wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 02:30 AM GMT

PDB ID	:	2HG3
Title	:	Reaction centre from Rhodobacter sphaeroides strain R-26.1 complexed with brominated phosphatidylcholine
Authors	:	Roszak, A.W.; Gardiner, A.T.; Isaacs, N.W.; Cogdell, R.J.
Deposited on	:	2006-06-26
Resolution	:	2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

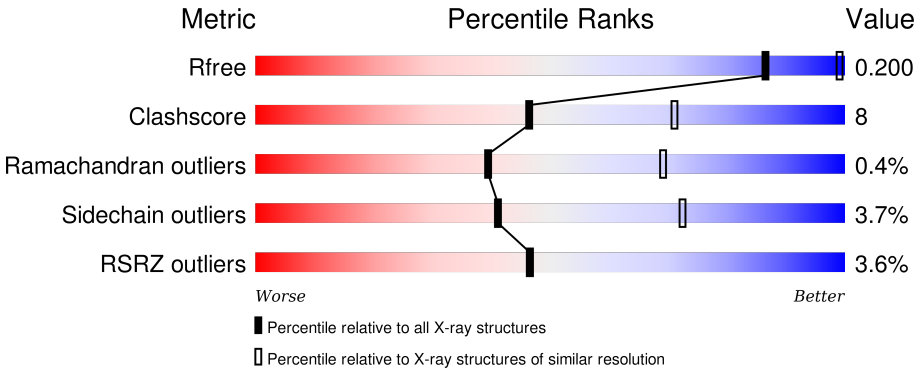
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	3%, 91%, 9%
2	M	307	5%, 84%, 14%
3	H	260	3%, 82%, 9%, 8%

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	HTO	L	705	-	-	-	X
11	CDL	M	800	-	-	-	X
12	PC9	M	801	-	-	-	X
12	PC9	M	802	-	-	-	X
13	LDA	H	903	-	-	-	X
13	LDA	L	905	-	-	-	X
13	LDA	L	906	-	-	-	X
13	LDA	L	908	-	-	-	X
13	LDA	L	909	-	-	-	X
13	LDA	M	907	-	-	-	X
13	LDA	M	920	-	-	-	X
14	GOL	H	706	-	-	-	X
14	GOL	L	707	-	-	-	X
14	GOL	L	708	-	-	-	X
6	PO4	L	701	-	-	-	X
6	PO4	M	703	-	-	X	-
9	U10	L	502	-	-	-	X

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 7921 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	4	0
			2246	1516	357	365	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	14	0
			2477	1654	405	407	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	240	Total	C	N	O	S	0	8	0
			1851	1181	321	338	11			

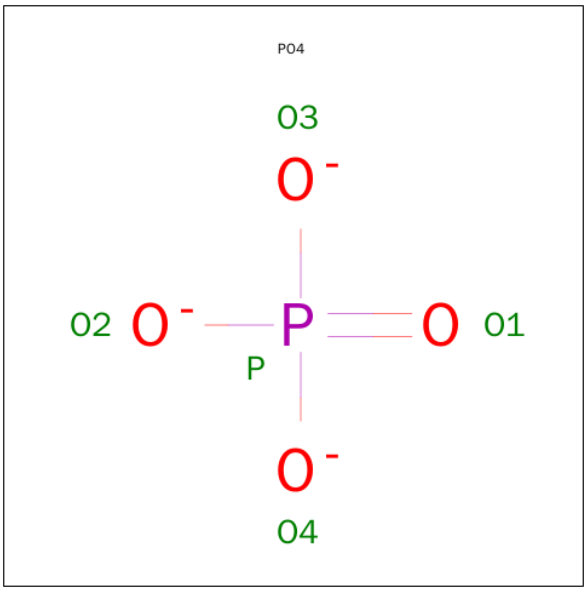
- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

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).

