



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:33 PM GMT

PDB ID : 3ZUW  
Title : PHOTOSYNTHETIC REACTION CENTRE MUTANT WITH TYR L128 REPLACED WITH HIS  
Authors : Gibasiewicz, K.; Pajzderska, M.; Potter, J.A.; Fyfe, P.K.; Dobek, A.; Brettel, K.; Jones, M.R.  
Deposited on : 2011-07-20  
Resolution : 2.31 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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

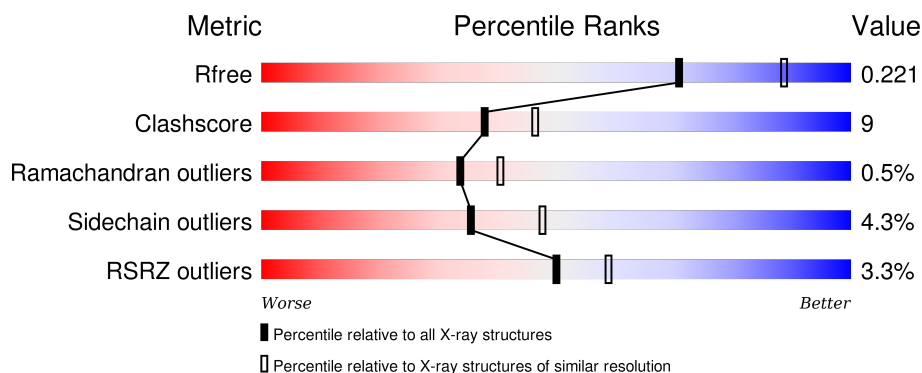
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.31 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	4425 (2.34-2.30)
Clashscore	102246	5057 (2.34-2.30)
Ramachandran outliers	100387	5008 (2.34-2.30)
Sidechain outliers	100360	5007 (2.34-2.30)
RSRZ outliers	91569	4432 (2.34-2.30)

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.

Mol	Chain	Length	Quality of chain
1	H	260	<div> <div>5%</div> <div>78% 12% • 7%</div> </div>
2	L	281	<div> <div>3%</div> <div>88% 9% •</div> </div>
3	M	307	<div> <div>2%</div> <div>86% 11% ••</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
4	LDA	H	1256	-	-	-	X
4	LDA	L	1284	-	-	X	-
4	LDA	M	1308	-	-	-	X
4	LDA	M	1310	-	-	-	X
6	BPH	L	1285	X	-	-	-
6	BPH	M	1311	X	-	-	-
7	U10	L	1286	-	-	-	X
9	PO4	M	1306	-	-	-	X

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7456 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 H CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	241	Total	C	N	O	S	0	0	1
			1830	1169	315	337	9			

- Molecule 2 is a protein called REACTION CENTER PROTEIN L CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	281	Total	C	N	O	S	0	0	0
			2230	1504	357	361	8			

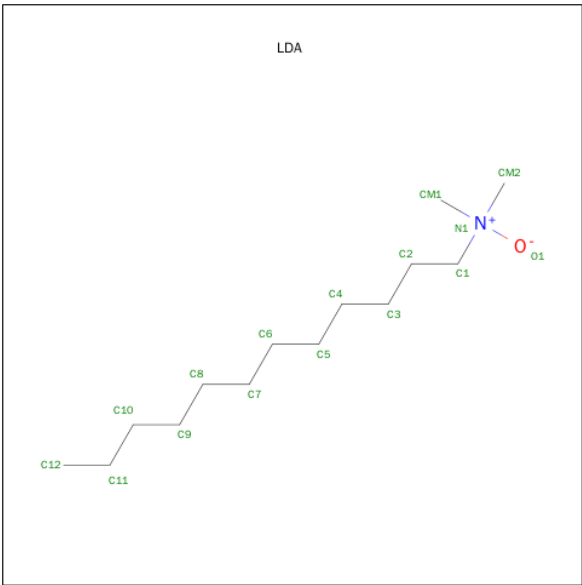
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	128	HIS	TYR	ENGINEERED MUTATION	UNP P0C0Y8

- Molecule 3 is a protein called REACTION CENTER PROTEIN M CHAIN.

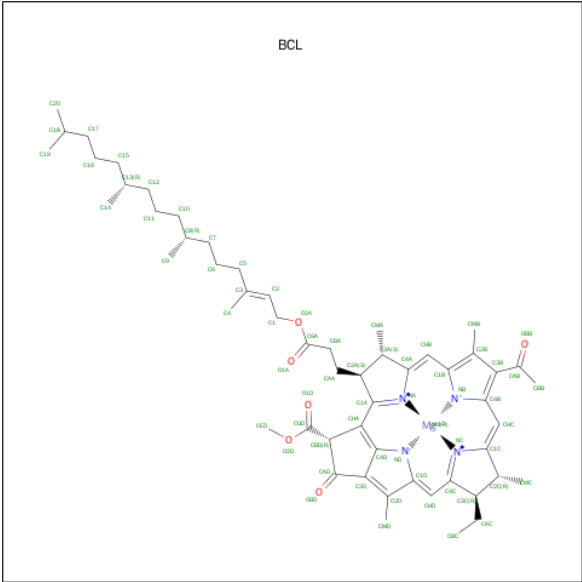
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	302	Total	C	N	O	S	0	1	0
			2414	1610	397	397	10			

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



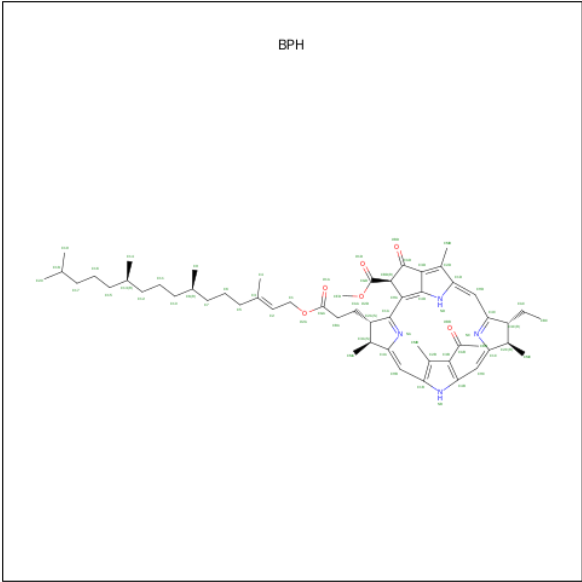
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total C N O 16 14 1 1	0	0
4	H	1	Total C 12 12	0	0
4	H	1	Total C N O 16 14 1 1	0	0
4	H	1	Total C N O 16 14 1 1	0	0
4	H	1	Total C N O 16 14 1 1	0	0
4	L	1	Total C N O 16 14 1 1	0	0
4	M	1	Total C N O 16 14 1 1	0	0
4	M	1	Total C N O 16 14 1 1	0	0
4	M	1	Total C N O 16 14 1 1	0	0

- Molecule 5 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C<sub>55</sub>H<sub>74</sub>MgN<sub>4</sub>O<sub>6</sub>).



