Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:08 PM GMT

PDB ID	:	4HBH
Title	:	Bacterial Photosynthetic Reaction Center from Rhodobacter sphaeroides with ILE M265 replaced with ASN
Authors	:	Mattis, A.J.; Wraight, C.A.
Deposited on	:	2012-09-28
Resolution	:	2.93 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:

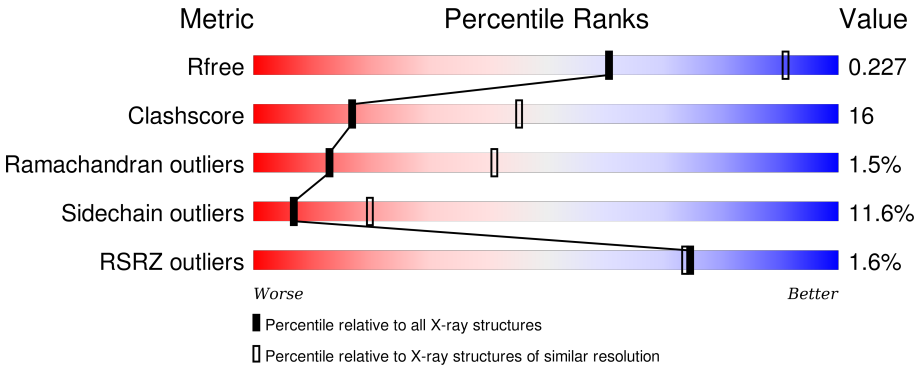
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.93 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	2057 (2.98-2.90)
Clashscore	102246	2308 (2.98-2.90)
Ramachandran outliers	100387	2245 (2.98-2.90)
Sidechain outliers	100360	2247 (2.98-2.90)
RSRZ outliers	91569	2065 (2.98-2.90)

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	2% 71% 24%
2	M	313	% 70% 22%
3	H	260	2% 67% 19% 5% 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	X
6	U10	L	305	-	-	X	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6919 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	0	0
			2209	1490	350	361	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
			2390	1594	391	395	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	265	ASN	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

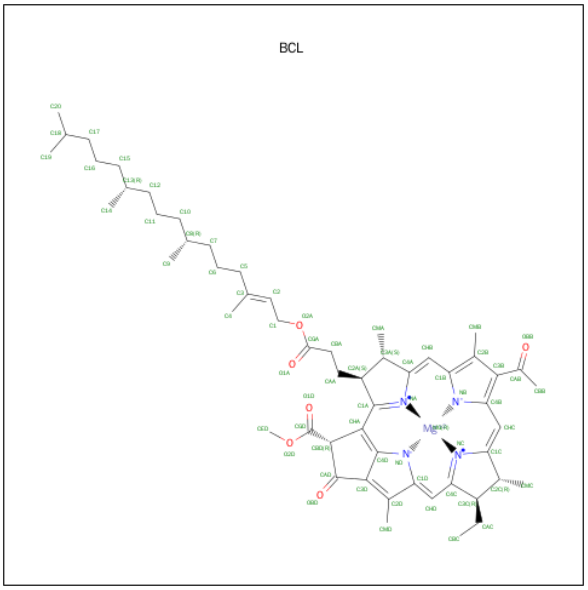
- Molecule 3 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	238	Total	C	N	O	S	0	0	0
			1792	1146	305	332	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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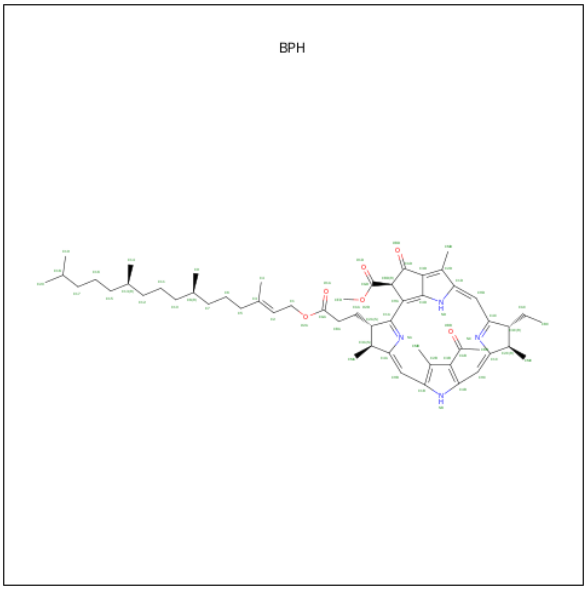
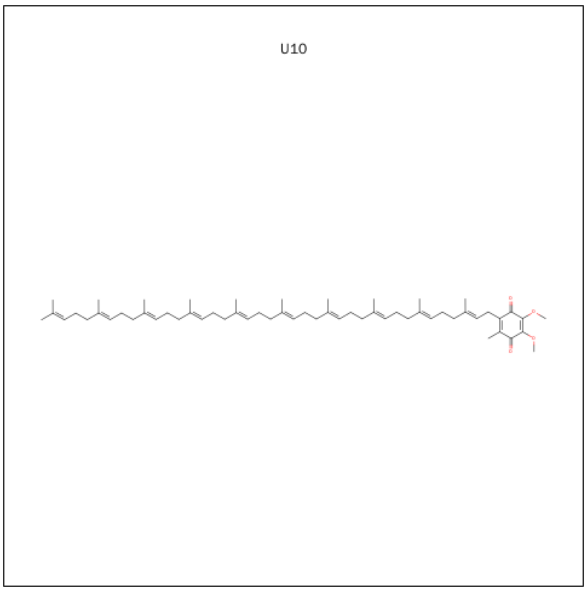
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	M	1	Total	C	Mg	N	O	0	0
			55	44	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- 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
			53	43	4	6		

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

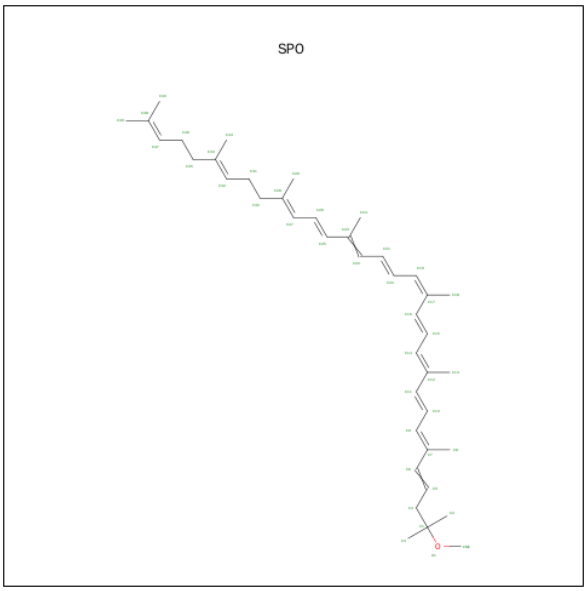


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	1	Total C O 26 22 4	0	0
6	L	1	Total C O 26 22 4	0	0
6	M	1	Total C O 48 44 4	0	0

- 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 35 34 1	0	0

- Molecule 9 is water.