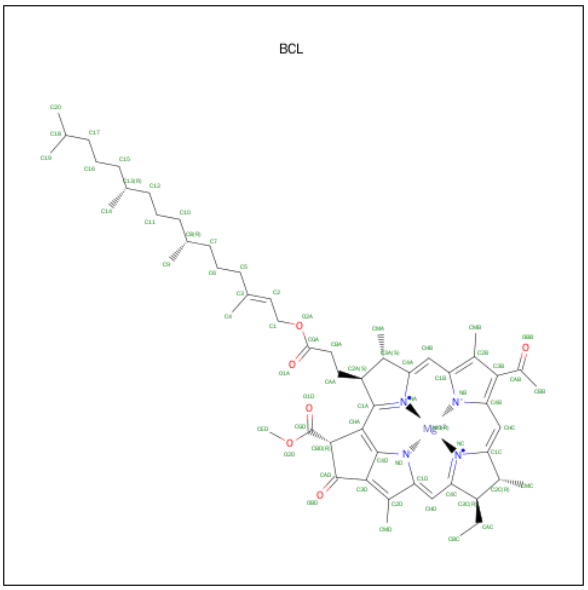
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total	K	0	0
			1	1		

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



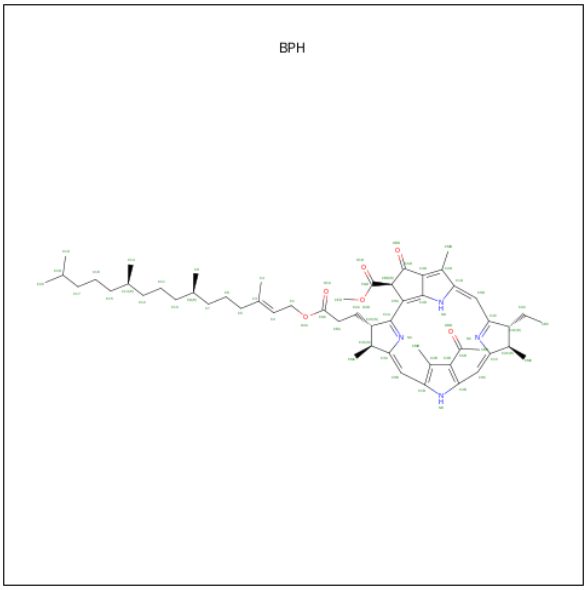
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	1	Total O P 5 4 1	0	0
6	L	1	Total O P 5 4 1	0	0
6	M	1	Total O P 5 4 1	0	0
6	M	1	Total O P 5 4 1	0	0

- Molecule 7 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



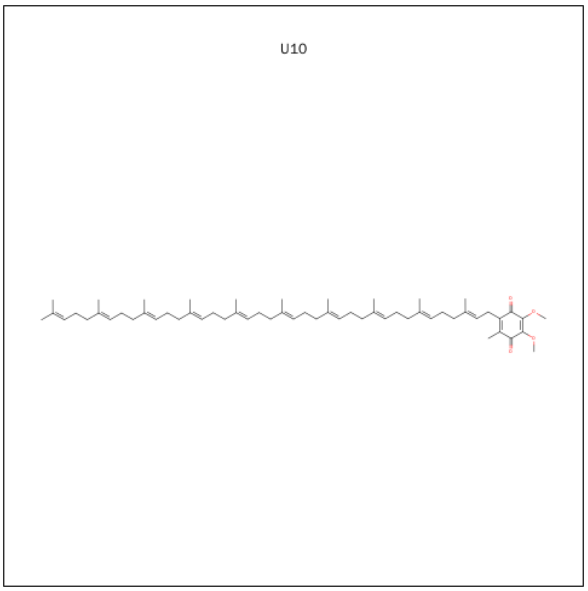
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 8 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