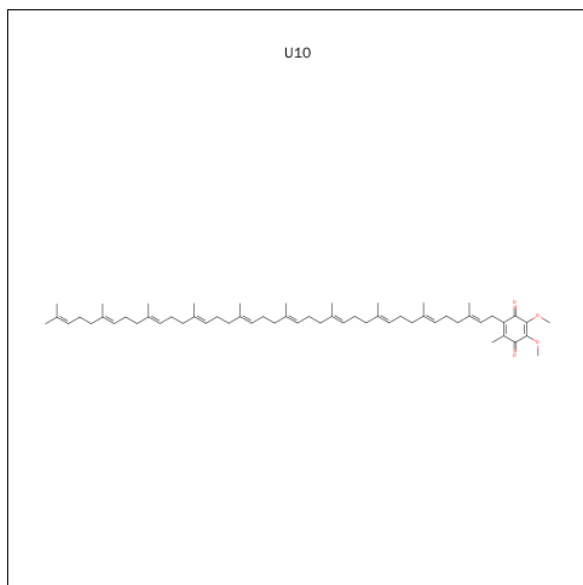
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- 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>).

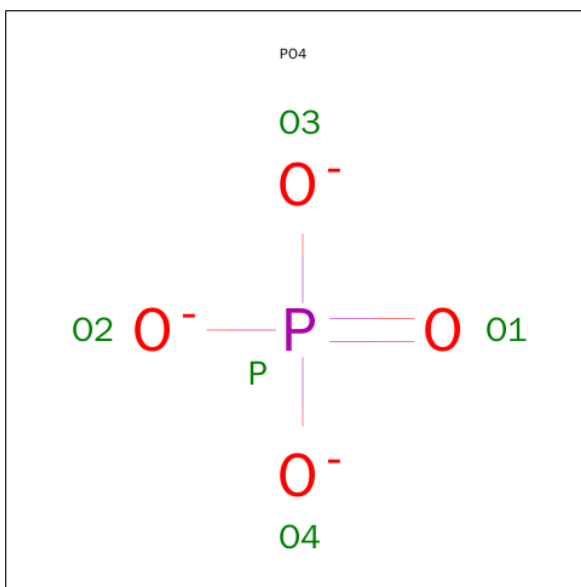


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	1	0
			48	44	4		
7	M	1	Total	C	O	0	0
			48	44	4		

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

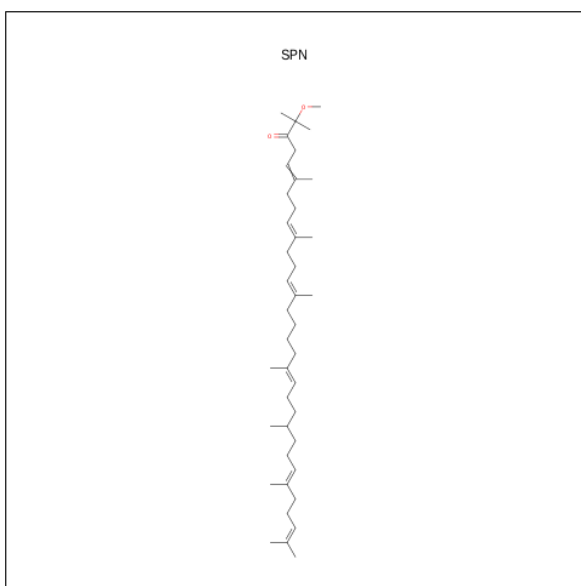
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	M	1	Total	Fe	0	0
			1	1		

- Molecule 9 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

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



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

- Molecule 11 is water.

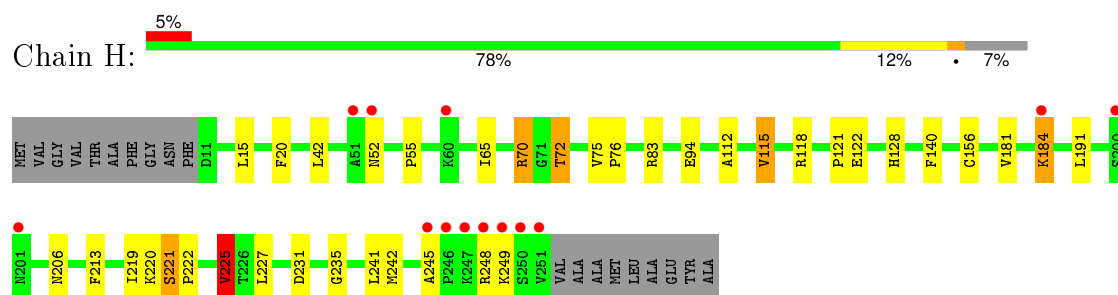


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	H	152	Total 152	O 152	0	0
11	L	81	Total 81	O 81	0	0
11	M	65	Total 65	O 65	0	0

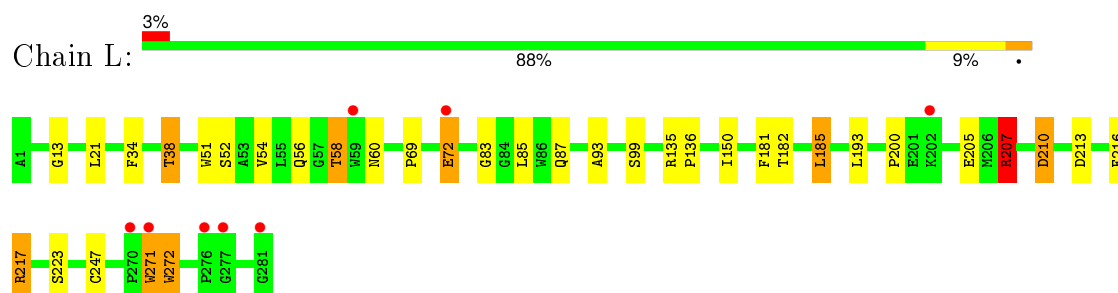
### 3 Residue-property plots

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.