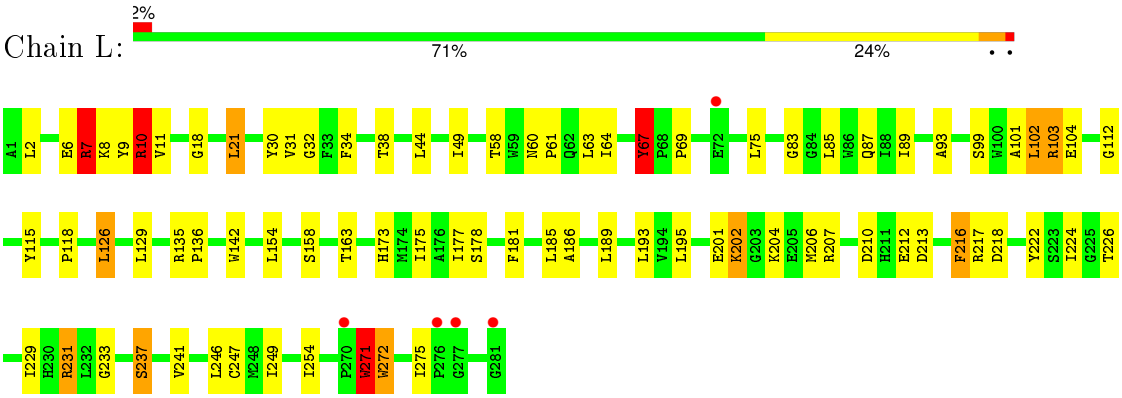
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	L	8	Total O 8 8	0	0
9	M	11	Total O 11 11	0	0
9	H	2	Total O 2 2	0	0

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.

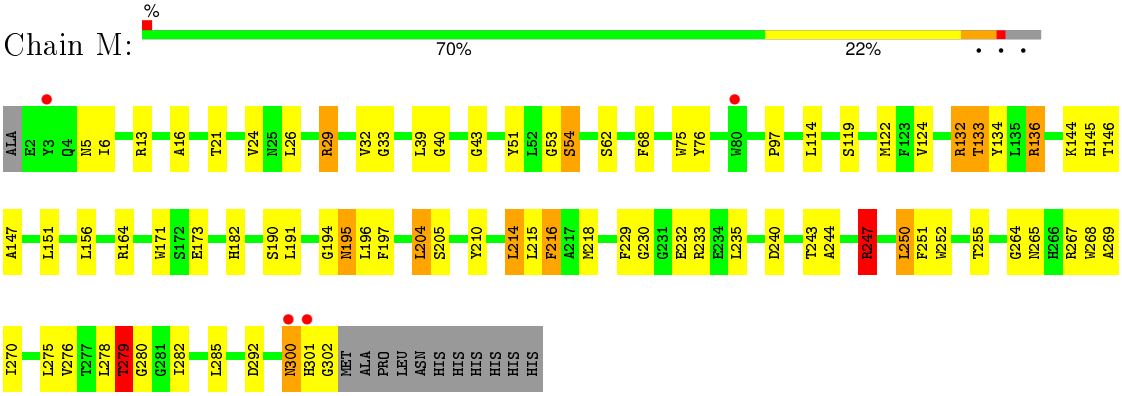
- Molecule 1: Reaction center protein L chain

Chain L:



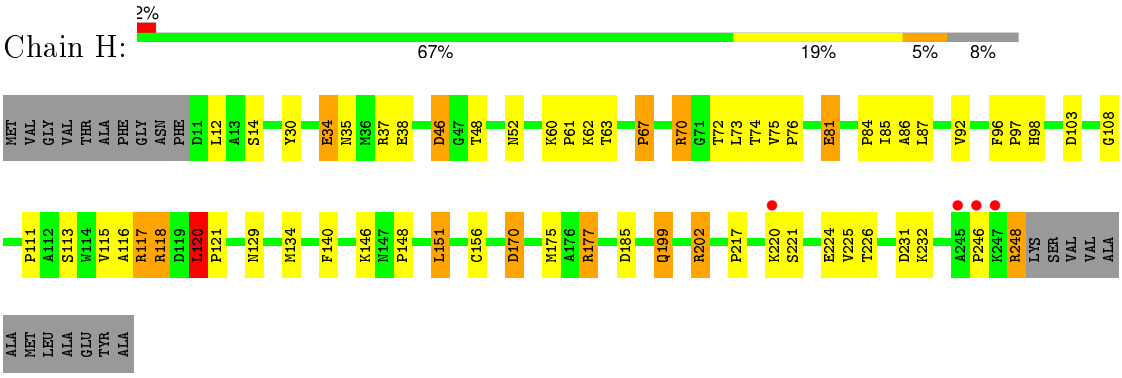
- Molecule 2: Reaction center protein M chain

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	139.72Å 139.72Å 183.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	121.00 – 2.93 19.84 – 2.93	Depositor EDS
% Data completeness (in resolution range)	99.6 (121.00-2.93) 100.0 (19.84-2.93)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.03 (at 2.93Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.185 , 0.226 0.187 , 0.227	Depositor DCC
R_{free} test set	2250 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	59.0	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 43.3	EDS
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 44997 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6919	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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	1.02	1/2295 (0.0%)	0.97	9/3144 (0.3%)
2	M	0.98	0/2480	0.94	4/3386 (0.1%)
3	H	0.99	0/1840	1.02	5/2511 (0.2%)
All	All	1.00	1/6615 (0.0%)	0.97	18/9041 (0.2%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	67	TYR	CD2-CE2	5.75	1.48	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	247	ARG	NE-CZ-NH1	9.40	125.00	120.30
1	L	231	ARG	NE-CZ-NH1	7.26	123.93	120.30
3	H	120	LEU	CA-CB-CG	6.83	131.01	115.30
2	M	21	THR	C-N-CA	-6.45	105.58	121.70
2	M	132	ARG	NE-CZ-NH1	-6.30	117.15	120.30
1	L	126	LEU	CB-CG-CD2	-6.13	100.58	111.00
1	L	231	ARG	NE-CZ-NH2	-5.77	117.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	81	GLU	C-N-CA	-5.77	107.28	121.70
1	L	7	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	L	10	ARG	NE-CZ-NH2	-5.52	117.54	120.30
3	H	170	ASP	CB-CG-OD1	5.50	123.25	118.30
1	L	10	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	L	103	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	L	7	ARG	NE-CZ-NH2	-5.22	117.69	120.30
3	H	46	ASP	CB-CG-OD1	5.13	122.92	118.30
2	M	204	LEU	CB-CG-CD1	5.10	119.67	111.00
1	L	31	VAL	C-N-CA	-5.08	111.63	122.30
3	H	67	PRO	C-N-CA	-5.05	109.06	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	32	GLY	Peptide
2	M	278	LEU	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	2209	0	2144	76	0
2	M	2390	0	2281	63	0
3	H	1792	0	1760	44	0
4	L	132	0	148	7	0
4	M	121	0	124	19	0
5	L	65	0	76	9	0
5	M	53	0	49	7	0
6	L	52	0	56	47	0
6	M	48	0	63	6	0
7	M	1	0	0	0	0
8	M	35	0	46	6	0
9	H	2	0	0	0	0
9	L	8	0	0	2	0
9	M	11	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6919	0	6747	224	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 16.