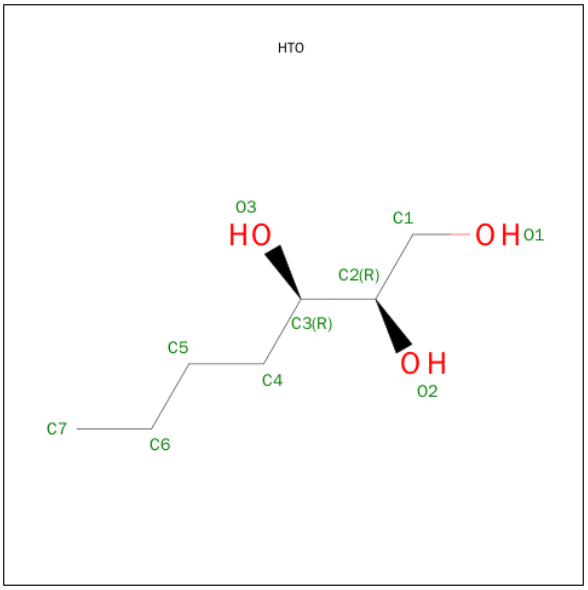
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	M	1	Total	C	N	O	0	0
			65	55	4	6		
8	L	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 9 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



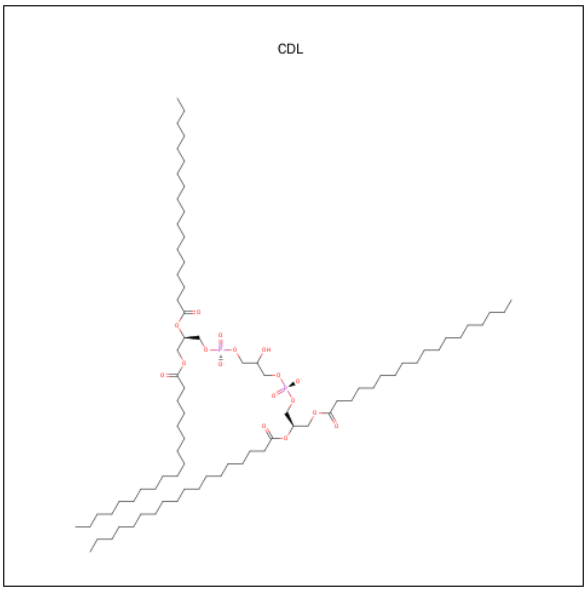
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	M	1	Total C O 48 44 4	0	0
9	L	1	Total C O 48 44 4	0	0

- Molecule 10 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: $C_7H_{16}O_3$).



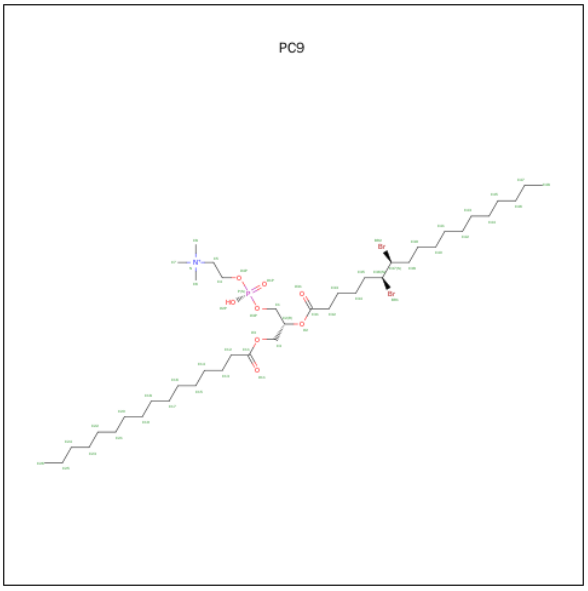
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	L	1	Total C O 10 7 3	0	0

