



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2018 – 05:47 pm GMT

PDB ID : 1E6D  
Title : PHOTOSYNTHETIC REACTION CENTER MUTANT WITH TRP M115 REPLACED WITH PHE (CHAIN M, WM115F) PHE M197 REPLACED WITH ARG (CHAIN M, FM197R)  
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Deposited on : 2000-08-11  
Resolution : 2.30 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30686

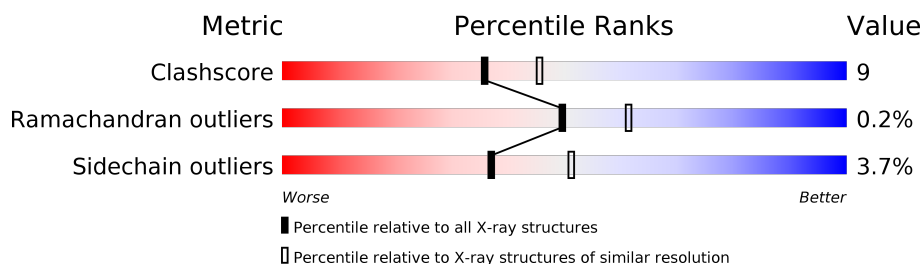
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
Clashscore	122078	5071 (2.30-2.30)
Ramachandran outliers	120005	5021 (2.30-2.30)
Sidechain outliers	119972	5020 (2.30-2.30)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	H	260	
2	L	281	
3	M	307	

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	PO4	M	1801	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	BCL	L	1304	X	-	-	-
5	BCL	M	1301	X	-	-	-
6	BPH	M	1401	X	-	-	-

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7334 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 PHOTOSYNTHETIC REACTION CENTER H SUBUNIT.

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

- Molecule 2 is a protein called PHOTOSYNTHETIC REACTION CENTER L SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	281	Total	C	N	O	S	0	0	0
			2232	1507	355	362	8			

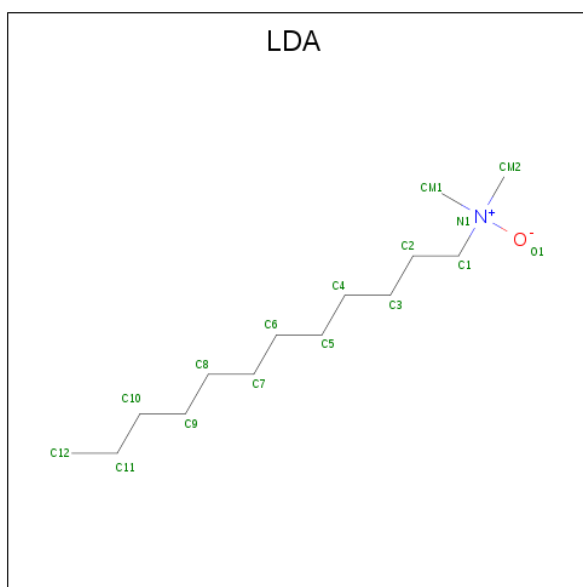
- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER M SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	302	Total	C	N	O	S	0	0	0
			2405	1602	396	397	10			

There are 2 discrepancies between the modelled and reference sequences:

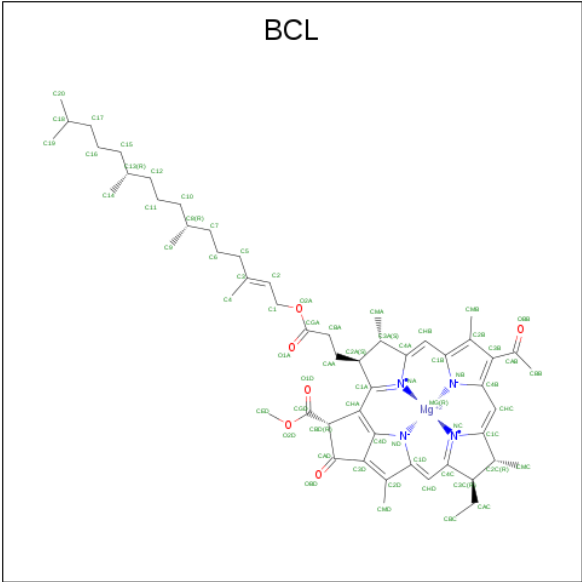
Chain	Residue	Modelled	Actual	Comment	Reference
M	197	ARG	PHE	engineered mutation	UNP P02953
M	115	PHE	TRP	engineered mutation	UNP P02953

- Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: C<sub>14</sub>H<sub>31</sub>NO).



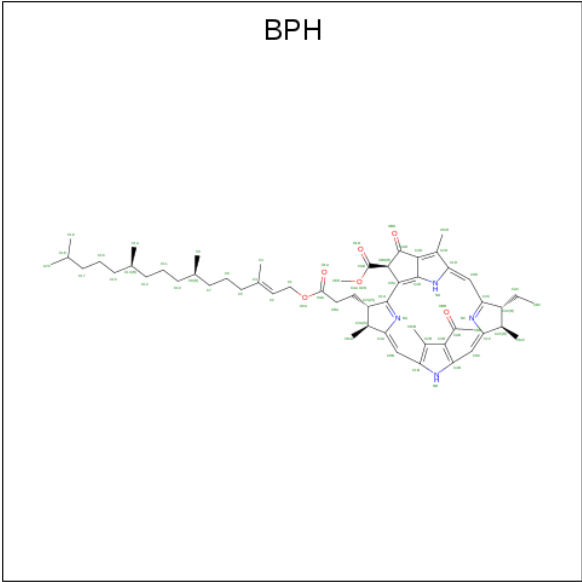
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	N	O	0	0
			16	14	1	1		
4	H	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 5 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula:  $C_{55}H_{74}MgN_4O_6$ ).



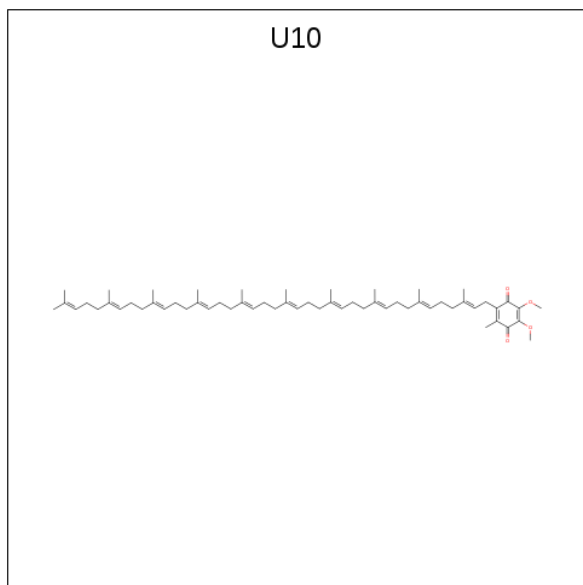
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 6 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: C<sub>55</sub>H<sub>76</sub>N<sub>4</sub>O<sub>6</sub>).