All (224) 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)
6:L:304:U10:C3M	6:L:305:U10:H1M1	1.29	1.60
6:L:304:U10:C3M	6:L:305:U10:C1M	2.23	1.15
3:H:117:ARG:HG2	3:H:117:ARG:HH11	1.07	1.09
6:L:304:U10:H3M1	6:L:305:U10:C1M	1.84	1.06
6:L:304:U10:H3M3	6:L:305:U10:H1M1	1.34	1.06
1:L:7:ARG:HH11	3:H:98:HIS:CD2	1.73	1.06
6:L:304:U10:H1M2	6:L:305:U10:H122	1.43	1.01
6:L:304:U10:H3M1	6:L:305:U10:H1M1	1.01	1.01
1:L:38:THR:HG22	1:L:99:SER:HB3	1.44	1.00
6:L:304:U10:H4M2	6:L:304:U10:H3M3	1.39	1.00
4:M:403:BCL:HHC	4:M:403:BCL:CBB	1.93	0.99
6:L:304:U10:O3	6:L:305:U10:H72	1.64	0.98
2:M:119:SER:HB3	8:M:406:SPO:H32	1.48	0.95
5:L:303:BPH:HBB2	2:M:210:TYR:HB3	1.53	0.90
1:L:216:PHE:CD2	6:L:305:U10:H8	2.05	0.89
3:H:117:ARG:HG2	3:H:117:ARG:NH1	1.88	0.87
3:H:117:ARG:HH11	3:H:117:ARG:CG	1.88	0.86
2:M:275:LEU:O	2:M:279:THR:HB	1.75	0.85
1:L:69:PRO:HG2	1:L:142:TRP:HB2	1.59	0.84
1:L:38:THR:HG22	1:L:99:SER:CB	2.06	0.84
1:L:186:ALA:HA	6:L:304:U10:C4M	2.07	0.83
5:M:404:BPH:HHC	5:M:404:BPH:HBB3	1.59	0.83
2:M:197:PHE:CZ	4:M:403:BCL:HBB2	2.15	0.82
6:L:304:U10:H3M3	6:L:305:U10:C1M	2.02	0.81
1:L:224:ILE:H	6:L:305:U10:H71	1.45	0.81
4:M:403:BCL:HHC	4:M:403:BCL:HBB3	1.62	0.81
6:L:304:U10:C3M	6:L:305:U10:C8	2.60	0.79
2:M:197:PHE:HZ	4:M:403:BCL:HBB2	1.43	0.79
3:H:129:ASN:ND2	3:H:224:GLU:HG2	1.98	0.78
4:M:403:BCL:HHC	4:M:403:BCL:HBB2	1.66	0.78
2:M:279:THR:HG22	2:M:280:GLY:N	1.99	0.78
5:L:303:BPH:HHC	5:L:303:BPH:HBB3	1.66	0.78
6:L:304:U10:H3M3	6:L:304:U10:C4M	2.14	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:60:ASN:HD22	1:L:61:PRO:CD	1.97	0.78
6:L:304:U10:O2	6:L:305:U10:H103	1.85	0.77
6:L:304:U10:O3	6:L:305:U10:C7	2.32	0.77
1:L:186:ALA:HA	6:L:304:U10:H4M1	1.67	0.76
2:M:240:ASP:O	3:H:117:ARG:NH1	2.19	0.75
1:L:189:LEU:HD12	6:L:304:U10:H4M3	1.68	0.75
1:L:213:ASP:O	1:L:217:ARG:HG3	1.87	0.75
2:M:279:THR:HG22	2:M:280:GLY:H	1.52	0.75
2:M:164:ARG:NH1	2:M:173:GLU:HG3	2.01	0.75
1:L:7:ARG:NH1	3:H:98:HIS:CD2	2.52	0.75
1:L:60:ASN:ND2	1:L:61:PRO:HD2	2.01	0.74
6:L:304:U10:C1M	6:L:305:U10:H122	2.18	0.73
3:H:70:ARG:NH2	3:H:121:PRO:O	2.20	0.73
4:L:302:BCL:HMB1	4:L:302:BCL:HBB2	1.71	0.72
4:L:302:BCL:HMB1	4:L:302:BCL:CBB	2.20	0.72
3:H:46:ASP:OD1	3:H:48:THR:HB	1.89	0.72
6:L:304:U10:O3	6:L:305:U10:C8	2.38	0.71
2:M:164:ARG:HH12	2:M:173:GLU:HG3	1.56	0.71
1:L:60:ASN:HD22	1:L:61:PRO:HD2	1.56	0.70
1:L:38:THR:CG2	1:L:99:SER:HB3	2.20	0.70
4:M:401:BCL:CBB	4:M:401:BCL:HHC	2.22	0.70
1:L:231:ARG:HD3	2:M:5:ASN:O	1.91	0.70
4:M:401:BCL:HBB2	4:M:401:BCL:HHC	1.74	0.70
3:H:37:ARG:O	3:H:38:GLU:HG2	1.90	0.70
2:M:53:GLY:O	2:M:54:SER:HB2	1.91	0.69
3:H:148:PRO:HA	3:H:151:LEU:HD22	1.74	0.69
3:H:156:CYS:SG	3:H:248:ARG:HA	2.32	0.69
1:L:224:ILE:HG22	6:L:305:U10:C7	2.22	0.69
1:L:216:PHE:CG	6:L:305:U10:H8	2.28	0.69
3:H:34:GLU:OE2	3:H:37:ARG:NH1	2.26	0.69
1:L:7:ARG:HH11	3:H:98:HIS:HD2	1.38	0.68
1:L:34:PHE:O	1:L:38:THR:HG23	1.93	0.68
2:M:97:PRO:HG2	2:M:171:TRP:HB2	1.75	0.68
2:M:32:VAL:HG12	2:M:33:GLY:O	1.93	0.68
3:H:70:ARG:O	3:H:118:ARG:NH2	2.26	0.67
5:L:303:BPH:CBB	2:M:210:TYR:HB3	2.24	0.67
1:L:201:GLU:O	1:L:202:LYS:HB2	1.94	0.67
6:L:304:U10:O2	6:L:305:U10:C10	2.43	0.67
1:L:181:PHE:HB3	5:M:404:BPH:HBB2	1.76	0.66
6:L:304:U10:O3	6:L:305:U10:H1M1	1.95	0.66
3:H:118:ARG:CD	3:H:120:LEU:HD22	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:181:PHE:HB3	5:M:404:BPH:CBB	2.28	0.64