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



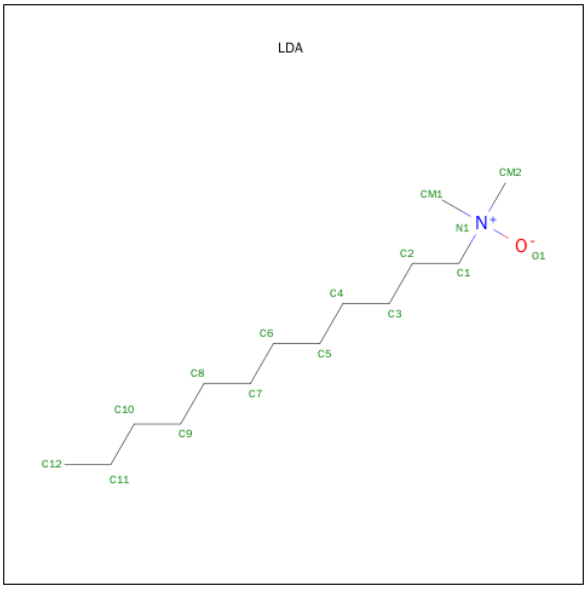
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
11	M	1	81	62	17	2	0	0

- Molecule 12 is (7R,14S)-14,15-DIBROMO-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (three-letter code: PC9) (formula: $C_{42}H_{83}Br_2NO_8P$).



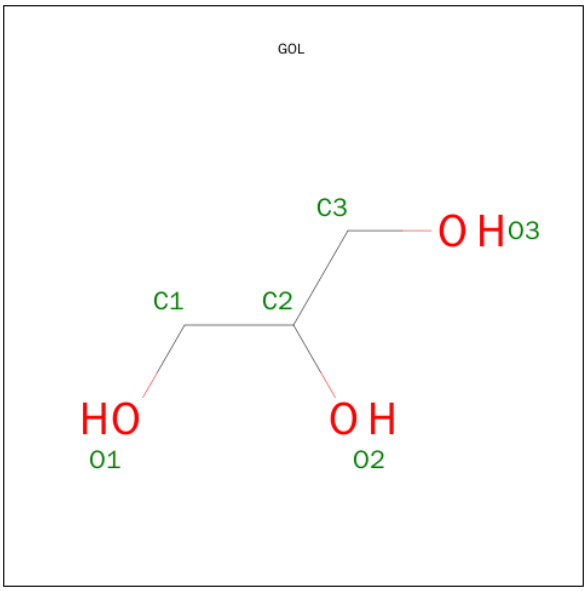
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	Br	C	N	O	P		
12	M	1	54	2	42	1	8	1	0	0
			Total	Br	C	N	O	P		
12	M	1	54	2	42	1	8	1	0	0

- Molecule 13 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



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

- Molecule 14 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

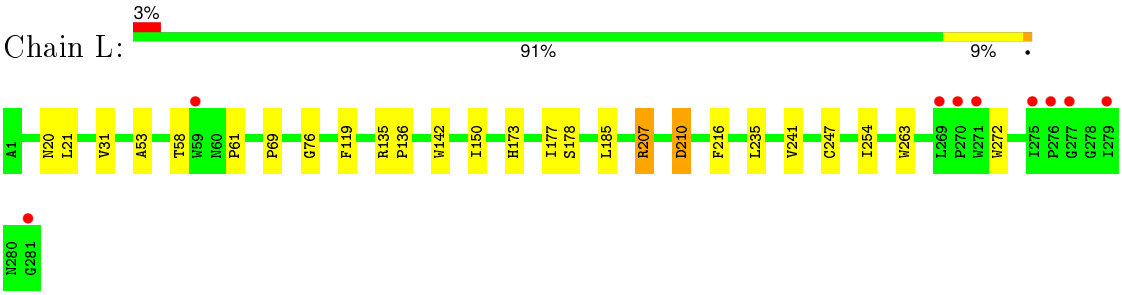
- Molecule 15 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	H	207	Total O 207 207	0	0
15	L	104	Total O 104 104	0	0
15	M	141	Total O 141 141	0	0