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

- Molecule 7 is UBIQUINONE-10 (three-letter code: U10) (formula: C<sub>59</sub>H<sub>90</sub>O<sub>4</sub>).

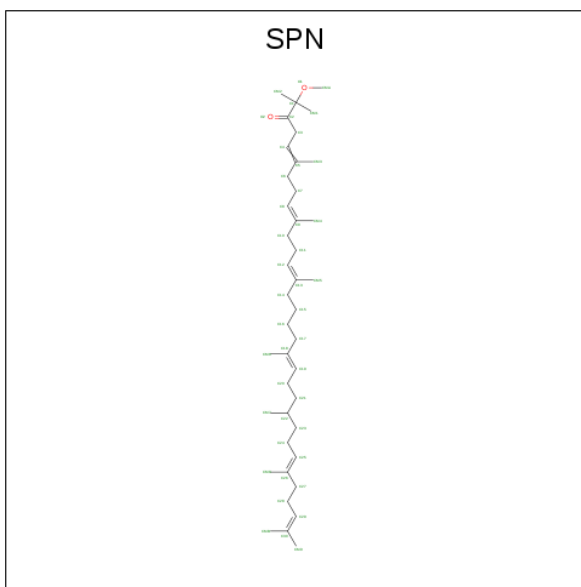


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	0	0
			48	44	4		
7	M	1	Total	C	O	0	0
			48	44	4		

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

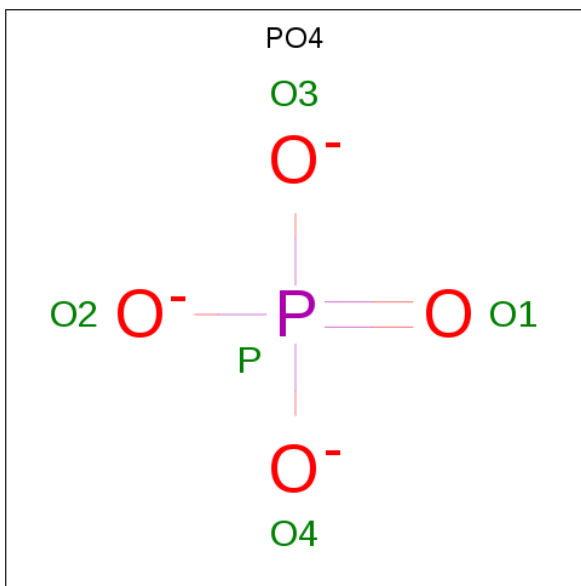
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	M	1	Total	Fe	0	0
			1	1		

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



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

- Molecule 10 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



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

- Molecule 11 is water.




Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	H	1	Total O 1 1	0	0
11	H	94	Total O 94 94	0	0
11	L	1	Total O 1 1	0	0
11	L	1	Total O 1 1	0	0
11	L	47	Total O 47 47	0	0
11	M	2	Total O 2 2	0	0
11	M	1	Total O 1 1	0	0
11	M	65	Total O 65 65	0	0

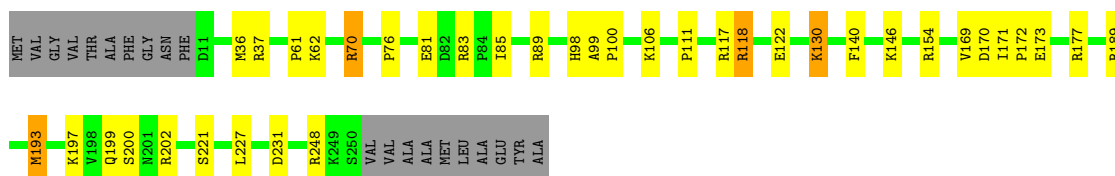
### 3 Residue-property plots [i](#)

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.


Note EDS was not executed.

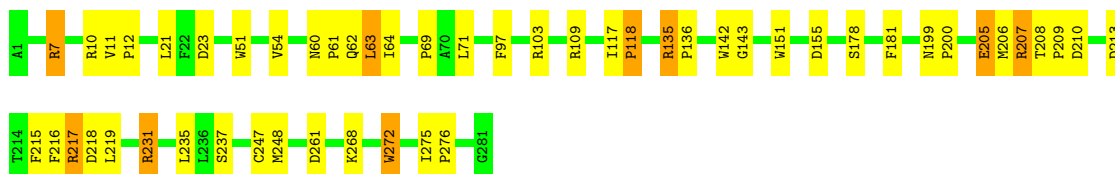
#### • Molecule 1: PHOTOSYNTHETIC REACTION CENTER H SUBUNIT

Chain H: 




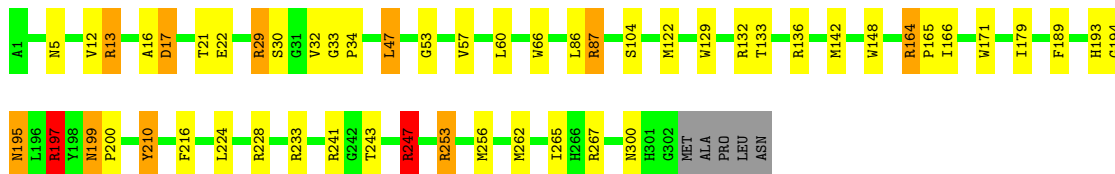
#### • Molecule 2: PHOTOSYNTHETIC REACTION CENTER L SUBUNIT

Chain L: 



#### • Molecule 3: PHOTOSYNTHETIC REACTION CENTER M SUBUNIT

Chain M: 



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	141.20Å 141.20Å 187.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	26.40 – 2.30	Depositor
% Data completeness (in resolution range)	94.5 (26.40-2.30)	Depositor
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.174 , 0.200	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7334	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

## 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, BPH, PO4, FE, SPN, U10

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	H	0.74	0/1877	1.29	14/2553 (0.5%)
2	L	0.73	1/2320 (0.0%)	1.12	15/3175 (0.5%)
3	M	0.70	0/2495	1.11	17/3404 (0.5%)
All	All	0.72	1/6692 (0.0%)	1.17	46/9132 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	237	SER	CA-CB	5.00	1.60	1.52