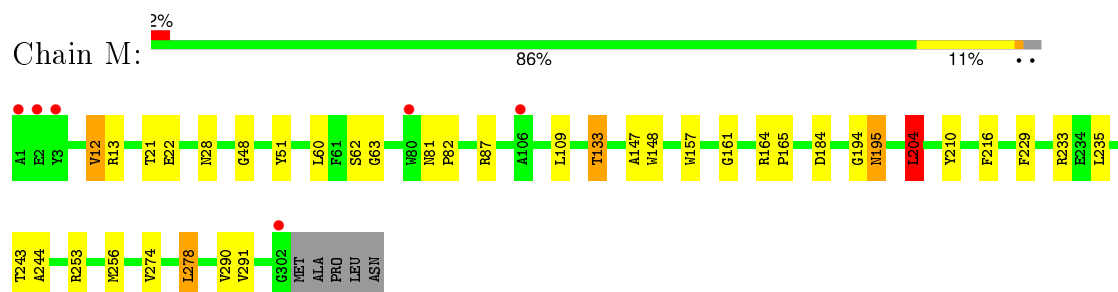
#### • Molecule 1: REACTION CENTER PROTEIN H CHAIN



#### • Molecule 2: REACTION CENTER PROTEIN L CHAIN



#### • Molecule 3: REACTION CENTER PROTEIN M CHAIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.87Å 139.87Å 184.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	17.87 – 2.31 14.94 – 2.31	Depositor EDS
% Data completeness (in resolution range)	98.0 (17.87-2.31) 95.2 (14.94-2.31)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.37 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.192 , 0.224 0.189 , 0.221	Depositor DCC
$R_{free}$ test set	4341 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.2	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 61.0	EDS
Estimated twinning fraction	0.016 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 86983 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7456	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, 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	1.02	1/1878 (0.1%)	0.92	5/2555 (0.2%)
2	L	1.00	1/2318 (0.0%)	0.84	4/3172 (0.1%)
3	M	0.93	0/2511	0.79	4/3427 (0.1%)
All	All	0.98	2/6707 (0.0%)	0.84	13/9154 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	94	GLU	CG-CD	7.51	1.63	1.51
2	L	72	GLU	CG-CD	5.28	1.59	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	217	ARG	NE-CZ-NH1	8.16	124.38	120.30
3	M	233	ARG	NE-CZ-NH1	-6.35	117.13	120.30
3	M	204	LEU	CB-CG-CD1	6.09	121.35	111.00
1	H	225	VAL	CG1-CB-CG2	6.07	120.61	110.90
1	H	225	VAL	CB-CA-C	-6.04	99.93	111.40
2	L	210	ASP	CB-CG-OD1	5.59	123.34	118.30
2	L	207	ARG	NE-CZ-NH2	-5.59	117.51	120.30
3	M	12	VAL	CG1-CB-CG2	5.39	119.52	110.90
1	H	115	VAL	CG1-CB-CG2	5.21	119.23	110.90
3	M	184	ASP	CB-CG-OD1	5.16	122.94	118.30
2	L	185	LEU	CB-CG-CD2	5.15	119.76	111.00
1	H	83	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	H	83	ARG	NE-CZ-NH2	-5.01	117.80	120.30

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	H	1830	0	1836	30	0
2	L	2230	0	2185	27	0
3	M	2414	0	2330	30	0
4	H	76	0	147	9	0
4	L	16	0	31	9	0
4	M	48	0	93	9	0
5	L	132	0	148	5	0
5	M	132	0	148	17	0
6	L	65	0	76	7	0
6	M	65	0	76	10	0
7	L	48	0	58	16	0
7	M	48	0	63	1	0
8	M	1	0	0	0	0
9	M	10	0	0	1	0
10	M	43	0	70	7	0
11	H	152	0	0	10	0
11	L	81	0	0	2	0
11	M	65	0	0	0	0
All	All	7456	0	7261	133	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 (133) 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:H:52:ASN:HB3	11:H:2041:HOH:O	1.48	1.10
7:L:1286:U10:C46	7:L:1286:U10:H351	1.84	1.08
1:H:220:LYS:HE3	11:H:2095:HOH:O	1.62	0.99
1:H:242:MET:HE3	2:L:13:GLY:HA3	1.41	0.98
6:L:1285:BPH:HHC	6:L:1285:BPH:HBB3	1.46	0.96
3:M:253[B]:ARG:HH22	4:M:1309:LDA:HM23	1.37	0.90
1:H:184:LYS:HD3	1:H:184:LYS:O	1.72	0.89
5:M:1303:BCL:CBB	5:M:1303:BCL:HMB1	2.08	0.84
1:H:242:MET:HE2	11:H:2151:HOH:O	1.80	0.80

