Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:07 PM GMT

PDB ID	:	4H9L
Title	:	Bacterial Photosynthetic Reaction Center from Rhodobacter sphaeroides with ILE M265 replaced with SER
Authors	:	Mattis, A.J.; Wraight, C.A.
Deposited on	:	2012-09-24
Resolution	:	2.77 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:

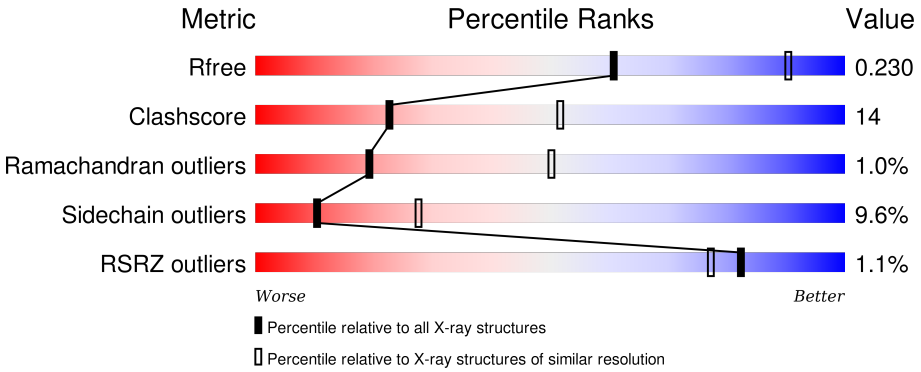
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.77 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	3004 (2.80-2.76)
Clashscore	102246	3480 (2.80-2.76)
Ramachandran outliers	100387	3423 (2.80-2.76)
Sidechain outliers	100360	3425 (2.80-2.76)
RSRZ outliers	91569	3016 (2.80-2.76)

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	% 68% 26% 5%
2	M	313	% 72% 19% 5%
3	H	260	% 71% 15% 6% 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
5	BPH	L	303	X	-	-	-
6	U10	L	304	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6916 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	280	Total	C	N	O	S	0	0	0
			2195	1484	347	356	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	301	Total	C	N	O	S	0	0	0
			2375	1586	390	389	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	265	SER	ILE	ENGINEERED MUTATION	UNP P0C0Y9
M	303	MET	-	EXPRESSION TAG	UNP P0C0Y9
M	304	ALA	-	EXPRESSION TAG	UNP P0C0Y9
M	305	PRO	-	EXPRESSION TAG	UNP P0C0Y9
M	306	LEU	-	EXPRESSION TAG	UNP P0C0Y9
M	307	ASN	-	EXPRESSION TAG	UNP P0C0Y9
M	308	HIS	-	EXPRESSION TAG	UNP P0C0Y9
M	309	HIS	-	EXPRESSION TAG	UNP P0C0Y9
M	310	HIS	-	EXPRESSION TAG	UNP P0C0Y9
M	311	HIS	-	EXPRESSION TAG	UNP P0C0Y9
M	312	HIS	-	EXPRESSION TAG	UNP P0C0Y9
M	313	HIS	-	EXPRESSION TAG	UNP P0C0Y9

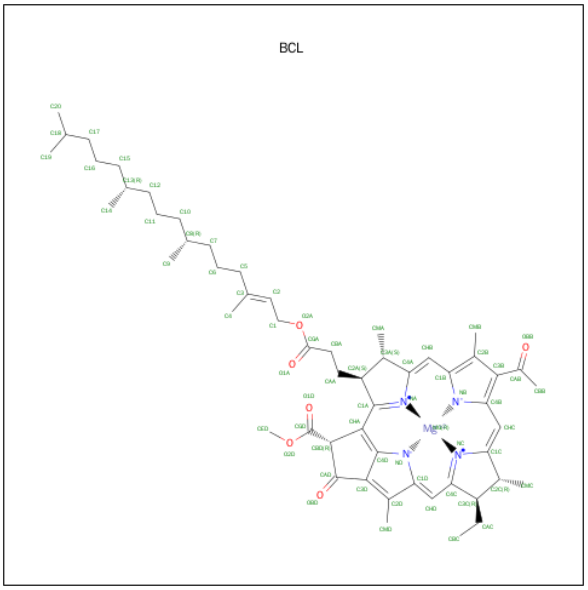
- Molecule 3 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	238	Total	C	N	O	S	0	0	0
			1786	1143	303	331	9			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	1	MET	-	EXPRESSION TAG	UNP P0C0Y7
H	2	VAL	-	EXPRESSION TAG	UNP P0C0Y7
H	3	GLY	-	EXPRESSION TAG	UNP P0C0Y7
H	4	VAL	-	EXPRESSION TAG	UNP P0C0Y7
H	5	THR	-	EXPRESSION TAG	UNP P0C0Y7
H	6	ALA	-	EXPRESSION TAG	UNP P0C0Y7
H	7	PHE	-	EXPRESSION TAG	UNP P0C0Y7
H	8	GLY	-	EXPRESSION TAG	UNP P0C0Y7
H	9	ASN	-	EXPRESSION TAG	UNP P0C0Y7
H	10	PHE	-	EXPRESSION TAG	UNP P0C0Y7
H	251	VAL	-	EXPRESSION TAG	UNP P0C0Y7
H	252	VAL	-	EXPRESSION TAG	UNP P0C0Y7
H	253	ALA	-	EXPRESSION TAG	UNP P0C0Y7
H	254	ALA	-	EXPRESSION TAG	UNP P0C0Y7
H	255	MET	-	EXPRESSION TAG	UNP P0C0Y7
H	256	LEU	-	EXPRESSION TAG	UNP P0C0Y7
H	257	ALA	-	EXPRESSION TAG	UNP P0C0Y7
H	258	GLU	-	EXPRESSION TAG	UNP P0C0Y7
H	259	TYR	-	EXPRESSION TAG	UNP P0C0Y7
H	260	ALA	-	EXPRESSION TAG	UNP P0C0Y7