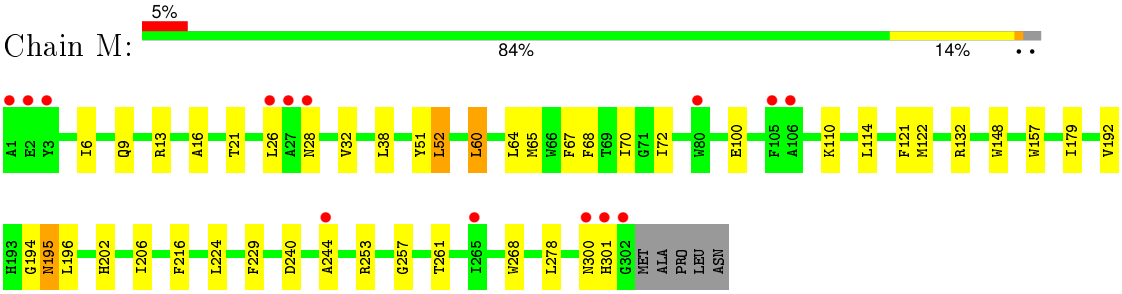
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

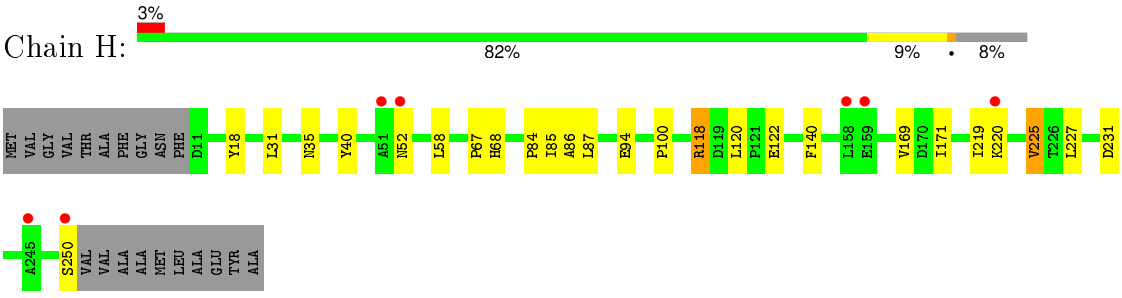
- Molecule 1: Reaction center protein L chain



- 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	139.84Å 139.84Å 184.34Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.35 – 2.70 34.35 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (34.35-2.70) 99.7 (34.35-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.57 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.164 , 0.199 0.169 , 0.200	Depositor DCC
R_{free} test set	2852 reflections (5.22%)	DCC
Wilson B-factor (Å^2)	53.8	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 78.2	EDS
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 57529 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7921	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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, PC9, CDL, BPH, K, HTO, 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	0.85	0/2351	0.77	3/3217 (0.1%)
2	M	0.88	0/2628	0.79	1/3584 (0.0%)
3	H	0.96	2/1945 (0.1%)	0.83	0/2642
All	All	0.89	2/6924 (0.0%)	0.79	4/9443 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	94	GLU	CG-CD	6.36	1.61	1.51
3	H	94	GLU	CD-OE2	6.10	1.32	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	210	ASP	CB-CG-OD1	6.91	124.52	118.30
1	L	207	ARG	NE-CZ-NH2	5.59	123.10	120.30
1	L	207	ARG	NE-CZ-NH1	-5.51	117.54	120.30
2	M	240	ASP	CB-CG-OD1	5.16	122.95	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	2246	0	2207	14	0
2	M	2477	0	2389	39	0
3	H	1851	0	1866	16	0
4	M	1	0	0	0	0
5	H	1	0	0	0	0
6	L	10	0	0	0	0
6	M	10	0	0	2	0
7	L	132	0	148	5	0
7	M	132	0	148	14	0
8	L	65	0	76	3	0
8	M	65	0	76	4	0
9	L	48	0	63	8	0
9	M	48	0	63	1	0
10	L	10	0	16	0	0
11	M	81	0	106	3	0
12	M	108	0	160	23	0
13	H	64	0	124	7	0
13	L	64	0	124	10	0
13	M	32	0	62	7	0
14	H	12	0	16	0	0
14	L	12	0	16	0	0
15	H	207	0	0	0	0
15	L	104	0	0	0	0
15	M	141	0	0	5	0
All	All	7921	0	7660	116	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.