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:1286:U10:C46	7:L:1286:U10:C35	2.61	0.79
5:L:1283:BCL:HMB1	5:L:1283:BCL:HBB2	1.63	0.78
6:M:1311:BPH:HBB3	6:M:1311:BPH:HHC	1.65	0.76
1:H:181:VAL:HG21	1:H:191:LEU:HD12	1.66	0.76
4:H:1253:LDA:H121	4:L:1284:LDA:H121	1.66	0.75
3:M:253[B]:ARG:NH2	4:M:1309:LDA:HM23	2.01	0.74
6:L:1285:BPH:HBB2	3:M:210:TYR:HB3	1.68	0.74
5:M:1303:BCL:HBB2	5:M:1303:BCL:HMB1	1.70	0.74
5:L:1283:BCL:HMB1	5:L:1283:BCL:CBB	2.19	0.73
2:L:272:TRP:CD1	3:M:87:ARG:HG3	2.23	0.73
7:L:1286:U10:C45	5:M:1303:BCL:C20	2.67	0.72
4:H:1253:LDA:H121	4:L:1284:LDA:C12	2.19	0.71
2:L:181:PHE:HB3	6:M:1311:BPH:HBB2	1.71	0.71
5:M:1304:BCL:CBB	5:M:1304:BCL:HMB1	2.22	0.69
6:L:1285:BPH:HHC	6:L:1285:BPH:CBB	2.23	0.68
4:M:1308:LDA:H91	4:M:1309:LDA:H121	1.75	0.67
2:L:34:PHE:O	2:L:38:THR:HG23	1.94	0.67
2:L:181:PHE:CD2	6:M:1311:BPH:HBB1	2.30	0.67
9:M:1307:PO4:O4	4:M:1310:LDA:HM11	1.95	0.67
3:M:161:GLY:HA3	10:M:1312:SPN:H201	1.76	0.66
2:L:51:TRP:O	2:L:54:VAL:HG22	1.96	0.66
1:H:72:THR:HG23	11:H:2058:HOH:O	1.95	0.65
3:M:278:LEU:HD11	4:M:1310:LDA:H122	1.79	0.64
2:L:93:ALA:HA	6:L:1285:BPH:H9C2	1.81	0.62
7:L:1286:U10:C26	7:L:1286:U10:C33	2.79	0.61
2:L:272:TRP:NE1	3:M:87:ARG:HG3	2.16	0.61
1:H:72:THR:CG2	11:H:2058:HOH:O	2.48	0.60
3:M:157:TRP:CZ2	10:M:1312:SPN:H22	2.36	0.60
5:L:1282:BCL:CBB	5:L:1282:BCL:HMB1	2.32	0.60
2:L:38:THR:HG22	2:L:99:SER:HB3	1.85	0.59
5:M:1303:BCL:HBB3	5:M:1303:BCL:HMB1	1.82	0.59
6:M:1311:BPH:HBC3	6:M:1311:BPH:HHD	1.85	0.58
7:L:1286:U10:C45	5:M:1303:BCL:H202	2.33	0.58
4:H:1253:LDA:H112	4:L:1284:LDA:H123	1.86	0.58
6:L:1285:BPH:HBB1	3:M:210:TYR:CD2	2.39	0.57
2:L:181:PHE:HB3	6:M:1311:BPH:CBB	2.35	0.57
6:M:1311:BPH:H111	6:M:1311:BPH:H161	1.85	0.57
7:L:1286:U10:H422	7:L:1286:U10:H361	1.88	0.56
4:H:1253:LDA:C12	4:L:1284:LDA:C12	2.83	0.56
5:M:1304:BCL:HBB2	5:M:1304:BCL:HMB1	1.86	0.56
2:L:34:PHE:O	2:L:38:THR:CG2	2.53	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:1286:U10:C43	7:L:1286:U10:H361	2.35	0.56
7:L:1286:U10:C45	5:M:1303:BCL:H203	2.36	0.55
3:M:290:VAL:HG12	3:M:291:VAL:HG23	1.89	0.55
1:H:42:LEU:HD11	4:M:1309:LDA:HM12	1.87	0.55
5:M:1303:BCL:H172	10:M:1312:SPN:H72	1.89	0.54
3:M:21:THR:O	3:M:22:GLU:C	2.45	0.54
1:H:220:LYS:CE	11:H:2095:HOH:O	2.36	0.54
4:H:1252:LDA:H62	4:H:1254:LDA:H62	1.88	0.54
5:M:1304:BCL:HAA2	5:M:1304:BCL:HBD	1.88	0.54
2:L:223:SER:HA	7:L:1286:U10:H103	1.89	0.54
7:L:1286:U10:H361	7:L:1286:U10:C42	2.38	0.53
7:L:1286:U10:H451	5:M:1303:BCL:H202	1.89	0.53
1:H:241:LEU:O	1:H:248:ARG:NH2	2.42	0.53
1:H:242:MET:CE	11:H:2151:HOH:O	2.45	0.53
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.92	0.52
4:L:1284:LDA:HM12	11:L:2081:HOH:O	2.10	0.51
1:H:115:VAL:HG13	3:M:243:THR:N	2.27	0.50
2:L:271:TRP:N	2:L:271:TRP:CD1	2.79	0.50
1:H:75:VAL:HA	1:H:76:PRO:C	2.33	0.49
1:H:219:ILE:HG21	1:H:225:VAL:HG13	1.95	0.49
3:M:157:TRP:CE2	10:M:1312:SPN:H22	2.48	0.49
4:H:1253:LDA:C12	4:L:1284:LDA:H121	2.37	0.49
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.93	0.49
3:M:133:THR:CG2	3:M:147:ALA:HA	2.42	0.49
7:L:1286:U10:H451	5:M:1303:BCL:C20	2.41	0.48
5:L:1282:BCL:HBB3	5:L:1282:BCL:HMB1	1.95	0.48
6:M:1311:BPH:HBC3	6:M:1311:BPH:CHD	2.43	0.47
2:L:216:PHE:CD1	7:L:1286:U10:H102	2.49	0.47
5:M:1304:BCL:HHC	5:M:1304:BCL:OBB	2.14	0.47
1:H:181:VAL:CG2	1:H:191:LEU:HD12	2.39	0.47
3:M:133:THR:HG21	3:M:147:ALA:HA	1.97	0.47
1:H:70:ARG:NH2	1:H:121:PRO:O	2.47	0.47
2:L:83:GLY:O	2:L:87:GLN:HG3	2.15	0.47
2:L:38:THR:HG22	2:L:99:SER:CB	2.44	0.46
1:H:220:LYS:NZ	11:H:2094:HOH:O	2.35	0.46
1:H:112:ALA:HA	1:H:235:GLY:O	2.16	0.46
4:H:1253:LDA:C12	4:L:1284:LDA:H123	2.45	0.46
2:L:193:LEU:HD23	7:L:1286:U10:C2	2.47	0.45
3:M:161:GLY:HA3	10:M:1312:SPN:HM72	1.98	0.45
5:M:1303:BCL:CAB	10:M:1312:SPN:H162	2.47	0.45
6:L:1285:BPH:CHC	6:L:1285:BPH:CBB	2.89	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:52:SER:HB2	2:L:85:LEU:HD13	1.99	0.45
5:L:1283:BCL:H172	5:L:1283:BCL:H13	1.74	0.44
7:L:1286:U10:H452	5:M:1303:BCL:C20	2.48	0.44
4:H:1253:LDA:C11	4:L:1284:LDA:H123	2.47	0.44
3:M:235:LEU:HD23	3:M:235:LEU:HA	1.85	0.44
1:H:55:PRO:HB2	4:H:1254:LDA:H52	2.00	0.43
3:M:133:THR:CG2	3:M:147:ALA:HB2	2.48	0.43
3:M:63:GLY:HA3	6:M:1311:BPH:H5C1	2.01	0.43
3:M:164:ARG:HB3	3:M:165:PRO:HD3	2.01	0.43
1:H:140:PHE:HA	3:M:13:ARG:O	2.18	0.43
6:L:1285:BPH:H112	6:L:1285:BPH:H7C2	1.89	0.43
2:L:207:ARG:N	2:L:207:ARG:HD2	2.32	0.42
1:H:118:ARG:NH2	11:H:2093:HOH:O	2.52	0.42
1:H:221:SER:HA	1:H:222:PRO:HD3	1.83	0.42
2:L:182:THR:OG1	5:M:1303:BCL:H2	2.20	0.42
10:M:1312:SPN:HM41	10:M:1312:SPN:H111	1.85	0.42
6:M:1311:BPH:HHC	6:M:1311:BPH:CBB	2.43	0.42
3:M:148:TRP:HB3	4:M:1310:LDA:H62	2.00	0.42
4:M:1308:LDA:H91	4:M:1309:LDA:C12	2.48	0.42
1:H:128:HIS:HD2	11:H:2102:HOH:O	2.02	0.42
1:H:65:ILE:HG22	2:L:205:GLU:HG2	2.01	0.42
6:M:1311:BPH:CBC	6:M:1311:BPH:HHH	2.50	0.42
2:L:85:LEU:HD23	2:L:85:LEU:HA	1.92	0.42
3:M:256:MET:CE	7:M:1313:U10:H102	2.49	0.42
7:L:1286:U10:H1M1	7:L:1286:U10:H71	1.71	0.41
2:L:200:PRO:HB3	2:L:207:ARG:HD3	2.02	0.41
3:M:194:GLY:O	3:M:195:ASN:HB3	2.21	0.41
5:M:1303:BCL:C7	5:M:1303:BCL:C4	2.99	0.41
2:L:69:PRO:HB2	11:L:2019:HOH:O	2.19	0.41
3:M:81:ASN:HA	3:M:82:PRO:HD2	1.84	0.41
3:M:28:ASN:HB2	3:M:51:TYR:CE2	2.55	0.41
2:L:58:THR:HB	2:L:60:ASN:H	1.86	0.41
1:H:20:PHE:CD1	1:H:20:PHE:C	2.93	0.41
3:M:133:THR:HG23	3:M:147:ALA:HB2	2.02	0.41
2:L:213:ASP:O	2:L:217:ARG:HG3	2.20	0.41
1:H:191:LEU:HD11	1:H:213:PHE:HE2	1.85	0.40
4:L:1284:LDA:HM13	4:L:1284:LDA:H21	1.90	0.40
3:M:148:TRP:HA	3:M:148:TRP:CE3	2.56	0.40
1:H:70:ARG:HD2	1:H:70:ARG:HH11	1.69	0.40
1:H:156:CYS:HB3	1:H:206:ASN:O	2.22	0.40
3:M:204:LEU:HD13	4:M:1308:LDA:H12	2.04	0.40

