



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 22, 2018 – 01:26 AM EST

PDB ID : 2HHK  
Title : Reaction centre from Rhodobacter sphaeroides strain R-26.1 complexed with dibrominated phosphatidylglycerol  
Authors : Roszak, A.W.; Gardiner, A.T.; Isaacs, N.W.; Cogdell, R.J.  
Deposited on : 2006-06-28  
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

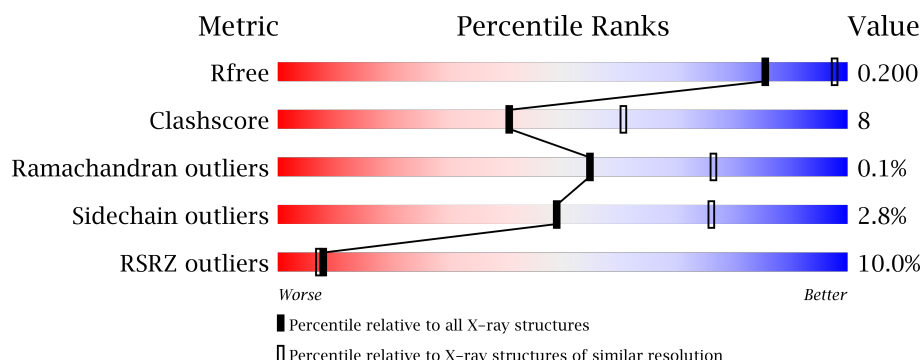
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	L	281	<div> <div>12%</div> <div>94%</div> <div>• •</div> </div>
2	M	307	<div> <div>12%</div> <div>89%</div> <div>9%</div> <div>• •</div> </div>
3	H	260	<div> <div>4%</div> <div>78%</div> <div>13%</div> <div>• 7%</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
11	CDL	M	800	-	-	-	X
12	PGK	M	802	-	-	-	X
13	LDA	H	901	-	-	X	X
13	LDA	H	903	-	-	X	X
13	LDA	M	902	-	-	-	X
13	LDA	M	907	-	-	-	X
13	LDA	M	920	-	-	-	X
15	PGT	H	801[A]	-	-	-	X
15	PGT	H	801[B]	-	-	-	X
6	U10	L	502	-	-	-	X
7	GOL	H	706	-	-	-	X
7	GOL	L	707	-	-	-	X
7	GOL	L	708	-	-	-	X
7	GOL	L	709	-	-	X	X

## 2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 7824 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	281	Total	C	N	O	S	0	1	0
			2235	1510	356	361	8			

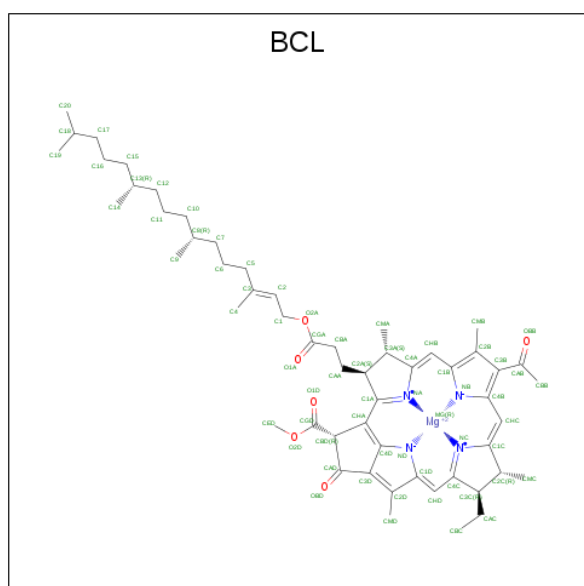
- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	302	Total	C	N	O	S	0	10	0
			2448	1633	402	402	11			

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

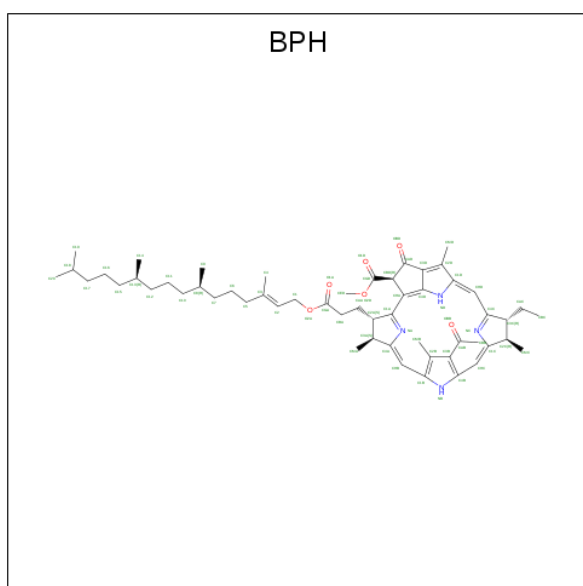
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	241	Total	C	N	O	S	0	8	0
			1862	1189	323	339	11			

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



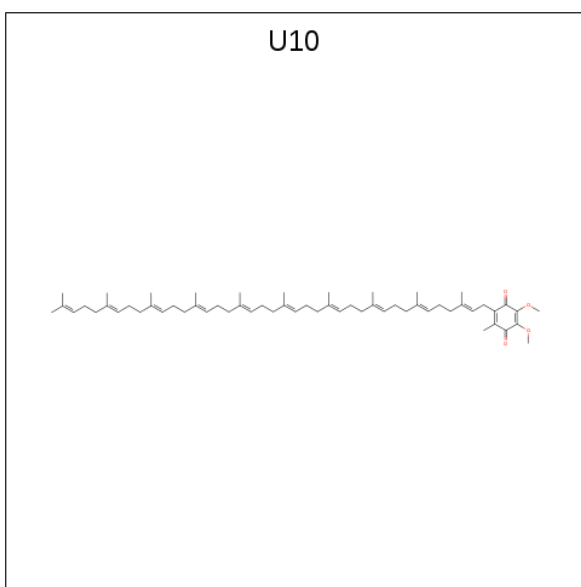
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 5 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula:  $C_{55}H_{76}N_4O_6$ ).



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

- Molecule 6 is UBIQUINONE-10 (three-letter code: U10) (formula:  $C_{59}H_{90}O_4$ ).



