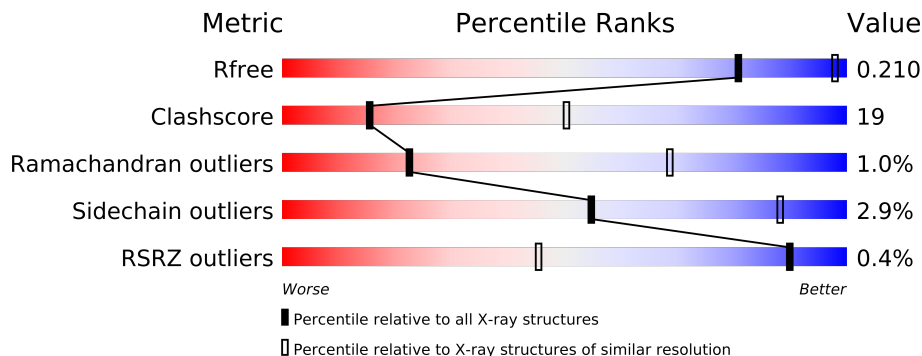
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	L	281	
2	M	314	
3	H	260	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
10	CDL	M	800	-	X
4	BCL	M	501	-	X
5	U10	L	504	-	X
5	U10	M	505	-	X
6	LDA	H	703	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
6	LDA	L	709	-	X
6	LDA	M	701	-	X
6	LDA	M	704	-	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 hydrogen and 0 are deuterium.

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			

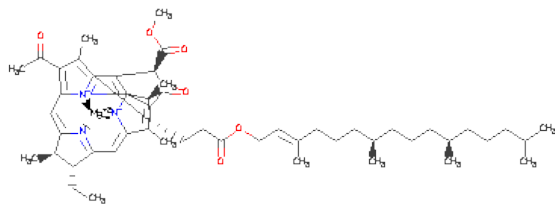
There are 8 discrepancies between the modelled and reference sequences:

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.

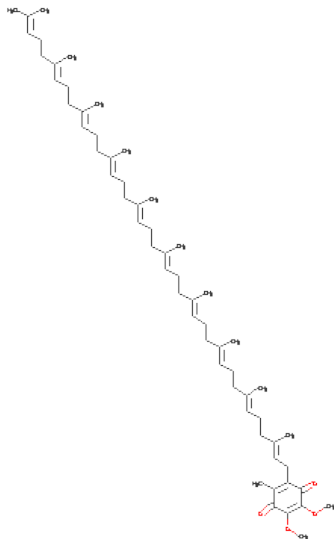
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	240	Total	C	N	O	S	0	0	0
			1829	1169	314	337	9			

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



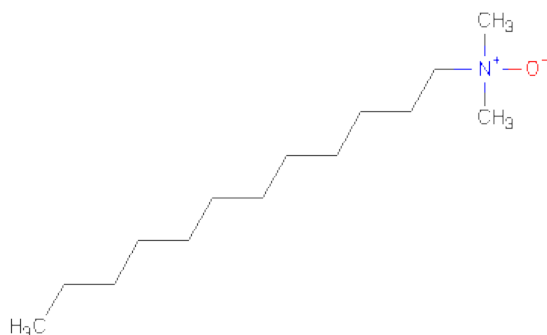
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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



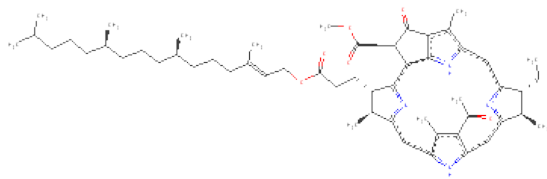
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	L	1	Total	C	O	0	0
			48	44	4		
5	M	1	Total	C	O	0	0
			48	44	4		

- 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: $C_{55}H_{76}N_4O_6$).



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).

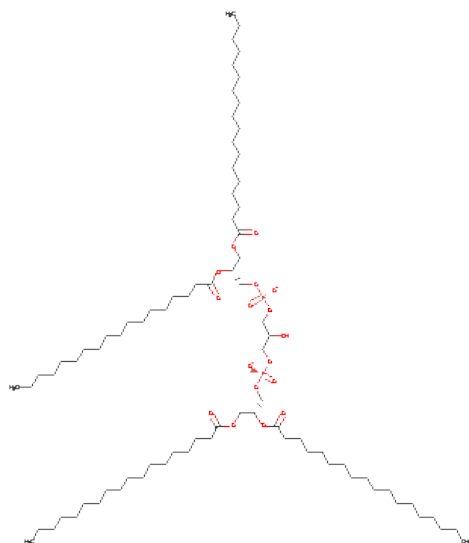
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	M	1	Total	Fe	0	0
			1	1		

- Molecule 9 is SPEROIDENONE (three-letter code: SPN) (formula: C₄₁H₇₀O₂).



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.

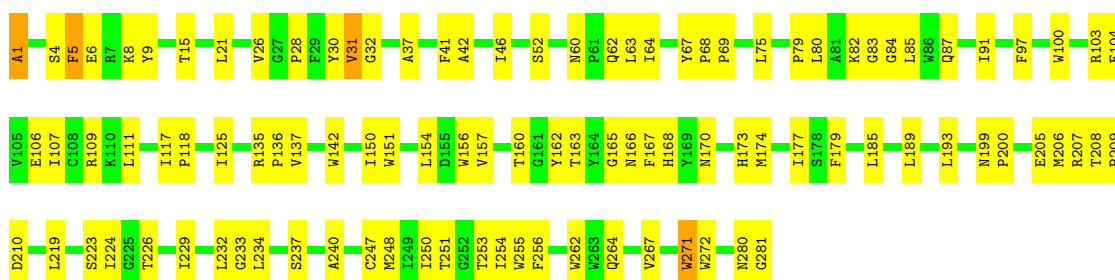
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	L	28	Total	O	0	0
			28	28		
11	M	27	Total	O	0	0
			27	27		
11	H	33	Total	O	0	0
			33	33		

3 Residue-property plots

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.