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:122:GLU:HB2	1:H:227:LEU:HD21	2.03	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	H	239/260 (92%)	232 (97%)	6 (2%)	1 (0%)	39	48
2	L	279/281 (99%)	267 (96%)	12 (4%)	0	100	100
3	M	301/307 (98%)	285 (95%)	13 (4%)	3 (1%)	19	20
All	All	819/848 (97%)	784 (96%)	31 (4%)	4 (0%)	34	40

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	245	ALA
3	M	48	GLY
3	M	195	ASN
3	M	109	LEU

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	195/208 (94%)	187 (96%)	8 (4%)	37	50
2	L	220/220 (100%)	208 (94%)	12 (6%)	27	36
3	M	237/240 (99%)	229 (97%)	8 (3%)	44	59
All	All	652/668 (98%)	624 (96%)	28 (4%)	35	48

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	15	LEU
1	H	70	ARG
1	H	72	THR
1	H	184	LYS
1	H	221	SER
1	H	225	VAL
1	H	231	ASP
1	H	249	LYS
2	L	21	LEU
2	L	38	THR
2	L	56	GLN
2	L	58	THR
2	L	72	GLU
2	L	150	ILE
2	L	185	LEU
2	L	207	ARG
2	L	210	ASP
2	L	247	CYS
2	L	271	TRP
2	L	272	TRP
3	M	12	VAL
3	M	60	LEU
3	M	62	SER
3	M	133	THR
3	M	204	LEU
3	M	216	PHE
3	M	274	VAL
3	M	278	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	M	301	HIS

### 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 21 ligands modelled in this entry, 1 is monoatomic - leaving 20 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	1252	-	15,15,15	3.56	1 (6%)	16,17,17	0.79	0
4	LDA	H	1253	-	11,11,15	0.28	0	10,10,17	0.62	0
4	LDA	H	1254	-	15,15,15	3.61	2 (13%)	16,17,17	0.37	0
4	LDA	H	1255	-	15,15,15	3.75	2 (13%)	16,17,17	0.95	1 (6%)
4	LDA	H	1256	-	15,15,15	3.56	1 (6%)	16,17,17	0.92	1 (6%)
5	BCL	L	1282	2	53,74,74	0.65	0	57,115,115	1.45	7 (12%)
5	BCL	L	1283	2	53,74,74	0.81	0	57,115,115	1.72	11 (19%)
4	LDA	L	1284	-	15,15,15	3.55	1 (6%)	16,17,17	0.72	0
6	BPH	L	1285	-	64,70,70	1.43	10 (15%)	73,101,101	1.67	11 (15%)
7	U10	L	1286	-	46,47,63	3.33	13 (28%)	54,59,79	2.00	16 (29%)
5	BCL	M	1303	3	53,74,74	0.68	0	57,115,115	1.57	9 (15%)
5	BCL	M	1304	3	53,74,74	0.69	0	57,115,115	1.70	11 (19%)
9	PO4	M	1306	-	4,4,4	0.50	0	6,6,6	0.27	0
9	PO4	M	1307	-	4,4,4	1.26	1 (25%)	6,6,6	0.25	0
4	LDA	M	1308	-	15,15,15	4.07	1 (6%)	16,17,17	1.46	4 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	LDA	M	1309	-	15,15,15	4.06	2 (13%)	16,17,17	1.10	1 (6%)
4	LDA	M	1310	-	15,15,15	3.40	1 (6%)	16,17,17	1.14	2 (12%)
6	BPH	M	1311	-	64,70,70	1.34	8 (12%)	73,101,101	1.63	15 (20%)
10	SPN	M	1312	-	41,42,42	0.77	1 (2%)	41,52,52	2.07	10 (24%)
7	U10	M	1313	-	48,48,63	3.07	12 (25%)	58,61,79	2.04	16 (27%)