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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	0	0
			6	3	3		
7	L	1	Total	C	O	0	0
			6	3	3		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	0	0
			6	3	3		
7	H	1	Total	C	O	0	0
			6	3	3		

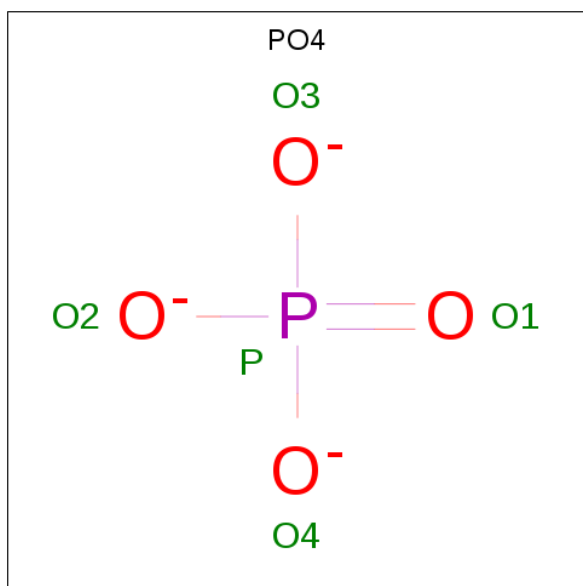
- Molecule 8 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	M	1	Total	Cl	0	0
			1	1		

- Molecule 10 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



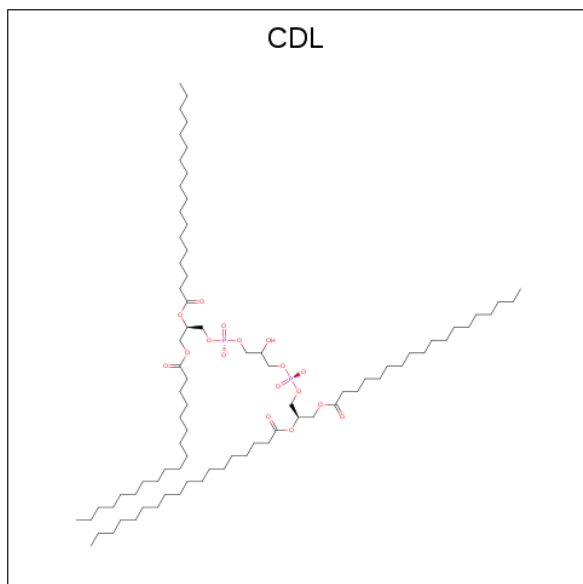
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	M	1	Total	O	P	0	0
			5	4	1		
10	M	1	Total	O	P	0	0
			5	4	1		
10	M	1	Total	O	P	0	0
			5	4	1		

*Continued on next page...*

*Continued from previous page...*

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

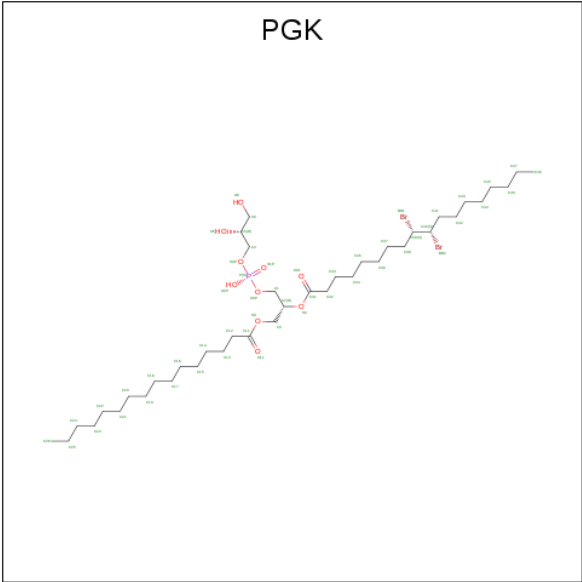
- Molecule 11 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



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

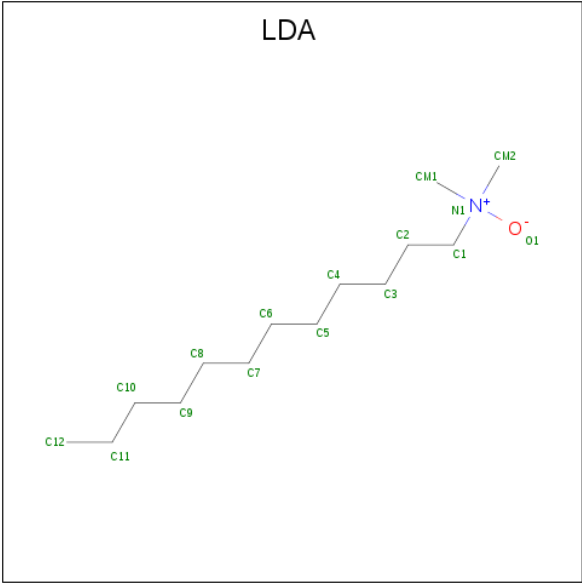
- Molecule 12 is (1R)-2-{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (9S,10S)-9,10-DIBROMOOCTADECANOATE (three-letter code: PGK) (formula:  $C_{40}H_{77}Br_2O_{10}P$ ).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	M	1	Total	Br	C	O	P	0	0
			53	2	40	10	1		

- Molecule 13 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
13	M	1	Total	C	N	O	0	0
			16	14	1	1		
13	M	1	Total	C	N	O	0	0
			16	14	1	1		

Continued on next page...

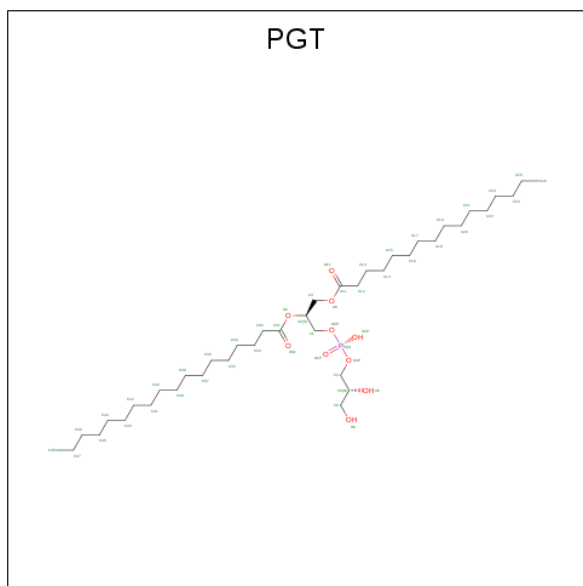
*Continued from previous page...*

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

- Molecule 14 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	H	1	Total	K	0	0
			1	1		

- Molecule 15 is (1S)-2-{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PGT) (formula: C<sub>40</sub>H<sub>79</sub>O<sub>10</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	H	1	Total	C	O	P	0	1
			102	80	20	2		

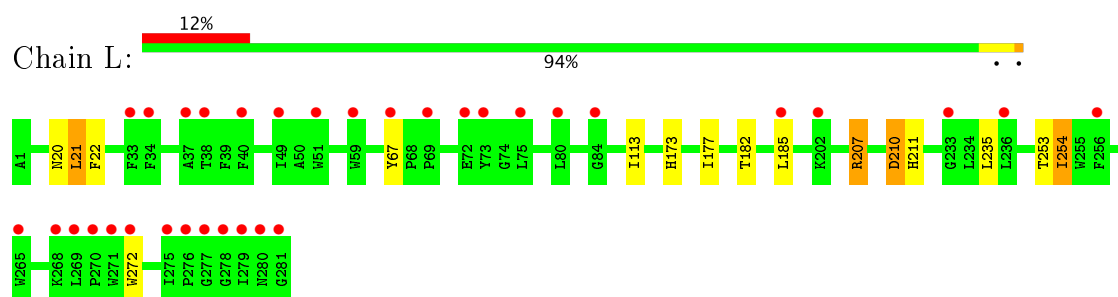
- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	L	92	Total 92	O 92	0	0
16	M	119	Total 119	O 119	0	0
16	H	199	Total 199	O 199	0	0