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	70	ARG	CD-NE-CZ	18.85	149.99	123.60
2	L	135	ARG	NE-CZ-NH2	-10.14	115.23	120.30
3	M	210	TYR	CB-CG-CD1	8.25	125.95	121.00
3	M	247	ARG	NE-CZ-NH2	7.74	124.17	120.30
1	H	117	ARG	NE-CZ-NH2	7.22	123.91	120.30
2	L	10	ARG	NE-CZ-NH2	7.18	123.89	120.30
1	H	154	ARG	NE-CZ-NH2	7.12	123.86	120.30
3	M	132	ARG	NE-CZ-NH2	7.01	123.80	120.30
2	L	135	ARG	CD-NE-CZ	6.93	133.30	123.60
2	L	109	ARG	NE-CZ-NH2	6.82	123.71	120.30
3	M	29	ARG	NE-CZ-NH2	6.76	123.68	120.30
3	M	197	ARG	NE-CZ-NH2	6.76	123.68	120.30
3	M	164	ARG	NE-CZ-NH2	6.66	123.63	120.30
3	M	87	ARG	NE-CZ-NH2	6.66	123.63	120.30
3	M	228	ARG	NE-CZ-NH2	6.61	123.61	120.30
3	M	233	ARG	NE-CZ-NH2	6.58	123.59	120.30
1	H	202	ARG	NE-CZ-NH2	6.48	123.54	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	210	TYR	CB-CG-CD2	-6.48	117.11	121.00
1	H	37	ARG	NE-CZ-NH2	6.48	123.54	120.30
1	H	177	ARG	NE-CZ-NH2	6.44	123.52	120.30
3	M	13	ARG	NE-CZ-NH2	6.44	123.52	120.30
3	M	136	ARG	NE-CZ-NH2	6.39	123.50	120.30
2	L	7	ARG	NE-CZ-NH2	6.36	123.48	120.30
2	L	103	ARG	NE-CZ-NH2	6.25	123.43	120.30
3	M	267	ARG	NE-CZ-NH2	6.24	123.42	120.30
1	H	189	ARG	NE-CZ-NH2	6.19	123.39	120.30
1	H	118	ARG	NE-CZ-NH2	6.19	123.39	120.30
3	M	241	ARG	NE-CZ-NH2	6.18	123.39	120.30
3	M	262	MET	CG-SD-CE	6.15	110.04	100.20
2	L	231	ARG	NE-CZ-NH2	6.14	123.37	120.30
1	H	193	MET	CA-CB-CG	6.10	123.67	113.30
2	L	135	ARG	NE-CZ-NH1	6.03	123.32	120.30
3	M	253	ARG	NE-CZ-NH2	6.02	123.31	120.30
2	L	237	SER	CA-CB-OG	-5.93	95.19	111.20
2	L	217	ARG	NE-CZ-NH2	5.92	123.26	120.30
1	H	89	ARG	NE-CZ-NH2	5.87	123.24	120.30
1	H	248	ARG	NE-CZ-NH2	5.81	123.21	120.30
2	L	205	GLU	OE1-CD-OE2	5.81	130.27	123.30
3	M	17	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	H	36	MET	CG-SD-CE	5.67	109.28	100.20
2	L	23	ASP	CB-CG-OD1	5.63	123.37	118.30
2	L	206	MET	CG-SD-CE	5.55	109.09	100.20
2	L	213	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	H	70	ARG	CG-CD-NE	5.41	123.17	111.80
2	L	118	PRO	N-CA-CB	5.30	109.66	103.30
1	H	130	LYS	CB-CG-CD	5.15	124.99	111.60

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1829	0	1836	17	0
2	L	2232	0	2187	36	0
3	M	2405	0	2324	44	0
4	H	32	0	62	0	0
4	M	80	0	155	11	0
5	L	132	0	148	5	0
5	M	132	0	148	14	0
6	L	65	0	75	6	0
6	M	65	0	76	10	0
7	L	48	0	63	9	0
7	M	48	0	63	3	0
8	M	1	0	0	0	0
9	M	43	0	69	2	0
10	M	10	0	0	3	0
11	H	95	0	0	1	0
11	L	49	0	0	8	0
11	M	68	0	0	1	0
All	All	7334	0	7206	124	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 9.

