Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:30 AM GMT

PDB ID	:	2HG9
Title	:	Reaction centre from Rhodobacter sphaeroides strain R-26.1 complexed with tetrabrominated phosphatidylcholine
Authors	:	Roszak, A.W.; Gardiner, A.T.; Isaacs, N.W.; Cogdell, R.J.
Deposited on	:	2006-06-26
Resolution	:	2.45 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
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 ①) were used in the production of this report:

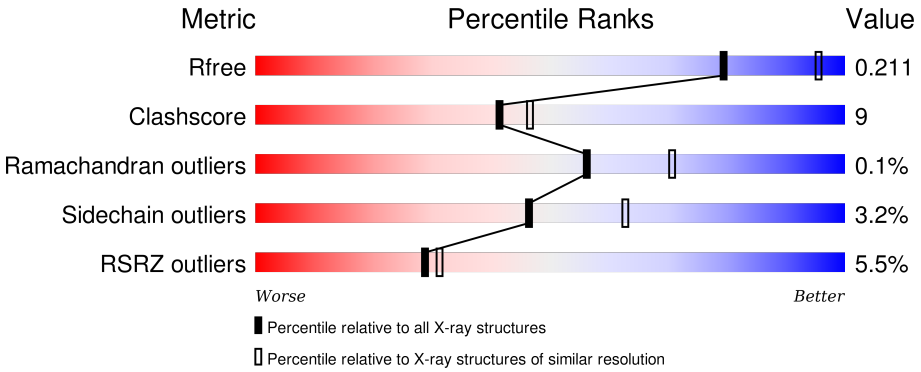
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.45 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	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	5% 93% 7%
2	M	307	8% 85% 11%
3	H	260	2% 81% 10% 7%

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	U10	L	502	-	-	-	X
11	CDL	M	800	-	-	-	X
12	PC7	H	801	-	-	-	X
13	PCK	M	802	-	-	X	X
14	LDA	H	901	-	-	-	X
14	LDA	H	908	-	-	X	X
14	LDA	M	907	-	-	-	X
14	LDA	M	920	-	-	-	X
15	GOL	H	705	-	-	-	X
15	GOL	H	708	-	-	-	X
6	PO4	H	704	-	-	-	X
6	PO4	L	703	-	-	-	X

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 7843 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	3	0
			2237	1511	356	362	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	12	0
			2450	1631	402	406	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	9	0
			1862	1189	323	339	11			

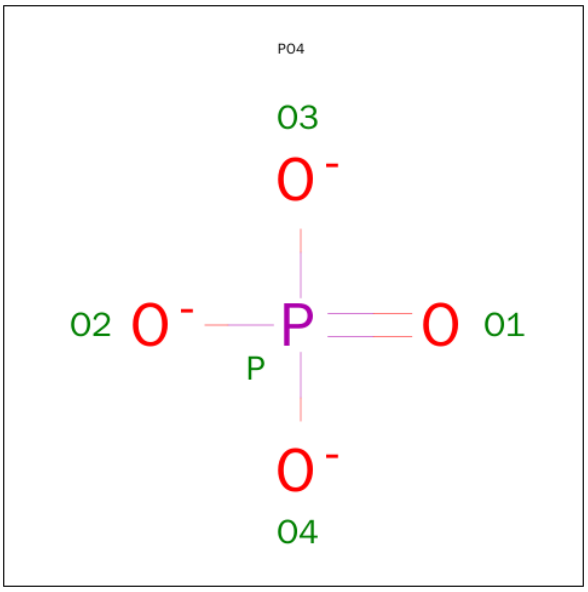
- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

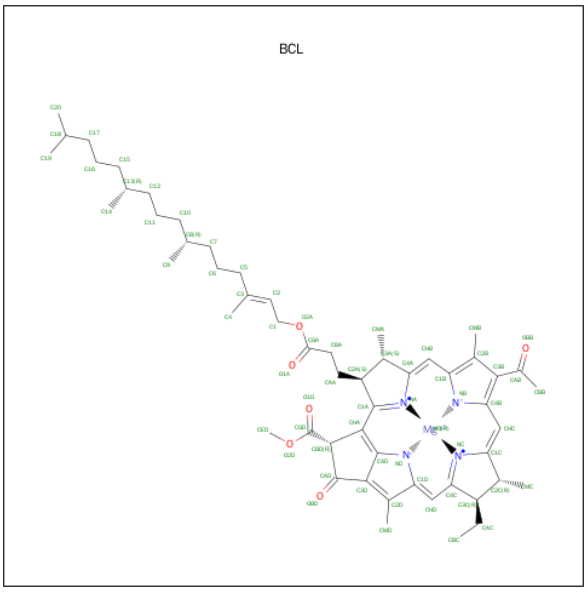


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	M	1	Total O P 5 4 1	0	0
6	M	1	Total O P 5 4 1	0	0
6	L	1	Total O P 5 4 1	0	0
6	H	1	Total O P 5 4 1	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

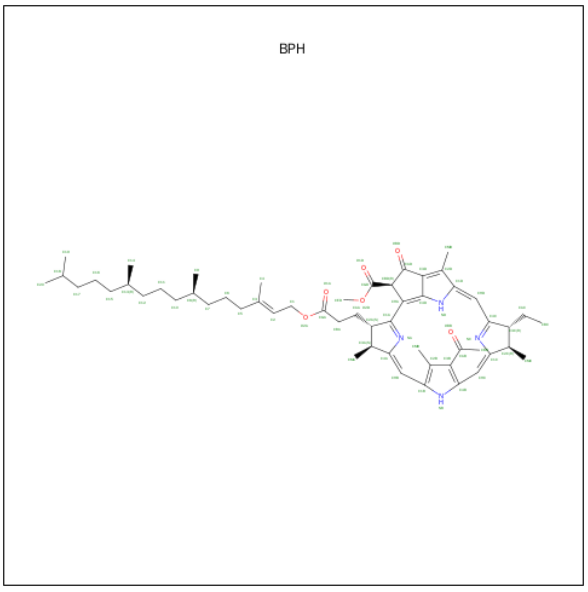
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	1	Total Cl 1 1	0	0
7	M	1	Total Cl 1 1	0	0

- Molecule 8 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



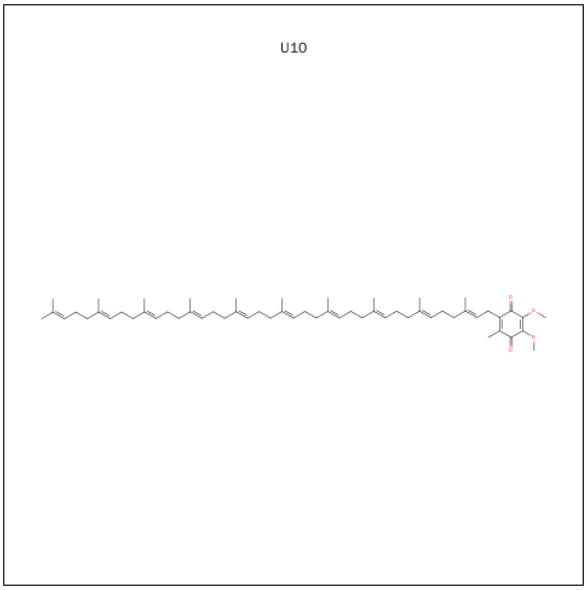
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
8	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
8	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
8	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 9 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