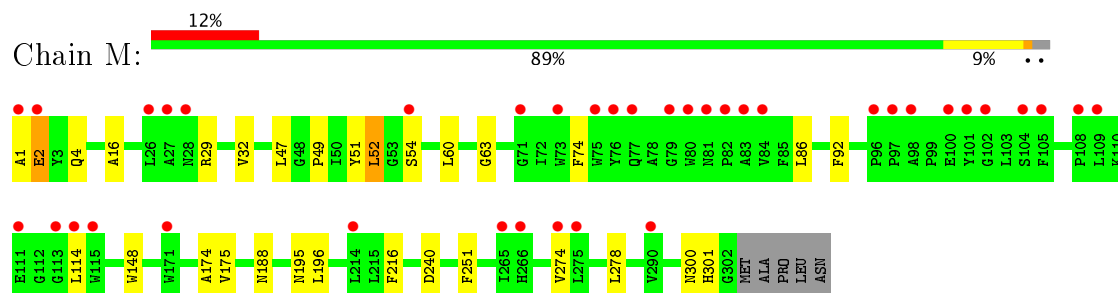
### 3 Residue-property plots [i](#)

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.

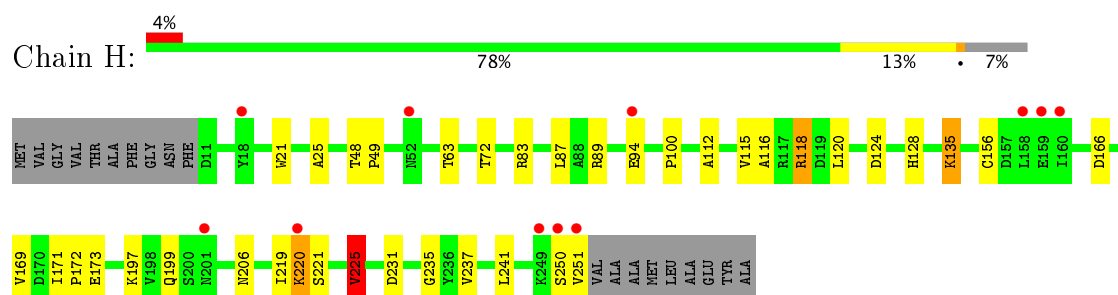
#### • Molecule 1: Reaction center protein L chain



#### • Molecule 2: Reaction center protein M chain



#### • Molecule 3: Reaction center protein H chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.42Å 139.42Å 183.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.00 – 2.50 45.63 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.00-2.50) 99.5 (45.63-2.50)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.62 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.172 , 0.197 0.177 , 0.200	Depositor DCC
$R_{free}$ test set	3548 reflections (5.22%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.2	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 97.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7824	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, GOL, LDA, CL, CDL, BPH, K, PGK, PGT, FE, U10, PO4

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	0.88	0/2328	0.73	1/3186 (0.0%)
2	M	0.87	0/2592	0.78	1/3536 (0.0%)
3	H	0.93	5/1953 (0.3%)	0.82	4/2652 (0.2%)
All	All	0.89	5/6873 (0.1%)	0.78	6/9374 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	M	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	173	GLU	CD-OE2	5.32	1.31	1.25
3	H	237	VAL	CB-CG2	5.12	1.63	1.52
3	H	221[A]	SER	CB-OG	5.07	1.48	1.42
3	H	221[B]	SER	CB-OG	5.07	1.48	1.42
3	H	94	GLU	CG-CD	5.05	1.59	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	210	ASP	CB-CG-OD1	6.50	124.15	118.30
3	H	124	ASP	CB-CG-OD1	6.31	123.98	118.30
3	H	225	VAL	CB-CA-C	-5.53	100.90	111.40
3	H	89	ARG	NE-CZ-NH2	-5.40	117.60	120.30
2	M	240	ASP	CB-CG-OD1	5.20	122.98	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	83	ARG	NE-CZ-NH1	5.05	122.83	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	M	1	ALA	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2235	0	2196	10	0
2	M	2448	0	2367	26	0
3	H	1862	0	1883	25	0
4	L	132	0	148	6	0
4	M	132	0	148	20	0
5	L	65	0	75	0	0
5	M	65	0	76	4	0
6	L	48	0	63	4	0
6	M	48	0	63	1	0
7	H	6	0	8	0	0
7	L	18	0	24	5	0
8	M	1	0	0	0	0
9	M	1	0	0	0	0
10	H	5	0	0	0	0
10	M	15	0	0	1	0
11	M	81	0	106	3	0
12	M	53	0	74	11	0
13	H	48	0	93	25	0
13	M	48	0	93	12	0
14	H	1	0	0	0	0
15	H	102	0	156	20	0
16	H	199	0	0	4	0
16	L	92	0	0	2	0
16	M	119	0	0	2	0
All	All	7824	0	7573	123	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 8.