- 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	C	Mg	N	O	0	0
			66	55	1	4	6		
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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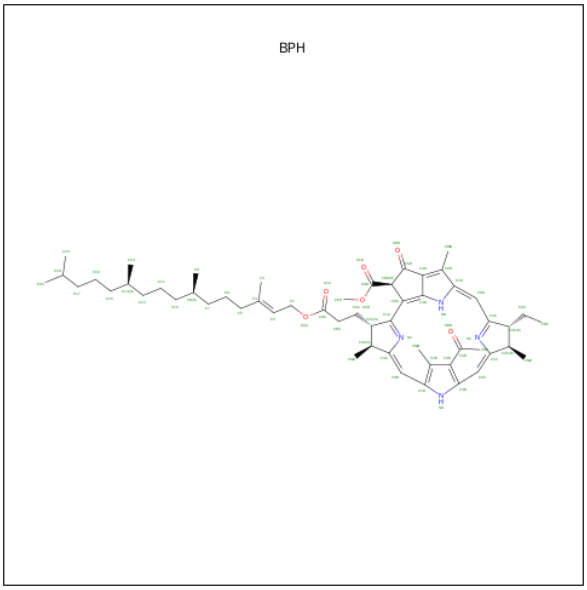
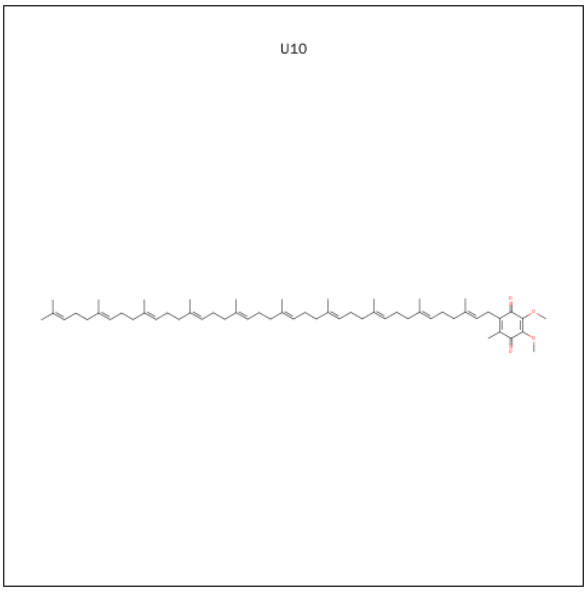
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	M	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- 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
			50	40	4	6		

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

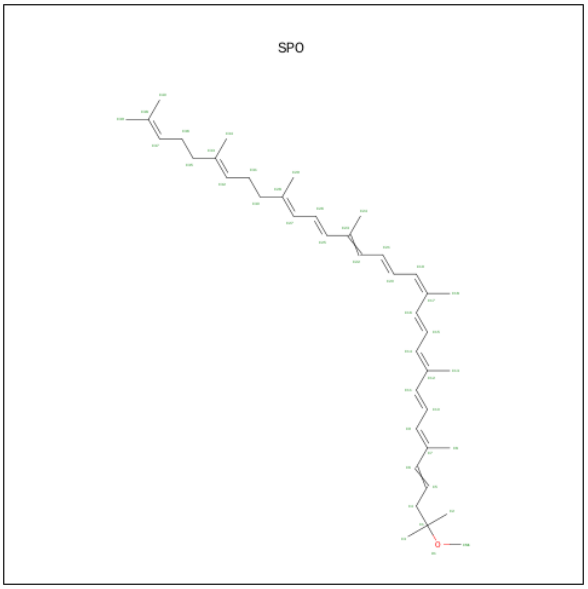


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	1	Total C O 16 12 4	0	0
6	M	1	Total C O 48 44 4	0	0

- Molecule 7 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 8 is SPHEROIDENE (three-letter code: SPO) (formula: $C_{41}H_{60}O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	M	1	Total C O 33 32 1	0	0

- Molecule 9 is water.

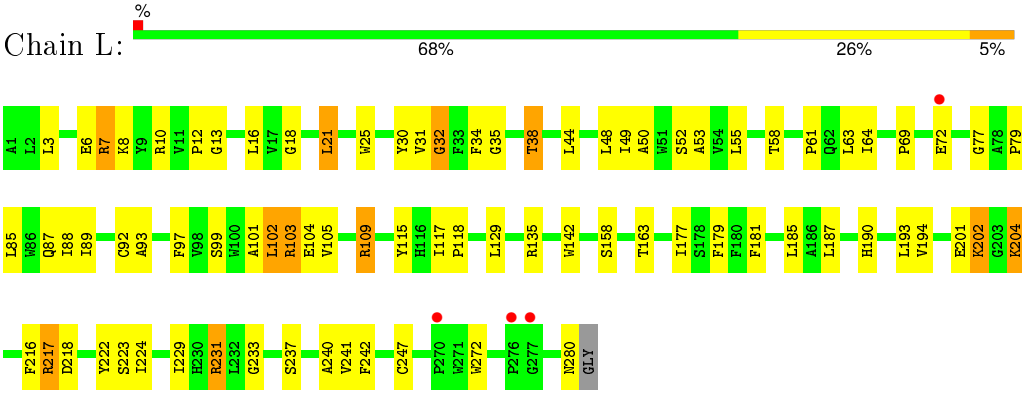
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	L	26	Total O 26 26	0	0
9	M	30	Total O 30 30	0	0
9	H	42	Total O 42 42	0	0

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.

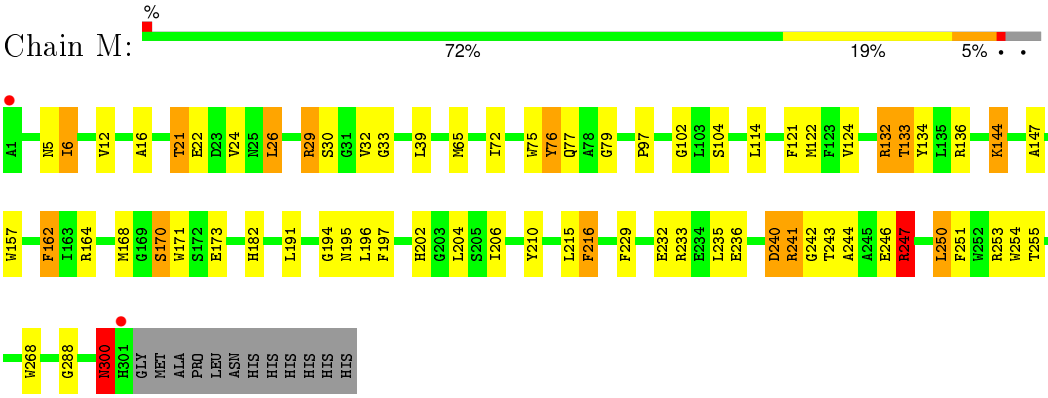
- Molecule 1: Reaction center protein L chain

Chain L:



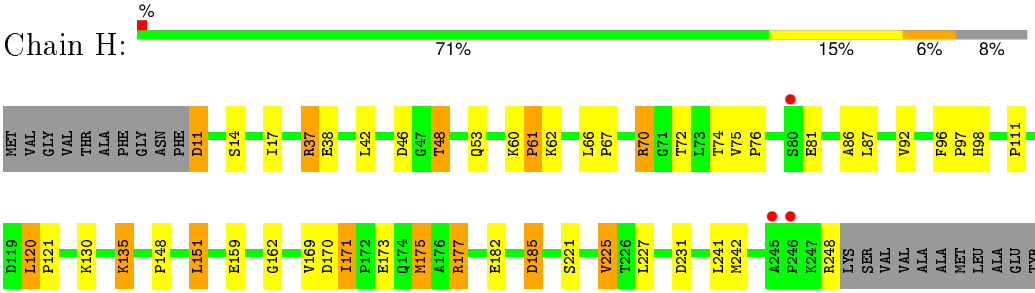
- Molecule 2: Reaction center protein M chain

Chain M:



- Molecule 3: Reaction center protein H chain

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	140.19Å 140.19Å 184.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.90 – 2.77 19.90 – 2.77	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.90-2.77) 99.9 (19.90-2.77)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.45 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.191 , 0.227 0.194 , 0.230	Depositor DCC
R_{free} test set	2682 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	56.5	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 44.3	EDS
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 53634 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6916	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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, BPH, U10, FE, SPO

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	1.18	1/2281 (0.0%)	1.10	14/3125 (0.4%)
2	M	1.13	3/2466 (0.1%)	1.07	12/3369 (0.4%)
3	H	1.11	0/1834	1.17	13/2504 (0.5%)
All	All	1.14	4/6581 (0.1%)	1.11	39/8998 (0.4%)

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
1	L	0	1
2	M	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	258	PHE	CE1-CZ	5.79	1.48	1.37
2	M	236	GLU	CG-CD	5.49	1.60	1.51
2	M	162	PHE	CD1-CE1	5.44	1.50	1.39
1	L	242	PHE	CE1-CZ	5.43	1.47	1.37

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	217	ARG	NE-CZ-NH1	11.40	126.00	120.30
3	H	177	ARG	NE-CZ-NH2	-10.61	114.99	120.30
3	H	177	ARG	NE-CZ-NH1	10.29	125.45	120.30
1	L	231	ARG	NE-CZ-NH2	-10.10	115.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	103	ARG	NE-CZ-NH2	-9.52	115.54	120.30
3	H	117	ARG	NE-CZ-NH1	9.52	125.06	120.30
1	L	217	ARG	NE-CZ-NH2	-8.96	115.82	120.30
2	M	241	ARG	NE-CZ-NH1	8.19	124.40	120.30
2	M	6	ILE	CG1-CB-CG2	-8.06	93.67	111.40
1	L	231	ARG	NE-CZ-NH1	7.96	124.28	120.30
2	M	132	ARG	NE-CZ-NH1	-7.82	116.39	120.30
2	M	240	ASP	CB-CG-OD1	7.78	125.30	118.30
2	M	144	LYS	CD-CE-NZ	-7.71	93.97	111.70
1	L	7	ARG	NE-CZ-NH2	-7.66	116.47	120.30
2	M	21	THR	C-N-CA	-7.56	102.81	121.70
3	H	117	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	L	135	ARG	NE-CZ-NH1	6.85	123.72	120.30
2	M	29	ARG	NE-CZ-NH1	6.71	123.66	120.30
3	H	225	VAL	CB-CA-C	-6.67	98.73	111.40
1	L	7	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	L	102	LEU	CB-CG-CD1	6.47	122.01	111.00
2	M	241	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	L	207	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	L	103	ARG	NE-CZ-NH1	6.30	123.45	120.30
2	M	233	ARG	NE-CZ-NH1	-6.26	117.17	120.30
2	M	247	ARG	NE-CZ-NH1	6.20	123.40	120.30
3	H	11	ASP	CB-CG-OD1	-6.16	112.75	118.30
2	M	29	ARG	NE-CZ-NH2	-6.13	117.24	120.30
3	H	185	ASP	CB-CG-OD1	-6.04	112.86	118.30
2	M	22	GLU	CB-CA-C	5.85	122.10	110.40
1	L	207	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	L	204	LYS	CD-CE-NZ	-5.73	98.52	111.70
3	H	66	LEU	C-N-CD	5.67	140.30	128.40
3	H	67	PRO	C-N-CA	-5.46	108.06	121.70
3	H	37	ARG	NE-CZ-NH2	-5.39	117.60	120.30
3	H	11	ASP	CB-CG-OD2	5.31	123.08	118.30
3	H	37	ARG	NE-CZ-NH1	5.23	122.92	120.30
3	H	81	GLU	C-N-CA	-5.20	108.69	121.70
1	L	31	VAL	C-N-CA	-5.07	111.65	122.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	32	GLY	Peptide
2	M	300	ASN	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	2195	0	2125	66	0
2	M	2375	0	2270	64	0
3	H	1786	0	1747	42	0
4	L	132	0	148	11	0
4	M	117	0	115	22	0
5	L	65	0	76	8	0
5	M	50	0	43	5	0
6	L	16	0	12	6	0
6	M	48	0	63	6	0
7	M	1	0	0	0	0
8	M	33	0	43	6	0
9	H	42	0	0	1	0
9	L	26	0	0	1	0
9	M	30	0	0	1	0
All	All	6916	0	6642	183	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 14.