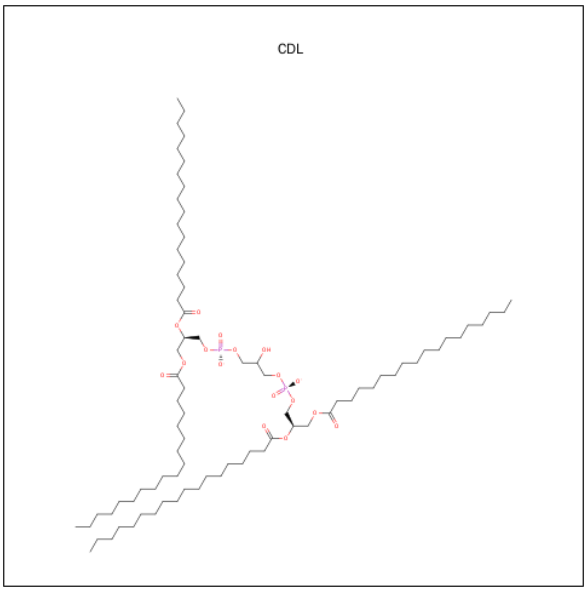
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	M	1	Total	C	N	O	0	0
			65	55	4	6		
9	L	1	Total	C	N	O	0	0
			65	55	4	6		

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



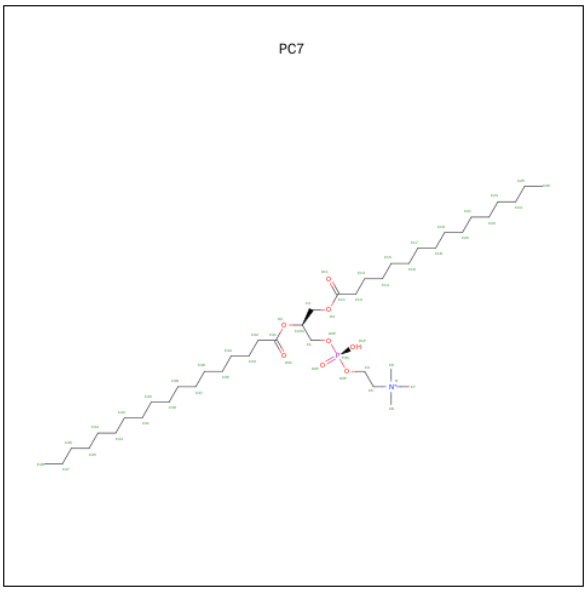
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	M	1	Total	C	O	0	0
			48	44	4		
10	L	1	Total	C	O	0	0
			48	44	4		

- 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		

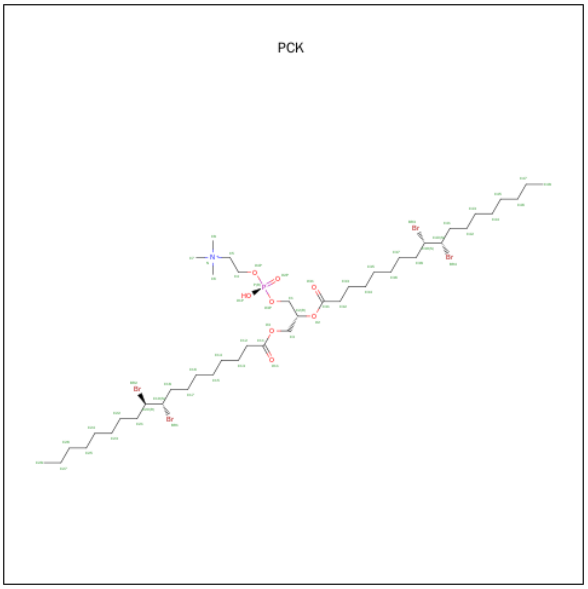
- Molecule 12 is (7S)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (three-letter code: PC7) (formula: $C_{42}H_{85}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	H	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

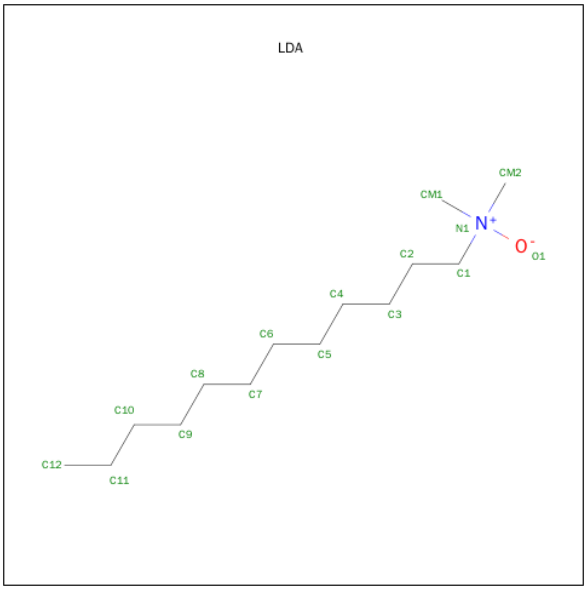
- Molecule 13 is (7R,18S,19R)-18,19-DIBROMO-7-{[(9S,10S)-9,10-DIBROMOOCTADECAN

OYL]OXY}-4-HYDROXY-N,N,N-TRIMETHYL-10-OXO-3,5,9-TRIOXA-4-PHOSPHAHE PTACOSAN-1-AMINIUM 4-OXIDE (three-letter code: PCK) (formula: $C_{44}H_{85}Br_4NO_8P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
13	M	1	Total	Br	C	N	O	P	0	0
			58	4	44	1	8	1		

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



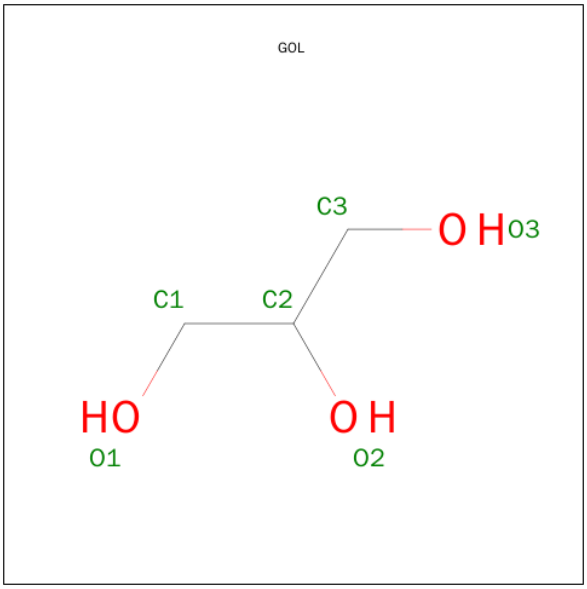
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	H	1	Total	C	N	O	0	0
			16	14	1	1		

Continued on next page...