All (124) 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)
3:M:243:THR:O	3:M:247:ARG:HG2	1.58	1.02
5:M:1303:BCL:H191	4:M:1706:LDA:H121	1.47	0.97
6:L:1402:BPH:HHC	6:L:1402:BPH:HBB3	1.51	0.93
2:L:215:PHE:HB2	3:M:142:MET:HE1	1.50	0.93
4:M:1701:LDA:H91	4:M:1702:LDA:H121	1.54	0.88
7:L:1502:U10:H4M1	11:L:3004:HOH:O	1.75	0.85
1:H:171:ILE:HB	1:H:172:PRO:HD3	1.59	0.83
5:M:1303:BCL:C19	4:M:1706:LDA:H121	2.14	0.77
3:M:243:THR:OG1	3:M:247:ARG:HD3	1.85	0.76
2:L:261:ASP:OD2	11:L:2047:HOH:O	2.05	0.73
5:L:1302:BCL:CBB	5:L:1302:BCL:HMB1	2.19	0.72
2:L:231:ARG:HD3	3:M:5:ASN:O	1.89	0.72
3:M:189:PHE:O	3:M:193:HIS:HD2	1.73	0.71
1:H:197:LYS:HE2	1:H:199:GLN:HE21	1.55	0.70
2:L:69:PRO:HG2	2:L:142:TRP:HB2	1.72	0.70
4:M:1701:LDA:H91	4:M:1702:LDA:C12	2.21	0.70
3:M:148:TRP:CD1	4:M:1703:LDA:HM22	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:217:ARG:NH1	11:L:2037:HOH:O	2.24	0.70
2:L:272:TRP:CD1	3:M:87:ARG:HG3	2.28	0.68
3:M:199:ASN:HD22	3:M:199:ASN:C	1.98	0.67
7:L:1502:U10:H3M3	11:L:2041:HOH:O	1.96	0.66
2:L:215:PHE:HB2	3:M:142:MET:CE	2.25	0.66
6:L:1402:BPH:CHC	6:L:1402:BPH:HBB3	2.26	0.65
6:M:1401:BPH:HHC	6:M:1401:BPH:HBB3	1.80	0.64
5:M:1301:BCL:H141	9:M:1600:SPN:H101	1.79	0.64
1:H:146:LYS:NZ	1:H:200:SER:O	2.31	0.63
6:L:1402:BPH:HBB2	3:M:210:TYR:HB3	1.81	0.62
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.81	0.62
3:M:243:THR:O	3:M:247:ARG:CG	2.43	0.61
2:L:208:THR:HB	2:L:209:PRO:HD2	1.81	0.61
3:M:60:LEU:HA	6:M:1401:BPH:H4C2	1.84	0.60
4:M:1703:LDA:CM2	10:M:1801:PO4:O3	2.50	0.59
3:M:148:TRP:HD1	4:M:1703:LDA:HM22	1.65	0.59
5:M:1301:BCL:HMB1	5:M:1301:BCL:HBB2	1.85	0.59
5:L:1302:BCL:HMB1	5:L:1302:BCL:HBB3	1.84	0.58
2:L:71:LEU:HD23	2:L:143:GLY:HA3	1.85	0.58
2:L:60:ASN:O	2:L:64:ILE:HG13	2.05	0.56
7:L:1502:U10:H3M1	11:L:2036:HOH:O	2.05	0.56
5:M:1301:BCL:CBB	5:M:1301:BCL:HMB1	2.36	0.55
6:L:1402:BPH:HHC	6:L:1402:BPH:CBB	2.32	0.54
2:L:218:ASP:OD1	3:M:29:ARG:HD3	2.07	0.54
2:L:231:ARG:HG2	3:M:224:LEU:HD21	1.90	0.54
3:M:265:ILE:HG21	7:M:1501:U10:H3M2	1.90	0.54
1:H:118:ARG:HD2	11:H:2055:HOH:O	2.08	0.53
5:M:1303:BCL:HBB3	5:M:1303:BCL:HMB1	1.89	0.53
3:M:189:PHE:O	3:M:193:HIS:CD2	2.59	0.53
4:M:1703:LDA:HM11	10:M:1800:PO4:O4	2.10	0.52
2:L:60:ASN:OD1	2:L:61:PRO:HD2	2.10	0.52
3:M:164:ARG:HB3	3:M:165:PRO:HD3	1.91	0.52
3:M:32:VAL:HG12	3:M:33:GLY:O	2.09	0.52
2:L:181:PHE:CD2	6:M:1401:BPH:HBB1	2.45	0.52
5:L:1302:BCL:HBB2	5:L:1302:BCL:HMB1	1.92	0.52
3:M:66:TRP:CD1	3:M:122:MET:HB2	2.46	0.51
2:L:207:ARG:HD2	2:L:207:ARG:N	2.26	0.50
3:M:194:GLY:O	3:M:195:ASN:HB3	2.10	0.50
5:M:1301:BCL:H102	5:M:1303:BCL:H202	1.93	0.50
7:L:1502:U10:C3M	11:L:2041:HOH:O	2.56	0.50
6:M:1401:BPH:HHH	6:M:1401:BPH:HBC3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:1502:U10:H202	5:M:1301:BCL:H43	1.94	0.49
2:L:135:ARG:HD2	2:L:248:MET:O	2.12	0.49
1:H:173:GLU:HG2	11:L:2042:HOH:O	2.11	0.49
1:H:169:VAL:HG23	1:H:171:ILE:HD13	1.93	0.49
1:H:171:ILE:HB	1:H:172:PRO:CD	2.37	0.49
5:L:1304:BCL:OBB	5:L:1304:BCL:HHC	2.13	0.49
2:L:219:LEU:HD11	3:M:133:THR:HG22	1.95	0.49
3:M:129:TRP:CH2	4:M:1706:LDA:H102	2.49	0.48
5:M:1301:BCL:C3B	9:M:1600:SPN:H152	2.43	0.48
2:L:272:TRP:NE1	3:M:87:ARG:HG3	2.29	0.48
2:L:181:PHE:HB3	6:M:1401:BPH:CBB	2.44	0.47
1:H:111:PRO:O	3:M:247:ARG:NH2	2.44	0.47
7:L:1502:U10:H301	7:L:1502:U10:H322	1.41	0.47
2:L:200:PRO:HB3	2:L:207:ARG:HD3	1.97	0.47
2:L:178:SER:HB3	7:L:1502:U10:H222	1.97	0.47
2:L:215:PHE:CD1	3:M:142:MET:HE3	2.51	0.46
1:H:62:LYS:NZ	2:L:199:ASN:HD21	2.14	0.46
3:M:129:TRP:O	3:M:133:THR:HG23	2.16	0.46
6:L:1402:BPH:CHC	6:L:1402:BPH:CBB	2.91	0.46
1:H:140:PHE:HA	3:M:13:ARG:O	2.16	0.46
6:M:1401:BPH:CHC	6:M:1401:BPH:HBB3	2.45	0.46
3:M:166:ILE:HD11	3:M:171:TRP:CH2	2.51	0.45
2:L:117:ILE:HB	2:L:118:PRO:HD3	1.98	0.45
6:M:1401:BPH:H192	6:M:1401:BPH:H161	1.61	0.45
5:M:1301:BCL:H152	5:M:1301:BCL:H111	1.69	0.45
7:L:1502:U10:H1M1	7:L:1502:U10:C8	2.45	0.45
4:M:1706:LDA:H123	4:M:1706:LDA:H92	1.52	0.45
1:H:98:HIS:HD2	2:L:7:ARG:HH21	1.65	0.45
2:L:97:PHE:CE1	5:L:1302:BCL:H121	2.51	0.45
1:H:61:PRO:HA	1:H:76:PRO:HD2	2.00	0.44
1:H:81:GLU:HG3	1:H:85:ILE:HD11	1.99	0.44
2:L:62:GLN:HB2	2:L:151:TRP:CD1	2.52	0.44
3:M:148:TRP:HA	3:M:148:TRP:CE3	2.53	0.44
3:M:256:MET:CE	7:M:1501:U10:H102	2.47	0.44
3:M:199:ASN:HD22	3:M:200:PRO:N	2.15	0.43
3:M:247:ARG:HG2	3:M:247:ARG:H	1.54	0.43
1:H:122:GLU:HB2	1:H:227:LEU:HD21	2.01	0.43
3:M:265:ILE:HD12	3:M:265:ILE:HA	1.85	0.43
3:M:300:ASN:N	3:M:300:ASN:OD1	2.50	0.43
1:H:130:LYS:HE3	1:H:170:ASP:OD1	2.19	0.43
6:L:1402:BPH:H3A	6:L:1402:BPH:HBA2	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:1401:BPH:HHD	6:M:1401:BPH:CBC	2.49	0.43
3:M:34:PRO:O	3:M:47:LEU:HB2	2.18	0.43
7:L:1502:U10:H272	7:L:1502:U10:H251	1.43	0.42
2:L:155:ASP:OD1	3:M:197:ARG:NH1	2.37	0.42
2:L:51:TRP:O	2:L:54:VAL:HG22	2.20	0.42
3:M:53:GLY:O	3:M:57:VAL:HG23	2.20	0.42
7:M:1501:U10:H322	7:M:1501:U10:H28	1.73	0.41
2:L:205:GLU:OE2	11:L:2032:HOH:O	2.21	0.41
5:M:1301:BCL:H141	5:M:1301:BCL:H162	1.84	0.41
2:L:275:ILE:HA	2:L:276:PRO:HD3	1.91	0.41
4:M:1703:LDA:HM23	10:M:1801:PO4:P	2.61	0.41
3:M:179:ILE:HG23	5:M:1301:BCL:HED1	2.01	0.41
3:M:17:ASP:OD2	11:M:2016:HOH:O	2.22	0.41
3:M:164:ARG:N	3:M:165:PRO:HD2	2.35	0.41
3:M:16:ALA:HB1	3:M:32:VAL:HG21	2.03	0.41
3:M:21:THR:O	3:M:22:GLU:C	2.57	0.41
1:H:98:HIS:CD2	2:L:7:ARG:HH21	2.38	0.41
2:L:181:PHE:HB3	6:M:1401:BPH:HBB2	2.03	0.41
6:M:1401:BPH:CHD	6:M:1401:BPH:HBC3	2.50	0.41
2:L:11:VAL:HB	2:L:12:PRO:HD2	2.02	0.41
5:M:1301:BCL:H101	5:M:1301:BCL:H61	1.68	0.41
2:L:63:LEU:HD12	2:L:63:LEU:HA	1.88	0.40
1:H:99:ALA:HA	1:H:100:PRO:HD3	1.87	0.40
3:M:194:GLY:O	3:M:195:ASN:CB	2.69	0.40
5:M:1301:BCL:H3A	5:M:1301:BCL:HBA1	1.92	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	H	238/260 (92%)	233 (98%)	5 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	279/281 (99%)	271 (97%)	8 (3%)	0	100	100
3	M	300/307 (98%)	290 (97%)	8 (3%)	2 (1%)	24	29
All	All	817/848 (96%)	794 (97%)	21 (3%)	2 (0%)	49	61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	30	SER
3	M	195	ASN