All (183) 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:197:PHE:CZ	4:M:403:BCL:HBB2	1.94	1.03
1:L:38:THR:HG22	1:L:99:SER:CB	1.89	1.02
1:L:49:ILE:HG13	1:L:89:ILE:HD13	1.41	1.02
1:L:38:THR:HG22	1:L:99:SER:HB2	1.06	1.02
2:M:197:PHE:HZ	4:M:403:BCL:HBB2	1.24	1.02
1:L:7:ARG:HH11	3:H:98:HIS:CD2	1.77	1.01
6:M:405:U10:H322	6:M:405:U10:H272	1.42	1.00
6:L:304:U10:C8	6:L:304:U10:H1M1	1.88	0.99
5:M:404:BPH:HHC	5:M:404:BPH:HBB3	1.45	0.98
5:L:303:BPH:HBB3	5:L:303:BPH:HHC	1.51	0.90
1:L:69:PRO:HG2	1:L:142:TRP:HB2	1.53	0.90
2:M:164:ARG:HH12	2:M:173:GLU:HG3	1.41	0.86
4:M:403:BCL:HHC	4:M:403:BCL:HBB3	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:242:GLY:CA	3:H:117:ARG:HD2	2.07	0.84
1:L:7:ARG:HH11	3:H:98:HIS:HD2	1.26	0.83
2:M:197:PHE:HZ	4:M:403:BCL:CBB	1.90	0.83
4:M:403:BCL:HHC	4:M:403:BCL:CBB	2.08	0.83
2:M:242:GLY:HA2	3:H:117:ARG:HD2	1.63	0.78
6:M:405:U10:C32	6:M:405:U10:H272	2.13	0.78
4:M:401:BCL:CBB	8:M:406:SPO:H243	2.13	0.78
5:M:404:BPH:HHC	5:M:404:BPH:CBB	2.13	0.78
1:L:38:THR:CG2	1:L:99:SER:HB2	2.02	0.78
6:L:304:U10:C1M	6:L:304:U10:C8	2.61	0.78
4:L:302:BCL:HBB2	4:L:302:BCL:HMB1	1.69	0.75
2:M:32:VAL:HG12	2:M:33:GLY:O	1.87	0.75
4:L:302:BCL:HMB1	4:L:302:BCL:CBB	2.16	0.75
5:L:303:BPH:HBB2	2:M:210:TYR:HB3	1.69	0.74
1:L:34:PHE:O	1:L:38:THR:HG23	1.86	0.74
1:L:201:GLU:O	1:L:202:LYS:CB	2.34	0.74
4:M:401:BCL:HBB2	8:M:406:SPO:H243	1.69	0.74
3:H:70:ARG:NH2	3:H:121:PRO:O	2.21	0.73
5:L:303:BPH:CBB	5:L:303:BPH:HHC	2.19	0.72
2:M:133:THR:HG22	2:M:147:ALA:HB2	1.73	0.71
2:M:164:ARG:HH12	2:M:173:GLU:CG	2.03	0.70
1:L:231:ARG:HD3	2:M:5:ASN:O	1.90	0.70
1:L:218:ASP:OD1	2:M:29:ARG:HD3	1.92	0.69
2:M:240:ASP:O	3:H:117:ARG:NH1	2.24	0.69
2:M:133:THR:HG21	2:M:147:ALA:HA	1.76	0.68
1:L:49:ILE:HG13	1:L:89:ILE:CD1	2.19	0.67
3:H:148:PRO:HA	3:H:151:LEU:HD22	1.76	0.66
1:L:181:PHE:HB3	5:M:404:BPH:HBB2	1.79	0.65
4:M:401:BCL:CBB	4:M:401:BCL:HHC	2.27	0.64
2:M:97:PRO:HG2	2:M:171:TRP:HB2	1.80	0.63
2:M:21:THR:HG23	2:M:26:LEU:HD11	1.79	0.63
1:L:7:ARG:NH1	3:H:98:HIS:HD2	1.96	0.63
2:M:132:ARG:HH11	2:M:132:ARG:HG2	1.63	0.63
1:L:13:GLY:HA3	3:H:242:MET:HE3	1.82	0.62
4:L:301:BCL:HBB3	4:L:301:BCL:HMB1	1.82	0.61
1:L:69:PRO:CG	1:L:142:TRP:HB2	2.30	0.61
3:H:96:PHE:HB3	3:H:97:PRO:CD	2.31	0.61
1:L:87:GLN:NE2	1:L:142:TRP:CD1	2.69	0.61
2:M:164:ARG:NH1	2:M:173:GLU:CG	2.64	0.60
2:M:197:PHE:CE1	4:M:403:BCL:HBB2	2.35	0.60
1:L:69:PRO:HD3	1:L:83:GLY:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:164:ARG:NH1	2:M:173:GLU:HG3	2.14	0.60
2:M:133:THR:CG2	2:M:147:ALA:HA	2.32	0.60
1:L:85:LEU:O	1:L:89:ILE:HG13	2.03	0.59
4:M:401:BCL:HBB1	8:M:406:SPO:H243	1.83	0.59
2:M:134:TYR:CE2	2:M:144:LYS:HG2	2.37	0.59
2:M:300:ASN:OD1	2:M:300:ASN:N	2.36	0.58
1:L:103:ARG:NH2	2:M:255:THR:O	2.35	0.58
2:M:242:GLY:HA3	3:H:117:ARG:HD2	1.87	0.57
1:L:79:PRO:O	1:L:80:LEU:C	2.44	0.56
4:M:401:BCL:HBB3	4:M:401:BCL:HHC	1.87	0.56
3:H:96:PHE:HB3	3:H:97:PRO:HD2	1.88	0.56
1:L:210:ASP:OD1	1:L:210:ASP:N	2.39	0.56
1:L:224:ILE:H	6:L:304:U10:H72	1.71	0.56
1:L:187:LEU:HD13	2:M:216:PHE:CG	2.41	0.55
3:H:70:ARG:O	3:H:118:ARG:NH2	2.40	0.55
1:L:48:LEU:CD1	1:L:88:ILE:HG22	2.37	0.55
3:H:98:HIS:HE1	9:H:325:HOH:O	1.90	0.55
1:L:7:ARG:HD2	3:H:98:HIS:CD2	2.42	0.54
4:M:401:BCL:OBB	4:M:401:BCL:HMB1	2.08	0.54
4:L:301:BCL:CBB	4:L:301:BCL:HMB1	2.36	0.54
2:M:16:ALA:HB1	2:M:32:VAL:HG21	1.88	0.54
1:L:177:ILE:HG12	4:L:301:BCL:HMB3	1.90	0.54
4:M:403:BCL:H11	5:M:404:BPH:HBB3	1.90	0.54
2:M:76:TYR:C	2:M:76:TYR:CD1	2.82	0.53
3:H:37:ARG:O	3:H:38:GLU:HG2	2.09	0.53
2:M:232:GLU:OE1	2:M:232:GLU:N	2.36	0.53
3:H:170:ASP:HB2	3:H:177:ARG:HD2	1.91	0.53
2:M:232:GLU:OE2	3:H:177:ARG:NH2	2.42	0.53
4:M:403:BCL:HBB3	4:M:403:BCL:CHC	2.35	0.52
4:M:403:BCL:H11	5:M:404:BPH:CBB	2.39	0.52
1:L:52:SER:HB2	1:L:85:LEU:HD13	1.91	0.52
1:L:49:ILE:CG1	1:L:89:ILE:HD13	2.28	0.52
4:M:403:BCL:HAA2	4:M:403:BCL:HBD	1.90	0.52
2:M:194:GLY:O	2:M:195:ASN:HB3	2.08	0.52
1:L:8:LYS:HA	3:H:87:LEU:HD11	1.92	0.52
2:M:136:ARG:HA	2:M:136:ARG:NE	2.25	0.51
1:L:55:LEU:HD13	1:L:81:ALA:HB2	1.91	0.51
4:M:401:BCL:HBB3	4:M:403:BCL:H41	1.91	0.51
1:L:280:ASN:C	9:L:421:HOH:O	2.49	0.51
3:H:70:ARG:NH2	3:H:120:LEU:HB3	2.25	0.51