Continued from previous page...

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

- Molecule 15 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	H	1	Total C O 6 3 3	0	0
15	H	1	Total C O 6 3 3	0	0
15	M	1	Total C O 6 3 3	0	0
15	H	1	Total C O 6 3 3	0	0
15	H	1	Total C O 6 3 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	M	1	Total	C	O	0	0
			6	3	3		

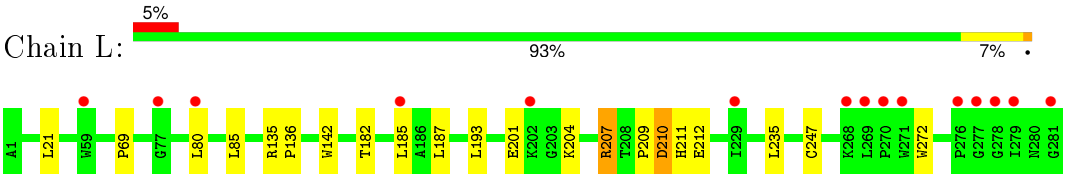
- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	H	208	Total	O	0	0
			208	208		
16	L	100	Total	O	0	0
			100	100		
16	M	133	Total	O	0	0
			133	133		

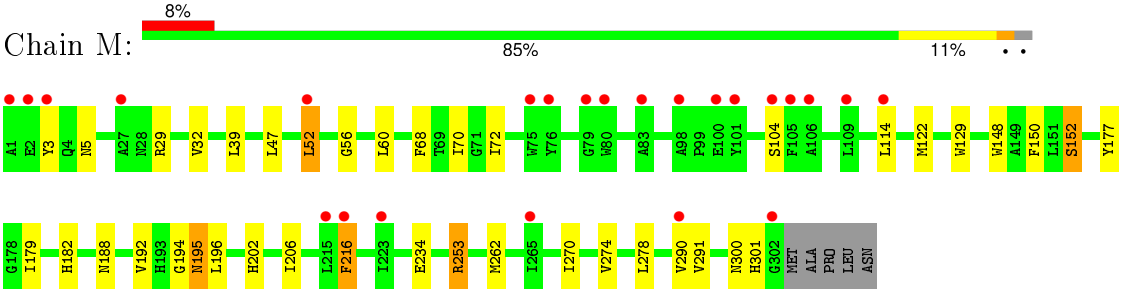
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

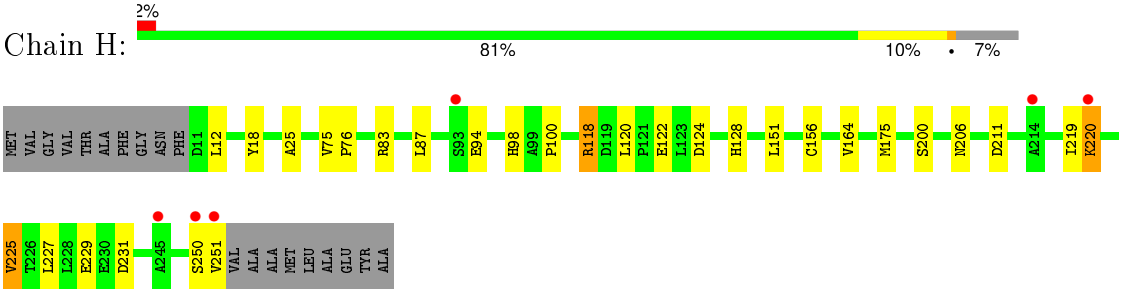
- Molecule 1: Reaction center protein L chain



- Molecule 2: Reaction center protein M chain



- Molecule 3: Reaction center protein H chain



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	139.55Å 139.55Å 184.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.36 – 2.45 39.36 – 2.45	Depositor EDS
% Data completeness (in resolution range)	98.0 (39.36-2.45) 98.0 (39.36-2.45)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.30 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.179 , 0.209 0.183 , 0.211	Depositor DCC
R_{free} test set	3709 reflections (5.19%)	DCC
Wilson B-factor (Å^2)	49.9	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 83.3	EDS
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 75227 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7843	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, GOL, LDA, CL, CDL, BPH, K, PC7, PCK, 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	0.90	0/2342	0.73	1/3205 (0.0%)
2	M	0.90	1/2601 (0.0%)	0.80	3/3548 (0.1%)
3	H	0.95	3/1961 (0.2%)	0.84	4/2663 (0.2%)
All	All	0.92	4/6904 (0.1%)	0.79	8/9416 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	94	GLU	CG-CD	6.20	1.61	1.51
3	H	94	GLU	CB-CG	5.59	1.62	1.52
3	H	94	GLU	CD-OE2	5.30	1.31	1.25
2	M	152	SER	CB-OG	5.05	1.48	1.42

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	124	ASP	CB-CG-OD1	7.74	125.27	118.30
3	H	124	ASP	CB-CG-OD2	-6.80	112.18	118.30
2	M	253[A]	ARG	NE-CZ-NH2	6.00	123.30	120.30
2	M	253[B]	ARG	NE-CZ-NH2	6.00	123.30	120.30
3	H	83	ARG	NE-CZ-NH2	-5.78	117.41	120.30
2	M	29	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	L	210	ASP	CB-CG-OD1	5.37	123.13	118.30
3	H	211	ASP	CB-CG-OD1	5.19	122.97	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2237	0	2202	10	0
2	M	2450	0	2370	38	0
3	H	1862	0	1884	21	0
4	M	1	0	0	0	0
5	H	1	0	0	0	0
6	H	5	0	0	0	0
6	L	5	0	0	0	0
6	M	10	0	0	0	0
7	L	1	0	0	0	0
7	M	1	0	0	1	0
8	L	132	0	148	8	0
8	M	132	0	148	20	0
9	L	65	0	75	3	0
9	M	65	0	76	4	0
10	L	48	0	63	4	0
10	M	48	0	63	1	0
11	M	81	0	106	2	0
12	H	52	0	84	6	0
13	M	58	0	80	24	0
14	H	64	0	124	19	0
14	M	48	0	93	9	0
15	H	24	0	32	2	0
15	M	12	0	16	0	0
16	H	208	0	0	0	0
16	L	100	0	0	0	0
16	M	133	0	0	7	0
All	All	7843	0	7564	128	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 (128) 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)
14:M:902:LDA:H121	14:H:908:LDA:H121	1.37	1.04