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	195/208 (94%)	189 (97%)	6 (3%)	43	59
2	L	220/220 (100%)	211 (96%)	9 (4%)	33	46
3	M	236/240 (98%)	227 (96%)	9 (4%)	36	50
All	All	651/668 (98%)	627 (96%)	24 (4%)	37	51

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	70	ARG
1	H	83	ARG
1	H	106	LYS
1	H	193	MET
1	H	221	SER
1	H	231	ASP
2	L	21	LEU
2	L	63	LEU
2	L	207	ARG
2	L	210	ASP
2	L	216	PHE
2	L	235	LEU

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Mol	Chain	Res	Type
2	L	247	CYS
2	L	268	LYS
2	L	272	TRP
3	M	12	VAL
3	M	47	LEU
3	M	86	LEU
3	M	104	SER
3	M	197	ARG
3	M	199	ASN
3	M	216	PHE
3	M	247	ARG
3	M	253	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	98	HIS
2	L	183	ASN
2	L	199	ASN
3	M	28	ASN
3	M	187	ASN
3	M	193	HIS
3	M	199	ASN
3	M	299	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	LDA	H	1704	-	12,15,15	2.15	1 (8%)	14,17,17	0.95	1 (7%)
4	LDA	H	1707	-	12,15,15	2.17	1 (8%)	14,17,17	0.72	0
5	BCL	L	1302	2	58,74,74	1.65	8 (13%)	66,115,115	2.06	22 (33%)
5	BCL	L	1304	2	58,74,74	1.72	9 (15%)	66,115,115	2.32	20 (30%)
6	BPH	L	1402	-	65,70,70	1.48	9 (13%)	75,101,101	2.06	22 (29%)
7	U10	L	1502	-	48,48,63	2.01	16 (33%)	56,61,79	1.64	10 (17%)
5	BCL	M	1301	3	58,74,74	1.75	8 (13%)	66,115,115	2.16	21 (31%)
5	BCL	M	1303	3	58,74,74	1.63	9 (15%)	66,115,115	1.92	18 (27%)
6	BPH	M	1401	-	65,70,70	1.37	10 (15%)	75,101,101	2.15	20 (26%)
7	U10	M	1501	-	48,48,63	1.86	15 (31%)	56,61,79	1.52	8 (14%)
9	SPN	M	1600	-	40,42,42	3.70	18 (45%)	51,52,52	2.37	19 (37%)
4	LDA	M	1701	-	12,15,15	2.16	1 (8%)	14,17,17	0.92	1 (7%)
4	LDA	M	1702	-	12,15,15	2.39	1 (8%)	14,17,17	0.75	0
4	LDA	M	1703	-	12,15,15	2.17	1 (8%)	14,17,17	1.04	1 (7%)
4	LDA	M	1705	-	12,15,15	2.13	1 (8%)	14,17,17	0.77	0
4	LDA	M	1706	-	12,15,15	2.35	1 (8%)	14,17,17	0.95	0
10	PO4	M	1800	-	4,4,4	3.25	1 (25%)	6,6,6	1.64	1 (16%)
10	PO4	M	1801	-	4,4,4	2.25	1 (25%)	6,6,6	1.13	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LDA	H	1704	-	-	0/13/13/13	0/0/0/0
4	LDA	H	1707	-	-	0/13/13/13	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BCL	L	1302	2	-	0/37/137/137	0/0/9/9
5	BCL	L	1304	2	1/1/21/25	0/37/137/137	0/0/9/9
6	BPH	L	1402	-	-	0/52/105/105	0/5/6/6
7	U10	L	1502	-	-	0/45/69/87	0/1/1/1
5	BCL	M	1301	3	1/1/21/25	0/37/137/137	0/0/9/9
5	BCL	M	1303	3	-	0/37/137/137	0/0/9/9
6	BPH	M	1401	-	1/1/18/22	0/52/105/105	0/5/6/6
7	U10	M	1501	-	-	0/45/69/87	0/1/1/1
9	SPN	M	1600	-	-	0/50/51/51	0/0/0/0
4	LDA	M	1701	-	-	0/13/13/13	0/0/0/0
4	LDA	M	1702	-	-	0/13/13/13	0/0/0/0
4	LDA	M	1703	-	-	0/13/13/13	0/0/0/0
4	LDA	M	1705	-	-	0/13/13/13	0/0/0/0
4	LDA	M	1706	-	-	0/13/13/13	0/0/0/0
10	PO4	M	1800	-	-	0/0/0/0	0/0/0/0
10	PO4	M	1801	-	-	0/0/0/0	0/0/0/0