3:H:118:ARG:HD2	3:H:120:LEU:HD22	1.79	0.64
2:M:194:GLY:O	2:M:195:ASN:HB3	1.98	0.64
3:H:120:LEU:HB3	3:H:121:PRO:CD	2.28	0.64
4:L:301:BCL:CBB	4:L:301:BCL:HMB1	2.28	0.63
1:L:69:PRO:HD3	1:L:83:GLY:O	1.98	0.63
1:L:60:ASN:ND2	1:L:61:PRO:CD	2.59	0.63
1:L:49:ILE:HG13	1:L:89:ILE:HD13	1.80	0.63
2:M:205:SER:HA	2:M:279:THR:HG21	1.80	0.62
2:M:243:THR:O	2:M:247:ARG:HG2	1.98	0.62
1:L:224:ILE:HG22	6:L:305:U10:H71	1.80	0.62
4:M:401:BCL:HBB3	4:M:403:BCL:H41	1.82	0.62
6:L:304:U10:H4M2	6:L:305:U10:C1M	2.30	0.61
3:H:129:ASN:HD21	3:H:224:GLU:HG2	1.65	0.61
2:M:133:THR:HG22	2:M:147:ALA:HB2	1.83	0.61
2:M:164:ARG:HH12	2:M:173:GLU:CG	2.12	0.61
1:L:7:ARG:NH1	3:H:98:HIS:HD2	1.97	0.61
1:L:241:VAL:HG21	5:L:303:BPH:HBC2	1.83	0.61
2:M:279:THR:CG2	2:M:280:GLY:N	2.63	0.61
1:L:216:PHE:CE2	6:L:304:U10:H3M2	2.36	0.60
2:M:119:SER:CB	8:M:406:SPO:H32	2.28	0.60
1:L:201:GLU:O	1:L:202:LYS:CB	2.49	0.60
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.83	0.60
4:L:301:BCL:HBB3	4:L:301:BCL:HMB1	1.83	0.59
6:L:304:U10:H3M1	6:L:305:U10:C8	2.31	0.59
4:M:403:BCL:HAA2	4:M:403:BCL:HBD	1.83	0.59
1:L:186:ALA:HA	6:L:304:U10:H4M3	1.84	0.59
2:M:164:ARG:NH1	2:M:173:GLU:CG	2.66	0.58
1:L:181:PHE:CD2	5:M:404:BPH:HBB1	2.38	0.58
1:L:49:ILE:CG1	1:L:89:ILE:HD13	2.33	0.58
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.39	0.57
2:M:76:TYR:CD2	2:M:76:TYR:C	2.78	0.57
1:L:226:THR:HG22	6:L:305:U10:H3M3	1.87	0.57
1:L:231:ARG:HD2	2:M:6:ILE:O	2.05	0.56
3:H:170:ASP:OD2	3:H:177:ARG:NH1	2.31	0.56
2:M:51:TYR:O	2:M:132:ARG:NH2	2.34	0.56
2:M:136:ARG:NE	2:M:136:ARG:HA	2.21	0.56
2:M:247:ARG:NH2	3:H:111:PRO:O	2.36	0.56
1:L:241:VAL:CG2	5:L:303:BPH:HBC2	2.35	0.56
6:L:304:U10:C3M	6:L:305:U10:C7	2.84	0.55
1:L:60:ASN:O	1:L:64:ILE:HG13	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:304:U10:C2	6:L:305:U10:C9	2.84	0.55
3:H:199:GLN:OE1	3:H:202:ARG:HD2	2.07	0.55
2:M:197:PHE:HZ	4:M:403:BCL:CBB	2.18	0.54
3:H:62:LYS:O	3:H:74:THR:HA	2.07	0.54
1:L:222:TYR:CD2	6:L:305:U10:C10	2.91	0.54
4:M:401:BCL:CBB	8:M:406:SPO:H243	2.38	0.53
1:L:186:ALA:CA	6:L:304:U10:H4M1	2.39	0.53
1:L:216:PHE:CD2	6:L:305:U10:C8	2.86	0.53
1:L:272:TRP:HA	1:L:275:ILE:CD1	2.39	0.53
6:L:304:U10:H4M2	6:L:305:U10:H1M2	1.91	0.53
2:M:194:GLY:O	2:M:195:ASN:CB	2.57	0.53
5:L:303:BPH:HBB1	2:M:210:TYR:CD2	2.42	0.53
2:M:133:THR:CG2	2:M:147:ALA:HA	2.39	0.52
1:L:101:ALA:O	1:L:104:GLU:HB2	2.09	0.52
1:L:271:TRP:HD1	1:L:271:TRP:H	1.54	0.52
2:M:232:GLU:OE2	3:H:177:ARG:NH2	2.42	0.52
1:L:103:ARG:NH2	2:M:255:THR:O	2.37	0.52
6:M:405:U10:H322	6:M:405:U10:H272	1.92	0.52
2:M:134:TYR:CE2	2:M:144:LYS:HG2	2.45	0.51
1:L:30:TYR:O	1:L:103:ARG:NH1	2.40	0.51
1:L:175:ILE:O	1:L:178:SER:HB3	2.10	0.51
1:L:9:TYR:O	1:L:11:VAL:N	2.40	0.51
4:M:403:BCL:HBB3	4:M:403:BCL:CHC	2.36	0.51
3:H:63:THR:HA	3:H:73:LEU:O	2.10	0.50
2:M:251:PHE:CD1	2:M:251:PHE:C	2.85	0.50
5:M:404:BPH:CHC	5:M:404:BPH:HBB3	2.37	0.50
2:M:24:VAL:HG11	2:M:29:ARG:NH1	2.27	0.50
1:L:222:TYR:HD2	6:L:305:U10:H101	1.77	0.49
1:L:233:GLY:HA3	2:M:216:PHE:CE1	2.47	0.49
4:L:301:BCL:HBB2	4:M:403:BCL:NA	2.27	0.49
2:M:264:GLY:HA3	3:H:35:ASN:OD1	2.12	0.49
1:L:218:ASP:OD1	2:M:29:ARG:HD3	2.13	0.49
3:H:118:ARG:HD3	3:H:120:LEU:HD22	1.95	0.49
6:M:405:U10:H8	6:M:405:U10:H1M1	1.95	0.48
2:M:300:ASN:C	2:M:302:GLY:H	2.15	0.48
1:L:34:PHE:CE1	1:L:102:LEU:HD23	2.49	0.48
4:L:301:BCL:CGA	4:L:302:BCL:HBC1	2.43	0.48