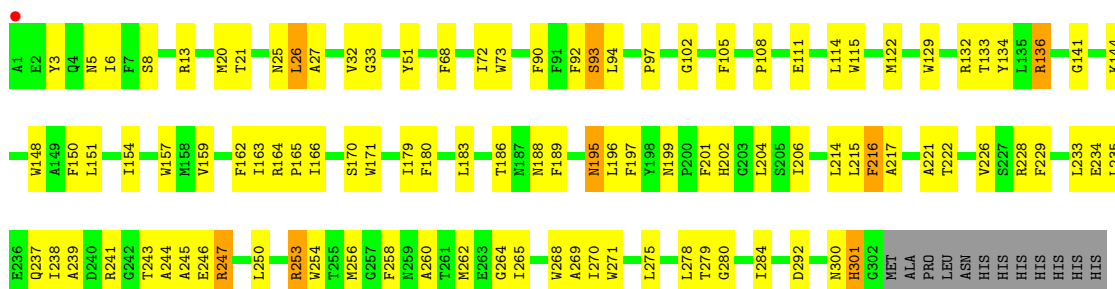
- Molecule 1: Reaction center protein L chain

Chain L:



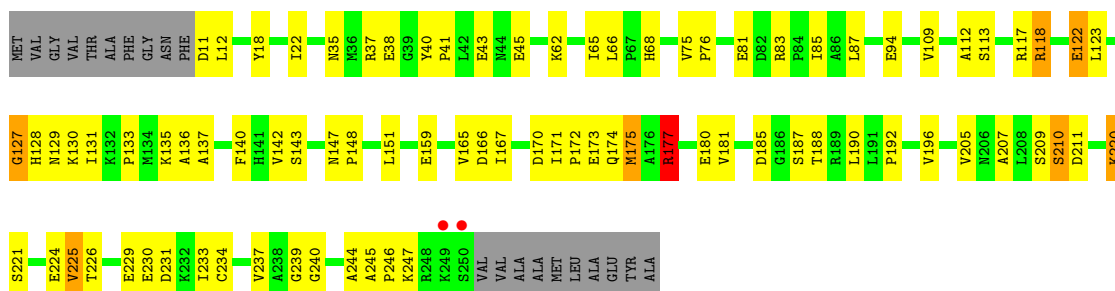
- Molecule 2: Reaction center protein M chain

Chain M:



- Molecule 3: Reaction center protein H chain

Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	60.3	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 32.5	EDS
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 34022 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7226	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

5 Model quality i

5.1 Standard geometry i

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	M	27	0	0	5	0
All	All	7226	0	7213	267	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 19.