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	1252	-	-	0/13/13/13	0/0/0/0
4	LDA	H	1253	-	-	0/9/9/13	0/0/0/0
4	LDA	H	1254	-	-	0/13/13/13	0/0/0/0
4	LDA	H	1255	-	-	0/13/13/13	0/0/0/0
4	LDA	H	1256	-	-	0/13/13/13	0/0/0/0
5	BCL	L	1282	2	-	0/37/137/137	0/0/9/9
5	BCL	L	1283	2	-	0/37/137/137	0/0/9/9
4	LDA	L	1284	-	-	0/13/13/13	0/0/0/0
6	BPH	L	1285	-	2/2/18/22	0/54/105/105	0/1/6/6
7	U10	L	1286	-	-	0/41/65/87	0/1/1/1
5	BCL	M	1303	3	-	0/37/137/137	0/0/9/9
5	BCL	M	1304	3	-	0/37/137/137	0/0/9/9
9	PO4	M	1306	-	-	0/0/0/0	0/0/0/0
9	PO4	M	1307	-	-	0/0/0/0	0/0/0/0
4	LDA	M	1308	-	-	0/13/13/13	0/0/0/0
4	LDA	M	1309	-	-	0/13/13/13	0/0/0/0
4	LDA	M	1310	-	-	0/13/13/13	0/0/0/0
6	BPH	M	1311	-	2/2/18/22	0/54/105/105	0/1/6/6
10	SPN	M	1312	-	-	0/50/51/51	0/0/0/0
7	U10	M	1313	-	-	0/45/69/87	0/1/1/1

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	1309	LDA	O1-N1	-15.44	1.24	1.39
4	M	1308	LDA	O1-N1	-15.42	1.24	1.39
4	H	1255	LDA	O1-N1	-14.26	1.26	1.39
4	H	1254	LDA	O1-N1	-13.75	1.26	1.39
4	H	1252	LDA	O1-N1	-13.66	1.26	1.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1256	LDA	O1-N1	-13.64	1.26	1.39
4	L	1284	LDA	O1-N1	-13.56	1.26	1.39
4	M	1310	LDA	O1-N1	-13.02	1.27	1.39
7	L	1286	U10	C27-C26	-9.24	1.07	1.51
7	L	1286	U10	O4-C4	-3.90	1.26	1.37
6	L	1285	BPH	C1A-NA	-3.69	1.29	1.37
7	M	1313	U10	O3-C3	-3.59	1.27	1.37
7	M	1313	U10	O4-C4	-3.50	1.27	1.37
6	M	1311	BPH	C1A-NA	-3.40	1.29	1.37
7	L	1286	U10	O3-C3	-3.09	1.28	1.37
6	M	1311	BPH	C1B-C2B	-3.07	1.39	1.45
6	M	1311	BPH	C4C-NC	-3.02	1.30	1.37
6	L	1285	BPH	C3B-C4B	-2.87	1.36	1.43
6	M	1311	BPH	CHB-C4A	-2.76	1.35	1.40
7	M	1313	U10	C4-C5	-2.74	1.41	1.48
7	L	1286	U10	C3-C2	-2.73	1.41	1.48
6	L	1285	BPH	C1B-C2B	-2.65	1.39	1.45
4	M	1309	LDA	C1-N1	-2.53	1.46	1.51
7	L	1286	U10	C6-C5	-2.41	1.39	1.46
4	H	1255	LDA	C1-N1	-2.35	1.47	1.51
9	M	1307	PO4	P-O3	-2.31	1.45	1.53
6	L	1285	BPH	CMD-C2D	-2.22	1.47	1.51
6	L	1285	BPH	C4C-NC	-2.19	1.32	1.37
6	M	1311	BPH	C3D-C2D	-2.18	1.34	1.40
4	H	1254	LDA	C1-N1	-2.16	1.47	1.51
7	L	1286	U10	C4-C5	-2.12	1.42	1.48
7	M	1313	U10	C3-C2	-2.08	1.42	1.48
6	M	1311	BPH	C3B-C4B	-2.00	1.38	1.43
7	M	1313	U10	C6-C1	2.02	1.40	1.35
6	L	1285	BPH	CHB-C1B	2.19	1.43	1.38
10	M	1312	SPN	C4-C5	2.37	1.37	1.33
6	L	1285	BPH	C2-C3	2.43	1.37	1.33
6	L	1285	BPH	C3D-C4D	3.55	1.45	1.41
6	L	1285	BPH	CHD-C4C	3.98	1.48	1.38
6	L	1285	BPH	CHA-C1A	4.28	1.47	1.37
6	M	1311	BPH	CHA-C1A	4.33	1.47	1.37
6	M	1311	BPH	CHD-C4C	4.61	1.49	1.38
7	L	1286	U10	C33-C34	4.63	1.48	1.33
7	L	1286	U10	C43-C44	5.25	1.48	1.32
7	M	1313	U10	C38-C39	5.43	1.49	1.32
7	L	1286	U10	C8-C9	6.91	1.46	1.33
7	M	1313	U10	C23-C24	7.07	1.46	1.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	1313	U10	C8-C9	7.16	1.47	1.33
7	L	1286	U10	C23-C24	7.19	1.47	1.33
7	M	1313	U10	C18-C19	7.35	1.47	1.33
7	M	1313	U10	C28-C29	7.60	1.47	1.33
7	M	1313	U10	C13-C14	8.07	1.48	1.33
7	L	1286	U10	C13-C14	8.21	1.49	1.33
7	L	1286	U10	C18-C19	8.51	1.49	1.33
7	M	1313	U10	C33-C34	8.64	1.49	1.33
7	L	1286	U10	C38-C39	8.69	1.50	1.33