6:L:304:U10:H3M1	6:L:305:U10:C7	2.44	0.48
1:L:18:GLY:O	1:L:21:LEU:HB2	2.14	0.48
2:M:40:GLY:HA2	2:M:43:GLY:O	2.13	0.48
4:M:401:BCL:HBB2	8:M:406:SPO:H243	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:404:BPH:HHD	5:M:404:BPH:HBC3	1.96	0.47
6:L:304:U10:O2	6:L:305:U10:C9	2.63	0.47
2:M:133:THR:HG21	2:M:147:ALA:HA	1.96	0.47
2:M:214:LEU:HD22	2:M:218:MET:SD	2.54	0.47
6:L:304:U10:C2	6:L:305:U10:C11	2.93	0.47
1:L:10:ARG:NH2	9:L:404:HOH:O	2.47	0.47
2:M:16:ALA:HB1	2:M:32:VAL:HG21	1.97	0.47
1:L:8:LYS:NZ	3:H:81:GLU:OE1	2.40	0.47
6:M:405:U10:C32	6:M:405:U10:H272	2.45	0.47
1:L:83:GLY:O	1:L:87:GLN:HG3	2.16	0.46
2:M:250:LEU:HA	2:M:250:LEU:HD12	1.82	0.46
1:L:216:PHE:CE2	6:L:305:U10:H112	2.51	0.46
4:M:401:BCL:HMB1	4:M:401:BCL:OBB	2.15	0.46
6:L:304:U10:H72	6:L:305:U10:C13	2.45	0.46
3:H:37:ARG:C	3:H:38:GLU:HG2	2.35	0.46
3:H:37:ARG:NH2	3:H:60:LYS:O	2.49	0.46
1:L:115:TYR:O	1:L:118:PRO:HG2	2.16	0.46
5:L:303:BPH:HBB1	2:M:210:TYR:CG	2.51	0.45
2:M:230:GLY:O	2:M:233:ARG:HG3	2.16	0.45
3:H:61:PRO:HA	3:H:76:PRO:HD2	1.99	0.45
5:M:404:BPH:H4C1	5:M:404:BPH:H6C1	1.71	0.45
2:M:68:PHE:HE1	8:M:406:SPO:H31	1.81	0.45
2:M:133:THR:HG22	2:M:147:ALA:CB	2.45	0.45
4:M:403:BCL:H2C	4:M:403:BCL:HBC2	1.76	0.45
1:L:38:THR:HG22	1:L:99:SER:HB2	1.96	0.45
4:M:403:BCL:HAA2	4:M:403:BCL:CBD	2.47	0.45
6:M:405:U10:H1M1	6:M:405:U10:C8	2.46	0.45
3:H:30:TYR:O	3:H:34:GLU:HB2	2.16	0.44
1:L:75:LEU:HA	1:L:75:LEU:HD23	1.79	0.44
1:L:193:LEU:HG	1:L:212:GLU:HG2	1.98	0.44
1:L:229:ILE:HD13	6:L:305:U10:H1M2	1.99	0.44
1:L:67:TYR:CD1	1:L:67:TYR:N	2.86	0.44
2:M:197:PHE:CE1	4:M:403:BCL:HBB2	2.53	0.43
6:L:304:U10:C1	6:L:305:U10:H122	2.47	0.43
2:M:13:ARG:O	3:H:140:PHE:HA	2.19	0.43
1:L:135:ARG:HB3	1:L:136:PRO:HD3	2.00	0.43
1:L:93:ALA:HA	5:L:303:BPH:H9C2	2.00	0.43
3:H:96:PHE:HB3	3:H:97:PRO:CD	2.47	0.43
3:H:118:ARG:CD	3:H:120:LEU:CD2	2.97	0.42
3:H:84:PRO:O	3:H:85:ILE:HD13	2.18	0.42
1:L:224:ILE:HG22	6:L:305:U10:H72	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:120:LEU:HA	3:H:226:THR:HG22	2.00	0.42
3:H:103:ASP:OD1	3:H:103:ASP:C	2.58	0.42
6:L:304:U10:C2	6:L:305:U10:H111	2.50	0.42
1:L:112:GLY:HA2	9:L:401:HOH:O	2.19	0.42
2:M:145:HIS:O	2:M:146:THR:C	2.58	0.41
2:M:114:LEU:HA	2:M:114:LEU:HD23	1.82	0.41
1:L:222:TYR:CD2	6:L:305:U10:H101	2.56	0.41
3:H:115:VAL:HG22	3:H:117:ARG:HG3	2.03	0.41
1:L:2:LEU:HD13	1:L:6:GLU:HG2	2.03	0.41
1:L:85:LEU:O	1:L:89:ILE:HG13	2.21	0.41
2:M:268:TRP:CD1	6:M:405:U10:H111	2.55	0.41
3:H:75:VAL:HA	3:H:76:PRO:C	2.40	0.41
2:M:269:ALA:O	2:M:270:ILE:C	2.57	0.41
8:M:406:SPO:H183	8:M:406:SPO:H15	1.88	0.41
1:L:206:MET:O	3:H:67:PRO:HG3	2.20	0.41
1:L:272:TRP:HA	1:L:275:ILE:HD12	2.02	0.41
2:M:282:ILE:HG13	2:M:282:ILE:H	1.74	0.41
2:M:243:THR:OG1	2:M:247:ARG:HD2	2.20	0.41
1:L:271:TRP:CD1	1:L:271:TRP:N	2.82	0.41
1:L:163:THR:O	1:L:163:THR:HG22	2.21	0.41
2:M:276:VAL:O	2:M:279:THR:HG22	2.21	0.40
2:M:252:TRP:CD1	6:M:405:U10:C6	3.03	0.40
2:M:190:SER:HB2	4:M:403:BCL:H3C	2.03	0.40
4:L:302:BCL:C19	5:L:303:BPH:H6C1	2.52	0.40
3:H:108:GLY:O	3:H:113:SER:HA	2.22	0.40
3:H:85:ILE:O	3:H:87:LEU:N	2.48	0.40
1:L:195:LEU:HD11	2:M:267:ARG:HG2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	279/281 (99%)	253 (91%)	22 (8%)	4 (1%)	14	43
2	M	299/313 (96%)	276 (92%)	19 (6%)	4 (1%)	15	45
3	H	236/260 (91%)	218 (92%)	14 (6%)	4 (2%)	11	37
All	All	814/854 (95%)	747 (92%)	55 (7%)	12 (2%)	13	41

