Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:37 PM GMT

PDB ID	:	1PSS
Title	:	CRYSTALLOGRAPHIC ANALYSES OF SITE-DIRECTED MUTANTS OF THE PHOTOSYNTHETIC REACTION CENTER FROM RHODOBACTER SPHAEROIDES
Authors	:	Chirino, A.J.; Feher, G.; Rees, D.C.
Deposited on	:	1993-12-13
Resolution	:	3.00 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 (i) symbol.

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

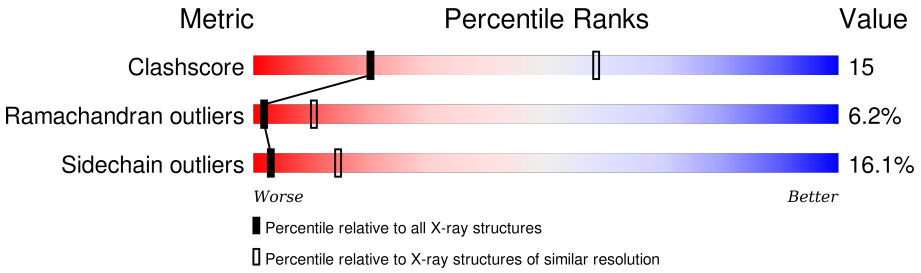
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 3.00 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))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	266	65% 28% 6%
2	M	296	57% 32% 9%
3	H	237	46% 36% 14%

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	BCL	M	3	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	BPH	L	271	X	-	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6789 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 PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	266	Total	C	N	O	S	0	0	0
			2121	1433	336	344	8			

- Molecule 2 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	296	Total	C	N	O	S	0	0	0
			2362	1579	386	387	10			

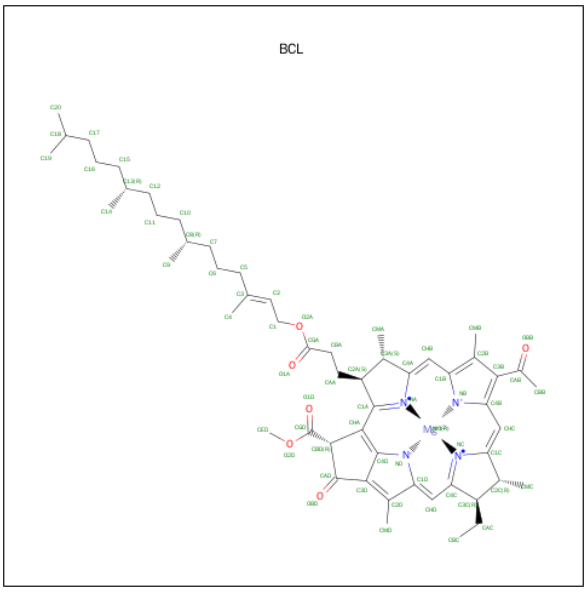
- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	237	Total	C	N	O	S	0	0	0
			1807	1156	310	332	9			

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

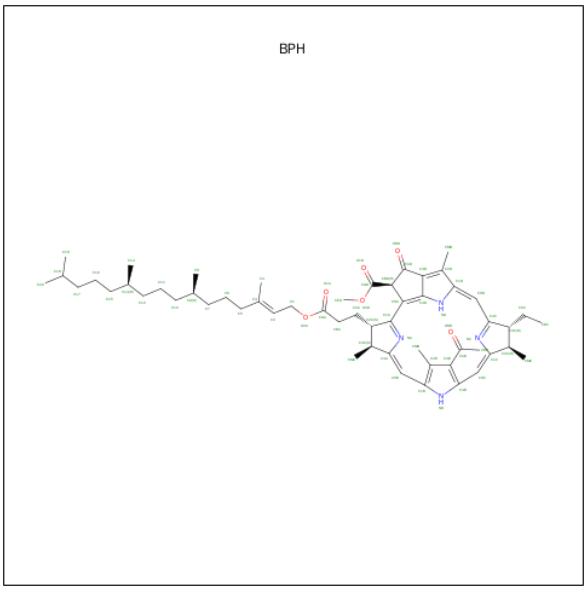
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	1	Total	Fe	0	0
			1	1		