All (267) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:300:ASN:O	2:M:301:HIS:CB	2.38	0.71
2:M:245:ALA:O	11:M:1032:HOH:O	2.08	0.71
3:H:122:GLU:OE2	3:H:130:LYS:HD2	1.90	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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
2:M:222:THR:O	2:M:226:VAL:HG22	1.94	0.67
1:L:117:ILE:HB	1:L:118:PRO:HD3	1.74	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:157:TRP:HB2	4:M:502:BCL:H62	1.81	0.61
2:M:13:ARG:O	3:H:140:PHE:HA	1.99	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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
4:M:501:BCL:HMB1	4:M:501:BCL:HBB2	1.85	0.57
1:L:199:ASN:N	1:L:200:PRO:HD3	2.20	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
1:L:185:LEU:C	1:L:185:LEU:HD23	2.29	0.54
3:H:40:TYR:HA	3:H:41:PRO:C	2.28	0.54
1:L:168:HIS:HE1	2:M:186:THR:HB	1.73	0.54
3:H:122:GLU:OE1	3:H:130:LYS:HD3	2.09	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:219:LEU:HD11	2:M:133:THR:HG22	1.90	0.52
4:L:502:BCL:H203	4:L:501:BCL:H102	1.91	0.52
6:M:701:LDA:H101	6:H:703:LDA:C12	2.39	0.52
1:L:205:GLU:HA	3:H:65:ILE:HB	1.92	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
2:M:197:PHE:HZ	4:M:502:BCL:HBB2	1.74	0.52
3:H:209:SER:O	3:H:210:SER:C	2.48	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:M:73:TRP:HB2	2:M:114:LEU:HD23	1.93	0.51
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
2:M:202:HIS:CE1	2:M:206:ILE:HD11	2.47	0.50
3:H:75:VAL:HA	3:H:76:PRO:C	2.30	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
1:L:91:ILE:CG1	6:L:709:LDA:H91	2.42	0.49
3:H:229:GLU:O	3:H:233:ILE:HG13	2.13	0.49
2:M:199:ASN:HB3	2:M:202:HIS:HB3	1.94	0.49
4:L:502:BCL:HAA2	4:L:501:BCL:HAC1	1.93	0.49
3:H:129:ASN:HD22	3:H:224:GLU:HG2	1.78	0.49
2:M:154:ILE:HG23	2:M:157:TRP:CE3	2.47	0.49
3:H:190:LEU:HD12	3:H:233:ILE:CD1	2.43	0.49
3:H:109:VAL:HA	3:H:113:SER:HB3	1.94	0.49
2:M:270:ILE:CG2	2:M:271:TRP:N	2.76	0.49
3:H:62:LYS:O	3:H:62:LYS:HG3	2.12	0.48
3:H:240:GLY:O	3:H:244:ALA:HB3	2.13	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
1:L:69:PRO:HG2	1:L:142:TRP:HB2	1.94	0.48
3:H:190:LEU:CD1	3:H:225:VAL:CG1	2.91	0.48
2:M:215:LEU:CD2	2:M:269:ALA:HA	2.44	0.48
1:L:250:ILE:HB	1:L:254:ILE:HD11	1.95	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
4:L:502:BCL:CHC	4:L:502:BCL:OBB	2.55	0.47
1:L:262:TRP:C	1:L:264:GLN:H	2.18	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:248:MET:HE2	4:L:502:BCL:HMD1	1.95	0.47
6:M:701:LDA:H101	6:H:703:LDA:H121	1.97	0.47
1:L:37:ALA:O	1:L:41:PHE:CD2	2.68	0.47
1:L:83:GLY:O	1:L:87:GLN:HG3	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:M:180:PHE:O	2:M:183:LEU:HB2	2.14	0.47
1:L:248:MET:HE2	4:L:502:BCL:OBD	2.15	0.47
3:H:37:ARG:HH11	3:H:76:PRO:HD3	1.79	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
2:M:129:TRP:O	2:M:133:THR:HG23	2.15	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
3:H:129:ASN:ND2	3:H:224:GLU:HG2	2.31	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:190:LEU:HD11	3:H:225:VAL:HG13	2.00	0.44
3:H:142:VAL:CG2	3:H:147:ASN:ND2	2.79	0.44
1:L:166:ASN:OD1	1:L:168:HIS:HB2	2.16	0.44
2:M:215:LEU:HD21	2:M:269:ALA:HA	1.99	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: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
2:M:157:TRP:NE1	9:M:600:SPN:H202	2.33	0.44
1:L:173:HIS:O	1:L:177:ILE:HG13	2.17	0.44
3:H:192:PRO:HD2	3:H:237:VAL:HG21	2.00	0.44
2:M:216:PHE:HD1	2:M:216:PHE:O	2.01	0.44
2:M:265:ILE:HG21	5:M:505:U10:H3M3	1.99	0.44
1:L:253:THR:OG1	1:L:254:ILE:N	2.51	0.44
2:M:73:TRP:HB2	2:M:114:LEU:CD2	2.47	0.44
1:L:193:LEU:HD23	5:L:504:U10:C3M	2.48	0.44
3:H:18:TYR:O	3:H:22:ILE:HG13	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:233:GLY:HA3	2:M:216:PHE:CD1	2.53	0.43
2:M:134:TYR:CE1	2:M:144:LYS:HG2	2.53	0.43
1:L:234:LEU:HD13	2:M:221:ALA:HB2	2.00	0.43
5:M:505:U10:H28	5:M:505:U10:H322	1.47	0.43
1:L:30:TYR:HB2	2:M:254:TRP:HB3	2.01	0.43
2:M:235:LEU:O	2:M:238:ILE:HB	2.18	0.43
1:L:179:PHE:CZ	5:L:504:U10:H23	2.53	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:156:TRP:O	1:L:160:THR:OG1	2.29	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
4:M:502:BCL:H121	4:M:502:BCL:H162	1.85	0.42
3:H:185:ASP:OD1	3:H:187:SER:OG	2.29	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
2:M:90:PHE:CD1	2:M:179:ILE:HG21	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
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
1:L:79:PRO:HG2	1:L:82:LYS:HB2	2.02	0.41
1:L:168:HIS:CD2	4:L:502:BCL:HMC2	2.55	0.41
1:L:157:VAL:CG1	4:M:502:BCL:HBB1	2.50	0.41
3:H:135:LYS:HG2	3:H:166:ASP:OD2	2.21	0.41
1:L:6:GLU:OE1	2:M:253:ARG:NH1	2.54	0.41
1:L:224:ILE:HG22	5:L:504:U10:C5	2.51	0.41
2:M:134:TYR:CD2	2:M:134:TYR:C	2.94	0.41
4:L:501:BCL:H122	4:L:501:BCL:H161	1.80	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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:173:GLU:O	3:H:174:GLN:C	2.58	0.41
4:M:501:BCL:C4A	4:M:501:BCL:HBA1	2.50	0.41
2:M:157:TRP:CE2	9:M:600:SPN:HM73	2.56	0.41
3:H:66:LEU:HD13	3:H:118:ARG:NH2	2.36	0.41
1:L:5:PHE:CD1	1:L:5:PHE:C	2.94	0.41
2:M:237:GLN:OE1	2:M:245:ALA:HB2	2.20	0.40
1:L:97:PHE:CD1	1:L:97:PHE:N	2.88	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
3:H:148:PRO:HA	3:H:151:LEU:HD12	2.03	0.40
7:M:504:BPH:H8	4:M:502:BCL:H191	2.04	0.40
1:L:5:PHE:O	1:L:5:PHE:CD1	2.73	0.40
1:L:167:PHE:HB3	4:L:502:BCL:HMC3	2.04	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:223:SER:OG	5:L:504:U10:C4M	2.69	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

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	279/281 (99%)	249 (89%)	28 (10%)	2 (1%)	30	76
2	M	300/314 (96%)	275 (92%)	21 (7%)	4 (1%)	18	60
3	H	238/260 (92%)	220 (92%)	16 (7%)	2 (1%)	27	74
All	All	817/855 (96%)	744 (91%)	65 (8%)	8 (1%)	22	68

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%)	56	89
2	M	236/247 (96%)	232 (98%)	4 (2%)	73	94
3	H	195/208 (94%)	186 (95%)	9 (5%)	37	78
All	All	649/673 (96%)	630 (97%)	19 (3%)	55	88

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
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

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Mol	Chain	Res	Type
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 ⓘ