2:M:241:ARG:HD3	2:M:246:GLU:HG2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:251:PHE:CD1	2:M:251:PHE:C	2.84	0.51
1:L:3:LEU:HD12	2:M:250:LEU:HD13	1.92	0.51
2:M:133:THR:HG22	2:M:147:ALA:CB	2.40	0.50
1:L:50:ALA:O	1:L:53:ALA:HB3	2.12	0.50
3:H:117:ARG:NH2	3:H:227:LEU:HD22	2.27	0.50
9:M:504:HOH:O	3:H:175:MET:HE1	2.10	0.50
1:L:18:GLY:O	1:L:21:LEU:HB2	2.12	0.50
2:M:24:VAL:HG11	2:M:29:ARG:NH1	2.27	0.50
3:H:241:LEU:O	3:H:248:ARG:NH2	2.45	0.49
4:L:302:BCL:H191	5:L:303:BPH:H6C1	1.95	0.49
3:H:62:LYS:O	3:H:74:THR:HA	2.12	0.49
2:M:102:GLY:HA2	2:M:170:SER:HB2	1.95	0.49
4:L:302:BCL:H193	5:L:303:BPH:H112	1.95	0.49
3:H:37:ARG:NH2	3:H:60:LYS:O	2.46	0.49
2:M:202:HIS:CE1	2:M:206:ILE:HD11	2.47	0.49
2:M:268:TRP:CD1	6:M:405:U10:H111	2.47	0.49
1:L:179:PHE:HB3	1:L:240:ALA:HB2	1.94	0.48
1:L:12:PRO:O	3:H:242:MET:HE1	2.13	0.48
3:H:14:SER:HA	3:H:17:ILE:HG22	1.94	0.48
2:M:164:ARG:NH1	2:M:173:GLU:HG2	2.28	0.48
3:H:175:MET:CE	3:H:177:ARG:NH2	2.76	0.48
1:L:101:ALA:O	1:L:104:GLU:N	2.46	0.48
1:L:6:GLU:OE2	1:L:10:ARG:HD2	2.13	0.48
2:M:260:ALA:O	6:M:405:U10:H4M3	2.14	0.48
6:M:405:U10:H322	6:M:405:U10:C27	2.23	0.47
1:L:105:VAL:O	1:L:109:ARG:HG3	2.13	0.47
3:H:130:LYS:HZ1	3:H:173:GLU:HG3	1.78	0.47
6:L:304:U10:H4M3	6:L:304:U10:H3M3	1.96	0.47
2:M:132:ARG:NH1	2:M:132:ARG:HG2	2.26	0.47
1:L:115:TYR:O	1:L:118:PRO:HG2	2.15	0.47
2:M:206:ILE:HG12	4:M:403:BCL:HMB3	1.96	0.47
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.96	0.47
1:L:193:LEU:HD23	6:L:304:U10:H3M3	1.97	0.46
5:L:303:BPH:HBB1	2:M:210:TYR:CD2	2.50	0.46
3:H:46:ASP:OD1	3:H:48:THR:OG1	2.33	0.46
1:L:222:TYR:CG	1:L:223:SER:N	2.83	0.46
4:L:301:BCL:HBB2	4:M:403:BCL:NA	2.31	0.46
2:M:76:TYR:O	2:M:79:GLY:N	2.32	0.45
2:M:133:THR:CG2	2:M:147:ALA:CA	2.94	0.45
2:M:157:TRP:CD1	8:M:406:SPO:H26	2.51	0.45
3:H:75:VAL:HA	3:H:76:PRO:C	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:253:ARG:HB2	2:M:259:ASN:OD1	2.16	0.45
2:M:247:ARG:NH2	3:H:111:PRO:O	2.47	0.45
3:H:148:PRO:O	3:H:151:LEU:HB2	2.16	0.44
2:M:157:TRP:NE1	8:M:406:SPO:H26	2.33	0.44
1:L:77:GLY:HA2	1:L:87:GLN:OE1	2.18	0.44
1:L:241:VAL:HG21	5:L:303:BPH:H2C	1.98	0.44
3:H:42:LEU:N	3:H:53:GLN:OE1	2.51	0.44
3:H:60:LYS:HA	3:H:61:PRO:HD2	1.71	0.44
3:H:148:PRO:HA	3:H:151:LEU:CD2	2.46	0.44
4:L:301:BCL:H202	4:L:301:BCL:H161	1.85	0.43
1:L:52:SER:HB2	1:L:85:LEU:CD1	2.48	0.43
1:L:84:GLY:HA2	1:L:87:GLN:HG3	2.00	0.43
1:L:117:ILE:HB	1:L:118:PRO:CD	2.48	0.43
2:M:243:THR:N	3:H:115:VAL:HG13	2.34	0.43
1:L:163:THR:HG22	1:L:163:THR:O	2.19	0.43
1:L:30:TYR:O	1:L:103:ARG:NH1	2.52	0.42
1:L:101:ALA:O	1:L:104:GLU:HB2	2.19	0.42
1:L:6:GLU:OE2	1:L:10:ARG:NH1	2.43	0.42
3:H:162:GLY:HA3	3:H:182:GLU:O	2.19	0.42
3:H:151:LEU:HD12	3:H:151:LEU:HA	1.80	0.42
2:M:133:THR:CG2	2:M:147:ALA:HB2	2.47	0.42
1:L:30:TYR:HB2	2:M:254:TRP:HB3	2.01	0.42
1:L:97:PHE:CE1	4:L:301:BCL:H121	2.54	0.42
4:M:403:BCL:H2C	4:M:403:BCL:HBC2	1.82	0.42
1:L:93:ALA:HA	5:L:303:BPH:H9C2	2.02	0.41
4:M:403:BCL:HHC	4:M:403:BCL:HBB2	1.98	0.41
2:M:21:THR:HG23	2:M:26:LEU:CD1	2.47	0.41
2:M:114:LEU:HD23	2:M:114:LEU:HA	1.87	0.41
2:M:168:MET:SD	2:M:288:GLY:O	2.79	0.41
1:L:83:GLY:O	1:L:87:GLN:HG3	2.20	0.41
1:L:25:TRP:CD1	1:L:30:TYR:HA	2.56	0.41
2:M:162:PHE:HB2	8:M:406:SPO:C31	2.50	0.41
6:M:405:U10:C32	6:M:405:U10:C27	2.90	0.41
1:L:193:LEU:O	1:L:194:VAL:C	2.59	0.41
2:M:65:MET:HB3	2:M:121:PHE:CE2	2.56	0.41
4:L:301:BCL:CGA	4:L:302:BCL:HBC1	2.51	0.41
1:L:32:GLY:CA	1:L:35:GLY:H	2.33	0.41
1:L:231:ARG:HD2	2:M:6:ILE:O	2.21	0.41
1:L:231:ARG:CD	2:M:5:ASN:O	2.65	0.41
3:H:175:MET:HE2	3:H:177:ARG:NH2	2.35	0.41
1:L:44:LEU:HD23	1:L:92:CYS:SG	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:169:VAL:HG23	3:H:171:ILE:CD1	2.51	0.41
1:L:61:PRO:HA	1:L:64:ILE:HD12	2.03	0.41
1:L:190:HIS:HD1	6:L:304:U10:H3M1	1.85	0.40
1:L:233:GLY:HA3	2:M:216:PHE:CE1	2.56	0.40
2:M:197:PHE:CZ	4:M:403:BCL:CBB	2.75	0.40
1:L:12:PRO:O	3:H:242:MET:CE	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	278/281 (99%)	244 (88%)	32 (12%)	2 (1%)	26	60
2	M	299/313 (96%)	276 (92%)	21 (7%)	2 (1%)	26	60
3	H	236/260 (91%)	220 (93%)	12 (5%)	4 (2%)	11	33
All	All	813/854 (95%)	740 (91%)	65 (8%)	8 (1%)	19	50