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:47[A]:LEU:HD22	13:M:802:PCK:BR4	2.11	1.04
10:L:502:U10:H351	10:L:502:U10:H38	1.41	1.03
13:M:802:PCK:H252	13:M:802:PCK:H211	1.35	1.02
2:M:122:MET:SD	14:M:920:LDA:H122	2.01	1.01
8:M:311:BCL:H93	13:M:802:PCK:H482	1.42	1.00
2:M:188[B]:ASN:OD1	16:M:1416:HOH:O	1.80	0.98
2:M:47[B]:LEU:HD23	13:M:802:PCK:BR4	2.26	0.90
13:M:802:PCK:BR1	13:M:802:PCK:H442	2.30	0.87
13:M:802:PCK:H252	13:M:802:PCK:C21	2.08	0.83
14:M:902:LDA:H121	14:H:908:LDA:C12	2.08	0.82
13:M:802:PCK:H161	13:M:802:PCK:BR3	2.36	0.81
2:M:60[B]:LEU:HD23	9:M:401:BPH:H4C1	1.63	0.81
10:L:502:U10:H351	10:L:502:U10:C38	2.11	0.80
14:H:903:LDA:CM2	14:H:904:LDA:O1	2.30	0.80
8:M:313:BCL:H191	13:M:802:PCK:H262	1.64	0.80
14:H:903:LDA:HM22	14:H:904:LDA:H21	1.66	0.76
13:M:802:PCK:H211	13:M:802:PCK:C25	2.10	0.76
14:M:902:LDA:C12	14:H:908:LDA:H121	2.16	0.74
12:H:801:PC7:H451	14:H:901:LDA:H121	1.68	0.74
8:M:311:BCL:C7	8:M:311:BCL:H41	2.18	0.72
8:M:311:BCL:HBB2	8:M:311:BCL:HMB1	1.71	0.71
8:M:311:BCL:CBB	8:M:311:BCL:HMB1	2.22	0.70
2:M:47[A]:LEU:CD2	13:M:802:PCK:BR4	2.94	0.70
8:M:311:BCL:H102	8:M:311:BCL:H41	1.75	0.67
14:H:903:LDA:HM23	14:H:904:LDA:O1	1.93	0.67
12:H:801:PC7:H451	14:H:901:LDA:C12	2.23	0.66
13:M:802:PCK:BR1	13:M:802:PCK:C44	2.99	0.66
8:M:311:BCL:H92	13:M:802:PCK:H261	1.78	0.66
8:M:311:BCL:H41	8:M:311:BCL:H71	1.78	0.65
2:M:52:LEU:HD11	2:M:60[A]:LEU:CD2	2.26	0.64
2:M:253[B]:ARG:NH2	16:M:1251:HOH:O	2.31	0.64
2:M:301[A]:HIS:CE1	16:M:1031:HOH:O	2.51	0.63
3:H:220[A]:LYS:NZ	3:H:229:GLU:OE2	2.32	0.62
2:M:68:PHE:O	2:M:72:ILE:HD13	2.00	0.62
2:M:56:GLY:O	2:M:60[A]:LEU:HD13	2.00	0.61
3:H:219:ILE:HG21	3:H:225:VAL:HG13	1.82	0.61
12:H:801:PC7:H73	14:H:908:LDA:H122	1.82	0.61
2:M:179:ILE:HG23	8:M:311:BCL:HED1	1.83	0.61
8:L:312:BCL:CBB	8:L:312:BCL:HMB1	2.32	0.60
2:M:47[B]:LEU:CD2	13:M:802:PCK:BR4	3.02	0.60
2:M:262:MET:HA	2:M:262:MET:HE3	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:70:ILE:HG21	14:M:920:LDA:HM13	1.84	0.58
8:M:311:BCL:C4	8:M:311:BCL:H71	2.34	0.57
8:M:311:BCL:H93	13:M:802:PCK:C48	2.27	0.57
8:L:314:BCL:HBB2	8:L:314:BCL:HMB1	1.85	0.56
1:L:201:GLU:OE2	1:L:204[B]:LYS:NZ	2.33	0.56
3:H:128[B]:HIS:ND1	15:H:708:GOL:H32	2.21	0.55
13:M:802:PCK:H271	13:M:802:PCK:BR1	2.61	0.55
8:M:313:BCL:HMB1	8:M:313:BCL:CBB	2.37	0.54
11:M:800:CDL:CA5	11:M:800:CDL:OA8	2.56	0.54
1:L:182:THR:OG1	8:M:311:BCL:H2	2.08	0.54
2:M:262:MET:HE3	2:M:262:MET:CA	2.38	0.53
2:M:39:LEU:HD23	14:M:907:LDA:H101	1.90	0.52
8:M:311:BCL:H92	13:M:802:PCK:C26	2.40	0.51
8:M:313:BCL:H191	13:M:802:PCK:C26	2.37	0.51
3:H:25:ALA:HB2	14:H:908:LDA:H61	1.92	0.51
3:H:18:TYR:CD1	14:H:908:LDA:HM23	2.46	0.51
8:L:314:BCL:HBB3	9:L:402:BPH:H141	1.92	0.50
8:L:312:BCL:CGA	8:L:314:BCL:HBC1	2.42	0.50
2:M:177:TYR:OH	14:M:920:LDA:H123	2.11	0.50
8:M:311:BCL:C9	13:M:802:PCK:H461	2.42	0.49
7:M:711:CL:CL	16:M:1177:HOH:O	2.57	0.49
1:L:69:PRO:HG2	1:L:142:TRP:HB2	1.94	0.49
14:H:904:LDA:H32	14:H:904:LDA:HM13	1.95	0.49
12:H:801:PC7:C7	14:H:908:LDA:H122	2.44	0.48