There are no RNA chains 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 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	-	15,15,15	4.76	4 (26%)	17,17,17	1.26	2 (11%)
4	BCL	L	501	-	74,74,74	1.57	14 (18%)	97,115,115	1.71	15 (15%)
4	BCL	L	502	1	74,74,74	1.61	13 (17%)	97,115,115	1.90	17 (17%)
5	U10	L	504	-	48,48,63	2.02	15 (31%)	59,61,79	3.09	17 (28%)
6	LDA	L	709	-	15,15,15	4.57	2 (13%)	17,17,17	3.73	1 (5%)
4	BCL	M	501	2	74,74,74	1.56	15 (20%)	97,115,115	2.14	24 (24%)
4	BCL	M	502	2	74,74,74	1.43	11 (14%)	97,115,115	1.46	14 (14%)
7	BPH	M	503	-	70,70,70	1.47	13 (18%)	94,101,101	1.79	22 (23%)
7	BPH	M	504	-	70,70,70	1.56	13 (18%)	94,101,101	2.13	34 (36%)
5	U10	M	505	-	48,48,63	2.60	23 (47%)	59,61,79	1.39	10 (16%)
9	SPN	M	600	-	42,42,42	4.15	17 (40%)	52,52,52	2.73	18 (34%)
6	LDA	M	701	-	15,15,15	4.89	2 (13%)	17,17,17	5.43	1 (5%)
6	LDA	M	704	-	15,15,15	3.75	1 (6%)	17,17,17	4.37	1 (5%)
10	CDL	M	800	-	80,80,99	1.36	4 (5%)	92,92,111	0.99	4 (4%)

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	0/41/137/137	0/0/9/9
4	BCL	L	502	1	-	0/41/137/137	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	1/41/137/137	0/0/9/9
4	BCL	M	502	2	-	0/41/137/137	0/0/9/9
7	BPH	M	503	-	2/2/18/22	0/49/105/105	0/0/6/6
7	BPH	M	504	-	1/1/18/22	0/49/105/105	0/0/6/6
5	U10	M	505	-	-	0/45/69/87	0/1/1/1
9	SPN	M	600	-	-	0/51/51/51	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	-	1/1/9/9	0/91/91/110	0/0/0/0