All (123) 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)
2:M:301[A]:HIS:HE1	16:M:1031:HOH:O	1.41	1.03
4:M:311:BCL:C9	4:M:311:BCL:H41	1.91	0.99
4:M:311:BCL:C7	4:M:311:BCL:H41	1.92	0.98
13:M:902:LDA:C12	13:H:903:LDA:C12	2.43	0.96
13:M:902:LDA:C12	13:H:903:LDA:H123	1.96	0.95
4:M:311:BCL:C4	4:M:311:BCL:H92	1.98	0.94
13:M:902:LDA:H122	13:H:903:LDA:C12	1.98	0.93
13:M:902:LDA:H122	13:H:903:LDA:H123	1.49	0.93
4:M:311:BCL:H92	4:M:311:BCL:H41	1.48	0.92
7:L:709:GOL:H2	3:H:241:LEU:HD13	1.54	0.89
15:H:801[A]:PGT:C44	13:H:901:LDA:H121	2.05	0.86
15:H:801[A]:PGT:C43	13:H:901:LDA:H121	2.05	0.85
4:M:313:BCL:H201	12:M:802:PGK:H252	1.59	0.84
4:M:311:BCL:HBB2	4:M:311:BCL:HMB1	1.63	0.81
4:M:311:BCL:CBB	4:M:311:BCL:HMB1	2.13	0.79
4:M:311:BCL:H41	4:M:311:BCL:H71	1.64	0.77
13:M:902:LDA:H123	13:H:903:LDA:C12	2.15	0.77
3:H:250:SER:O	3:H:251:VAL:HG23	1.85	0.76
6:L:502:U10:H153	12:M:802:PGK:H482	1.69	0.74
15:H:801[A]:PGT:H442	13:H:901:LDA:C12	2.20	0.71
4:M:311:BCL:C8	4:M:311:BCL:H41	2.20	0.71
2:M:16:ALA:HB1	2:M:32:VAL:HG11	1.73	0.69
1:L:254:ILE:C	1:L:254:ILE:HD12	2.13	0.69
4:L:314:BCL:HBB2	4:L:314:BCL:HMB1	1.74	0.68
15:H:801[B]:PGT:C32	15:H:801[B]:PGT:H12	2.22	0.68
15:H:801[A]:PGT:H362	15:H:801[A]:PGT:H321	1.75	0.68
1:L:182:THR:OG1	4:M:311:BCL:H2	1.94	0.68
15:H:801[A]:PGT:H442	13:H:901:LDA:H121	1.72	0.68
3:H:220[B]:LYS:NZ	16:H:1209:HOH:O	2.25	0.67
6:L:502:U10:H153	12:M:802:PGK:C48	2.25	0.66
3:H:219:ILE:HG21	3:H:225:VAL:HG13	1.78	0.66
15:H:801[B]:PGT:C43	13:H:901:LDA:H121	2.24	0.66
15:H:801[B]:PGT:C44	13:H:901:LDA:H121	2.26	0.65
4:M:313:BCL:C20	12:M:802:PGK:H252	2.26	0.64
4:M:311:BCL:C4	4:M:311:BCL:C9	2.63	0.64
15:H:801[A]:PGT:H412	13:H:903:LDA:H111	1.82	0.62
15:H:801[A]:PGT:H432	13:H:901:LDA:H121	1.81	0.62

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:902:LDA:H122	13:H:903:LDA:H122	1.80	0.62
11:M:800:CDL:H231	13:H:904:LDA:HM12	1.82	0.60
2:M:174:ALA:HB1	13:M:920:LDA:H121	1.83	0.60
2:M:175:VAL:H	13:M:920:LDA:H123	1.66	0.60
4:M:311:BCL:H191	12:M:802:PGK:BR2	2.57	0.60
4:M:311:BCL:H42	4:M:311:BCL:H92	1.84	0.60
3:H:118[B]:ARG:HE	3:H:120:LEU:HD12	1.68	0.57
13:M:902:LDA:C12	13:H:903:LDA:H122	2.33	0.57
2:M:148:TRP:HA	2:M:148:TRP:CE3	2.40	0.57
4:M:311:BCL:C4	4:M:311:BCL:H71	2.33	0.57
3:H:21:TRP:CD1	15:H:801[B]:PGT:H5	2.41	0.56
4:L:314:BCL:CBB	4:L:314:BCL:HMB1	2.37	0.55
11:M:800:CDL:C23	13:H:904:LDA:HM12	2.37	0.54
4:M:311:BCL:H8	12:M:802:PGK:H471	1.91	0.52
2:M:60[A]:LEU:HD23	5:M:401:BPH:H4C1	1.92	0.52
15:H:801[B]:PGT:H322	15:H:801[B]:PGT:H12	1.92	0.52
7:L:709:GOL:H2	3:H:241:LEU:CD1	2.35	0.51
2:M:278[B]:LEU:HD11	11:M:800:CDL:H811	1.91	0.51
3:H:197[A]:LYS:NZ	3:H:199:GLN:HE21	2.09	0.51
15:H:801[B]:PGT:H431	13:H:901:LDA:H121	1.90	0.50
6:L:502:U10:C15	12:M:802:PGK:H482	2.41	0.50
2:M:175:VAL:N	13:M:920:LDA:H123	2.26	0.50
3:H:169:VAL:HG23	3:H:171:ILE:HD13	1.93	0.50
3:H:87:LEU:HD23	3:H:100:PRO:HA	1.93	0.50
2:M:51:TYR:O	2:M:52:LEU:HD23	2.11	0.50
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.47	0.50
4:L:312:BCL:CBB	4:L:312:BCL:HMB1	2.43	0.48
2:M:188[B]:ASN:ND2	16:M:1077:HOH:O	2.43	0.48
3:H:220[B]:LYS:NZ	16:H:1100:HOH:O	2.41	0.48
2:M:54:SER:OG	10:M:703:PO4:O2	2.32	0.47
2:M:175:VAL:H	13:M:920:LDA:C12	2.27	0.47
15:H:801[A]:PGT:H442	13:H:901:LDA:H123	1.96	0.47
6:L:502:U10:H4M3	6:L:502:U10:H3M2	1.96	0.47
15:H:801[A]:PGT:C41	13:H:903:LDA:H111	2.44	0.47
1:L:113:ILE:O	7:L:709:GOL:H11	2.15	0.47
2:M:175:VAL:HB	13:M:920:LDA:H123	1.97	0.47
2:M:29:ARG:O	12:M:802:PGK:H42	2.15	0.47
4:L:312:BCL:HHC	4:L:312:BCL:OBB	2.15	0.46
1:L:113:ILE:O	7:L:709:GOL:C1	2.63	0.46
4:M:313:BCL:HMB1	4:M:313:BCL:CBB	2.45	0.46
3:H:63:THR:CG2	3:H:72:THR:HB	2.46	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:207:ARG:HG2	1:L:211:HIS:CG	2.51	0.46
7:L:709:GOL:C2	3:H:241:LEU:HD13	2.36	0.46
3:H:156[A]:CYS:HB3	3:H:206:ASN:O	2.16	0.45
3:H:156[B]:CYS:HB3	3:H:206:ASN:O	2.16	0.45
4:M:313:BCL:HAA2	4:M:313:BCL:HBD	1.99	0.45
2:M:148:TRP:HA	2:M:148:TRP:HE3	1.81	0.45
3:H:128[B]:HIS:HE1	16:H:1109:HOH:O	1.99	0.45
5:M:401:BPH:CBC	5:M:401:BPH:HHD	2.47	0.45
12:M:802:PGK:H121	12:M:802:PGK:H31	1.53	0.45
1:L:21:LEU:HD13	1:L:22:PHE:CE1	2.52	0.44
3:H:135:LYS:HB3	3:H:135:LYS:HE3	1.57	0.44
15:H:801[A]:PGT:H362	15:H:801[A]:PGT:C32	2.46	0.44
2:M:63:GLY:HA3	5:M:401:BPH:H5C2	1.99	0.44
4:L:312:BCL:HMB1	4:L:312:BCL:HBB3	1.99	0.44
2:M:47:LEU:HD22	12:M:802:PGK:BR2	2.73	0.43
15:H:801[B]:PGT:H322	15:H:801[B]:PGT:H351	1.58	0.43
15:H:801[A]:PGT:H432	13:H:903:LDA:H112	2.00	0.43
2:M:196:LEU:HD12	2:M:196:LEU:HA	1.91	0.43
3:H:128[B]:HIS:HD2	16:H:1280:HOH:O	2.01	0.42
1:L:67:TYR:HB3	16:L:1167:HOH:O	2.19	0.42
3:H:135:LYS:HB3	3:H:166:ASP:OD2	2.20	0.42
1:L:253:THR:OG1	1:L:254:ILE:N	2.51	0.42
4:M:313:BCL:H201	12:M:802:PGK:C25	2.40	0.42
2:M:74:PHE:CD1	2:M:92:PHE:HB3	2.54	0.42
3:H:48:THR:HB	3:H:49:PRO:HD2	2.02	0.42
3:H:25:ALA:HB2	13:H:903:LDA:H52	2.01	0.42
15:H:801[A]:PGT:C44	13:H:901:LDA:C12	2.81	0.42
2:M:2:GLU:HG3	2:M:2:GLU:H	1.53	0.42
2:M:2:GLU:O	2:M:4:GLN:NE2	2.52	0.42
3:H:115:VAL:HG12	3:H:116:ALA:N	2.35	0.42
13:H:901:LDA:H22	13:H:901:LDA:HM11	1.80	0.42
2:M:32:VAL:HG12	2:M:49:PRO:HD3	2.02	0.42
6:M:501:U10:H322	6:M:501:U10:H28	1.80	0.41
3:H:112:ALA:HA	3:H:235:GLY:O	2.20	0.41
15:H:801[B]:PGT:C41	13:H:903:LDA:H111	2.50	0.41
1:L:20:ASN:ND2	16:L:1300:HOH:O	2.52	0.41
4:L:312:BCL:CGA	4:L:314:BCL:HBC1	2.51	0.41
3:H:118[B]:ARG:NE	3:H:120:LEU:HD12	2.35	0.41
3:H:171:ILE:HB	3:H:172:PRO:HD3	2.01	0.41
2:M:251:PHE:CD1	2:M:251:PHE:C	2.94	0.41
2:M:52:LEU:HD11	2:M:60[A]:LEU:HD12	2.02	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:401:BPH:HBC3	5:M:401:BPH:HHD	2.02	0.40
4:M:311:BCL:HMB1	4:M:311:BCL:HBB3	2.00	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	280/281 (100%)	274 (98%)	6 (2%)	0	100	100
2	M	310/307 (101%)	298 (96%)	11 (4%)	1 (0%)	44	66
3	H	247/260 (95%)	242 (98%)	5 (2%)	0	100	100
All	All	837/848 (99%)	814 (97%)	22 (3%)	1 (0%)	55	76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	195	ASN