- Molecule 5 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



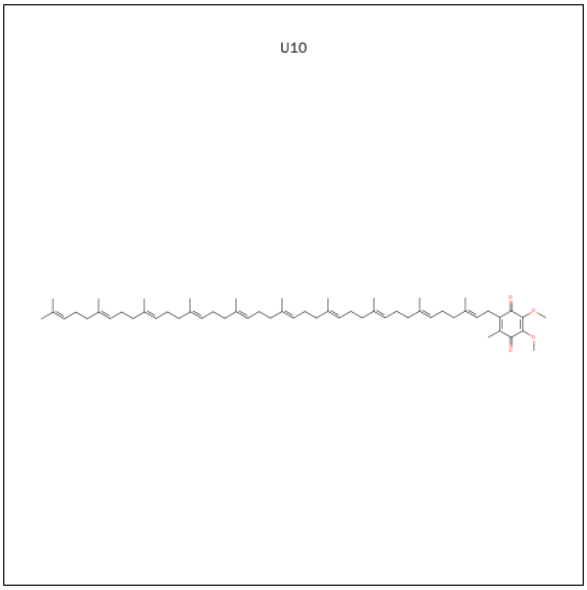
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	M	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	M	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		

- Molecule 6 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



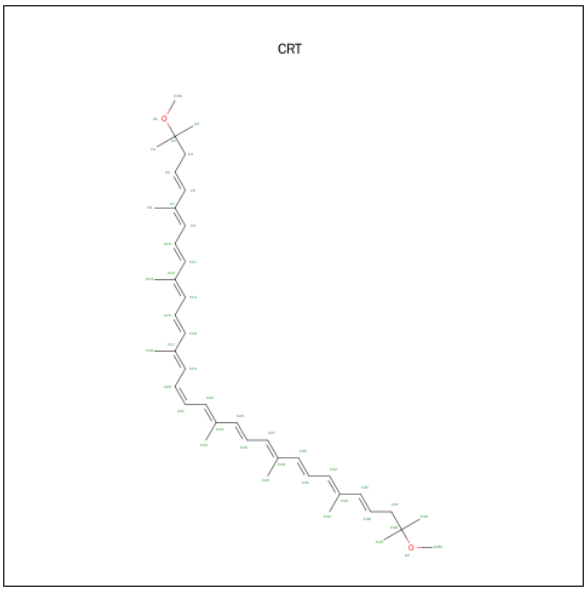
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	M	1	Total	C	N	O	0	0
			65	55	4	6		
6	L	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 7 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	M	1	Total	C	O	0	0
			51	47	4		
7	L	1	Total	C	O	0	0
			41	37	4		

- Molecule 8 is SPIRILLOXANTHIN (three-letter code: CRT) (formula: $C_{42}H_{60}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	M	1	Total	C	O	0	0
			42	41	1		

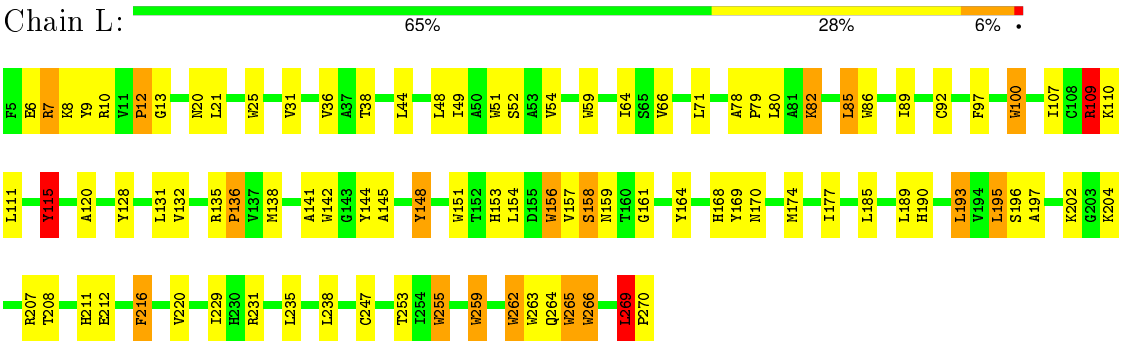
3 Residue-property plots (i)