All (147) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	701	LDA	O1-N1	-18.71	1.21	1.39
6	H	703	LDA	O1-N1	-17.65	1.22	1.39
6	L	709	LDA	O1-N1	-17.44	1.22	1.39
6	M	704	LDA	O1-N1	-14.43	1.25	1.39
9	M	600	SPN	C4-C5	10.60	1.54	1.32
9	M	600	SPN	C19-C18	10.48	1.54	1.32
9	M	600	SPN	C8-C9	10.05	1.53	1.32
9	M	600	SPN	C12-C13	9.73	1.52	1.32
5	M	505	U10	C27-C28	-8.21	1.26	1.50
9	M	600	SPN	C3-C2	7.88	1.61	1.51
5	M	505	U10	O3-C3	7.00	1.54	1.36
10	M	800	CDL	C43-C42	-6.59	1.52	1.55
10	M	800	CDL	C58-C57	-6.57	1.52	1.55
9	M	600	SPN	C3-C4	-6.02	1.41	1.50
7	M	504	BPH	C1D-CHD	5.23	1.41	1.35
9	M	600	SPN	C17-C18	-5.18	1.39	1.51
10	M	800	CDL	C84-C83	-5.08	1.53	1.55
9	M	600	SPN	C10-C9	-5.08	1.39	1.51
4	L	502	BCL	O2D-CED	-4.80	1.33	1.45
10	M	800	CDL	C24-C23	-4.73	1.53	1.55
9	M	600	SPN	C14-C13	-4.72	1.40	1.51
5	L	504	U10	C31-C29	4.65	1.62	1.51
4	M	502	BCL	C3B-C4B	4.64	1.47	1.40
9	M	600	SPN	C6-C5	-4.55	1.40	1.51
4	M	501	BCL	O2D-CGD	4.47	1.45	1.33
4	L	502	BCL	C3B-C4B	4.45	1.47	1.40
5	L	504	U10	O4-C4	4.31	1.47	1.36
5	M	505	U10	C17-C18	-4.30	1.38	1.50
7	M	503	BPH	C1D-CHD	4.28	1.40	1.35
4	L	501	BCL	O2D-CGD	4.26	1.44	1.33
4	L	501	BCL	C3B-C4B	4.15	1.46	1.40
4	M	502	BCL	C4C-NC	4.12	1.41	1.32
5	L	504	U10	C13-C14	4.05	1.41	1.32
4	L	502	BCL	C4C-NC	4.01	1.41	1.32
4	L	502	BCL	C1A-NA	3.99	1.41	1.32
9	M	600	SPN	C20-C19	-3.99	1.39	1.50
4	L	501	BCL	MG-ND	-3.98	1.96	2.05
9	M	600	SPN	C25-C26	3.96	1.40	1.32
4	L	502	BCL	O2A-CGA	3.92	1.45	1.33
4	L	501	BCL	C1A-NA	3.91	1.40	1.32
4	M	501	BCL	C4C-NC	3.91	1.40	1.32
4	M	502	BCL	C1B-C2B	3.89	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	501	BCL	C4C-NC	3.85	1.40	1.32
4	L	501	BCL	C1B-C2B	3.84	1.45	1.40
7	M	504	BPH	C4B-NB	3.84	1.40	1.36
7	M	503	BPH	C1B-NB	3.79	1.40	1.36
5	M	505	U10	C33-C34	3.79	1.40	1.32
4	M	501	BCL	C3B-C4B	3.74	1.46	1.40
5	M	505	U10	C37-C38	-3.73	1.39	1.50
5	L	504	U10	C23-C24	3.72	1.40	1.32
5	M	505	U10	C22-C23	-3.71	1.39	1.50
4	L	502	BCL	C1-C2	-3.70	1.36	1.49
7	M	504	BPH	O2A-CGA	3.62	1.44	1.33
6	H	703	LDA	CM1-N1	-3.59	1.43	1.49
7	M	504	BPH	O2D-CGD	3.59	1.42	1.33
7	M	503	BPH	O2D-CGD	3.57	1.42	1.33
5	M	505	U10	O4-C4	3.56	1.45	1.36
5	L	504	U10	C7-C8	-3.54	1.45	1.50
4	M	501	BCL	O2A-CGA	3.53	1.44	1.33
9	M	600	SPN	C7-C8	-3.51	1.40	1.50
9	M	600	SPN	C11-C12	-3.48	1.40	1.50
4	M	502	BCL	C1B-NB	3.45	1.38	1.34
5	M	505	U10	C8-C9	3.41	1.39	1.32
5	M	505	U10	C23-C24	3.38	1.39	1.32
5	L	504	U10	C8-C9	3.34	1.39	1.32
4	M	502	BCL	C2-C3	3.30	1.39	1.32
4	M	501	BCL	MG-NA	3.28	2.16	2.07
5	M	505	U10	C35-C34	3.26	1.59	1.50
4	M	501	BCL	C1B-C2B	3.25	1.44	1.40
7	M	503	BPH	O2A-CGA	3.24	1.43	1.33
4	M	501	BCL	C1B-NB	3.18	1.38	1.34
4	L	501	BCL	C2-C3	3.17	1.39	1.32
5	L	504	U10	C18-C19	3.16	1.39	1.32
5	L	504	U10	O3-C3	3.13	1.44	1.36
5	L	504	U10	C32-C33	-3.11	1.41	1.50
6	H	703	LDA	C1-N1	-3.11	1.45	1.51
4	M	502	BCL	C4B-NB	3.10	1.38	1.34
4	L	502	BCL	MG-NA	3.09	2.16	2.07
7	M	503	BPH	C2-C3	3.04	1.39	1.32
5	M	505	U10	C36-C34	3.02	1.58	1.51
4	L	501	BCL	MG-NA	2.94	2.15	2.07
5	M	505	U10	C13-C14	2.93	1.38	1.32
4	M	501	BCL	C1A-NA	2.93	1.38	1.32
7	M	503	BPH	C3B-C4B	2.93	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	502	BCL	MG-NA	2.92	2.15	2.07
4	M	502	BCL	C1A-NA	2.89	1.38	1.32
9	M	600	SPN	O1-CMA	2.88	1.52	1.43
4	L	502	BCL	C1B-C2B	2.84	1.43	1.40
4	M	501	BCL	C4B-NB	2.84	1.38	1.34
5	L	504	U10	O3-C3M	-2.83	1.38	1.45
4	M	501	BCL	C2-C3	2.82	1.38	1.32
5	M	505	U10	C18-C19	2.82	1.38	1.32
4	L	502	BCL	C4B-NB	2.82	1.38	1.34
7	M	504	BPH	C2-C3	2.81	1.38	1.32
5	M	505	U10	C38-C39	2.80	1.40	1.34
7	M	504	BPH	C1B-NB	2.79	1.39	1.36
9	M	600	SPN	C29-C30	2.73	1.41	1.32
5	L	504	U10	C38-C39	2.72	1.40	1.34
4	M	501	BCL	CAA-C2A	2.70	1.59	1.54
7	M	503	BPH	C4C-NC	2.70	1.41	1.34
7	M	504	BPH	O2D-CED	-2.67	1.38	1.45
4	L	501	BCL	C4B-NB	2.66	1.37	1.34
5	M	505	U10	C41-C39	2.61	1.54	1.40
7	M	504	BPH	C3B-C4B	2.59	1.44	1.40
7	M	503	BPH	CAA-C2A	2.56	1.58	1.54
7	M	504	BPH	C4D-ND	-2.52	1.34	1.38
9	M	600	SPN	C21-C22	-2.51	1.39	1.52
5	L	504	U10	C28-C29	2.48	1.37	1.32
4	L	501	BCL	CMB-C2B	-2.48	1.46	1.51
4	M	501	BCL	CHC-C1C	2.45	1.42	1.36
5	L	504	U10	C41-C39	2.43	1.53	1.40
5	M	505	U10	C30-C29	2.43	1.56	1.50
7	M	504	BPH	C4C-NC	2.43	1.40	1.34
7	M	503	BPH	O1D-CGD	2.41	1.27	1.21
5	M	505	U10	C15-C14	2.40	1.56	1.50
7	M	503	BPH	C4B-NB	2.37	1.39	1.36
5	M	505	U10	O4-C4M	-2.37	1.39	1.45
4	L	501	BCL	O2A-CGA	2.36	1.40	1.33
7	M	504	BPH	C15-C13	2.33	1.65	1.52
7	M	503	BPH	O2D-CED	-2.32	1.39	1.45
6	H	703	LDA	CM2-N1	-2.32	1.45	1.49
4	L	501	BCL	C1B-NB	2.30	1.37	1.34
4	L	502	BCL	C4-C3	2.28	1.56	1.50
4	M	501	BCL	C2C-C3C	-2.28	1.47	1.54
5	L	504	U10	C27-C28	-2.27	1.44	1.50
7	M	504	BPH	C2C-C3C	-2.27	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	501	BCL	CMA-C3A	2.27	1.58	1.53
4	L	502	BCL	C2-C3	2.23	1.37	1.32
4	L	501	BCL	C4D-C3D	2.22	1.44	1.41
7	M	504	BPH	CAA-C2A	2.19	1.58	1.54
4	M	502	BCL	O2D-CED	-2.18	1.39	1.45
5	M	505	U10	C28-C29	2.17	1.37	1.32
5	M	505	U10	C40-C39	2.16	1.55	1.48
6	M	701	LDA	CM2-N1	-2.15	1.46	1.49
6	L	709	LDA	CM2-N1	-2.14	1.46	1.49
5	M	505	U10	O3-C3M	-2.14	1.40	1.45
4	L	502	BCL	MG-NC	2.11	2.13	2.07
4	L	501	BCL	C3D-CAD	-2.09	1.43	1.47
5	M	505	U10	O2-C2	2.09	1.28	1.23
7	M	503	BPH	C3B-C2B	-2.08	1.34	1.40
4	M	502	BCL	C4D-C3D	2.08	1.44	1.41
5	M	505	U10	C7-C8	-2.08	1.47	1.50
7	M	503	BPH	C4D-C3D	2.06	1.44	1.41
4	M	501	BCL	C4D-C3D	2.02	1.44	1.41
4	L	502	BCL	CMC-C2C	-2.02	1.48	1.53
5	L	504	U10	C15-C14	2.01	1.55	1.50
4	M	502	BCL	O2A-CGA	2.01	1.39	1.33