The worst 5 of 116 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)
12:M:801:PC9:H261	13:H:903:LDA:H121	1.33	1.05
2:M:257:GLY:O	12:M:801:PC9:H32	1.64	0.98
7:M:311:BCL:H41	12:M:802:PC9:H441	1.45	0.97
3:H:118[B]:ARG:HD3	3:H:120:LEU:HD12	1.65	0.79
3:H:84:PRO:O	3:H:85:ILE:HD13	1.85	0.76

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	283/281 (101%)	272 (96%)	10 (4%)	1 (0%)	39	69
2	M	314/307 (102%)	298 (95%)	15 (5%)	1 (0%)	46	75
3	H	246/260 (95%)	240 (98%)	5 (2%)	1 (0%)	39	69
All	All	843/848 (99%)	810 (96%)	30 (4%)	3 (0%)	39	69

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	195	ASN
3	H	86	ALA
1	L	31	VAL

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	224/220 (102%)	215 (96%)	9 (4%)	38	69
2	M	250/240 (104%)	239 (96%)	11 (4%)	35	65
3	H	203/208 (98%)	197 (97%)	6 (3%)	48	79
All	All	677/668 (101%)	651 (96%)	26 (4%)	41	71

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	60[A]	LEU
2	M	114	LEU
3	H	231	ASP
2	M	60[B]	LEU
2	M	100	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	274	ASN
2	M	28	ASN
3	H	68	HIS

5.3.3 RNA (i)

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, 2 are monoatomic - leaving 30 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	$\#\|Z\| > 2$
14	GOL	H	706	-	5,5,5	0.33	0	5,5,5	0.91	0
14	GOL	H	709	-	5,5,5	0.52	0	5,5,5	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	LDA	H	901	-	15,15,15	3.65	2 (13%)	16,17,17	0.86	1 (6%)
13	LDA	H	902	-	15,15,15	3.60	1 (6%)	16,17,17	0.76	1 (6%)
13	LDA	H	903	-	15,15,15	3.72	1 (6%)	16,17,17	1.05	2 (12%)
13	LDA	H	904	-	15,15,15	3.82	2 (13%)	16,17,17	0.53	0
7	BCL	L	312	1	53,74,74	0.80	0	57,115,115	1.20	7 (12%)
7	BCL	L	314	1	53,74,74	0.76	0	57,115,115	1.74	13 (22%)
8	BPH	L	402	-	64,70,70	0.78	1 (1%)	73,101,101	1.31	11 (15%)
9	U10	L	502	-	48,48,63	1.33	7 (14%)	58,61,79	1.97	15 (25%)
6	PO4	L	701	-	4,4,4	0.47	0	6,6,6	0.27	0
6	PO4	L	702	-	4,4,4	2.40	2 (50%)	6,6,6	0.32	0
10	HTO	L	705	-	9,9,9	0.59	0	8,10,10	0.72	0
14	GOL	L	707	-	5,5,5	0.66	0	5,5,5	1.00	0
14	GOL	L	708	-	5,5,5	0.52	0	5,5,5	0.38	0
13	LDA	L	905	-	15,15,15	3.61	1 (6%)	16,17,17	0.75	0
13	LDA	L	906	-	15,15,15	3.01	1 (6%)	16,17,17	0.53	0
13	LDA	L	908	-	15,15,15	3.52	2 (13%)	16,17,17	0.74	0
13	LDA	L	909	-	15,15,15	3.60	1 (6%)	16,17,17	1.12	2 (12%)
7	BCL	M	311	2	53,74,74	0.83	1 (1%)	57,115,115	1.78	17 (29%)
7	BCL	M	313	2	53,74,74	0.89	2 (3%)	57,115,115	1.42	10 (17%)
8	BPH	M	401	-	64,70,70	0.98	4 (6%)	73,101,101	1.70	16 (21%)
9	U10	M	501	-	48,48,63	1.07	3 (6%)	58,61,79	1.95	13 (22%)
6	PO4	M	703	-	4,4,4	0.38	0	6,6,6	0.27	0
6	PO4	M	704	-	4,4,4	0.95	0	6,6,6	0.31	0
11	CDL	M	800	-	80,80,99	1.26	4 (5%)	82,92,111	1.41	10 (12%)
12	PC9	M	801	-	53,53,53	1.11	6 (11%)	59,63,63	1.52	9 (15%)
12	PC9	M	802	-	53,53,53	1.01	4 (7%)	59,63,63	1.49	7 (11%)
13	LDA	M	907	-	15,15,15	3.33	1 (6%)	16,17,17	1.32	2 (12%)
13	LDA	M	920	-	15,15,15	3.17	1 (6%)	16,17,17	1.44	2 (12%)