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.

Note EDS was not executed.

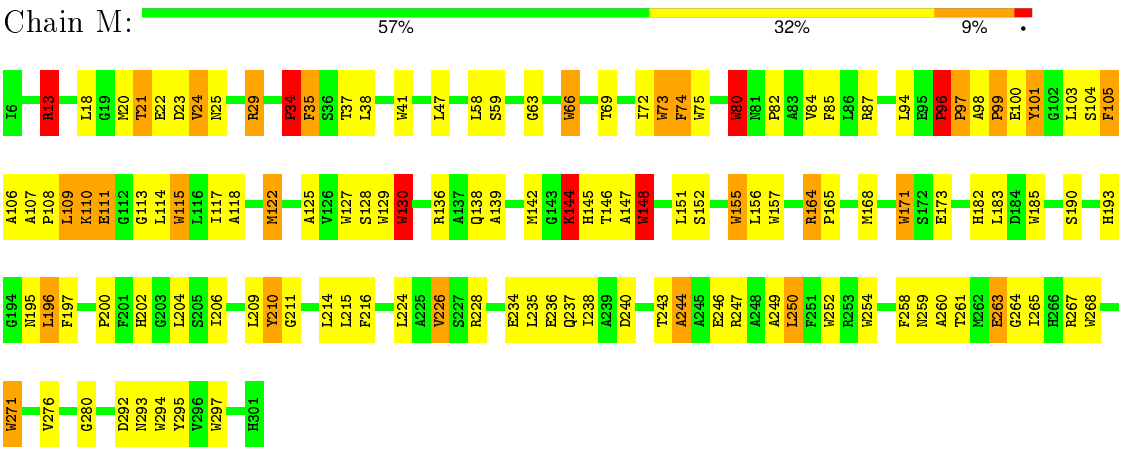
• Molecule 1: PHOTOSYNTHETIC REACTION CENTER

Chain L:



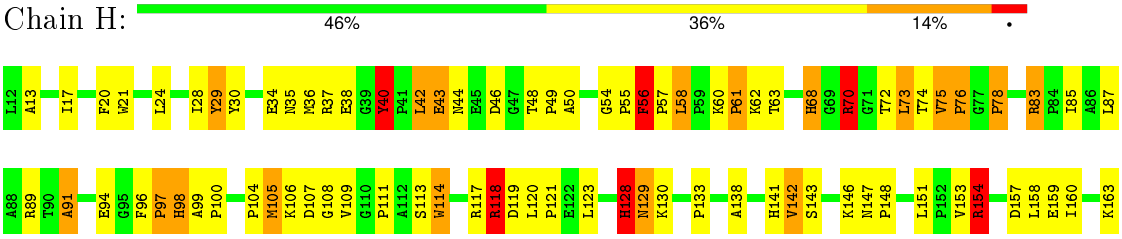
• Molecule 2: PHOTOSYNTHETIC REACTION CENTER

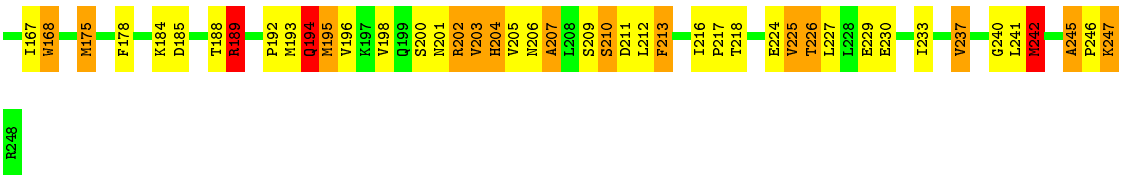
Chain M:



• Molecule 3: PHOTOSYNTHETIC REACTION CENTER

Chain H:




I167
W168
M175
F178
K184
D185
T188
R189
P192
M193
Q194
M195
V196
K197
V198
Q199
S200
N201
R202
V203
H204
V205
N206
A207
L208
S209
S210
D211
L212
F213
I216
P217
T218
E224
V225
T226
L227
L228
E229
E230
I233
V237
G240
L241
N242
A245
P246
K247
R248

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	138.00Å 77.50Å 141.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.223 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6789	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

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, FE, CRT, U10

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	0.84	0/2204	1.63	51/3014 (1.7%)
2	M	0.92	0/2453	1.79	83/3348 (2.5%)
3	H	0.81	0/1855	1.69	33/2523 (1.3%)
All	All	0.86	0/6512	1.71	167/8885 (1.9%)

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
3	H	0	2
All	All	0	4

There are no bond length outliers.

All (167) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	13	ARG	NE-CZ-NH1	13.43	127.01	120.30
2	M	41	TRP	CD1-CG-CD2	9.38	113.81	106.30
2	M	171	TRP	CD1-CG-CD2	9.22	113.67	106.30
1	L	262	TRP	CD1-CG-CD2	9.06	113.55	106.30
1	L	142	TRP	CD1-CG-CD2	8.96	113.46	106.30
2	M	157	TRP	CD1-CG-CD2	8.90	113.42	106.30
2	M	294	TRP	CD1-CG-CD2	8.76	113.31	106.30
2	M	130	TRP	CE2-CD2-CG	-8.66	100.37	107.30
1	L	86	TRP	CD1-CG-CD2	8.58	113.16	106.30
2	M	75	TRP	CD1-CG-CD2	8.49	113.09	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	25	TRP	CD1-CG-CD2	8.49	113.09	106.30
1	L	142	TRP	CE2-CD2-CG	-8.40	100.58	107.30
3	H	21	TRP	CD1-CG-CD2	8.37	112.99	106.30
2	M	130	TRP	CD1-CG-CD2	8.35	112.98	106.30
1	L	151	TRP	CD1-CG-CD2	8.35	112.98	106.30
1	L	100	TRP	CD1-CG-CD2	8.18	112.84	106.30
2	M	75	TRP	CE2-CD2-CG	-8.18	100.76	107.30
2	M	171	TRP	CE2-CD2-CG	-8.18	100.76	107.30
2	M	66	TRP	CD1-CG-CD2	8.17	112.84	106.30
2	M	294	TRP	CE2-CD2-CG	-8.14	100.79	107.30
2	M	164	ARG	NE-CZ-NH1	8.11	124.35	120.30
2	M	129	TRP	CD1-CG-CD2	8.08	112.76	106.30
2	M	41	TRP	CE2-CD2-CG	-8.03	100.87	107.30
3	H	114	TRP	CD1-CG-CD2	7.93	112.64	106.30
2	M	115	TRP	CD1-CG-CD2	7.86	112.59	106.30
2	M	185	TRP	CD1-CG-CD2	7.86	112.59	106.30
1	L	263	TRP	CE2-CD2-CG	-7.86	101.01	107.30