All (180) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	701	LDA	C2-C1-N1	22.31	152.25	113.80
6	M	704	LDA	C2-C1-N1	17.86	144.58	113.80
5	L	504	U10	C32-C33-C34	16.31	162.97	127.80
6	L	709	LDA	C2-C1-N1	15.22	140.03	113.80
4	L	502	BCL	OBB-CAB-C3B	10.93	136.48	120.07
9	M	600	SPN	CM6-C18-C17	7.68	127.06	115.39
4	M	501	BCL	C1-C2-C3	7.51	139.54	126.19
7	M	504	BPH	O2D-CGD-CBD	7.20	126.00	111.33
5	L	504	U10	C27-C28-C29	7.11	143.13	127.80
9	M	600	SPN	CM5-C13-C14	7.05	126.10	115.39
7	M	503	BPH	O2D-CGD-CBD	6.88	125.34	111.33
4	M	501	BCL	OBB-CAB-C3B	6.88	130.39	120.07
4	L	501	BCL	O2D-CGD-CBD	6.87	125.31	111.33
5	L	504	U10	C3M-O3-C3	6.65	139.07	116.48
4	M	501	BCL	C4-C3-C5	-6.63	105.31	115.39
4	L	501	BCL	OBB-CAB-C3B	6.17	129.33	120.07
7	M	504	BPH	C1-C2-C3	5.67	136.28	126.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	501	BCL	O1D-CGD-CBD	-5.47	113.20	124.42
9	M	600	SPN	C6-C5-C4	-5.39	110.71	121.08
5	L	504	U10	C30-C29-C31	5.23	123.34	115.39
7	M	504	BPH	C16-C15-C13	5.15	129.98	115.14
9	M	600	SPN	C17-C18-C19	-5.12	111.22	121.08
4	M	502	BCL	O2D-CGD-CBD	4.92	121.34	111.33
5	L	504	U10	C31-C29-C28	-4.89	111.67	121.08
4	L	502	BCL	C4B-C3B-CAB	-4.86	105.81	127.09
4	M	501	BCL	CAA-C2A-C3A	-4.67	102.00	113.04
7	M	503	BPH	O2A-CGA-O1A	-4.66	110.69	123.43
4	M	501	BCL	O2A-CGA-CBA	4.62	126.47	111.94
9	M	600	SPN	C3-C4-C5	-4.52	119.13	126.76
9	M	600	SPN	C20-C19-C18	-4.49	118.11	127.80
4	M	501	BCL	OBD-CAD-CBD	-4.46	119.20	125.94
7	M	503	BPH	O2D-CGD-O1D	-4.40	114.85	123.79
5	L	504	U10	O5-C5-C6	-4.33	113.71	121.67
9	M	600	SPN	C7-C8-C9	-4.29	118.53	127.80
4	L	502	BCL	O2D-CGD-CBD	4.29	120.07	111.33
4	M	501	BCL	O2A-CGA-O1A	-4.28	111.75	123.43
9	M	600	SPN	C11-C12-C13	-4.25	118.63	127.80
9	M	600	SPN	CM7-C22-C21	4.25	126.62	111.02
9	M	600	SPN	CM4-C9-C10	4.23	121.82	115.39
4	M	502	BCL	OBB-CAB-C3B	4.14	126.28	120.07
4	M	501	BCL	C5-C3-C2	4.12	129.00	121.08
9	M	600	SPN	C10-C9-C8	-4.03	113.32	121.08
4	M	501	BCL	O2D-CGD-CBD	3.99	119.45	111.33
4	L	501	BCL	OBB-CAB-CBB	-3.96	110.29	120.13
6	H	703	LDA	C2-C1-N1	3.89	120.51	113.80
9	M	600	SPN	C14-C13-C12	-3.88	113.61	121.08
7	M	504	BPH	O2D-CGD-O1D	-3.86	115.95	123.79
7	M	504	BPH	CAA-C2A-C3A	-3.86	103.92	113.04
5	M	505	U10	C27-C28-C29	3.80	135.99	127.80
7	M	504	BPH	C6-C5-C3	3.77	121.73	112.78
4	L	502	BCL	OBB-CAB-CBB	-3.70	110.93	120.13
4	M	502	BCL	O1D-CGD-CBD	-3.70	116.83	124.42
4	M	501	BCL	CMB-C2B-C1B	-3.70	122.93	128.62
9	M	600	SPN	C16-C17-C18	3.64	121.43	112.78
7	M	503	BPH	CAA-C2A-C3A	-3.64	104.44	113.04
5	M	505	U10	C26-C27-C28	-3.63	101.23	111.62
7	M	504	BPH	CED-O2D-CGD	3.53	124.41	116.02
7	M	503	BPH	C2C-C1C-NC	-3.50	108.19	112.90
7	M	503	BPH	OBD-CAD-CBD	-3.49	120.67	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	504	U10	C16-C14-C13	3.47	127.77	121.08
4	M	501	BCL	C2C-C3C-C4C	3.46	105.85	101.05
7	M	504	BPH	C3C-C4C-CHD	3.44	128.98	121.83
7	M	504	BPH	C2C-C1C-NC	-3.41	108.31	112.90
7	M	503	BPH	O2A-CGA-CBA	3.40	122.64	111.94
4	M	502	BCL	O2A-CGA-CBA	3.39	122.59	111.94
7	M	504	BPH	CBC-CAC-C3C	3.31	121.76	113.61
5	L	504	U10	O2-C2-C3	-3.23	113.80	120.96
7	M	504	BPH	C11-C12-C13	-3.18	105.98	115.14
5	L	504	U10	C20-C19-C21	-3.17	110.57	115.39
4	L	502	BCL	O2A-CGA-CBA	3.15	121.84	111.94
4	L	501	BCL	CMD-C2D-C3D	3.14	129.91	124.97
7	M	504	BPH	O1D-CGD-CBD	-3.13	118.02	124.42
7	M	503	BPH	CAC-C3C-C2C	3.12	121.05	113.89
4	L	501	BCL	CMB-C2B-C1B	-3.11	123.83	128.62
4	M	501	BCL	O2D-CGD-O1D	-3.11	117.47	123.79
4	L	502	BCL	C3A-C4A-NA	-3.07	107.20	110.95
7	M	504	BPH	CMB-C2B-C1B	-3.05	124.00	128.65
10	M	800	CDL	OB8-CB6-CB4	3.03	116.78	108.83
4	L	502	BCL	CBB-CAB-C3B	-3.03	111.44	120.30
4	L	502	BCL	OBD-CAD-CBD	-3.00	121.41	125.94
4	L	502	BCL	C2B-C3B-CAB	2.99	137.65	127.43
4	M	501	BCL	C4B-CHC-C1C	-2.90	124.02	130.06
4	L	501	BCL	C4A-NA-C1A	2.90	110.52	106.52
4	M	501	BCL	OBB-CAB-CBB	-2.90	112.94	120.13
7	M	503	BPH	C3A-C4A-NA	-2.89	109.01	112.90
4	L	502	BCL	C4A-NA-C1A	2.87	110.48	106.52
7	M	504	BPH	CMB-C2B-C3B	2.87	129.49	124.97
4	L	501	BCL	C3C-C4C-NC	-2.86	107.92	111.60
4	M	501	BCL	CMD-C2D-C3D	2.86	129.47	124.97