14:H:903:LDA:HM22	14:H:904:LDA:O1	2.13	0.48
2:M:150:PHE:N	9:M:401:BPH:HMD3	2.28	0.47
10:M:501:U10:O3	10:M:501:U10:H4M2	2.14	0.47
8:L:312:BCL:HMB1	8:L:312:BCL:HBB3	1.95	0.47
2:M:270:ILE:HD13	11:M:800:CDL:H711	1.97	0.47
3:H:18:TYR:HD1	14:H:908:LDA:HM23	1.80	0.47
2:M:3:TYR:CZ	2:M:5:ASN:HA	2.50	0.47
2:M:52:LEU:HD11	2:M:60[A]:LEU:HD21	1.96	0.46
9:L:402:BPH:HBB3	9:L:402:BPH:CMB	2.46	0.46
2:M:290:VAL:HG21	3:H:12:LEU:HD23	1.97	0.46
1:L:187:LEU:HD13	2:M:216:PHE:CG	2.51	0.46
16:M:1078:HOH:O	3:H:175:MET:HE1	2.16	0.46
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.97	0.46
2:M:52:LEU:HD11	2:M:60[B]:LEU:HD12	1.97	0.46
8:M:313:BCL:HMB1	8:M:313:BCL:HBB3	1.96	0.46
2:M:148:TRP:HA	2:M:148:TRP:CE3	2.51	0.46
2:M:152:SER:OG	2:M:278:LEU:HG	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:68:PHE:CE1	2:M:72:ILE:HD11	2.51	0.45
3:H:122:GLU:HB2	3:H:227:LEU:HD21	1.99	0.45
2:M:234:GLU:OE2	2:M:262:MET:HE1	2.17	0.45
3:H:219:ILE:HG21	3:H:225:VAL:CG1	2.47	0.45
12:H:801:PC7:H41	12:H:801:PC7:H11	1.99	0.45
2:M:202:HIS:CE1	2:M:206:ILE:HD11	2.52	0.45
9:M:401:BPH:H4C3	13:M:802:PCK:BR2	2.73	0.44
3:H:25:ALA:HB2	14:H:908:LDA:C6	2.47	0.44
12:H:801:PC7:H11	12:H:801:PC7:C4	2.47	0.44
8:L:314:BCL:H202	9:L:402:BPH:H7C2	2.00	0.44
2:M:52:LEU:HD11	2:M:60[A]:LEU:HD22	2.00	0.44
1:L:193:LEU:HD23	10:L:502:U10:C2	2.48	0.43
3:H:156[B]:CYS:HB3	3:H:206:ASN:O	2.18	0.43
8:M:313:BCL:C20	13:M:802:PCK:H242	2.49	0.43
3:H:156[A]:CYS:HB3	3:H:206:ASN:O	2.18	0.43
3:H:118[B]:ARG:NE	3:H:120:LEU:HD12	2.34	0.43
8:L:312:BCL:NA	8:M:313:BCL:HBB2	2.34	0.43
14:H:904:LDA:HM13	14:H:904:LDA:C3	2.48	0.43
2:M:188[A]:ASN:ND2	16:M:1416:HOH:O	2.49	0.43
13:M:802:PCK:H252	13:M:802:PCK:C20	2.49	0.42
3:H:87:LEU:HD23	3:H:100:PRO:HA	2.01	0.42
3:H:151:LEU:O	3:H:164:VAL:HG23	2.19	0.42
9:M:401:BPH:CMB	9:M:401:BPH:HBB3	2.48	0.42
1:L:207:ARG:CG	1:L:211:HIS:CG	3.03	0.42
1:L:207:ARG:HG2	1:L:211:HIS:CG	2.55	0.42
8:L:314:BCL:CBB	8:L:314:BCL:HMB1	2.50	0.42
10:L:502:U10:C35	10:L:502:U10:C38	2.92	0.42
2:M:129:TRP:CH2	13:M:802:PCK:BR2	3.28	0.42
14:H:903:LDA:H102	14:H:904:LDA:H101	2.02	0.42
2:M:301[A]:HIS:HE1	16:M:1031:HOH:O	1.95	0.41
14:M:902:LDA:C11	14:H:908:LDA:H121	2.49	0.41
8:M:313:BCL:H18	13:M:802:PCK:C24	2.51	0.41
1:L:209:PRO:HA	1:L:212:GLU:OE1	2.20	0.41
1:L:80:LEU:O	1:L:85:LEU:HD12	2.20	0.41
2:M:290:VAL:HG12	2:M:291:VAL:HG23	2.03	0.41
3:H:75:VAL:HA	3:H:76:PRO:C	2.40	0.41
14:M:902:LDA:H21	14:M:902:LDA:HM13	1.85	0.41
13:M:802:PCK:H62	13:M:802:PCK:H41	1.83	0.41
3:H:128[B]:HIS:CE1	15:H:708:GOL:H32	2.55	0.41
3:H:118[B]:ARG:HE	3:H:120:LEU:HD12	1.86	0.41
2:M:194:GLY:O	2:M:195:ASN:HB3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:87:LEU:HD13	3:H:98:HIS:HB2	2.01	0.40
3:H:250:SER:O	3:H:251:VAL:HG23	2.21	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	282/281 (100%)	275 (98%)	7 (2%)	0	100 100
2	M	312/307 (102%)	300 (96%)	11 (4%)	1 (0%)	46 57
3	H	248/260 (95%)	245 (99%)	3 (1%)	0	100 100
All	All	842/848 (99%)	820 (97%)	21 (2%)	1 (0%)	56 71