### 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	L	221/220 (100%)	214 (97%)	7 (3%)	44	71
2	M	246/240 (102%)	240 (98%)	6 (2%)	54	80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	H	204/208 (98%)	197 (97%)	7 (3%)	42	69
All	All	671/668 (100%)	651 (97%)	20 (3%)	49	74

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	21	LEU
1	L	185	LEU
1	L	207	ARG
1	L	210	ASP
1	L	235	LEU
1	L	254	ILE
1	L	272	TRP
2	M	2	GLU
2	M	52	LEU
2	M	86	LEU
2	M	114	LEU
2	M	216	PHE
2	M	274	VAL
3	H	118[A]	ARG
3	H	118[B]	ARG
3	H	135	LYS
3	H	220[A]	LYS
3	H	220[B]	LYS
3	H	225	VAL
3	H	231	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	M	28	ASN
3	H	199	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 29 ligands modelled in this entry, 3 are monoatomic - leaving 26 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
10	PO4	H	704	-	4,4,4	0.75	0	6,6,6	0.60	0
7	GOL	H	706	-	5,5,5	0.25	0	5,5,5	0.81	0
15	PGT	H	801[A]	-	50,50,50	0.71	0	51,56,56	1.01	3 (5%)
15	PGT	H	801[B]	-	50,50,50	0.84	1 (2%)	51,56,56	1.15	5 (9%)
13	LDA	H	901	-	13,15,15	2.12	2 (15%)	14,17,17	0.91	0
13	LDA	H	903	-	13,15,15	2.23	1 (7%)	14,17,17	0.82	1 (7%)
13	LDA	H	904	-	13,15,15	2.37	2 (15%)	14,17,17	0.52	0
4	BCL	L	312	1	55,74,74	1.35	3 (5%)	65,115,115	1.44	11 (16%)
4	BCL	L	314	1	55,74,74	1.40	2 (3%)	65,115,115	1.56	12 (18%)
5	BPH	L	402	-	65,70,70	0.79	1 (1%)	75,101,101	1.26	9 (12%)
6	U10	L	502	-	48,48,63	1.07	4 (8%)	58,61,79	1.60	9 (15%)
7	GOL	L	707	-	5,5,5	0.33	0	5,5,5	0.47	0
7	GOL	L	708	-	5,5,5	0.47	0	5,5,5	0.56	0
7	GOL	L	709	-	5,5,5	0.62	0	5,5,5	0.65	0
4	BCL	M	311	2	55,74,74	1.18	2 (3%)	65,115,115	1.82	18 (27%)
4	BCL	M	313	2	55,74,74	1.45	3 (5%)	65,115,115	1.69	14 (21%)
5	BPH	M	401	-	65,70,70	0.87	1 (1%)	75,101,101	1.56	16 (21%)
6	U10	M	501	-	48,48,63	1.11	2 (4%)	58,61,79	1.42	8 (13%)
10	PO4	M	702	-	4,4,4	0.50	0	6,6,6	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	PO4	M	703	-	4,4,4	0.75	0	6,6,6	1.25	1 (16%)
10	PO4	M	705	-	4,4,4	0.70	0	6,6,6	0.69	0
11	CDL	M	800	-	80,80,99	1.23	4 (5%)	82,92,111	1.53	12 (14%)
12	PGK	M	802	-	52,52,52	0.85	3 (5%)	53,60,60	1.53	6 (11%)
13	LDA	M	902	-	13,15,15	2.23	1 (7%)	14,17,17	0.54	0
13	LDA	M	907	-	13,15,15	2.36	1 (7%)	14,17,17	0.89	1 (7%)
13	LDA	M	920	-	13,15,15	2.19	1 (7%)	14,17,17	1.15	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	PO4	H	704	-	-	0/0/0/0	0/0/0/0
7	GOL	H	706	-	-	0/4/4/4	0/0/0/0
15	PGT	H	801[A]	-	-	0/55/55/55	0/0/0/0
15	PGT	H	801[B]	-	-	0/55/55/55	0/0/0/0
13	LDA	H	901	-	-	0/13/13/13	0/0/0/0
13	LDA	H	903	-	-	0/13/13/13	0/0/0/0
13	LDA	H	904	-	-	0/13/13/13	0/0/0/0
4	BCL	L	312	1	-	0/37/137/137	0/0/9/9
4	BCL	L	314	1	-	0/37/137/137	0/0/9/9
5	BPH	L	402	-	-	0/54/105/105	0/1/6/6
6	U10	L	502	-	-	0/45/69/87	0/1/1/1
7	GOL	L	707	-	-	0/4/4/4	0/0/0/0
7	GOL	L	708	-	-	0/4/4/4	0/0/0/0
7	GOL	L	709	-	-	0/4/4/4	0/0/0/0
4	BCL	M	311	2	-	0/37/137/137	0/0/9/9
4	BCL	M	313	2	-	0/37/137/137	0/0/9/9
5	BPH	M	401	-	-	0/54/105/105	0/1/6/6
6	U10	M	501	-	-	0/45/69/87	0/1/1/1
10	PO4	M	702	-	-	0/0/0/0	0/0/0/0
10	PO4	M	703	-	-	0/0/0/0	0/0/0/0
10	PO4	M	705	-	-	0/0/0/0	0/0/0/0
11	CDL	M	800	-	-	0/91/91/110	0/0/0/0
12	PGK	M	802	-	-	0/60/60/60	0/0/0/0
13	LDA	M	902	-	-	0/13/13/13	0/0/0/0
13	LDA	M	907	-	-	0/13/13/13	0/0/0/0
13	LDA	M	920	-	-	0/13/13/13	0/0/0/0