7	M	503	BPH	C3C-C4C-CHD	2.86	127.77	121.83
7	M	503	BPH	C4-C3-C5	-2.84	111.08	115.39
4	L	502	BCL	O1D-CGD-CBD	-2.84	118.61	124.42
7	M	503	BPH	CMA-C3A-C4A	-2.83	103.93	112.94
4	L	502	BCL	CMB-C2B-C1B	-2.80	124.31	128.62
4	L	501	BCL	O2A-CGA-CBA	2.78	120.70	111.94
7	M	504	BPH	C17-C16-C15	2.76	127.16	113.02
5	M	505	U10	C25-C24-C26	-2.75	111.21	115.39
4	M	502	BCL	CED-O2D-CGD	2.74	122.54	116.02
4	M	502	BCL	C2C-C1C-NC	-2.74	107.61	110.95
10	M	800	CDL	CB6-CB4-CB3	-2.74	105.62	111.86
7	M	504	BPH	C3C-C4C-NC	-2.71	108.77	113.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	502	BCL	C4A-NA-C1A	2.70	110.25	106.52
4	M	501	BCL	CMA-C3A-C2A	-2.69	102.56	114.14
7	M	504	BPH	C11-C10-C8	2.69	122.90	115.14
4	M	502	BCL	OBD-CAD-CBD	-2.69	121.88	125.94
4	M	501	BCL	CGD-CBD-CHA	-2.66	101.91	110.96
4	M	502	BCL	C3C-C4C-NC	-2.66	108.18	111.60
5	L	504	U10	C7-C6-C5	-2.65	115.87	118.75
7	M	504	BPH	CMD-C2D-C3D	2.65	129.15	124.97
9	M	600	SPN	CM3-C5-C6	2.65	119.41	115.39
4	L	502	BCL	C4B-C3B-C2B	-2.63	103.78	106.97
7	M	504	BPH	O2A-CGA-O1A	-2.63	116.25	123.43
7	M	503	BPH	C3C-C4C-NC	-2.61	108.94	113.49
7	M	504	BPH	C2C-C3C-C4C	2.59	105.59	102.06
7	M	504	BPH	C5-C3-C2	-2.55	116.18	121.08
7	M	503	BPH	CED-O2D-CGD	2.51	121.99	116.02
4	M	502	BCL	C3A-C2A-C1A	2.48	104.58	101.08
4	M	501	BCL	C3C-C2C-C1C	2.48	105.21	101.40
7	M	503	BPH	CAA-C2A-C1A	-2.47	106.22	112.72
4	L	501	BCL	C4B-C3B-C2B	-2.44	104.01	106.97
7	M	504	BPH	CAA-C2A-C1A	-2.44	106.30	112.72
5	L	504	U10	C17-C18-C19	2.41	133.00	127.80
5	M	505	U10	C7-C8-C9	2.41	130.82	126.76
4	M	502	BCL	CMB-C2B-C1B	-2.40	124.93	128.62
4	M	502	BCL	C2D-C1D-ND	2.39	111.22	109.41
4	M	501	BCL	CMB-C2B-C3B	2.38	128.72	124.97
7	M	504	BPH	C3B-C4B-NB	2.38	109.78	107.10
4	L	501	BCL	CAC-C3C-C4C	-2.37	107.32	112.58
7	M	504	BPH	C14-C13-C12	2.35	119.64	111.02
7	M	504	BPH	C1D-C2D-C3D	-2.35	104.88	106.89
4	M	501	BCL	CHA-C1A-NA	-2.33	121.44	126.22
5	L	504	U10	C1-C6-C5	-2.31	117.35	120.26
5	L	504	U10	C12-C13-C14	-2.31	122.82	127.80
7	M	504	BPH	C3A-C4A-NA	-2.31	109.79	112.90
7	M	503	BPH	C3B-C4B-NB	2.31	109.71	107.10
5	L	504	U10	C21-C19-C18	2.31	125.52	121.08
4	M	502	BCL	C1-C2-C3	2.29	130.26	126.19
5	M	505	U10	C3M-O3-C3	2.29	124.26	116.48
4	M	501	BCL	C2D-C1D-ND	2.28	111.13	109.41
7	M	503	BPH	O1D-CGD-CBD	-2.27	119.77	124.42
4	L	502	BCL	C1-C2-C3	2.27	130.22	126.19
7	M	504	BPH	C3C-C2C-C1C	2.26	106.21	101.11
9	M	600	SPN	C7-C6-C5	2.26	120.22	112.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	501	BCL	O2A-CGA-O1A	-2.26	117.27	123.43
5	L	504	U10	C31-C32-C33	2.24	118.01	111.62
5	M	505	U10	C20-C19-C21	-2.23	111.99	115.39
7	M	504	BPH	C2A-C1A-NA	-2.23	109.29	112.61
4	M	501	BCL	C2A-C3A-C4A	2.21	104.80	101.40
4	L	502	BCL	C2A-C1A-NA	-2.21	108.80	111.24
7	M	504	BPH	C4A-NA-C1A	2.20	111.97	107.76
4	L	501	BCL	C2D-C1D-ND	2.20	111.07	109.41
5	L	504	U10	C15-C14-C13	-2.19	119.18	123.52
10	M	800	CDL	CA6-CA4-CA3	-2.19	106.88	111.86
7	M	504	BPH	C4-C3-C5	2.18	118.70	115.39
9	M	600	SPN	O1-C1-C2	-2.17	104.99	109.32
4	L	502	BCL	CED-O2D-CGD	2.17	121.19	116.02
4	M	502	BCL	C2A-C3A-C4A	2.17	104.74	101.40
5	M	505	U10	C31-C29-C28	-2.17	116.91	121.08
7	M	504	BPH	OBD-CAD-CBD	-2.15	122.69	125.94
7	M	504	BPH	CMA-C3A-C4A	-2.14	106.12	112.94
4	L	501	BCL	C2C-C1C-NC	-2.14	108.34	110.95
4	L	502	BCL	C2C-C3C-C4C	2.12	103.99	101.05
9	M	600	SPN	C15-C16-C17	2.12	121.27	113.28
7	M	503	BPH	O2A-C1-C2	-2.11	103.97	108.55
4	M	501	BCL	C1B-CHB-C4A	-2.11	125.68	130.06
5	M	505	U10	C4M-O4-C4	2.09	123.59	116.48
5	M	505	U10	C22-C23-C24	2.08	132.28	127.80
5	L	504	U10	O5-C5-C4	2.07	125.55	120.96
7	M	503	BPH	C2A-C3A-C4A	2.06	105.76	101.11
4	M	501	BCL	O1D-CGD-CBD	-2.06	120.21	124.42
7	M	504	BPH	CBD-CHA-C1A	2.06	128.97	123.62
7	M	503	BPH	CMB-C2B-C1B	-2.05	125.53	128.65
7	M	503	BPH	C3C-C2C-C1C	2.04	105.72	101.11
7	M	503	BPH	C2C-C3C-C4C	2.04	104.84	102.06
5	M	505	U10	C10-C9-C11	-2.04	112.29	115.39
4	L	501	BCL	OBD-CAD-CBD	-2.03	122.87	125.94
9	M	600	SPN	C11-C10-C9	2.02	119.42	112.74
6	H	703	LDA	O1-N1-CM2	2.01	111.72	109.01
7	M	504	BPH	C6-C7-C8	-2.01	109.35	115.14
10	M	800	CDL	OA8-CA7-OA9	-2.00	117.96	123.43