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	223/220 (101%)	216 (97%)	7 (3%)	47 64
2	M	248/240 (103%)	239 (96%)	9 (4%)	42 58

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	H	205/208 (99%)	198 (97%)	7 (3%)	44 61
All	All	676/668 (101%)	653 (97%)	23 (3%)	46 61

All (23) 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	247	CYS
1	L	272	TRP
2	M	32	VAL
2	M	52	LEU
2	M	104	SER
2	M	114	LEU
2	M	182	HIS
2	M	192	VAL
2	M	196	LEU
2	M	216	PHE
2	M	274	VAL
3	H	118[A]	ARG
3	H	118[B]	ARG
3	H	200	SER
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 (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	M	4	GLN
2	M	28	ASN
3	H	68	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 32 ligands modelled in this entry, 4 are monoatomic - leaving 28 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	PO4	H	704	-	4,4,4	0.30	0	6,6,6	0.30	0
15	GOL	H	705	-	5,5,5	0.50	0	5,5,5	0.65	0
15	GOL	H	706	-	5,5,5	0.30	0	5,5,5	1.01	0
15	GOL	H	708	-	5,5,5	0.27	0	5,5,5	0.49	0
15	GOL	H	709	-	5,5,5	0.44	0	5,5,5	0.46	0
12	PC7	H	801	-	51,51,51	0.85	2 (3%)	55,59,59	0.93	3 (5%)
14	LDA	H	901	-	15,15,15	3.79	2 (13%)	16,17,17	0.74	0
14	LDA	H	903	-	15,15,15	3.71	1 (6%)	16,17,17	0.69	0
14	LDA	H	904	-	15,15,15	3.69	2 (13%)	16,17,17	0.69	0
14	LDA	H	908	-	15,15,15	3.77	2 (13%)	16,17,17	1.15	2 (12%)
8	BCL	L	312	1	53,74,74	0.78	0	57,115,115	1.34	10 (17%)
8	BCL	L	314	1	53,74,74	0.84	0	57,115,115	1.77	15 (26%)
9	BPH	L	402	-	64,70,70	0.81	1 (1%)	73,101,101	1.36	8 (10%)
10	U10	L	502	-	48,48,63	1.10	4 (8%)	58,61,79	1.85	15 (25%)
6	PO4	L	703	-	4,4,4	0.34	0	6,6,6	0.28	0
8	BCL	M	311	2	53,74,74	0.70	0	57,115,115	1.48	10 (17%)
8	BCL	M	313	2	53,74,74	0.88	1 (1%)	57,115,115	1.51	11 (19%)
9	BPH	M	401	-	64,70,70	0.85	1 (1%)	73,101,101	1.44	11 (15%)
10	U10	M	501	-	48,48,63	0.96	4 (8%)	58,61,79	1.67	11 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	PO4	M	701	-	4,4,4	0.46	0	6,6,6	0.31	0
6	PO4	M	702	-	4,4,4	0.43	0	6,6,6	0.31	0
15	GOL	M	707	-	5,5,5	0.49	0	5,5,5	0.32	0
15	GOL	M	710	-	5,5,5	0.39	0	5,5,5	0.44	0
11	CDL	M	800	-	80,80,99	1.15	4 (5%)	82,92,111	1.16	6 (7%)
13	PCK	M	802	-	57,57,57	0.77	0	65,69,69	1.09	5 (7%)
14	LDA	M	902	-	15,15,15	3.80	2 (13%)	16,17,17	1.63	2 (12%)
14	LDA	M	907	-	15,15,15	3.79	2 (13%)	16,17,17	0.97	2 (12%)
14	LDA	M	920	-	15,15,15	3.72	1 (6%)	16,17,17	0.88	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
6	PO4	H	704	-	-	0/0/0/0	0/0/0/0
15	GOL	H	705	-	-	0/4/4/4	0/0/0/0
15	GOL	H	706	-	-	0/4/4/4	0/0/0/0
15	GOL	H	708	-	-	0/4/4/4	0/0/0/0
15	GOL	H	709	-	-	0/4/4/4	0/0/0/0
12	PC7	H	801	-	-	0/55/55/55	0/0/0/0
14	LDA	H	901	-	-	0/13/13/13	0/0/0/0
14	LDA	H	903	-	-	0/13/13/13	0/0/0/0
14	LDA	H	904	-	-	0/13/13/13	0/0/0/0
14	LDA	H	908	-	-	0/13/13/13	0/0/0/0
8	BCL	L	312	1	-	0/37/137/137	0/0/9/9
8	BCL	L	314	1	-	0/37/137/137	0/0/9/9
9	BPH	L	402	-	-	0/54/105/105	0/1/6/6
10	U10	L	502	-	-	0/45/69/87	0/1/1/1
6	PO4	L	703	-	-	0/0/0/0	0/0/0/0
8	BCL	M	311	2	-	0/37/137/137	0/0/9/9
8	BCL	M	313	2	-	0/37/137/137	0/0/9/9
9	BPH	M	401	-	-	0/54/105/105	0/1/6/6
10	U10	M	501	-	-	0/45/69/87	0/1/1/1
6	PO4	M	701	-	-	0/0/0/0	0/0/0/0
6	PO4	M	702	-	-	0/0/0/0	0/0/0/0
15	GOL	M	707	-	-	0/4/4/4	0/0/0/0
15	GOL	M	710	-	-	0/4/4/4	0/0/0/0
11	CDL	M	800	-	-	0/91/91/110	0/0/0/0
13	PCK	M	802	-	-	0/67/67/67	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	LDA	M	902	-	-	0/13/13/13	0/0/0/0
14	LDA	M	907	-	-	0/13/13/13	0/0/0/0
14	LDA	M	920	-	-	0/13/13/13	0/0/0/0

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	901	LDA	O1-N1	-14.38	1.25	1.39
14	H	908	LDA	O1-N1	-14.36	1.25	1.39
14	M	907	LDA	O1-N1	-14.34	1.25	1.39
14	H	903	LDA	O1-N1	-14.14	1.26	1.39
14	M	902	LDA	O1-N1	-14.11	1.26	1.39
14	M	920	LDA	O1-N1	-14.11	1.26	1.39
14	H	904	LDA	O1-N1	-13.97	1.26	1.39
14	M	902	LDA	C1-N1	-3.95	1.44	1.51
8	M	313	BCL	C3C-C4C	-3.65	1.46	1.51
14	H	904	LDA	C1-N1	-2.64	1.46	1.51
14	M	907	LDA	C1-N1	-2.46	1.46	1.51
14	H	901	LDA	C1-N1	-2.15	1.47	1.51
14	H	908	LDA	C1-N1	-2.03	1.47	1.51
10	M	501	U10	O4-C4	2.00	1.42	1.37
12	H	801	PC7	C3-C2	2.02	1.56	1.50
10	M	501	U10	C33-C34	2.13	1.37	1.33
10	L	502	U10	C28-C29	2.23	1.37	1.33
10	M	501	U10	O3-C3	2.27	1.43	1.37
9	L	402	BPH	CHC-C1C	2.28	1.40	1.36
10	M	501	U10	C13-C14	2.28	1.37	1.33
12	H	801	PC7	C1-C2	2.42	1.57	1.50
10	L	502	U10	C13-C14	2.73	1.38	1.33
10	L	502	U10	O4-C4	2.89	1.44	1.37
9	M	401	BPH	CHC-C1C	3.48	1.43	1.36
10	L	502	U10	O3-C3	3.85	1.47	1.37
11	M	800	CDL	OB8-CB7	4.14	1.45	1.33
11	M	800	CDL	OB6-CB5	4.33	1.47	1.34
11	M	800	CDL	OA6-CA5	4.47	1.47	1.34
11	M	800	CDL	OA8-CA7	4.53	1.47	1.33