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
14	GOL	H	706	-	-	0/4/4/4	0/0/0/0
14	GOL	H	709	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	LDA	H	901	-	-	0/13/13/13	0/0/0/0
13	LDA	H	902	-	-	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
7	BCL	L	312	1	-	0/37/137/137	0/0/9/9
7	BCL	L	314	1	-	0/37/137/137	0/0/9/9
8	BPH	L	402	-	-	0/54/105/105	0/1/6/6
9	U10	L	502	-	-	0/45/69/87	0/1/1/1
6	PO4	L	701	-	-	0/0/0/0	0/0/0/0
6	PO4	L	702	-	-	0/0/0/0	0/0/0/0
10	HTO	L	705	-	-	0/10/10/10	0/0/0/0
14	GOL	L	707	-	-	0/4/4/4	0/0/0/0
14	GOL	L	708	-	-	0/4/4/4	0/0/0/0
13	LDA	L	905	-	-	0/13/13/13	0/0/0/0
13	LDA	L	906	-	-	0/13/13/13	0/0/0/0
13	LDA	L	908	-	-	0/13/13/13	0/0/0/0
13	LDA	L	909	-	-	0/13/13/13	0/0/0/0
7	BCL	M	311	2	-	0/37/137/137	0/0/9/9
7	BCL	M	313	2	-	0/37/137/137	0/0/9/9
8	BPH	M	401	-	-	0/54/105/105	0/1/6/6
9	U10	M	501	-	-	0/45/69/87	0/1/1/1
6	PO4	M	703	-	-	0/0/0/0	0/0/0/0
6	PO4	M	704	-	-	0/0/0/0	0/0/0/0
11	CDL	M	800	-	-	0/91/91/110	0/0/0/0
12	PC9	M	801	-	-	0/60/60/60	0/0/0/0
12	PC9	M	802	-	-	0/60/60/60	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

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	H	904	LDA	O1-N1	-14.40	1.25	1.39
13	H	903	LDA	O1-N1	-14.28	1.26	1.39
13	H	901	LDA	O1-N1	-13.95	1.26	1.39
13	L	909	LDA	O1-N1	-13.78	1.26	1.39
13	L	905	LDA	O1-N1	-13.74	1.26	1.39

The worst 5 of 138 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	M	501	U10	C17-C18-C19	-4.83	117.25	127.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	M	501	U10	C32-C33-C34	-4.57	117.82	127.76
8	M	401	BPH	OBD-CAD-CBD	-4.53	119.09	125.94
9	L	502	U10	C25-C24-C23	-4.51	114.65	123.50
9	M	501	U10	C26-C27-C28	-4.31	100.39	111.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