1	L	25	TRP	CE2-CD2-CG	-7.83	101.03	107.30
2	M	252	TRP	CD1-CG-CD2	7.83	112.56	106.30
2	M	136	ARG	NE-CZ-NH1	7.79	124.19	120.30
3	H	168	TRP	CD1-CG-CD2	7.79	112.53	106.30
2	M	271	TRP	CD1-CG-CD2	7.78	112.52	106.30
1	L	266	TRP	CD1-CG-CD2	7.77	112.52	106.30
1	L	263	TRP	CD1-CG-CD2	7.73	112.48	106.30
2	M	66	TRP	CE2-CD2-CG	-7.62	101.20	107.30
1	L	255	TRP	CE2-CD2-CG	-7.59	101.22	107.30
1	L	156	TRP	CD1-CG-CD2	7.58	112.36	106.30
2	M	129	TRP	CE2-CD2-CG	-7.58	101.24	107.30
3	H	118	ARG	NE-CZ-NH1	7.55	124.07	120.30
2	M	185	TRP	CE2-CD2-CG	-7.53	101.27	107.30
1	L	86	TRP	CE2-CD2-CG	-7.53	101.28	107.30
2	M	271	TRP	CE2-CD2-CG	-7.49	101.31	107.30
3	H	168	TRP	CE2-CD2-CG	-7.47	101.32	107.30
1	L	156	TRP	CE2-CD2-CG	-7.47	101.33	107.30
3	H	21	TRP	CE2-CD2-CG	-7.46	101.34	107.30
2	M	148	TRP	CA-CB-CG	7.44	127.84	113.70
2	M	268	TRP	CE2-CD2-CG	-7.43	101.35	107.30
2	M	127	TRP	CD1-CG-CD2	7.42	112.24	106.30
1	L	259	TRP	CE2-CD2-CG	-7.39	101.39	107.30
2	M	115	TRP	CE2-CD2-CG	-7.39	101.39	107.30
1	L	59	TRP	CE2-CD2-CG	-7.38	101.39	107.30
1	L	151	TRP	CE2-CD2-CG	-7.37	101.40	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	100	TRP	CE2-CD2-CG	-7.37	101.41	107.30
2	M	268	TRP	CD1-CG-CD2	7.35	112.18	106.30
1	L	59	TRP	CD1-CG-CD2	7.33	112.16	106.30
1	L	262	TRP	CE2-CD2-CG	-7.32	101.45	107.30
2	M	252	TRP	CE2-CD2-CG	-7.32	101.45	107.30
1	L	255	TRP	CD1-CG-CD2	7.28	112.12	106.30
2	M	254	TRP	CD1-CG-CD2	7.25	112.10	106.30
3	H	114	TRP	CE2-CD2-CG	-7.23	101.52	107.30
2	M	254	TRP	CE2-CD2-CG	-7.18	101.56	107.30
2	M	73	TRP	CD1-CG-CD2	7.15	112.02	106.30
2	M	155	TRP	CE2-CD2-CG	-7.12	101.60	107.30
1	L	266	TRP	CE2-CD2-CG	-7.01	101.69	107.30
2	M	25	ASN	CA-C-N	-7.00	101.79	117.20
1	L	51	TRP	CD1-CG-CD2	7.00	111.90	106.30
2	M	297	TRP	CE2-CD2-CG	-6.97	101.72	107.30
2	M	80	TRP	CD1-CG-CD2	6.94	111.85	106.30
2	M	80	TRP	CE2-CD2-CG	-6.92	101.76	107.30
1	L	265	TRP	CE2-CD2-CG	-6.92	101.77	107.30
2	M	157	TRP	CE2-CD2-CG	-6.90	101.78	107.30
2	M	127	TRP	CE2-CD2-CG	-6.89	101.78	107.30
1	L	51	TRP	CE2-CD2-CG	-6.85	101.82	107.30
3	H	242	MET	CA-CB-CG	6.83	124.91	113.30
2	M	73	TRP	CE2-CD2-CG	-6.79	101.86	107.30
1	L	259	TRP	CD1-CG-CD2	6.78	111.73	106.30