All (111) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	1702	LDA	O1-N1	-8.23	1.22	1.42
4	M	1706	LDA	O1-N1	-8.04	1.22	1.42
4	M	1703	LDA	O1-N1	-7.47	1.23	1.42
4	H	1707	LDA	O1-N1	-7.45	1.23	1.42
4	M	1701	LDA	O1-N1	-7.43	1.23	1.42
4	H	1704	LDA	O1-N1	-7.40	1.24	1.42
4	M	1705	LDA	O1-N1	-7.34	1.24	1.42
9	M	1600	SPN	C3-C4	-5.96	1.41	1.50
9	M	1600	SPN	C10-C9	-5.91	1.38	1.51
7	L	1502	U10	C7-C8	-5.89	1.41	1.50
9	M	1600	SPN	C14-C13	-5.31	1.39	1.51
9	M	1600	SPN	C6-C5	-5.14	1.40	1.51
9	M	1600	SPN	C17-C18	-4.96	1.40	1.51
7	L	1502	U10	O4-C4M	-3.68	1.36	1.45
7	M	1501	U10	C7-C8	-3.28	1.45	1.50
6	L	1402	BPH	O2D-CED	-3.26	1.37	1.45
6	M	1401	BPH	O2D-CED	-3.18	1.37	1.45
7	M	1501	U10	O3-C3M	-3.10	1.37	1.45
9	M	1600	SPN	C20-C19	-2.90	1.40	1.50
9	M	1600	SPN	C11-C12	-2.88	1.40	1.50
9	M	1600	SPN	C7-C8	-2.87	1.40	1.50
5	M	1301	BCL	C2C-C3C	-2.71	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	1402	BPH	CAC-C3C	-2.67	1.48	1.53
7	L	1502	U10	O3-C3M	-2.62	1.39	1.45
5	M	1303	BCL	O2D-CED	-2.58	1.39	1.45
9	M	1600	SPN	C21-C22	-2.51	1.38	1.52
5	L	1304	BCL	C3B-C2B	-2.48	1.34	1.39
5	M	1303	BCL	C2C-C3C	-2.48	1.47	1.54
5	L	1302	BCL	C2C-C3C	-2.38	1.47	1.54
6	M	1401	BPH	C2C-C3C	-2.36	1.47	1.54
9	M	1600	SPN	C16-C15	-2.27	1.38	1.51
6	L	1402	BPH	C2C-C3C	-2.24	1.48	1.54
7	M	1501	U10	O4-C4M	-2.14	1.40	1.45
5	L	1302	BCL	O2D-CED	-2.09	1.40	1.45
7	L	1502	U10	C16-C14	2.02	1.55	1.51
7	M	1501	U10	C35-C34	2.03	1.55	1.50
7	M	1501	U10	C7-C6	2.03	1.54	1.51
6	M	1401	BPH	C2-C3	2.04	1.38	1.33
7	L	1502	U10	C23-C24	2.05	1.38	1.33
9	M	1600	SPN	O1-C1	2.07	1.51	1.41
7	L	1502	U10	C15-C14	2.08	1.56	1.50
5	M	1303	BCL	O1D-CGD	2.09	1.26	1.21
7	L	1502	U10	C36-C34	2.11	1.55	1.51
5	L	1302	BCL	C4-C3	2.11	1.56	1.50
5	L	1304	BCL	CAC-C3C	2.13	1.58	1.53
6	M	1401	BPH	CMA-C3A	2.17	1.58	1.53
6	M	1401	BPH	O1D-CGD	2.18	1.26	1.21
7	L	1502	U10	C25-C24	2.21	1.56	1.50
5	L	1304	BCL	O1D-CGD	2.23	1.26	1.21
7	L	1502	U10	C13-C14	2.23	1.38	1.33
7	M	1501	U10	C20-C19	2.27	1.56	1.50
7	M	1501	U10	C18-C19	2.30	1.38	1.33
5	M	1303	BCL	C4-C3	2.30	1.56	1.50
6	L	1402	BPH	OBB-CAB	2.31	1.28	1.23
5	L	1304	BCL	O2A-CGA	2.34	1.40	1.33
5	L	1302	BCL	O2A-CGA	2.38	1.40	1.33
6	L	1402	BPH	CAA-C2A	2.46	1.58	1.54
6	M	1401	BPH	OBB-CAB	2.50	1.28	1.23
6	M	1401	BPH	C4C-NC	2.50	1.42	1.37
6	L	1402	BPH	C2-C3	2.52	1.39	1.33
5	L	1304	BCL	CAA-C2A	2.59	1.59	1.54
7	M	1501	U10	C31-C29	2.63	1.57	1.51
7	M	1501	U10	C8-C9	2.65	1.39	1.33
6	M	1401	BPH	C3D-C4D	2.67	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	1303	BCL	C2-C3	2.67	1.39	1.33
7	L	1502	U10	C33-C34	2.68	1.39	1.33
7	M	1501	U10	C13-C14	2.76	1.39	1.33
7	M	1501	U10	C38-C39	2.79	1.40	1.32
7	L	1502	U10	C38-C39	2.81	1.40	1.32
5	L	1302	BCL	C2-C3	2.87	1.40	1.33
6	L	1402	BPH	CMA-C3A	2.87	1.59	1.53
5	M	1301	BCL	C2-C3	2.90	1.40	1.33
5	M	1303	BCL	O2A-CGA	2.93	1.41	1.33
7	L	1502	U10	C28-C29	3.03	1.40	1.33
7	L	1502	U10	C18-C19	3.04	1.40	1.33
9	M	1600	SPN	C29-C30	3.05	1.41	1.32
6	M	1401	BPH	O2A-CGA	3.19	1.42	1.33
7	L	1502	U10	C8-C9	3.21	1.40	1.33
7	M	1501	U10	O4-C4	3.29	1.45	1.36
5	M	1301	BCL	CAA-C2A	3.34	1.60	1.54
5	M	1301	BCL	CMA-C3A	3.37	1.60	1.53
5	L	1304	BCL	C2-C3	3.42	1.41	1.33
9	M	1600	SPN	O1-CMA	3.50	1.54	1.43
6	L	1402	BPH	O2A-CGA	3.57	1.43	1.33
9	M	1600	SPN	C25-C26	3.57	1.41	1.33
7	M	1501	U10	C23-C24	3.59	1.41	1.33
7	L	1502	U10	O4-C4	3.63	1.45	1.36
5	M	1301	BCL	O2A-CGA	3.68	1.44	1.33
7	L	1502	U10	O3-C3	3.74	1.46	1.36
7	M	1501	U10	C33-C34	3.96	1.42	1.33
6	M	1401	BPH	O2D-CGD	3.99	1.43	1.33
10	M	1801	PO4	P-O1	4.41	1.60	1.50
7	M	1501	U10	O3-C3	4.62	1.48	1.36
5	M	1303	BCL	CHB-C4A	4.74	1.39	1.33
5	L	1302	BCL	CHB-C4A	4.81	1.39	1.33
5	L	1302	BCL	O2D-CGD	4.84	1.45	1.33
5	M	1301	BCL	O2D-CGD	5.03	1.45	1.33
5	L	1304	BCL	O2D-CGD	5.13	1.46	1.33
5	M	1301	BCL	CHB-C4A	5.15	1.39	1.33
5	M	1303	BCL	O2D-CGD	5.23	1.46	1.33
6	L	1402	BPH	O2D-CGD	5.35	1.46	1.33
5	L	1304	BCL	CHB-C4A	5.49	1.39	1.33
5	L	1304	BCL	CHC-C1C	5.60	1.40	1.33
10	M	1800	PO4	P-O1	6.19	1.65	1.50
5	M	1303	BCL	CHC-C1C	6.41	1.40	1.33
5	M	1301	BCL	CHC-C1C	6.56	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	1302	BCL	CHC-C1C	7.12	1.41	1.33
9	M	1600	SPN	C19-C18	7.81	1.52	1.33
9	M	1600	SPN	C12-C13	8.21	1.53	1.33
9	M	1600	SPN	C4-C5	8.70	1.54	1.33
9	M	1600	SPN	C8-C9	9.38	1.56	1.33