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	202	LYS
2	M	279	THR
2	M	301	HIS
3	H	86	ALA
3	H	185	ASP
2	M	54	SER
1	L	237	SER
2	M	195	ASN
1	L	10	ARG
1	L	271	TRP
3	H	116	ALA
3	H	246	PRO

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	215/220 (98%)	192 (89%)	23 (11%)	8	24
2	M	231/246 (94%)	205 (89%)	26 (11%)	7	21
3	H	186/208 (89%)	162 (87%)	24 (13%)	5	15
All	All	632/674 (94%)	559 (88%)	73 (12%)	7	20

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	7	ARG

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Mol	Chain	Res	Type
1	L	21	LEU
1	L	44	LEU
1	L	58	THR
1	L	63	LEU
1	L	67	TYR
1	L	102	LEU
1	L	126	LEU
1	L	129	LEU
1	L	154	LEU
1	L	158	SER
1	L	185	LEU
1	L	204	LYS
1	L	207	ARG
1	L	210	ASP
1	L	216	PHE
1	L	237	SER
1	L	246	LEU
1	L	247	CYS
1	L	249	ILE
1	L	254	ILE
1	L	271	TRP
1	L	272	TRP
2	M	26	LEU
2	M	29	ARG
2	M	39	LEU
2	M	62	SER
2	M	75	TRP
2	M	122	MET
2	M	124	VAL
2	M	133	THR
2	M	136	ARG
2	M	151	LEU
2	M	156	LEU
2	M	182	HIS
2	M	191	LEU
2	M	196	LEU
2	M	204	LEU
2	M	214	LEU
2	M	215	LEU
2	M	216	PHE
2	M	235	LEU
2	M	247	ARG

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Mol	Chain	Res	Type
2	M	250	LEU
2	M	265	ASN
2	M	279	THR
2	M	285	LEU
2	M	292	ASP
2	M	300	ASN
3	H	12	LEU
3	H	14	SER
3	H	34	GLU
3	H	52	ASN
3	H	70	ARG
3	H	72	THR
3	H	92	VAL
3	H	117	ARG
3	H	118	ARG
3	H	120	LEU
3	H	134	MET
3	H	146	LYS
3	H	151	LEU
3	H	175	MET
3	H	177	ARG
3	H	199	GLN
3	H	202	ARG
3	H	217	PRO
3	H	220	LYS
3	H	221	SER
3	H	225	VAL
3	H	231	ASP
3	H	232	LYS
3	H	248	ARG

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	60	ASN
3	H	52	ASN
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 (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 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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	0.66	0	57,115,115	1.33	7 (12%)
4	BCL	L	302	-	53,74,74	0.80	1 (1%)	57,115,115	2.44	16 (28%)
5	BPH	L	303	-	64,70,70	1.48	10 (15%)	73,101,101	1.86	16 (21%)
6	U10	L	304	-	26,26,63	2.98	9 (34%)	31,34,79	2.32	9 (29%)
6	U10	L	305	-	26,26,63	3.38	13 (50%)	31,34,79	2.41	13 (41%)
4	BCL	M	401	-	42,63,74	0.90	2 (4%)	43,101,115	2.25	12 (27%)
4	BCL	M	403	-	53,74,74	0.68	0	57,115,115	1.74	12 (21%)
5	BPH	M	404	-	52,58,70	1.72	10 (19%)	58,86,101	2.21	22 (37%)
6	U10	M	405	-	48,48,63	3.22	12 (25%)	58,61,79	1.84	18 (31%)
8	SPO	M	406	-	33,34,41	1.26	3 (9%)	36,41,50	2.28	10 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BCL	L	301	-	-	0/37/137/137	0/0/9/9
4	BCL	L	302	-	-	0/37/137/137	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BPH	L	303	-	2/2/18/22	0/54/105/105	0/1/6/6
6	U10	L	304	-	-	0/19/43/87	0/1/1/1
6	U10	L	305	-	-	0/19/43/87	0/1/1/1
4	BCL	M	401	-	-	0/24/124/137	0/0/9/9
4	BCL	M	403	-	-	0/37/137/137	0/0/9/9
5	BPH	M	404	-	-	0/40/91/105	0/1/6/6
6	U10	M	405	-	-	0/45/69/87	0/1/1/1
8	SPO	M	406	-	-	0/39/39/47	0/0/0/0

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	304	U10	O4-C4	-4.94	1.24	1.37
6	L	304	U10	O3-C3	-4.51	1.25	1.37
6	L	305	U10	O4-C4	-4.29	1.25	1.37
6	M	405	U10	O4-C4	-4.23	1.25	1.37
5	M	404	BPH	C1B-C2B	-3.71	1.37	1.45
5	M	404	BPH	C4C-NC	-3.61	1.29	1.37
6	M	405	U10	O3-C3	-3.60	1.27	1.37
6	L	304	U10	C3-C2	-3.26	1.39	1.48
5	L	303	BPH	C4C-NC	-3.13	1.30	1.37
5	M	404	BPH	C1A-NA	-3.12	1.30	1.37
6	L	304	U10	C4-C5	-3.09	1.40	1.48
5	L	303	BPH	C1B-C2B	-2.90	1.39	1.45
5	L	303	BPH	C1A-NA	-2.78	1.31	1.37
5	L	303	BPH	CHB-C4A	-2.72	1.35	1.40
6	L	305	U10	C3-C2	-2.71	1.41	1.48
6	L	305	U10	O3-C3	-2.63	1.30	1.37
6	L	304	U10	C6-C5	-2.51	1.39	1.46
6	M	405	U10	C4-C5	-2.36	1.42	1.48
5	L	303	BPH	C3B-C4B	-2.25	1.38	1.43
6	L	305	U10	C4-C5	-2.24	1.42	1.48
5	M	404	BPH	CHB-C4A	-2.20	1.36	1.40
6	M	405	U10	C3-C2	-2.09	1.42	1.48
4	L	302	BCL	C1A-CHA	-2.06	1.34	1.43
5	M	404	BPH	C3B-C4B	-2.04	1.38	1.43
6	L	305	U10	C4-C3	2.01	1.44	1.35
5	L	303	BPH	C4A-NA	2.01	1.39	1.34
8	M	406	SPO	C26-C27	2.13	1.50	1.43
5	L	303	BPH	CHB-C1B	2.18	1.43	1.38
6	L	305	U10	C7-C8	2.20	1.54	1.50
4	M	401	BCL	C6-C5	2.30	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	404	BPH	CHB-C1B	2.31	1.43	1.38
6	L	305	U10	C16-C14	2.38	1.56	1.51
5	M	404	BPH	C2-C3	2.42	1.37	1.33
6	L	305	U10	C11-C9	2.55	1.57	1.51
5	M	404	BPH	O2A-CGA	2.62	1.41	1.33
8	M	406	SPO	C25-C23	2.71	1.51	1.45
4	M	401	BCL	C5-C3	2.77	1.57	1.51
6	M	405	U10	C6-C1	2.79	1.41	1.35
6	L	304	U10	C19-C18	2.82	1.48	1.28
6	L	305	U10	C19-C18	2.89	1.48	1.28
6	L	304	U10	C6-C1	2.94	1.42	1.35
6	L	305	U10	C6-C1	3.01	1.42	1.35
6	L	305	U10	C7-C6	3.31	1.57	1.51
5	L	303	BPH	C3D-C4D	3.32	1.45	1.41
8	M	406	SPO	C27-C28	3.74	1.38	1.34
5	L	303	BPH	CHA-C1A	4.06	1.46	1.37
5	M	404	BPH	CHD-C4C	4.35	1.49	1.38
5	M	404	BPH	CHA-C1A	4.68	1.48	1.37
5	L	303	BPH	CHD-C4C	5.08	1.51	1.38
6	M	405	U10	C38-C39	6.06	1.50	1.32
6	M	405	U10	C8-C9	6.55	1.45	1.33
6	M	405	U10	C18-C19	7.65	1.48	1.33
6	M	405	U10	C23-C24	7.77	1.48	1.33
6	L	304	U10	C8-C9	7.91	1.48	1.33
6	M	405	U10	C28-C29	8.03	1.48	1.33
6	L	304	U10	C13-C14	8.25	1.49	1.33
6	M	405	U10	C13-C14	8.29	1.49	1.33
6	M	405	U10	C33-C34	9.36	1.51	1.33
6	L	305	U10	C13-C14	9.82	1.52	1.33
6	L	305	U10	C8-C9	9.93	1.52	1.33