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	907	LDA	O1-N1	-8.26	1.25	1.42
13	H	904	LDA	O1-N1	-8.19	1.26	1.42
13	M	902	LDA	O1-N1	-7.83	1.26	1.42
13	H	903	LDA	O1-N1	-7.75	1.26	1.42
13	M	920	LDA	O1-N1	-7.54	1.27	1.42
13	H	901	LDA	O1-N1	-7.25	1.27	1.42
13	H	901	LDA	C1-N1	-2.33	1.46	1.51
12	M	802	PGK	O2-C2	-2.06	1.41	1.46
12	M	802	PGK	BR1-C39	-2.04	1.92	1.97
13	H	904	LDA	C1-N1	-2.03	1.46	1.51
4	M	313	BCL	C5-C3	2.02	1.55	1.51
6	L	502	U10	C33-C34	2.13	1.38	1.33
5	L	402	BPH	CHC-C1C	2.29	1.41	1.36
5	M	401	BPH	CHC-C1C	2.48	1.41	1.36
6	L	502	U10	O4-C4	2.53	1.43	1.36
6	L	502	U10	C13-C14	2.74	1.39	1.33
4	L	312	BCL	C4-C3	2.89	1.58	1.50
6	M	501	U10	O4-C4	2.99	1.44	1.36
15	H	801[B]	PGT	C1-C2	3.05	1.59	1.50
12	M	802	PGK	P-O1P	3.17	1.62	1.50
6	L	502	U10	O3-C3	4.07	1.47	1.36
6	M	501	U10	O3-C3	4.12	1.47	1.36
11	M	800	CDL	OA6-CA5	4.24	1.46	1.34
11	M	800	CDL	OB8-CB7	4.30	1.46	1.33
11	M	800	CDL	OB6-CB5	4.49	1.47	1.34
4	M	311	BCL	CHB-C4A	5.02	1.39	1.33
4	L	314	BCL	CHC-C1C	5.32	1.40	1.33
11	M	800	CDL	OA8-CA7	5.38	1.49	1.33
4	M	313	BCL	CHC-C1C	5.49	1.40	1.33
4	M	311	BCL	CHC-C1C	5.56	1.40	1.33
4	L	312	BCL	CHB-C4A	5.73	1.40	1.33
4	L	312	BCL	CHC-C1C	5.89	1.41	1.33
4	L	314	BCL	CHB-C4A	6.36	1.41	1.33
4	M	313	BCL	CHB-C4A	7.06	1.42	1.33

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	313	BCL	CMB-C2B-C1B	-5.91	119.38	128.46
12	M	802	PGK	BR1-C39-C40	-5.04	100.39	110.28
12	M	802	PGK	C3-C2-C1	-4.86	100.90	111.86
4	M	313	BCL	CAC-C3C-C2C	-4.67	102.49	114.24

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	312	BCL	CMB-C2B-C1B	-4.59	121.41	128.46
11	M	800	CDL	CA4-OA6-CA5	-4.37	107.55	117.88
6	L	502	U10	O2-C2-C3	-4.18	112.07	120.95
5	M	401	BPH	C1-C2-C3	-4.08	118.45	125.96
4	M	311	BCL	C4-C3-C2	-3.88	113.32	123.69
4	L	314	BCL	CAA-C2A-C3A	-3.87	102.21	112.81
4	M	311	BCL	CMB-C2B-C1B	-3.80	122.63	128.46
4	L	314	BCL	CAC-C3C-C2C	-3.75	104.81	114.24
15	H	801[B]	PGT	C2-O2-C31	-3.63	109.30	117.88
6	M	501	U10	C17-C18-C19	-3.55	118.77	127.68
4	M	311	BCL	CED-O2D-CGD	-3.52	107.73	115.97
6	M	501	U10	C22-C23-C24	-3.29	119.41	127.68
5	M	401	BPH	CAA-C2A-C3A	-3.29	103.80	112.81
6	L	502	U10	C12-C13-C14	-3.28	119.44	127.68
5	M	401	BPH	OBD-CAD-CBD	-3.26	121.02	125.94
4	L	312	BCL	CAA-C2A-C3A	-3.12	104.27	112.81
5	M	401	BPH	C4D-C3D-CAD	-3.10	106.00	107.78
13	M	920	LDA	CM2-N1-CM1	-3.09	105.07	110.99
4	L	314	BCL	C5-C3-C2	-3.02	114.92	121.10
6	M	501	U10	C26-C27-C28	-2.98	101.73	111.97
12	M	802	PGK	C2-O2-C31	-2.97	110.85	117.88
4	L	314	BCL	O1D-CGD-CBD	-2.91	119.38	124.60
6	M	501	U10	C32-C33-C34	-2.86	120.50	127.68
6	L	502	U10	C25-C24-C23	-2.83	116.15	123.69
6	M	501	U10	C7-C6-C5	-2.79	114.90	118.47
5	L	402	BPH	C1-C2-C3	-2.78	120.84	125.96
6	L	502	U10	C22-C23-C24	-2.76	120.75	127.68
4	L	312	BCL	CHA-C1A-NA	-2.76	119.78	126.18
4	M	313	BCL	O2D-CGD-O1D	-2.72	118.34	123.82
5	M	401	BPH	O2D-CGD-O1D	-2.67	118.44	123.82
6	L	502	U10	C7-C6-C5	-2.60	115.15	118.47
11	M	800	CDL	OB8-CB7-OB9	-2.55	117.23	123.55
4	L	314	BCL	CMB-C2B-C1B	-2.53	124.58	128.46
4	M	311	BCL	CHA-C1A-NA	-2.52	120.33	126.18
4	M	313	BCL	C4B-CHC-C1C	-2.51	125.15	130.12
13	M	907	LDA	CM2-N1-CM1	-2.50	106.20	110.99
11	M	800	CDL	C72-C71-CB7	-2.48	104.53	113.58
4	L	312	BCL	OBD-CAD-CBD	-2.47	122.21	125.94
4	L	312	BCL	CAC-C3C-C2C	-2.46	108.05	114.24
12	M	802	PGK	BR2-C40-C39	-2.42	105.55	110.28
5	L	402	BPH	CMA-C3A-C2A	-2.41	104.01	113.77
13	H	903	LDA	CM2-N1-CM1	-2.40	106.39	110.99