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	311	BCL	C4-C3-C2	-4.78	114.11	123.50
14	M	902	LDA	O1-N1-C1	-4.65	105.04	110.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	M	501	U10	C32-C33-C34	-4.53	117.92	127.76
10	L	502	U10	C35-C34-C33	-4.27	115.11	123.50
10	L	502	U10	C31-C29-C28	-4.24	113.02	121.05
8	M	313	BCL	CMB-C2B-C1B	-4.06	121.64	128.36
10	M	501	U10	C26-C27-C28	-4.06	101.06	111.69
10	M	501	U10	C31-C29-C28	-3.66	114.11	121.05
8	L	314	BCL	CMB-C2B-C1B	-3.65	122.32	128.36
8	L	312	BCL	CMB-C2B-C1B	-3.64	122.34	128.36
8	L	314	BCL	CAC-C3C-C2C	-3.63	105.00	114.13
10	M	501	U10	C17-C18-C19	-3.44	120.28	127.76
8	L	312	BCL	CAA-C2A-C3A	-3.41	103.41	113.22
8	L	314	BCL	O1D-CGD-CBD	-3.37	119.80	124.62
14	M	902	LDA	CM2-N1-CM1	-3.31	105.10	108.83
10	L	502	U10	O2-C2-C3	-3.27	113.71	120.79
10	L	502	U10	C7-C6-C5	-3.24	114.74	118.56
8	M	313	BCL	CAC-C3C-C2C	-3.22	106.02	114.13
10	L	502	U10	C12-C13-C14	-3.11	120.99	127.76
9	M	401	BPH	OBD-CAD-CBD	-3.09	121.27	125.94
8	L	314	BCL	CAA-C2A-C3A	-3.06	104.41	113.22
10	M	501	U10	C22-C23-C24	-3.03	121.17	127.76
8	M	313	BCL	O2D-CGD-O1D	-2.82	117.96	123.79
8	M	311	BCL	CMB-C2B-C1B	-2.77	123.79	128.36
9	L	402	BPH	O2D-CGD-O1D	-2.75	118.10	123.79
8	M	311	BCL	CHA-C1A-NA	-2.74	119.31	126.06
8	L	314	BCL	C5-C3-C2	-2.74	115.85	121.05
8	M	313	BCL	CHA-C1A-NA	-2.74	119.32	126.06
8	M	311	BCL	CAA-C2A-C3A	-2.72	105.40	113.22
10	L	502	U10	C15-C14-C13	-2.72	118.17	123.50
9	M	401	BPH	CBB-CAB-C3B	-2.68	114.57	120.52
8	M	313	BCL	CAC-C3C-C4C	-2.63	106.74	112.58
8	L	314	BCL	OBB-CAB-CBB	-2.62	113.86	120.13
10	M	501	U10	C7-C6-C5	-2.59	115.51	118.56
12	H	801	PC7	C2-O2-C31	-2.58	111.70	117.89
13	M	802	PCK	C18-C19-C20	-2.55	108.96	115.64
8	L	312	BCL	CHA-C1A-NA	-2.54	119.80	126.06
9	L	402	BPH	O2A-CGA-O1A	-2.50	117.04	123.49
8	L	312	BCL	OBD-CAD-CBD	-2.49	122.18	125.94
9	M	401	BPH	O1D-CGD-CBD	-2.48	121.07	124.62
8	M	313	BCL	C11-C10-C8	-2.47	107.29	115.49
10	L	502	U10	C1M-C1-C6	-2.47	118.82	124.10
9	L	402	BPH	C1C-NC-C4C	-2.44	107.94	110.44
10	L	502	U10	C22-C23-C24	-2.41	122.52	127.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	M	401	BPH	CAA-C2A-C3A	-2.38	106.37	113.22
11	M	800	CDL	OA8-CA7-OA9	-2.35	117.42	123.49
10	M	501	U10	C11-C9-C8	-2.32	116.65	121.05
10	L	502	U10	C25-C24-C23	-2.28	119.03	123.50
9	M	401	BPH	C3B-C4B-NB	-2.22	105.25	109.98
14	H	908	LDA	CM2-N1-CM1	-2.16	106.40	108.83
8	L	314	BCL	CAC-C3C-C4C	-2.15	107.80	112.58
9	M	401	BPH	CMA-C3A-C2A	-2.15	104.83	114.35
10	L	502	U10	C21-C19-C18	-2.13	117.01	121.05
11	M	800	CDL	OA6-CA5-OA7	-2.11	117.99	123.67
14	M	907	LDA	O1-N1-CM2	-2.09	106.26	109.05
8	L	312	BCL	CAA-C2A-C1A	-2.04	105.28	112.47
9	L	402	BPH	CMA-C3A-C2A	-2.04	105.33	114.35
8	L	314	BCL	CMC-C2C-C3C	-2.03	105.36	114.35
13	M	802	PCK	BR1-C19-C18	2.02	112.44	108.92
14	H	908	LDA	CM1-N1-C1	2.04	116.35	109.77
8	M	313	BCL	CMD-C2D-C3D	2.04	129.09	125.09
8	M	311	BCL	C2A-C1A-CHA	2.06	127.69	123.89
9	M	401	BPH	CMD-C2D-C3D	2.07	129.13	125.09
8	M	313	BCL	C2C-C3C-C4C	2.15	105.15	101.50
10	L	502	U10	C3M-O3-C3	2.15	124.27	116.61
8	L	312	BCL	CED-O2D-CGD	2.20	121.14	115.99
12	H	801	PC7	O3-C11-C12	2.23	118.69	111.90
8	L	314	BCL	CMB-C2B-C3B	2.23	129.46	125.09
8	M	313	BCL	C4-C3-C5	2.29	118.91	115.41
8	M	311	BCL	O2D-CGD-CBD	2.30	114.45	111.30
9	M	401	BPH	C3C-C4C-NC	2.32	110.25	107.93
10	M	501	U10	C10-C9-C11	2.32	118.95	115.41
10	L	502	U10	C36-C34-C33	2.34	125.48	121.05
8	M	311	BCL	C4-C3-C5	2.35	118.99	115.41
8	L	314	BCL	C4-C3-C5	2.36	119.01	115.41
8	M	313	BCL	CHC-C1C-NC	2.41	127.84	124.51
8	L	312	BCL	CMB-C2B-C3B	2.42	129.81	125.09
8	L	314	BCL	CBC-CAC-C3C	2.42	119.48	113.57
8	L	312	BCL	C2C-C3C-C4C	2.44	105.63	101.50
8	M	311	BCL	CAA-CBA-CGA	2.46	120.51	113.32
10	M	501	U10	C25-C24-C26	2.48	119.20	115.41
9	M	401	BPH	C1B-NB-C4B	2.53	111.51	106.51
8	L	312	BCL	C4-C3-C5	2.54	119.29	115.41
8	L	314	BCL	CMD-C2D-C3D	2.56	130.10	125.09
8	M	313	BCL	O1D-CGD-CBD	2.60	128.35	124.62
8	M	311	BCL	OBB-CAB-C3B	2.61	124.14	120.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	L	502	U10	C35-C34-C36	2.62	119.41	115.41
14	M	907	LDA	O1-N1-C1	2.69	113.31	110.27
9	L	402	BPH	CAC-C3C-C4C	2.72	119.64	112.67
11	M	800	CDL	OA8-CA7-C31	2.74	120.25	111.90
9	L	402	BPH	CAC-C3C-C2C	2.84	121.28	114.13
8	L	312	BCL	CBA-CAA-C2A	2.91	121.95	113.73
11	M	800	CDL	CA6-OA8-CA7	2.92	125.02	116.85
8	L	314	BCL	CAA-CBA-CGA	2.95	121.95	113.32
13	M	802	PCK	O2-C31-C32	2.96	117.95	111.53
13	M	802	PCK	O3-C11-C12	3.01	121.09	111.90
10	M	501	U10	C15-C14-C16	3.06	120.07	115.41
8	M	311	BCL	C5-C3-C2	3.08	126.90	121.05
12	H	801	PC7	O2-C31-C32	3.22	118.53	111.53
10	L	502	U10	C25-C24-C26	3.26	120.39	115.41
13	M	802	PCK	O3-C3-C2	3.28	117.53	108.69
8	L	314	BCL	OBB-CAB-C3B	3.32	125.26	120.00
10	M	501	U10	C30-C29-C31	4.15	121.74	115.41
9	M	401	BPH	CAC-C3C-C4C	4.19	123.44	112.67
11	M	800	CDL	OB6-CB5-C51	4.43	121.17	111.53
9	L	402	BPH	O2D-CGD-CBD	4.44	117.39	111.30
10	L	502	U10	C30-C29-C31	4.49	122.27	115.41
9	M	401	BPH	O2D-CGD-CBD	4.56	117.55	111.30
9	L	402	BPH	C3C-C4C-NC	4.67	112.61	107.93
11	M	800	CDL	OA6-CA5-C11	4.90	122.17	111.53
8	L	314	BCL	O2D-CGD-CBD	5.19	118.42	111.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