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	202	LYS
2	M	77	GLN
1	L	80	LEU
2	M	30	SER
3	H	61	PRO
3	H	135	LYS
3	H	185	ASP
3	H	86	ALA

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	213/220 (97%)	192 (90%)	21 (10%)	10 26
2	M	228/246 (93%)	204 (90%)	24 (10%)	8 23
3	H	184/208 (88%)	169 (92%)	15 (8%)	14 36
All	All	625/674 (93%)	565 (90%)	60 (10%)	10 28

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	16	LEU
1	L	21	LEU
1	L	38	THR
1	L	58	THR
1	L	63	LEU
1	L	72	GLU
1	L	102	LEU
1	L	109	ARG
1	L	129	LEU
1	L	158	SER
1	L	185	LEU
1	L	204	LYS
1	L	205	GLU
1	L	207	ARG
1	L	210	ASP
1	L	216	PHE
1	L	217	ARG
1	L	229	ILE
1	L	237	SER
1	L	247	CYS
1	L	272	TRP
2	M	12	VAL
2	M	26	LEU
2	M	39	LEU
2	M	72	ILE
2	M	75	TRP

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Mol	Chain	Res	Type
2	M	76	TYR
2	M	104	SER
2	M	122	MET
2	M	124	VAL
2	M	133	THR
2	M	151	LEU
2	M	156	LEU
2	M	170	SER
2	M	182	HIS
2	M	191	LEU
2	M	196	LEU
2	M	204	LEU
2	M	215	LEU
2	M	216	PHE
2	M	235	LEU
2	M	247	ARG
2	M	250	LEU
2	M	259	ASN
2	M	300	ASN
3	H	11	ASP
3	H	48	THR
3	H	70	ARG
3	H	72	THR
3	H	92	VAL
3	H	118	ARG
3	H	120	LEU
3	H	135	LYS
3	H	151	LEU
3	H	159	GLU
3	H	171	ILE
3	H	175	MET
3	H	221	SER
3	H	225	VAL
3	H	231	ASP

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

Mol	Chain	Res	Type
3	H	98	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	BCL	L	301	-	53,74,74	0.74	0	57,115,115	1.28	8 (14%)
4	BCL	L	302	-	53,74,74	0.74	0	57,115,115	2.16	12 (21%)
5	BPH	L	303	-	64,70,70	1.49	8 (12%)	73,101,101	1.68	7 (9%)
6	U10	L	304	-	16,16,63	1.81	6 (37%)	18,22,79	2.93	8 (44%)
4	BCL	M	401	-	38,59,74	0.83	1 (2%)	40,97,115	2.55	10 (25%)
4	BCL	M	403	-	53,74,74	0.74	0	57,115,115	1.73	15 (26%)
5	BPH	M	404	-	49,55,70	1.70	10 (20%)	56,83,101	2.32	19 (33%)
6	U10	M	405	-	48,48,63	3.41	12 (25%)	58,61,79	1.94	19 (32%)
8	SPO	M	406	-	31,32,41	1.59	4 (12%)	33,39,50	2.63	11 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BCL	L	301	-	-	0/37/137/137	0/0/9/9
4	BCL	L	302	-	-	0/37/137/137	0/0/9/9
5	BPH	L	303	-	2/2/18/22	0/54/105/105	0/1/6/6
6	U10	L	304	-	-	0/7/31/87	0/1/1/1
4	BCL	M	401	-	-	0/19/119/137	0/0/9/9
4	BCL	M	403	-	-	0/37/137/137	0/0/9/9
5	BPH	M	404	-	-	0/36/87/105	0/1/6/6
6	U10	M	405	-	-	0/45/69/87	0/1/1/1
8	SPO	M	406	-	-	0/37/37/47	0/0/0/0