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	1313	U10	C17-C18-C19	-4.98	116.93	127.76
7	L	1286	U10	C7-C8-C9	-4.72	118.70	126.70
6	M	1311	BPH	C2D-C1D-ND	-4.40	103.08	110.29
5	L	1283	BCL	C1D-CHD-C4C	-4.30	119.50	126.07
7	L	1286	U10	C25-C24-C23	-4.03	115.59	123.50
7	L	1286	U10	C1M-C1-C6	-3.97	115.61	124.10
7	M	1313	U10	C22-C23-C24	-3.88	119.32	127.76
5	M	1303	BCL	C4-C3-C2	-3.86	115.91	123.50
6	L	1285	BPH	C1C-NC-C4C	-3.85	106.49	110.44
6	L	1285	BPH	C2D-C1D-ND	-3.83	104.02	110.29
7	M	1313	U10	C32-C33-C34	-3.81	119.47	127.76
10	M	1312	SPN	C21-C20-C19	-3.74	101.92	112.40
7	M	1313	U10	C27-C28-C29	-3.70	119.71	127.76
5	L	1282	BCL	C1D-CHD-C4C	-3.67	120.47	126.07
7	L	1286	U10	C22-C23-C24	-3.52	120.10	127.76
6	L	1285	BPH	C4-C3-C5	-3.29	110.38	115.41
5	M	1304	BCL	O2D-CGD-O1D	-3.17	117.25	123.79
4	M	1308	LDA	O1-N1-CM1	-3.09	104.93	109.05
4	H	1255	LDA	O1-N1-C1	-3.03	106.87	110.27
6	M	1311	BPH	CAC-C3C-C2C	-2.99	106.62	114.13
5	M	1303	BCL	C1D-CHD-C4C	-2.97	121.53	126.07
7	L	1286	U10	C15-C14-C13	-2.96	117.69	123.50
5	L	1282	BCL	C11-C12-C13	-2.90	105.86	115.49
6	M	1311	BPH	CBA-CAA-C2A	-2.90	105.55	113.73
4	M	1310	LDA	O1-N1-CM1	-2.87	105.22	109.05
4	M	1308	LDA	O1-N1-CM2	-2.80	105.31	109.05
5	L	1283	BCL	O2D-CGD-O1D	-2.79	118.02	123.79
5	M	1303	BCL	C3C-C4C-CHD	-2.71	117.28	123.33
6	M	1311	BPH	C2B-C1B-NB	-2.70	105.68	109.73

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	1313	U10	C25-C24-C23	-2.69	118.22	123.50
6	L	1285	BPH	C2B-C1B-NB	-2.69	105.70	109.73
10	M	1312	SPN	C3-C4-C5	-2.67	122.17	126.70
10	M	1312	SPN	C14-C13-C12	-2.65	116.03	121.05
5	L	1283	BCL	O2A-CGA-O1A	-2.62	116.72	123.49
6	L	1285	BPH	C1D-CHD-C4C	-2.61	117.75	127.23
5	M	1304	BCL	C4-C3-C2	-2.61	118.38	123.50
4	H	1256	LDA	O1-N1-CM1	-2.57	105.62	109.05
7	L	1286	U10	O5-C5-C6	-2.56	116.86	121.68
5	L	1283	BCL	OBD-CAD-C3D	-2.56	123.13	128.35
5	M	1304	BCL	C1D-CHD-C4C	-2.55	122.17	126.07
4	M	1309	LDA	CM1-N1-C1	-2.52	101.64	109.77
5	M	1304	BCL	C11-C12-C13	-2.49	107.22	115.49
7	M	1313	U10	C11-C9-C8	-2.44	116.42	121.05
10	M	1312	SPN	C20-C19-C18	-2.44	122.45	127.76
5	L	1283	BCL	C3C-C4C-CHD	-2.42	117.94	123.33
7	M	1313	U10	C11-C12-C13	-2.25	105.80	111.69
5	M	1303	BCL	O1D-CGD-CBD	-2.24	121.42	124.62
5	L	1283	BCL	C5-C3-C2	-2.23	116.83	121.05
6	M	1311	BPH	CAA-C2A-C1A	-2.22	107.01	112.86
7	L	1286	U10	C10-C9-C8	-2.21	119.16	123.50
5	M	1304	BCL	CAA-C2A-C3A	-2.20	106.90	113.22
7	L	1286	U10	C37-C38-C39	-2.18	123.02	127.76
4	M	1310	LDA	O1-N1-CM2	-2.17	106.16	109.05
7	M	1313	U10	C30-C29-C28	-2.15	119.29	123.50
7	L	1286	U10	C12-C13-C14	-2.14	123.11	127.76
6	L	1285	BPH	C7-C6-C5	-2.12	106.79	113.06
5	M	1303	BCL	CMB-C2B-C1B	-2.12	124.86	128.36
6	L	1285	BPH	C3A-C4A-NA	-2.12	109.87	113.57
7	L	1286	U10	O2-C2-C3	-2.05	116.34	120.79
5	L	1282	BCL	CMB-C2B-C1B	-2.05	124.97	128.36
6	M	1311	BPH	C4-C3-C5	-2.04	112.29	115.41
5	L	1283	BCL	OBB-CAB-CBB	-2.01	115.32	120.13
6	M	1311	BPH	CHB-C1B-C2B	2.01	130.15	125.61
10	M	1312	SPN	CMB-C30-CM9	2.05	119.69	114.64
6	L	1285	BPH	C6-C5-C3	2.11	117.12	112.48
7	M	1313	U10	C31-C32-C33	2.12	117.23	111.69
6	M	1311	BPH	CMD-C2D-C3D	2.16	129.31	125.09
5	M	1304	BCL	CED-O2D-CGD	2.18	121.11	115.99
6	L	1285	BPH	C1B-NB-C4B	2.19	110.85	106.51
7	M	1313	U10	C41-C39-C40	2.22	120.09	114.64
6	M	1311	BPH	C4D-C3D-C2D	2.22	109.95	107.08