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	800	CDL	C74-C73-C72	-2.40	102.08	114.45
4	M	313	BCL	CHA-C1A-NA	-2.40	120.61	126.18
4	M	311	BCL	CAA-C2A-C3A	-2.35	106.38	112.81
5	M	401	BPH	C4-C3-C2	-2.34	117.43	123.69
4	L	314	BCL	CMC-C2C-C3C	-2.33	104.31	113.77
4	L	314	BCL	CAC-C3C-C4C	-2.32	107.43	112.58
5	L	402	BPH	O2D-CGD-O1D	-2.31	119.17	123.82
15	H	801[B]	PGT	O2-C31-O31	-2.30	117.94	123.68
5	M	401	BPH	C4B-C3B-CAB	-2.28	121.69	130.09
11	M	800	CDL	OA6-CA5-OA7	-2.27	118.01	123.68
5	M	401	BPH	C2B-C1B-NB	-2.25	106.49	109.82
4	M	311	BCL	C6-C5-C3	-2.21	107.65	112.66
5	M	401	BPH	CMA-C3A-C2A	-2.19	104.88	113.77
4	M	313	BCL	C16-C15-C13	-2.14	108.70	115.73
4	L	312	BCL	CMA-C3A-C2A	-2.14	105.08	113.77
4	M	311	BCL	CMA-C3A-C4A	-2.13	106.04	111.77
4	M	311	BCL	O1D-CGD-CBD	-2.13	120.77	124.60
6	L	502	U10	C1M-C1-C6	-2.13	119.88	124.20
4	M	313	BCL	C1-C2-C3	-2.12	122.04	125.96
5	L	402	BPH	CAA-C2A-C3A	-2.11	107.02	112.81
11	M	800	CDL	CB6-CB4-CB3	-2.11	107.10	111.86
12	M	802	PGK	C3-O3-C11	-2.10	110.82	117.13
4	M	311	BCL	OBD-CAD-CBD	-2.09	122.78	125.94
4	L	314	BCL	CMA-C3A-C2A	-2.08	105.33	113.77
4	L	312	BCL	CMA-C3A-C4A	-2.05	106.25	111.77
5	M	401	BPH	CAA-C2A-C1A	-2.05	106.98	112.28
4	M	313	BCL	O2D-CGD-CBD	2.01	114.89	111.30
10	M	703	PO4	O4-P-O3	2.03	115.36	107.90
4	M	313	BCL	CHC-C1C-NC	2.03	127.32	124.51
4	M	311	BCL	OBD-CAD-C3D	2.09	131.88	128.03
4	M	311	BCL	C4-C3-C5	2.12	118.97	115.29
5	M	401	BPH	C1B-NB-C4B	2.23	110.94	106.52
5	M	401	BPH	C3A-C2A-C1A	2.24	104.32	101.68
4	M	313	BCL	C2C-C3C-C4C	2.25	104.70	101.34
4	L	312	BCL	C4-C3-C5	2.31	119.30	115.29
4	M	311	BCL	CMB-C2B-C3B	2.33	129.21	124.89
5	M	401	BPH	C1-O2A-CGA	2.35	122.41	116.77
15	H	801[B]	PGT	O3-C3-C2	2.36	114.58	108.66
4	M	311	BCL	C1D-CHD-C4C	2.36	129.44	125.92
4	L	312	BCL	C1-O2A-CGA	2.37	122.46	116.77
5	L	402	BPH	CAC-C3C-C2C	2.40	120.26	114.24
4	L	314	BCL	C4-C3-C5	2.44	119.52	115.29

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	402	BPH	CAC-C3C-C4C	2.45	118.96	112.67
15	H	801[A]	PGT	O3-C11-C12	2.46	119.05	111.90
4	M	313	BCL	CMA-C3A-C4A	2.47	118.41	111.77
11	M	800	CDL	CA6-OA8-CA7	2.47	124.57	117.13
4	M	311	BCL	CAA-CBA-CGA	2.48	120.82	113.35
5	L	402	BPH	C1B-NB-C4B	2.49	111.45	106.52
4	L	314	BCL	C2C-C3C-C4C	2.49	105.08	101.34
5	M	401	BPH	C3C-C4C-NC	2.50	110.32	107.97
4	L	312	BCL	C2C-C3C-C4C	2.65	105.31	101.34
15	H	801[A]	PGT	O3-C3-C2	2.72	115.50	108.66
4	M	313	BCL	C4-C3-C5	2.75	120.06	115.29
15	H	801[B]	PGT	O3-C11-C12	2.82	120.11	111.90
6	M	501	U10	C41-C39-C40	2.83	121.20	114.60
5	L	402	BPH	O2D-CGD-CBD	2.90	116.48	111.30
4	L	314	BCL	CAA-CBA-CGA	2.92	122.13	113.35
6	M	501	U10	C30-C29-C31	3.01	120.50	115.29
6	M	501	U10	C15-C14-C16	3.07	120.61	115.29
6	L	502	U10	C30-C29-C31	3.11	120.68	115.29
11	M	800	CDL	OB8-CB7-C71	3.17	121.12	111.90
6	L	502	U10	C3M-O3-C3	3.21	127.91	116.44
4	M	311	BCL	C5-C3-C2	3.22	127.70	121.10
11	M	800	CDL	OA8-CA7-C31	3.38	121.72	111.90
4	L	314	BCL	O2D-CGD-CBD	3.48	117.53	111.30
5	M	401	BPH	CAC-C3C-C4C	3.64	122.03	112.67
5	L	402	BPH	C3C-C4C-NC	3.66	111.42	107.97
4	L	312	BCL	CMB-C2B-C3B	3.91	132.16	124.89
4	M	313	BCL	CMD-C2D-C3D	3.92	132.16	124.89
11	M	800	CDL	OA6-CA5-C11	4.06	119.98	111.55
4	M	311	BCL	O2D-CGD-CBD	4.06	118.56	111.30
4	M	311	BCL	OBB-CAB-C3B	4.08	127.73	119.95
4	M	313	BCL	CMB-C2B-C3B	4.09	132.48	124.89
15	H	801[B]	PGT	O2-C31-C32	4.11	120.08	111.55
4	M	311	BCL	C1-O2A-CGA	4.25	126.97	116.77
12	M	802	PGK	O2-C31-C32	4.29	120.45	111.55
15	H	801[A]	PGT	O2-C31-C32	4.30	120.47	111.55
11	M	800	CDL	OB8-CB6-CB4	4.48	119.91	108.66
6	L	502	U10	C25-C24-C26	4.48	123.07	115.29
5	M	401	BPH	O2D-CGD-CBD	4.64	119.59	111.30
11	M	800	CDL	OB6-CB5-C51	5.56	123.09	111.55