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	302	BCL	O1D-CGD-CBD	-9.90	110.44	124.62
6	L	304	U10	C7-C6-C5	-7.70	109.51	118.56
4	M	401	BCL	C4-C3-C2	-6.64	110.45	123.50
6	L	305	U10	C1-C6-C5	-6.12	113.14	120.12
8	M	406	SPO	C4-C5-C6	-5.51	116.83	124.67
6	L	304	U10	C7-C8-C9	-5.25	117.80	126.70
8	M	406	SPO	C20-C21-C22	-5.06	112.21	123.39
5	L	303	BPH	CBC-CAC-C3C	-4.24	103.19	113.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	404	BPH	C4-C3-C5	-3.99	109.31	115.41
5	M	404	BPH	CAC-C3C-C2C	-3.94	104.23	114.13
4	L	302	BCL	C1D-CHD-C4C	-3.71	120.41	126.07
6	M	405	U10	C17-C18-C19	-3.70	119.72	127.76
5	M	404	BPH	C2D-C1D-ND	-3.64	104.32	110.29
6	L	305	U10	C10-C9-C8	-3.63	116.38	123.50
8	M	406	SPO	C15-C16-C17	-3.62	115.65	126.32
8	M	406	SPO	C18-C17-C19	-3.56	117.64	122.90
6	L	305	U10	O2-C2-C3	-3.53	113.14	120.79
6	M	405	U10	C12-C13-C14	-3.51	120.13	127.76
5	L	303	BPH	CAC-C3C-C4C	-3.30	104.20	112.67
6	M	405	U10	C30-C29-C28	-3.28	117.06	123.50
6	L	304	U10	C12-C13-C14	-3.16	120.89	127.76
4	L	302	BCL	OBD-CAD-C3D	-3.11	122.00	128.35
5	L	303	BPH	C2D-C1D-ND	-3.10	105.21	110.29
4	L	302	BCL	C5-C3-C2	-3.05	115.26	121.05
6	L	304	U10	C10-C9-C8	-3.05	117.51	123.50
4	L	301	BCL	C1D-CHD-C4C	-3.00	121.49	126.07
5	M	404	BPH	C3A-C2A-C1A	-2.83	98.25	101.84
6	M	405	U10	C15-C14-C13	-2.81	117.99	123.50
6	M	405	U10	C22-C23-C24	-2.78	121.72	127.76
6	M	405	U10	C7-C8-C9	-2.74	122.06	126.70
4	L	301	BCL	O1D-CGD-CBD	-2.73	120.71	124.62
5	L	303	BPH	C2B-C1B-NB	-2.71	105.67	109.73
4	M	403	BCL	C1D-CHD-C4C	-2.70	121.95	126.07
4	M	401	BCL	OBD-CAD-C3D	-2.70	122.85	128.35
6	L	304	U10	O4-C4-C3	-2.69	112.51	124.17
5	M	404	BPH	OBD-CAD-CBD	-2.63	121.96	125.94
5	M	404	BPH	C4-C3-C2	-2.62	118.36	123.50
6	M	405	U10	C35-C34-C33	-2.61	118.38	123.50
5	L	303	BPH	CAA-CBA-CGA	-2.61	105.68	113.32
6	L	304	U10	O5-C5-C6	-2.55	116.89	121.68
4	M	403	BCL	O2D-CGD-O1D	-2.54	118.55	123.79
4	M	401	BCL	C1D-CHD-C4C	-2.52	122.22	126.07
6	L	305	U10	C15-C14-C13	-2.52	118.55	123.50
8	M	406	SPO	C24-C23-C22	-2.52	119.19	122.90
6	L	305	U10	C4-C3-C2	-2.42	114.47	120.73
5	M	404	BPH	C2B-C1B-NB	-2.41	106.12	109.73
4	M	401	BCL	O1D-CGD-CBD	-2.39	121.20	124.62
8	M	406	SPO	C15-C14-C12	-2.38	123.76	127.20
4	M	403	BCL	O2A-CGA-O1A	-2.38	117.36	123.49
6	M	405	U10	C27-C28-C29	-2.36	122.64	127.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	405	U10	C1M-C1-C6	-2.35	119.07	124.10
5	L	303	BPH	C4-C3-C5	-2.30	111.90	115.41
6	L	304	U10	C15-C14-C13	-2.29	119.01	123.50
4	L	302	BCL	O2A-CGA-O1A	-2.28	117.61	123.49
4	M	401	BCL	O1A-CGA-CBA	-2.25	114.74	123.72
4	L	301	BCL	C2A-C1A-CHA	-2.24	119.75	123.89
5	M	404	BPH	CMA-C3A-C4A	-2.24	105.70	113.01
4	M	403	BCL	C11-C10-C8	-2.22	108.12	115.49
5	M	404	BPH	C1C-NC-C4C	-2.19	108.19	110.44
4	L	302	BCL	CMB-C2B-C1B	-2.17	124.78	128.36
4	L	302	BCL	C11-C12-C13	-2.16	108.32	115.49
5	L	303	BPH	C1D-CHD-C4C	-2.15	119.42	127.23
6	M	405	U10	C26-C27-C28	-2.12	106.13	111.69
4	M	403	BCL	O1D-CGD-CBD	-2.11	121.60	124.62
4	M	403	BCL	CBC-CAC-C3C	-2.10	108.44	113.57
5	L	303	BPH	C3A-C4A-NA	-2.09	109.92	113.57
5	M	404	BPH	C3A-C4A-NA	-2.08	109.94	113.57
4	L	302	BCL	C2A-C1A-CHA	-2.06	120.09	123.89
4	M	401	BCL	O2D-CGD-O1D	-2.06	119.54	123.79
5	M	404	BPH	C3B-C4B-NB	-2.05	105.63	109.98
5	L	303	BPH	C3B-C4B-NB	-2.02	105.68	109.98
4	M	403	BCL	C3C-C4C-CHD	-2.01	118.85	123.33
8	M	406	SPO	C26-C25-C23	2.00	132.21	126.32
5	M	404	BPH	C3B-C2B-C1B	2.01	108.99	105.77
5	M	404	BPH	C1B-NB-C4B	2.02	110.51	106.51
5	M	404	BPH	C3D-CAD-CBD	2.09	110.55	107.60
6	M	405	U10	C37-C36-C34	2.10	119.55	112.71
6	M	405	U10	C20-C19-C21	2.12	118.64	115.41
5	M	404	BPH	C7-C6-C5	2.14	123.51	113.61
4	L	301	BCL	CHD-C4C-NC	2.15	127.55	125.06
6	M	405	U10	C3M-O3-C3	2.24	124.58	116.61
6	L	305	U10	C4M-O4-C4	2.25	124.62	116.61
5	M	404	BPH	C2A-C1A-NA	2.31	115.04	112.08
5	L	303	BPH	C1B-NB-C4B	2.35	111.17	106.51
4	L	301	BCL	C4-C3-C5	2.37	119.03	115.41
6	M	405	U10	C4M-O4-C4	2.45	125.32	116.61
4	L	302	BCL	CED-O2D-CGD	2.46	121.75	115.99
4	M	401	BCL	CHD-C4C-NC	2.48	127.94	125.06
6	L	305	U10	C6-C1-C2	2.52	123.07	120.42
5	L	303	BPH	C6-C7-C8	2.53	123.89	115.49
4	L	302	BCL	CHB-C4A-NA	2.55	128.04	124.51
6	L	305	U10	C11-C12-C13	2.57	118.42	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	404	BPH	CHC-C4B-NB	2.59	129.84	124.91
5	L	303	BPH	C4D-C3D-C2D	2.61	110.45	107.08
4	L	302	BCL	OBB-CAB-C3B	2.62	124.14	120.00
6	L	305	U10	C16-C17-C18	2.64	119.07	112.09
6	M	405	U10	C10-C9-C11	2.70	119.53	115.41
4	L	301	BCL	O2A-CGA-CBA	2.75	120.27	111.90
4	M	401	BCL	CHB-C4A-NA	2.77	128.34	124.51
5	L	303	BPH	CMD-C2D-C3D	2.81	130.58	125.09
4	M	403	BCL	CED-O2D-CGD	2.87	122.71	115.99
4	M	403	BCL	O2A-CGA-CBA	3.00	121.05	111.90
5	M	404	BPH	O2D-CGD-CBD	3.13	115.59	111.30
4	L	302	BCL	CHD-C4C-NC	3.15	128.71	125.06
6	L	304	U10	C15-C14-C16	3.18	120.26	115.41
5	M	404	BPH	CMD-C2D-C3D	3.18	131.31	125.09
4	L	302	BCL	C4-C3-C5	3.19	120.29	115.41
8	M	406	SPO	C29-C28-C30	3.23	120.34	115.41
4	M	401	BCL	O2A-CGA-CBA	3.34	122.09	111.90
4	L	302	BCL	O2A-CGA-CBA	3.50	122.56	111.90
4	M	403	BCL	OBB-CAB-C3B	3.50	125.55	120.00
4	L	301	BCL	O2D-CGD-CBD	3.56	116.19	111.30
6	L	305	U10	C15-C14-C16	3.69	121.04	115.41
5	M	404	BPH	C6-C5-C3	3.69	120.59	112.48
4	L	302	BCL	OBD-CAD-CBD	3.75	131.60	125.94
5	L	303	BPH	C11-C10-C8	3.81	128.13	115.49
6	L	304	U10	C10-C9-C11	3.84	121.28	115.41
6	L	305	U10	C11-C9-C8	3.85	128.35	121.05
6	L	305	U10	C8-C7-C6	3.88	123.30	111.64
8	M	406	SPO	C24-C23-C25	3.89	124.56	118.10
6	L	305	U10	C3M-O3-C3	3.99	130.78	116.61
6	M	405	U10	C15-C14-C16	4.07	121.62	115.41
4	M	403	BCL	CHD-C4C-NC	4.35	130.10	125.06
6	M	405	U10	C30-C29-C31	4.43	122.17	115.41
6	M	405	U10	C35-C34-C36	4.75	122.66	115.41
8	M	406	SPO	C16-C17-C19	5.19	127.34	118.98
4	M	401	BCL	C6-C5-C3	5.46	124.46	112.48
4	M	401	BCL	C5-C3-C2	5.48	131.44	121.05
4	M	401	BCL	O2D-CGD-CBD	5.78	119.23	111.30
5	L	303	BPH	C3C-C4C-NC	5.87	113.81	107.93
5	M	404	BPH	C5-C3-C2	5.94	132.32	121.05
4	M	403	BCL	O2D-CGD-CBD	6.23	119.85	111.30
5	L	303	BPH	C6-C5-C3	7.32	128.56	112.48
5	M	404	BPH	C3C-C4C-NC	7.52	115.46	107.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	302	BCL	O2D-CGD-CBD	9.36	124.14	111.30