All (164) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	1402	BPH	O2D-CGD-O1D	-5.59	112.73	123.82
6	M	1401	BPH	O1D-CGD-CBD	-5.50	114.37	124.58
5	M	1303	BCL	CAC-C3C-C4C	-5.43	100.52	112.58
9	M	1600	SPN	C10-C9-C8	-5.26	110.39	121.10
5	L	1304	BCL	C4B-C3B-CAB	-5.15	117.19	127.13
5	L	1304	BCL	O1D-CGD-CBD	-5.10	115.13	124.58
9	M	1600	SPN	C7-C8-C9	-4.91	115.50	127.66
5	M	1301	BCL	CMB-C2B-C1B	-4.75	121.17	128.46
9	M	1600	SPN	C3-C4-C5	-4.73	118.78	126.79
9	M	1600	SPN	C6-C5-C4	-4.71	111.52	121.10
6	M	1401	BPH	O2D-CGD-O1D	-4.62	114.65	123.82
5	L	1304	BCL	CMB-C2B-C1B	-4.47	121.59	128.46
5	L	1302	BCL	CAC-C3C-C4C	-4.32	103.00	112.58
5	M	1301	BCL	O2A-CGA-O1A	-4.21	113.31	123.58
6	L	1402	BPH	O2A-CGA-O1A	-4.13	113.49	123.58
5	M	1301	BCL	O2D-CGD-O1D	-4.09	115.70	123.82
5	M	1303	BCL	C4B-C3B-CAB	-4.04	119.33	127.13
9	M	1600	SPN	C17-C18-C19	-3.94	113.08	121.10
5	L	1304	BCL	CAC-C3C-C4C	-3.90	103.92	112.58
5	L	1302	BCL	OBD-CAD-CBD	-3.71	120.46	125.91
5	M	1301	BCL	CAA-C2A-C3A	-3.65	102.81	112.81
6	L	1402	BPH	OBD-CAD-CBD	-3.63	120.58	125.91
5	M	1301	BCL	OBD-CAD-CBD	-3.57	120.67	125.91
9	M	1600	SPN	C14-C13-C12	-3.44	114.10	121.10
5	L	1304	BCL	C1B-CHB-C4A	-3.36	123.47	130.12
5	M	1303	BCL	O1D-CGD-CBD	-3.33	118.41	124.58
5	L	1304	BCL	CAA-C2A-C3A	-3.32	103.72	112.81
5	M	1303	BCL	O2D-CGD-O1D	-3.30	117.27	123.82
5	L	1304	BCL	CAC-C3C-C2C	-3.27	106.01	114.24
5	L	1302	BCL	CAA-C2A-C3A	-3.26	103.88	112.81
4	H	1704	LDA	CM2-N1-CM1	-3.25	105.72	110.91
9	M	1600	SPN	C20-C19-C18	-3.23	119.66	127.66
5	L	1304	BCL	O2D-CGD-O1D	-3.16	117.56	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	1303	BCL	C4B-CHC-C1C	-3.12	123.94	130.12
5	L	1302	BCL	OBB-CAB-CBB	-3.08	113.22	120.15
5	L	1302	BCL	O2D-CGD-O1D	-3.08	117.72	123.82
9	M	1600	SPN	C11-C12-C13	-3.07	120.06	127.66
4	M	1703	LDA	CM2-N1-CM1	-3.06	106.03	110.91
6	L	1402	BPH	CMA-C3A-C4A	-3.02	103.30	112.37
7	M	1501	U10	C22-C23-C24	-2.97	120.30	127.66
5	M	1301	BCL	CMA-C3A-C2A	-2.97	101.79	113.81
5	L	1302	BCL	O2A-CGA-O1A	-2.92	116.46	123.58
10	M	1800	PO4	O2-P-O1	-2.92	98.47	110.93
5	M	1301	BCL	C4B-C3B-CAB	-2.85	121.62	127.13
7	L	1502	U10	C25-C24-C26	-2.77	110.50	115.29
7	L	1502	U10	C35-C34-C36	-2.77	110.51	115.29
5	M	1301	BCL	CAC-C3C-C4C	-2.76	106.46	112.58
5	M	1303	BCL	CMB-C2B-C1B	-2.76	124.22	128.46
6	L	1402	BPH	O1D-CGD-CBD	-2.74	119.50	124.58
6	M	1401	BPH	OBD-CAD-CBD	-2.74	121.89	125.91
6	L	1402	BPH	C4D-CHA-C1A	-2.73	123.78	130.51
5	M	1301	BCL	C1B-CHB-C4A	-2.71	124.74	130.12
4	M	1701	LDA	CM2-N1-CM1	-2.58	106.80	110.91
9	M	1600	SPN	C24-C23-C22	-2.54	108.67	116.23
6	L	1402	BPH	C3A-C4A-NA	-2.54	108.68	113.06
5	L	1302	BCL	CAC-C3C-C2C	-2.54	107.86	114.24
5	L	1302	BCL	C4B-C3B-CAB	-2.49	122.32	127.13
6	M	1401	BPH	CAA-C2A-C3A	-2.48	106.00	112.81
5	M	1301	BCL	OBB-CAB-CBB	-2.47	114.59	120.15
5	L	1302	BCL	CMA-C3A-C2A	-2.45	103.90	113.81
5	M	1303	BCL	O2A-CGA-O1A	-2.44	117.64	123.58
6	L	1402	BPH	CMA-C3A-C2A	-2.42	104.00	113.81
6	M	1401	BPH	CMA-C3A-C2A	-2.41	104.05	113.81
7	L	1502	U10	C15-C14-C16	-2.37	111.20	115.29
6	L	1402	BPH	C4-C3-C5	-2.35	111.23	115.29
6	M	1401	BPH	C4D-CHA-C1A	-2.33	124.76	130.51
6	M	1401	BPH	O2A-CGA-O1A	-2.31	117.95	123.58
6	M	1401	BPH	C4B-C3B-CAB	-2.30	121.98	130.22
7	M	1501	U10	C15-C14-C16	-2.28	111.35	115.29
5	M	1301	BCL	CMA-C3A-C4A	-2.26	105.71	111.77
6	L	1402	BPH	CAA-C2A-C3A	-2.24	106.67	112.81
7	M	1501	U10	C30-C29-C31	-2.23	111.43	115.29
6	L	1402	BPH	C4B-C3B-CAB	-2.21	122.28	130.22
5	L	1304	BCL	C1D-CHD-C4C	-2.19	122.65	125.92
5	L	1302	BCL	O1D-CGD-CBD	-2.18	120.53	124.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1304	BCL	C4B-CHC-C1C	-2.16	125.83	130.12
5	L	1302	BCL	CMB-C2B-C1B	-2.14	125.17	128.46
5	M	1301	BCL	CED-O2D-CGD	-2.14	111.04	115.97
6	M	1401	BPH	C4-C3-C5	-2.08	111.69	115.29
5	L	1302	BCL	C4B-CHC-C1C	-2.08	125.99	130.12
5	M	1303	BCL	C7-C6-C5	-2.08	107.51	113.17
6	M	1401	BPH	CMA-C3A-C4A	-2.05	106.22	112.37
9	M	1600	SPN	CM4-C9-C8	-2.04	118.34	123.70
5	M	1303	BCL	OBB-CAB-CBB	-2.01	115.62	120.15
5	L	1304	BCL	C3A-C2A-C1A	2.06	104.42	101.34
5	M	1303	BCL	C2C-C3C-C4C	2.11	104.50	101.34