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	405	U10	O3-C3	-4.23	1.25	1.37
5	L	303	BPH	C1A-NA	-3.71	1.29	1.37
6	M	405	U10	O4-C4	-3.55	1.27	1.37
5	M	404	BPH	C4C-NC	-3.26	1.30	1.37
5	M	404	BPH	CHB-C4A	-3.18	1.34	1.40
5	M	404	BPH	C1A-NA	-3.01	1.30	1.37
5	M	404	BPH	C1B-C2B	-2.90	1.39	1.45
6	L	304	U10	O3-C3	-2.70	1.29	1.37
5	L	303	BPH	C1B-C2B	-2.48	1.40	1.45
5	M	404	BPH	OBD-CAD	-2.46	1.18	1.22
6	L	304	U10	C3-C2	-2.45	1.41	1.48
6	M	405	U10	C3-C2	-2.42	1.41	1.48
6	L	304	U10	O4-C4	-2.28	1.31	1.37
5	L	303	BPH	C4C-NC	-2.25	1.32	1.37
5	M	404	BPH	C3B-C4B	-2.24	1.38	1.43
6	M	405	U10	C4-C5	-2.21	1.42	1.48
5	L	303	BPH	C4A-NA	2.02	1.39	1.34
4	M	401	BCL	O2A-CGA	2.09	1.39	1.33
8	M	406	SPO	C16-C17	2.11	1.50	1.45
8	M	406	SPO	C26-C27	2.30	1.50	1.43
6	M	405	U10	C6-C1	2.39	1.40	1.35
5	M	404	BPH	C5-C3	2.41	1.57	1.50
6	L	304	U10	C4-C3	2.42	1.46	1.35
5	L	303	BPH	CHB-C1B	2.65	1.44	1.38
5	L	303	BPH	C3D-C4D	2.80	1.45	1.41
5	M	404	BPH	C2-C3	2.84	1.41	1.32
8	M	406	SPO	C25-C23	3.14	1.52	1.45
6	L	304	U10	C7-C6	3.20	1.57	1.51
6	L	304	U10	C9-C8	3.24	1.51	1.28
5	L	303	BPH	CHA-C1A	4.13	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	404	BPH	CHA-C1A	4.25	1.47	1.37
5	M	404	BPH	CHD-C4C	4.61	1.49	1.38
8	M	406	SPO	C27-C28	5.55	1.40	1.34
5	L	303	BPH	CHD-C4C	5.58	1.52	1.38
6	M	405	U10	C38-C39	6.01	1.50	1.32
6	M	405	U10	C23-C24	7.09	1.46	1.33
6	M	405	U10	C8-C9	7.67	1.48	1.33
6	M	405	U10	C28-C29	8.26	1.49	1.33
6	M	405	U10	C18-C19	9.20	1.51	1.33
6	M	405	U10	C33-C34	9.32	1.51	1.33
6	M	405	U10	C13-C14	9.72	1.52	1.33