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	M	501	BCL	C8

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Mol	Chain	Res	Type	Atom
4	M	501	BCL	C13
7	M	503	BPH	C8
7	M	503	BPH	C13
10	M	800	CDL	CA4
4	L	501	BCL	C13
7	M	504	BPH	C13

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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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%)	-0.42	0 100 100	24, 43, 83, 99	0
2	M	302/314 (96%)	-0.38	1 (0%) 91 53	25, 51, 87, 109	0
3	H	240/260 (92%)	-0.34	2 (0%) 83 28	25, 48, 74, 109	0
All	All	823/855 (96%)	-0.38	3 (0%) 90 45	24, 47, 84, 109	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	249	LYS	2.3
2	M	1	ALA	2.2
3	H	250	SER	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	U10	L	504	48/63	0.50	10.19	76,89,95,96	0
6	LDA	M	704	16/16	0.34	7.48	90,97,121,122	0
6	LDA	M	701	16/16	0.24	5.33	57,75,79,82	0
10	CDL	M	800	81/100	0.37	5.07	25,68,82,85	81
6	LDA	L	709	16/16	0.62	3.53	104,109,119,120	0
9	SPN	M	600	43/43	0.30	2.83	44,64,91,94	0
5	U10	M	505	48/63	0.21	2.29	30,45,77,79	0
6	LDA	H	703	16/16	0.29	2.24	64,74,87,89	0
4	BCL	M	501	66/66	0.21	2.13	31,41,88,91	0
4	BCL	M	502	66/66	0.17	1.19	27,37,69,75	0
4	BCL	L	501	66/66	0.16	0.92	19,33,55,59	0
7	BPH	M	503	65/65	0.15	0.86	25,37,47,50	0
7	BPH	M	504	65/65	0.19	0.74	22,53,71,79	10
4	BCL	L	502	66/66	0.15	0.17	22,33,42,49	0
8	FE	M	500	1/1	0.10	-1.69	36,36,36,36	0

6.5 Other polymers ⓘ

There are no such residues in this entry.