19 monomers are involved in 75 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	H	902	LDA	1	0
13	H	903	LDA	6	0
13	H	904	LDA	2	0
7	L	312	BCL	3	0
7	L	314	BCL	3	0
8	L	402	BPH	3	0
9	L	502	U10	8	0
13	L	906	LDA	4	0
13	L	908	LDA	6	0
13	L	909	LDA	2	0
7	M	311	BCL	10	0
7	M	313	BCL	5	0
8	M	401	BPH	4	0
9	M	501	U10	1	0
6	M	703	PO4	2	0
11	M	800	CDL	3	0
12	M	801	PC9	14	0
12	M	802	PC9	9	0
13	M	920	LDA	7	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%)	-0.43	9 (3%) 51 51	42, 51, 63, 72	0
2	M	302/307 (98%)	-0.12	14 (4%) 36 35	40, 51, 61, 88	1 (0%)
3	H	240/260 (92%)	-0.27	7 (2%) 55 55	39, 51, 59, 83	0
All	All	823/848 (97%)	-0.27	30 (3%) 46 46	39, 51, 62, 88	1 (0%)

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	250	SER	4.7
1	L	271	TRP	4.2
2	M	1	ALA	3.9
1	L	270	PRO	3.6
2	M	2[A]	GLU	3.2

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
13	LDA	M	920	16/16	0.66	0.70	23.67	49,53,65,66	16
13	LDA	L	906	16/16	0.72	0.45	20.73	51,55,69,70	16
10	HTO	L	705	10/10	0.88	0.41	19.96	56,60,62,65	10
13	LDA	L	905	16/16	0.25	1.20	18.71	61,66,70,71	16
14	GOL	L	708	6/6	0.95	0.27	11.26	49,57,59,60	0
12	PC9	M	802	54/54	0.66	0.52	6.79	42,54,70,73	54
9	U10	L	502	48/63	0.73	0.45	5.63	37,56,66,67	48
13	LDA	L	909	16/16	0.50	0.45	5.18	50,54,71,73	16
11	CDL	M	800	81/100	0.74	0.38	4.99	50,69,80,87	81
12	PC9	M	801	54/54	0.71	0.48	4.75	30,52,79,80	54
14	GOL	H	706	6/6	0.95	0.45	4.55	59,62,63,65	6
13	LDA	H	903	16/16	0.54	0.47	3.91	49,55,63,63	16
6	PO4	L	701	5/5	0.88	0.32	3.21	65,65,66,67	5
13	LDA	M	907	16/16	0.82	0.30	2.96	60,64,70,71	16
14	GOL	L	707	6/6	0.85	0.28	2.24	58,61,62,66	6
7	BCL	M	311	66/66	0.96	0.21	1.51	41,51,103,104	0
8	BPH	M	401	65/65	0.90	0.20	1.14	44,52,96,97	0
13	LDA	L	908	16/16	0.75	0.44	1.05	51,59,72,73	16
9	U10	M	501	48/63	0.91	0.22	0.68	46,54,80,83	0
8	BPH	L	402	65/65	0.97	0.12	0.21	42,49,55,56	0
7	BCL	L	312	66/66	0.97	0.12	0.12	40,48,55,59	0
5	K	H	700	1/1	0.98	0.13	-0.07	52,52,52,52	0
7	BCL	M	313	66/66	0.97	0.14	-0.18	41,48,72,80	0
7	BCL	L	314	66/66	0.97	0.11	-0.33	38,46,66,73	0
6	PO4	L	702	5/5	0.93	0.16	-0.85	64,65,66,68	5
6	PO4	M	704	5/5	0.96	0.19	-0.87	54,54,56,58	5
4	FE	M	500	1/1	1.00	0.14	-1.57	52,52,52,52	0
13	LDA	H	904	16/16	0.80	0.44	-	60,62,66,66	16
14	GOL	H	709	6/6	0.70	0.24	-	50,51,52,53	6
13	LDA	H	901	16/16	0.56	0.49	-	52,55,66,66	16
13	LDA	H	902	16/16	0.56	0.59	-	64,66,72,72	16
6	PO4	M	703	5/5	0.75	0.38	-	64,65,66,67	5

6.5 Other polymers (i)

There are no such residues in this entry.