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	1308	LDA	O1-N1-C1	2.24	112.80	110.27
5	M	1304	BCL	C4-C3-C5	2.31	118.93	115.41
5	M	1303	BCL	O2A-CGA-CBA	2.35	119.06	111.90
5	L	1282	BCL	O2A-CGA-CBA	2.38	119.16	111.90
5	M	1304	BCL	CHB-C4A-NA	2.48	127.94	124.51
7	M	1313	U10	C4M-O4-C4	2.56	125.73	116.61
6	M	1311	BPH	C1B-NB-C4B	2.58	111.62	106.51
5	M	1303	BCL	C5-C3-C2	2.59	125.95	121.05
5	M	1304	BCL	O2A-CGA-CBA	2.60	119.82	111.90
6	M	1311	BPH	CAC-C3C-C4C	2.61	119.38	112.67
4	M	1308	LDA	CM1-N1-C1	2.61	118.20	109.77
6	M	1311	BPH	OBB-CAB-C3B	2.75	125.63	120.31
6	M	1311	BPH	C5-C3-C2	2.86	126.47	121.05
6	M	1311	BPH	C6-C5-C3	2.94	118.93	112.48
10	M	1312	SPN	CM8-C26-C27	2.94	119.90	115.41
7	L	1286	U10	C40-C39-C41	3.06	120.08	115.41
6	L	1285	BPH	OBB-CAB-C3B	3.08	126.25	120.31
7	L	1286	U10	C27-C26-C24	3.09	129.00	112.89
7	M	1313	U10	C15-C14-C16	3.13	120.18	115.41
5	L	1283	BCL	CHB-C4A-NA	3.14	128.85	124.51
5	L	1283	BCL	O2A-CGA-CBA	3.17	121.55	111.90
10	M	1312	SPN	CM3-C5-C6	3.24	120.36	115.41
5	L	1282	BCL	O2D-CGD-CBD	3.33	115.87	111.30
7	L	1286	U10	C10-C9-C11	3.38	120.57	115.41
7	M	1313	U10	C25-C24-C26	3.43	120.64	115.41
5	L	1282	BCL	C4-C3-C5	3.44	120.67	115.41
7	M	1313	U10	C35-C34-C36	3.56	120.85	115.41
10	M	1312	SPN	CM4-C9-C10	3.72	121.09	115.41
7	L	1286	U10	C15-C14-C16	3.79	121.20	115.41
5	M	1304	BCL	CHD-C4C-NC	3.81	129.47	125.06
7	L	1286	U10	C3M-O3-C3	4.04	130.98	116.61
5	L	1282	BCL	CHD-C4C-NC	4.07	129.78	125.06
5	M	1303	BCL	O2D-CGD-CBD	4.18	117.03	111.30
5	L	1283	BCL	CHD-C4C-NC	4.35	130.10	125.06
10	M	1312	SPN	CM6-C18-C17	4.39	122.11	115.41
5	M	1303	BCL	CHD-C4C-NC	4.58	130.37	125.06
7	M	1313	U10	C10-C9-C11	4.79	122.72	115.41
7	M	1313	U10	C30-C29-C31	4.82	122.77	115.41
7	L	1286	U10	C25-C24-C26	4.89	121.22	115.68
10	M	1312	SPN	CM5-C13-C14	5.47	123.77	115.41
6	M	1311	BPH	C3C-C4C-NC	5.51	113.45	107.93
5	L	1283	BCL	O2D-CGD-CBD	6.00	119.54	111.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	1304	BCL	O2D-CGD-CBD	6.80	120.62	111.30
6	L	1285	BPH	C3C-C4C-NC	7.36	115.30	107.93

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	L	1285	BPH	C8
6	L	1285	BPH	C13
6	M	1311	BPH	C8
6	M	1311	BPH	C13

There are no torsion outliers.

There are no ring outliers.

17 monomers are involved in 75 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1252	LDA	1	0
4	H	1253	LDA	7	0
4	H	1254	LDA	2	0
5	L	1282	BCL	2	0
5	L	1283	BCL	3	0
4	L	1284	LDA	9	0
6	L	1285	BPH	7	0
7	L	1286	U10	16	0
5	M	1303	BCL	13	0
5	M	1304	BCL	4	0
9	M	1307	PO4	1	0
4	M	1308	LDA	3	0
4	M	1309	LDA	5	0
4	M	1310	LDA	3	0
6	M	1311	BPH	10	0
10	M	1312	SPN	7	0
7	M	1313	U10	1	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

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	H	241/260 (92%)	-0.39	13 (5%) 29 38	26, 35, 52, 113	0
2	L	281/281 (100%)	-0.46	8 (2%) 56 66	24, 34, 64, 86	0
3	M	302/307 (98%)	-0.51	6 (1%) 68 76	22, 37, 61, 84	0
All	All	824/848 (97%)	-0.46	27 (3%) 50 59	22, 35, 61, 113	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	251	VAL	9.4
3	M	1	ALA	9.0
1	H	250	SER	8.5
1	H	245	ALA	5.4
1	H	249	LYS	5.4
1	H	246	PRO	5.1
2	L	281	GLY	4.5
3	M	2	GLU	3.7
2	L	59	TRP	3.6
3	M	3	TYR	3.5
3	M	302	GLY	3.4
2	L	276	PRO	2.9
1	H	247	LYS	2.8
2	L	270	PRO	2.8
2	L	271	TRP	2.8
2	L	202	LYS	2.7
2	L	72	GLU	2.6
3	M	106	ALA	2.6
1	H	200	SER	2.5
1	H	52	ASN	2.4
1	H	184	LYS	2.4
1	H	248	ARG	2.3
1	H	60	LYS	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	M	80	TRP	2.3
1	H	201	ASN	2.2
1	H	51	ALA	2.1
2	L	277	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
7	U10	L	1286	48/63	0.78	0.24	8.62	38,67,112,114	1
4	LDA	M	1310	16/16	0.51	0.25	6.81	59,64,92,93	0
4	LDA	H	1256	16/16	0.49	0.30	5.86	70,79,106,107	0
9	PO4	M	1306	5/5	0.95	0.22	2.38	66,68,71,72	0
4	LDA	M	1308	16/16	0.89	0.16	2.30	35,47,53,54	0
7	U10	M	1313	48/63	0.94	0.12	1.03	16,38,66,68	0
4	LDA	M	1309	16/16	0.94	0.12	0.97	42,53,65,65	0
5	BCL	M	1303	66/66	0.96	0.10	0.63	18,31,73,75	0
10	SPN	M	1312	43/43	0.93	0.12	0.60	26,42,72,80	0
6	BPH	L	1285	65/65	0.98	0.10	0.16	17,27,41,48	0
6	BPH	M	1311	65/65	0.96	0.10	-0.10	22,38,103,105	0
5	BCL	M	1304	66/66	0.97	0.08	-0.17	19,29,50,64	0
5	BCL	L	1282	66/66	0.97	0.08	-0.32	20,29,41,44	0
5	BCL	L	1283	66/66	0.97	0.08	-0.62	13,25,44,55	0
8	FE	M	1305	1/1	0.99	0.06	-1.66	26,26,26,26	0
9	PO4	M	1307	5/5	0.96	0.20	-	36,50,55,58	0
4	LDA	H	1253	12/16	0.86	0.15	-	64,67,73,74	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	LDA	H	1252	16/16	0.55	0.27	-	61,72,107,107	0
4	LDA	H	1255	16/16	0.75	0.23	-	74,81,92,93	0
4	LDA	L	1284	16/16	0.53	0.26	-	65,80,102,102	0
4	LDA	H	1254	16/16	0.52	0.29	-	68,81,117,117	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.