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

18 monomers are involved in 81 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	H	801[A]	PGT	12	0
15	H	801[B]	PGT	8	0
13	H	901	LDA	11	0
13	H	903	LDA	12	0
13	H	904	LDA	2	0
4	L	312	BCL	4	0
4	L	314	BCL	3	0
6	L	502	U10	4	0
7	L	709	GOL	5	0
4	M	311	BCL	15	0
4	M	313	BCL	5	0
5	M	401	BPH	4	0
6	M	501	U10	1	0
10	M	703	PO4	1	0
11	M	800	CDL	3	0
12	M	802	PGK	11	0
13	M	902	LDA	7	0
13	M	920	LDA	5	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	L	281/281 (100%)	0.48	33 (11%) 5 4	54, 62, 73, 80	0
2	M	302/307 (98%)	0.59	38 (12%) 4 3	54, 62, 73, 94	0
3	H	241/260 (92%)	0.16	11 (4%) 33 35	54, 62, 73, 100	0
All	All	824/848 (97%)	0.42	82 (9%) 8 7	54, 62, 73, 100	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	1	ALA	6.7
2	M	80	TRP	6.4
3	H	250	SER	6.2
3	H	251	VAL	5.7
1	L	277	GLY	5.0
3	H	249	LYS	4.8
1	L	270	PRO	4.7
1	L	202	LYS	4.5
2	M	79	GLY	4.4
1	L	281	GLY	4.2
1	L	269	LEU	4.2
2	M	28	ASN	4.2
1	L	271	TRP	4.1
2	M	75	TRP	3.9
1	L	278	GLY	3.8
2	M	265	ILE	3.7
1	L	275	ILE	3.6
3	H	52	ASN	3.5
2	M	101	TYR	3.4
1	L	51	TRP	3.4
1	L	279	ILE	3.4
2	M	100[A]	GLU	3.3
1	L	73	TYR	3.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	M	104	SER	3.2
2	M	114	LEU	3.2
3	H	158	LEU	3.2
2	M	102	GLY	3.1
3	H	159	GLU	3.1
1	L	80	LEU	3.1
2	M	97	PRO	3.0
2	M	82	PRO	3.0
1	L	33	PHE	3.0
1	L	185	LEU	3.0
1	L	268	LYS	2.9
2	M	81	ASN	2.9
1	L	75	LEU	2.9
2	M	71	GLY	2.9
2	M	84	VAL	2.8
1	L	84	GLY	2.8
2	M	108	PRO	2.8
1	L	276	PRO	2.8
2	M	2	GLU	2.7
1	L	38	THR	2.7
2	M	98	ALA	2.7
2	M	73	TRP	2.7
1	L	40	PHE	2.6
2	M	77	GLN	2.6
1	L	280	ASN	2.6
2	M	111	GLU	2.6
1	L	236	LEU	2.6
2	M	171	TRP	2.5
1	L	72	GLU	2.5
1	L	272	TRP	2.5
1	L	59	TRP	2.5
1	L	256	PHE	2.5
2	M	26	LEU	2.4
3	H	160	ILE	2.4
2	M	96	PRO	2.4
3	H	94	GLU	2.4
2	M	76	TYR	2.4
2	M	83	ALA	2.4
2	M	275	LEU	2.4
3	H	18	TYR	2.4
2	M	27	ALA	2.3
1	L	69	PRO	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	M	54	SER	2.2
2	M	113	GLY	2.2
1	L	49	ILE	2.2
1	L	265	TRP	2.2
3	H	201	ASN	2.2
2	M	290	VAL	2.2
2	M	105	PHE	2.2
2	M	274	VAL	2.1
1	L	37	ALA	2.1
1	L	34	PHE	2.1
3	H	220[A]	LYS	2.1
1	L	233	GLY	2.1
1	L	67	TYR	2.0
2	M	115	TRP	2.0
2	M	266	HIS	2.0
2	M	109	LEU	2.0
2	M	214	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
13	LDA	M	902	16/16	0.22	0.93	29.11	66,71,75,79	16
13	LDA	H	903	16/16	-0.13	1.34	21.19	73,75,78,78	16
13	LDA	M	907	16/16	0.75	0.48	19.45	69,72,77,77	16
15	PGT	H	801[B]	51/51	0.41	1.25	17.11	47,76,84,85	51

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
15	PGT	H	801[A]	51/51	0.41	1.25	16.87	45,73,81,82	51
7	GOL	L	708	6/6	0.81	0.32	11.66	60,66,68,68	6
13	LDA	M	920	16/16	0.61	0.62	10.89	41,60,78,80	16
11	CDL	M	800	81/100	0.64	0.49	6.82	49,74,88,90	81
6	U10	L	502	48/63	0.76	0.59	6.53	53,68,86,90	48
12	PGK	M	802	53/53	0.19	0.75	6.35	61,67,76,77	53
7	GOL	H	706	6/6	0.91	0.39	5.29	72,72,73,74	6
13	LDA	H	901	16/16	0.83	0.41	4.50	72,77,86,88	16
7	GOL	L	709	6/6	0.75	0.46	3.11	65,66,68,70	6
7	GOL	L	707	6/6	0.65	0.35	2.23	65,67,68,68	6
6	U10	M	501	48/63	0.84	0.31	1.75	56,69,90,93	0
4	BCL	M	313	66/66	0.94	0.20	1.16	51,59,84,95	0
5	BPH	M	401	65/65	0.90	0.20	0.53	56,62,116,118	0
4	BCL	L	314	66/66	0.93	0.19	0.47	50,59,75,80	0
4	BCL	M	311	66/66	0.95	0.20	0.37	55,62,119,120	0
4	BCL	L	312	66/66	0.93	0.17	0.25	49,59,70,78	0
5	BPH	L	402	65/65	0.93	0.17	0.09	50,62,66,68	0
10	PO4	M	702	5/5	0.95	0.21	-0.11	69,71,74,77	5
10	PO4	M	703	5/5	0.96	0.21	-0.77	59,59,63,64	5
8	FE	M	500	1/1	1.00	0.18	-0.91	59,59,59,59	0
14	K	H	700	1/1	0.96	0.10	-2.31	58,58,58,58	0
10	PO4	M	705	5/5	0.78	0.25	-	63,64,65,65	5
10	PO4	H	704	5/5	0.68	0.26	-	61,61,63,63	5
13	LDA	H	904	16/16	0.44	0.74	-	76,79,86,86	16
9	CL	M	701	1/1	0.93	0.32	-	73,73,73,73	1

## 6.5 Other polymers

There are no such residues in this entry.