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.

10 monomers are involved in 97 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	301	BCL	4	0
4	L	302	BCL	4	0
5	L	303	BPH	9	0
6	L	304	U10	34	0
6	L	305	U10	39	0
4	M	401	BCL	6	0
4	M	403	BCL	14	0
5	M	404	BPH	7	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	281/281 (100%)	-0.65	5 (1%)	71	70	30, 44, 77, 91	0
2	M	301/313 (96%)	-0.73	4 (1%)	79	79	29, 47, 75, 82	0
3	H	238/260 (91%)	-0.54	4 (1%)	73	72	34, 46, 61, 94	0
All	All	820/854 (96%)	-0.65	13 (1%)	74	74	29, 46, 74, 94	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	246	PRO	4.4
1	L	281	GLY	4.0
1	L	270	PRO	3.4
2	M	301	HIS	2.9
1	L	72	GLU	2.6
1	L	276	PRO	2.6
3	H	245	ALA	2.4
2	M	300	ASN	2.4
2	M	80	TRP	2.3
1	L	277	GLY	2.3
3	H	247	LYS	2.2
3	H	220	LYS	2.2
2	M	3	TYR	2.0

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
6	U10	L	305	26/63	0.70	0.40	27.97	46,55,66,67	26
6	U10	L	304	26/63	0.81	0.37	13.74	67,90,94,99	26
8	SPO	M	406	35/42	0.90	0.21	1.98	54,68,86,87	0
6	U10	M	405	48/63	0.91	0.17	1.49	41,52,83,85	0
4	BCL	M	401	55/66	0.94	0.15	1.22	33,39,69,71	0
4	BCL	M	403	66/66	0.97	0.15	1.07	32,41,55,70	0
4	BCL	L	301	66/66	0.97	0.15	0.70	29,39,43,55	0
5	BPH	M	404	53/65	0.97	0.12	0.16	33,46,59,64	0
5	BPH	L	303	65/65	0.98	0.12	0.15	26,35,40,46	0
4	BCL	L	302	66/66	0.98	0.09	-0.69	27,33,48,55	0
7	FE	M	402	1/1	0.99	0.07	-1.53	35,35,35,35	0

6.5 Other polymers

There are no such residues in this entry.