19 monomers are involved in 81 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	H	708	GOL	2	0
12	H	801	PC7	6	0
14	H	901	LDA	2	0
14	H	903	LDA	5	0
14	H	904	LDA	7	0
14	H	908	LDA	10	0
8	L	312	BCL	4	0
8	L	314	BCL	5	0
9	L	402	BPH	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	L	502	U10	4	0
8	M	311	BCL	13	0
8	M	313	BCL	7	0
9	M	401	BPH	4	0
10	M	501	U10	1	0
11	M	800	CDL	2	0
13	M	802	PCK	24	0
14	M	902	LDA	5	0
14	M	907	LDA	1	0
14	M	920	LDA	3	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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	L	281/281 (100%)	0.06	15 (5%) 30 33	43, 53, 66, 82	0
2	M	302/307 (98%)	0.24	24 (7%) 15 16	43, 53, 65, 89	0
3	H	241/260 (92%)	-0.19	6 (2%) 61 63	44, 53, 61, 95	0
All	All	824/848 (97%)	0.05	45 (5%) 29 31	43, 53, 65, 95	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	1	ALA	10.7
3	H	251	VAL	9.0
2	M	2[A]	GLU	6.3
3	H	250	SER	6.2
1	L	277	GLY	5.0
1	L	270	PRO	4.7
2	M	114	LEU	4.0
2	M	302	GLY	4.0
1	L	268	LYS	3.5
2	M	100[A]	GLU	3.4
2	M	80	TRP	3.3
1	L	59	TRP	3.2
1	L	185	LEU	3.2
2	M	104	SER	3.2
2	M	75	TRP	3.1
1	L	80	LEU	3.1
2	M	106	ALA	3.0
2	M	98	ALA	3.0
3	H	245	ALA	2.9
3	H	220[A]	LYS	2.9
2	M	105	PHE	2.9
1	L	269	LEU	2.9
2	M	101	TYR	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	L	276[A]	PRO	2.7
1	L	281	GLY	2.7
2	M	3	TYR	2.7
1	L	202	LYS	2.7
2	M	109	LEU	2.6
1	L	279	ILE	2.6
2	M	216	PHE	2.5
1	L	278	GLY	2.5
2	M	27	ALA	2.5
1	L	271	TRP	2.3
2	M	290	VAL	2.3
2	M	83	ALA	2.3
2	M	79	GLY	2.3
2	M	76	TYR	2.2
2	M	265	ILE	2.1
3	H	93	SER	2.1
3	H	214	ALA	2.1
2	M	215	LEU	2.1
2	M	223	ILE	2.1
1	L	77	GLY	2.1
1	L	229	ILE	2.0
2	M	52	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^{th} 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^2)	Q<0.9
15	GOL	H	708	6/6	0.72	1.10	47.74	47,49,50,52	6
14	LDA	M	920	16/16	0.62	0.80	20.92	42,46,59,59	16
12	PC7	H	801	52/52	0.44	0.68	14.77	24,60,69,69	52
15	GOL	H	705	6/6	0.87	0.41	10.88	48,58,59,61	6
13	PCK	M	802	58/58	0.22	0.74	9.11	60,69,82,84	58
11	CDL	M	800	81/100	0.63	0.51	8.25	43,67,79,82	81
14	LDA	H	908	16/16	0.45	0.61	7.31	45,51,61,61	16
6	PO4	H	704	5/5	0.87	0.30	6.80	71,73,74,75	5
10	U10	L	502	48/63	0.73	0.55	5.84	40,55,73,75	48
14	LDA	M	907	16/16	0.66	0.39	5.20	56,59,65,66	16
14	LDA	H	901	16/16	0.85	0.29	4.43	61,63,66,68	16
6	PO4	L	703	5/5	0.73	0.33	2.19	61,61,62,65	5
15	GOL	H	706	6/6	0.87	0.26	1.71	71,72,73,74	6
8	BCL	M	311	66/66	0.94	0.22	1.22	46,54,119,120	0
9	BPH	M	401	65/65	0.88	0.23	1.21	45,55,106,107	0
10	U10	M	501	48/63	0.89	0.24	1.16	49,61,81,84	0
8	BCL	L	312	66/66	0.96	0.16	0.84	42,50,63,67	0
8	BCL	M	313	66/66	0.96	0.19	0.78	42,50,79,87	0
9	BPH	L	402	65/65	0.96	0.15	0.14	40,52,60,61	0
8	BCL	L	314	66/66	0.97	0.15	-0.01	41,48,67,71	0
6	PO4	M	702	5/5	0.94	0.12	-0.69	53,53,54,55	5
5	K	H	700	1/1	0.93	0.11	-0.81	57,57,57,57	0
6	PO4	M	701	5/5	0.96	0.14	-2.01	57,58,62,62	5
4	FE	M	500	1/1	0.99	0.17	-2.26	51,51,51,51	0
14	LDA	H	904	16/16	0.37	0.63	-	53,54,58,58	16
14	LDA	M	902	16/16	0.72	0.62	-	59,64,67,68	16
15	GOL	M	707	6/6	0.75	0.23	-	49,50,52,52	6
7	CL	M	711	1/1	0.88	0.24	-	74,74,74,74	1
7	CL	L	712	1/1	0.72	0.35	-	66,66,66,66	1
15	GOL	H	709	6/6	0.88	0.19	-	55,56,57,58	6
14	LDA	H	903	16/16	0.47	0.44	-	56,61,64,65	16
15	GOL	M	710	6/6	0.63	0.33	-	55,57,58,60	6

6.5 Other polymers

There are no such residues in this entry.