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	302	BCL	O1D-CGD-CBD	-7.99	113.17	124.62
8	M	406	SPO	C18-C17-C19	-6.80	112.85	122.90
6	L	304	U10	C1-C6-C5	-5.41	113.95	120.12
8	M	406	SPO	C20-C21-C22	-5.37	111.51	123.39
6	M	405	U10	C17-C18-C19	-5.18	116.50	127.76
5	M	404	BPH	OBD-CAD-CBD	-5.00	118.39	125.94
4	L	302	BCL	C1D-CHD-C4C	-4.93	118.54	126.07
8	M	406	SPO	C4-C5-C6	-4.32	118.52	124.67
4	M	401	BCL	C1D-CHD-C4C	-4.00	119.97	126.07
5	M	404	BPH	C5-C3-C4	-3.86	105.15	114.64
6	L	304	U10	O5-C5-C4	-3.77	112.62	120.79
5	M	404	BPH	C2D-C1D-ND	-3.73	104.19	110.29
5	M	404	BPH	CAC-C3C-C2C	-3.71	104.80	114.13
5	M	404	BPH	C1C-NC-C4C	-3.68	106.67	110.44
4	M	401	BCL	O2D-CGD-O1D	-3.56	116.43	123.79
6	M	405	U10	C27-C28-C29	-3.49	120.17	127.76
6	M	405	U10	C7-C8-C9	-3.49	120.79	126.70
5	L	303	BPH	C4-C3-C5	-3.40	110.21	115.41
5	L	303	BPH	C2D-C1D-ND	-3.35	104.80	110.29
6	L	304	U10	O2-C2-C3	-3.28	113.68	120.79
4	L	302	BCL	C5-C3-C2	-3.10	115.17	121.05
6	L	304	U10	C1M-C1-C6	-2.98	117.73	124.10
4	M	403	BCL	O2D-CGD-O1D	-2.94	117.71	123.79
4	M	403	BCL	O2A-CGA-O1A	-2.74	116.43	123.49
5	M	404	BPH	O1D-CGD-CBD	-2.72	120.72	124.62
4	L	302	BCL	C3D-CAD-CBD	-2.60	103.92	107.60
4	M	403	BCL	CAC-C3C-C2C	-2.57	107.68	114.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	404	BPH	C2B-C1B-NB	-2.54	105.92	109.73
6	M	405	U10	C10-C9-C8	-2.50	118.59	123.50
4	M	401	BCL	O1A-CGA-CBA	-2.46	113.87	123.72
4	M	403	BCL	C6-C5-C3	-2.39	107.24	112.48
5	M	404	BPH	C3A-C2A-C1A	-2.39	98.82	101.84
4	M	403	BCL	C1D-CHD-C4C	-2.34	122.50	126.07
4	M	403	BCL	CGD-CBD-CAD	-2.33	102.72	110.62
4	L	302	BCL	C3C-C4C-CHD	-2.33	118.14	123.33
4	M	401	BCL	CBC-CAC-C3C	-2.27	108.03	113.57
6	M	405	U10	C22-C23-C24	-2.25	122.88	127.76
6	M	405	U10	C26-C27-C28	-2.25	105.80	111.69
4	M	403	BCL	CAA-C2A-C3A	-2.24	106.78	113.22
6	M	405	U10	C30-C29-C28	-2.19	119.20	123.50
6	M	405	U10	C25-C24-C23	-2.18	119.22	123.50
6	M	405	U10	C21-C22-C23	-2.18	105.98	111.69
4	L	301	BCL	O2A-CGA-O1A	-2.15	117.94	123.49
6	M	405	U10	C1M-C1-C6	-2.14	119.52	124.10
4	M	403	BCL	C11-C10-C8	-2.13	108.42	115.49
4	L	301	BCL	C1D-CHD-C4C	-2.12	122.83	126.07
4	M	403	BCL	C7-C6-C5	-2.09	106.89	113.06
5	M	404	BPH	C3B-C4B-NB	-2.09	105.55	109.98
4	L	301	BCL	CMB-C2B-C1B	-2.05	124.98	128.36
5	L	303	BPH	C3B-C4B-NB	-2.04	105.64	109.98
4	L	301	BCL	C14-C13-C15	-2.03	103.27	111.08
6	M	405	U10	C35-C34-C33	-2.00	119.57	123.50
8	M	406	SPO	C21-C20-C19	2.03	127.88	123.39
5	M	404	BPH	C2A-C1A-NA	2.04	114.70	112.08
6	M	405	U10	C37-C36-C34	2.12	119.63	112.71
4	M	403	BCL	CHB-C4A-NA	2.18	127.53	124.51
4	M	401	BCL	CHB-C4A-NA	2.21	127.57	124.51
8	M	406	SPO	O1-C1-C4	2.21	111.29	105.87
4	L	301	BCL	CHD-C4C-NC	2.22	127.64	125.06
6	M	405	U10	C36-C37-C38	2.27	117.62	111.69
6	L	304	U10	C6-C1-C2	2.27	122.81	120.42
8	M	406	SPO	C20-C19-C17	2.28	130.49	127.20
6	M	405	U10	C4M-O4-C4	2.28	124.73	116.61
4	L	302	BCL	OBD-CAD-CBD	2.33	129.45	125.94
5	L	303	BPH	CMD-C2D-C3D	2.33	129.65	125.09
4	M	401	BCL	OBD-CAD-CBD	2.36	129.50	125.94
5	M	404	BPH	CMB-C2B-C1B	2.39	128.95	125.06
8	M	406	SPO	C10-C9-C7	2.40	130.67	127.20
8	M	406	SPO	C24-C23-C25	2.42	122.13	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	302	BCL	CHC-C1C-NC	2.44	127.89	124.51
5	M	404	BPH	C1B-NB-C4B	2.47	111.39	106.51
4	L	302	BCL	O2A-CGA-CBA	2.53	119.61	111.90
4	L	302	BCL	CHB-C4A-NA	2.55	128.04	124.51
4	L	301	BCL	CAA-CBA-CGA	2.60	120.93	113.32
8	M	406	SPO	C29-C28-C30	2.65	118.68	115.68
5	L	303	BPH	C11-C10-C8	2.66	124.32	115.49
4	L	302	BCL	C4-C3-C5	2.70	119.53	115.41
6	L	304	U10	C3M-O3-C3	2.81	126.59	116.61
5	M	404	BPH	CAC-C3C-C4C	2.88	120.06	112.67
6	M	405	U10	C15-C14-C16	2.91	119.85	115.41
6	M	405	U10	C25-C24-C26	2.92	119.86	115.41
5	M	404	BPH	C4D-C3D-C2D	2.93	110.87	107.08
4	M	403	BCL	O2A-CGA-CBA	2.95	120.88	111.90
4	M	403	BCL	CED-O2D-CGD	2.96	122.92	115.99
4	M	401	BCL	O2A-CGA-CBA	3.00	121.05	111.90
5	M	404	BPH	CMD-C2D-C3D	3.01	130.98	125.09
4	L	301	BCL	O2A-CGA-CBA	3.08	121.27	111.90
4	M	403	BCL	CHD-C4C-NC	3.13	128.70	125.06
4	M	403	BCL	OBB-CAB-C3B	3.21	125.09	120.00
4	M	401	BCL	CHD-C4C-NC	3.28	128.86	125.06
6	L	304	U10	C4M-O4-C4	3.41	128.74	116.61
5	M	404	BPH	C3D-CAD-CBD	3.44	112.45	107.60
4	L	301	BCL	O2D-CGD-CBD	3.68	116.35	111.30
6	M	405	U10	C10-C9-C11	3.94	121.42	115.41
8	M	406	SPO	C21-C22-C23	4.00	132.98	127.20
6	M	405	U10	C30-C29-C31	4.04	121.58	115.41
4	L	302	BCL	CHD-C4C-NC	4.30	130.05	125.06
5	L	303	BPH	C3C-C4C-NC	4.50	112.43	107.93
5	M	404	BPH	O2D-CGD-CBD	4.55	117.54	111.30
5	M	404	BPH	C1-C2-C3	4.94	134.81	126.71
6	M	405	U10	C35-C34-C36	4.97	123.00	115.41
4	M	403	BCL	O2D-CGD-CBD	6.08	119.64	111.30
6	L	304	U10	C7-C6-C5	7.51	127.39	118.56
4	M	401	BCL	O2D-CGD-CBD	7.64	121.78	111.30
8	M	406	SPO	C16-C17-C19	7.76	131.48	118.98
5	M	404	BPH	C3C-C4C-NC	7.85	115.80	107.93
4	L	302	BCL	O2D-CGD-CBD	8.43	122.87	111.30
5	L	303	BPH	C6-C5-C3	8.66	131.48	112.48
4	M	401	BCL	C1-C2-C3	9.53	142.34	126.71

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	L	303	BPH	C8
5	L	303	BPH	C13

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 56 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	301	BCL	7	0
4	L	302	BCL	5	0
5	L	303	BPH	8	0
6	L	304	U10	6	0
4	M	401	BCL	7	0
4	M	403	BCL	16	0
5	M	404	BPH	5	0
6	M	405	U10	6	0
8	M	406	SPO	6	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	280/281 (99%)	-0.58	4 (1%)	78	72	33, 47, 84, 90	0
2	M	301/313 (96%)	-0.68	2 (0%)	89	86	33, 47, 77, 86	0
3	H	238/260 (91%)	-0.57	3 (1%)	79	74	35, 47, 62, 77	0
All	All	819/854 (95%)	-0.62	9 (1%)	82	77	33, 47, 77, 90	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	1	ALA	5.7
3	H	246	PRO	3.6
1	L	276	PRO	3.2
1	L	277	GLY	2.8
3	H	245	ALA	2.5
1	L	72	GLU	2.4
1	L	270	PRO	2.2
2	M	301	HIS	2.1
3	H	80	SER	2.1

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 (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
6	U10	L	304	16/63	0.84	0.27	7.43	57,71,81,90	0
4	BCL	M	403	66/66	0.96	0.15	1.40	34,45,63,69	0
8	SPO	M	406	33/42	0.90	0.20	1.19	54,63,94,95	0
4	BCL	L	301	66/66	0.96	0.16	0.88	35,45,51,56	0
6	U10	M	405	48/63	0.93	0.14	0.62	36,46,80,82	0
4	BCL	M	401	51/66	0.96	0.12	0.13	34,40,57,65	0
5	BPH	L	303	65/65	0.97	0.12	-0.03	24,37,47,51	0
5	BPH	M	404	50/65	0.96	0.10	-0.08	35,45,59,68	0
4	BCL	L	302	66/66	0.98	0.07	-0.89	23,33,58,66	0
7	FE	M	402	1/1	0.99	0.08	-0.90	40,40,40,40	0

6.5 Other polymers (i)

There are no such residues in this entry.