5	L	1302	BCL	CMD-C2D-C3D	2.13	128.75	124.88
5	M	1303	BCL	CMB-C2B-C3B	2.13	128.76	124.88
6	M	1401	BPH	C1-C2-C3	2.20	130.01	125.96
6	L	1402	BPH	C2A-C3A-C4A	2.25	105.83	101.33
5	L	1302	BCL	CHC-C1C-NC	2.26	127.64	124.51
7	M	1501	U10	C30-C29-C28	2.27	129.65	123.70
6	L	1402	BPH	C3C-C2C-C1C	2.27	105.53	101.87
5	L	1302	BCL	C3C-C2C-C1C	2.27	105.53	101.87
5	M	1303	BCL	CHC-C1C-NC	2.30	127.70	124.51
5	M	1301	BCL	CHD-C4C-NC	2.36	127.70	125.08
6	L	1402	BPH	C3A-C2A-C1A	2.36	104.47	101.68
5	L	1304	BCL	OBB-CAB-C3B	2.38	124.41	119.95
5	L	1302	BCL	CED-O2D-CGD	2.39	121.47	115.97
7	M	1501	U10	C3M-O3-C3	2.41	125.02	116.45
5	M	1301	BCL	CMD-C2D-C3D	2.43	129.30	124.88
5	L	1304	BCL	C2A-C1A-CHA	2.43	128.20	123.92
6	M	1401	BPH	O2A-CGA-CBA	2.44	118.98	111.92
6	M	1401	BPH	C1-O2A-CGA	2.45	122.41	116.77
9	M	1600	SPN	C7-C6-C5	2.48	121.03	112.85
7	M	1501	U10	C7-C8-C9	2.48	130.99	126.79
5	M	1303	BCL	C3A-C2A-C1A	2.54	105.15	101.34
5	L	1304	BCL	CMD-C2D-C3D	2.54	129.51	124.88
6	M	1401	BPH	C3C-C2C-C1C	2.56	106.01	101.87
5	M	1303	BCL	CHD-C4C-NC	2.65	128.02	125.08
6	M	1401	BPH	C3A-C4A-CHB	2.68	126.29	121.75
5	M	1303	BCL	C3C-C2C-C1C	2.71	106.25	101.87
9	M	1600	SPN	C15-C14-C13	2.72	119.42	112.82
5	L	1304	BCL	O2A-CGA-CBA	2.75	119.86	111.92
5	M	1301	BCL	C3C-C2C-C1C	2.77	106.34	101.87
9	M	1600	SPN	C16-C15-C14	2.77	123.29	113.23
5	L	1304	BCL	C4A-NA-C1A	2.78	109.90	106.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1304	BCL	C2C-C3C-C4C	2.81	105.55	101.34
9	M	1600	SPN	C11-C10-C9	2.82	122.17	112.85
7	L	1502	U10	C3M-O3-C3	2.82	126.50	116.45
5	M	1301	BCL	C2C-C3C-C4C	2.96	105.77	101.34
6	L	1402	BPH	C1-C2-C3	2.98	131.45	125.96
6	L	1402	BPH	C3A-C4A-CHB	2.99	126.81	121.75
5	L	1304	BCL	CMB-C2B-C3B	2.99	130.33	124.88
6	M	1401	BPH	CMC-C2C-C1C	3.00	120.47	112.09
5	M	1301	BCL	C4A-NA-C1A	3.01	110.20	106.32
6	L	1402	BPH	C2C-C3C-C4C	3.06	105.92	101.34
7	L	1502	U10	C22-C23-C24	3.09	135.31	127.66
6	L	1402	BPH	CAC-C3C-C2C	3.11	122.04	114.24
5	L	1302	BCL	C2C-C3C-C4C	3.13	106.03	101.34
6	L	1402	BPH	C4A-NA-C1A	3.25	110.79	108.16
7	L	1502	U10	C8-C7-C6	3.28	120.99	111.95
7	L	1502	U10	C32-C33-C34	3.32	135.87	127.66
9	M	1600	SPN	CM6-C18-C17	3.35	121.06	115.29
5	M	1303	BCL	C4A-NA-C1A	3.36	110.66	106.32
9	M	1600	SPN	CM3-C5-C6	3.44	121.22	115.29
7	L	1502	U10	C12-C13-C14	3.51	136.34	127.66
5	M	1301	BCL	CMB-C2B-C3B	3.56	131.35	124.88
6	M	1401	BPH	CED-O2D-CGD	3.64	124.36	115.97
5	L	1302	BCL	C1-O2A-CGA	3.64	125.15	116.77
9	M	1600	SPN	CM7-C22-C21	3.65	124.65	111.36
6	M	1401	BPH	C2C-C3C-C4C	3.74	106.94	101.34
5	M	1301	BCL	OBB-CAB-C3B	3.85	127.18	119.95
5	L	1302	BCL	OBB-CAB-C3B	4.02	127.49	119.95
7	M	1501	U10	C4M-O4-C4	4.11	131.09	116.45
5	L	1302	BCL	C4A-NA-C1A	4.12	111.63	106.32
5	L	1302	BCL	O2A-CGA-CBA	4.12	123.84	111.92
9	M	1600	SPN	CM4-C9-C10	4.14	122.43	115.29
6	M	1401	BPH	C4A-NA-C1A	4.19	111.55	108.16
6	L	1402	BPH	O2A-CGA-CBA	4.21	124.09	111.92
6	L	1402	BPH	CBC-CAC-C3C	4.22	123.05	113.45
7	L	1502	U10	C7-C8-C9	4.26	134.00	126.79
5	M	1303	BCL	O2A-CGA-CBA	4.35	124.51	111.92
9	M	1600	SPN	CM5-C13-C14	4.60	123.22	115.29
5	L	1302	BCL	O2D-CGD-CBD	5.34	120.75	111.28
5	M	1303	BCL	O2D-CGD-CBD	5.81	121.58	111.28
7	M	1501	U10	C27-C28-C29	5.82	142.07	127.66
7	L	1502	U10	C4M-O4-C4	5.83	137.21	116.45
5	M	1301	BCL	O2A-CGA-CBA	5.91	129.02	111.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1304	BCL	C1-O2A-CGA	6.29	131.27	116.77
5	M	1301	BCL	O2D-CGD-CBD	6.30	122.46	111.28
5	L	1304	BCL	O2D-CGD-CBD	8.32	126.04	111.28
6	L	1402	BPH	O2D-CGD-CBD	8.66	126.63	111.28
6	M	1401	BPH	O2D-CGD-CBD	10.64	130.15	111.28

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	M	1301	BCL	C13
5	L	1304	BCL	C13
6	M	1401	BPH	C8

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	1302	BCL	4	0
5	L	1304	BCL	1	0
6	L	1402	BPH	6	0
7	L	1502	U10	9	0
5	M	1301	BCL	11	0
5	M	1303	BCL	4	0
6	M	1401	BPH	10	0
7	M	1501	U10	3	0
9	M	1600	SPN	2	0
4	M	1701	LDA	2	0
4	M	1702	LDA	2	0
4	M	1703	LDA	5	0
4	M	1706	LDA	4	0
10	M	1800	PO4	1	0
10	M	1801	PO4	2	0

## 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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.