3	H	37	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	L	164	TYR	CB-CG-CD2	-6.72	116.97	121.00
2	M	155	TRP	CD1-CG-CD2	6.69	111.65	106.30
1	L	156	TRP	CG-CD2-CE3	6.69	139.92	133.90
2	M	101	TYR	CA-CB-CG	6.67	126.08	113.40
3	H	141	HIS	O-C-N	6.65	133.35	122.70
2	M	29	ARG	NE-CZ-NH1	6.59	123.60	120.30
3	H	29	TYR	CB-CG-CD1	-6.59	117.05	121.00
2	M	297	TRP	CD1-CG-CD2	6.55	111.54	106.30
1	L	109	ARG	NE-CZ-NH1	6.45	123.53	120.30
3	H	154	ARG	NE-CZ-NH2	-6.36	117.12	120.30
3	H	42	LEU	CA-C-N	-6.36	103.21	117.20
3	H	91	ALA	N-CA-C	6.34	128.12	111.00
2	M	66	TRP	CG-CD2-CE3	6.31	139.58	133.90
3	H	204	HIS	N-CA-C	6.27	127.92	111.00
3	H	189	ARG	NE-CZ-NH1	6.22	123.41	120.30
2	M	261	THR	CA-CB-CG2	6.14	121.00	112.40
2	M	252	TRP	CG-CD2-CE3	6.12	139.40	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	202	ARG	NE-CZ-NH1	6.09	123.35	120.30
3	H	154	ARG	NE-CZ-NH1	6.07	123.33	120.30
2	M	294	TRP	CG-CD2-CE3	6.06	139.35	133.90
2	M	75	TRP	CG-CD2-CE3	6.04	139.33	133.90
2	M	297	TRP	CG-CD2-CE3	6.03	139.32	133.90
1	L	59	TRP	CG-CD2-CE3	6.02	139.32	133.90
1	L	115	TYR	N-CA-C	6.00	127.21	111.00
1	L	265	TRP	CD1-CG-CD2	5.98	111.08	106.30
3	H	175	MET	CA-CB-CG	5.98	123.46	113.30
3	H	141	HIS	CA-C-N	-5.96	104.08	117.20
3	H	168	TRP	CG-CD2-CE3	5.95	139.26	133.90
3	H	74	THR	CA-C-N	-5.94	104.14	117.20
1	L	7	ARG	NE-CZ-NH1	5.90	123.25	120.30
2	M	144	LYS	N-CA-C	5.89	126.90	111.00
3	H	128	HIS	CA-C-N	-5.88	104.28	117.20
1	L	142	TRP	CG-CD2-CE3	5.87	139.18	133.90
2	M	261	THR	N-CA-CB	-5.85	99.19	110.30
2	M	196	LEU	CA-CB-CG	5.84	128.72	115.30
2	M	157	TRP	CG-CD1-NE1	-5.82	104.28	110.10
1	L	25	TRP	CG-CD2-CE3	5.76	139.09	133.90
2	M	34	PRO	N-CA-C	5.76	127.08	112.10
2	M	268	TRP	CG-CD2-CE3	5.71	139.04	133.90
1	L	263	TRP	CG-CD2-CE3	5.68	139.01	133.90
2	M	130	TRP	CB-CG-CD1	-5.67	119.63	127.00
2	M	297	TRP	CB-CG-CD1	-5.65	119.65	127.00
1	L	148	TYR	CB-CG-CD2	-5.65	117.61	121.00
1	L	142	TRP	CB-CG-CD1	-5.64	119.67	127.00
1	L	216	PHE	CA-CB-CG	-5.62	100.42	113.90
1	L	25	TRP	CB-CG-CD1	-5.57	119.76	127.00
2	M	226	VAL	N-CA-CB	-5.57	99.25	111.50
2	M	66	TRP	CB-CG-CD1	-5.55	119.78	127.00
2	M	155	TRP	CB-CG-CD1	-5.52	119.83	127.00
2	M	210	TYR	CB-CG-CD2	-5.52	117.69	121.00
2	M	250	LEU	CB-CG-CD1	-5.50	101.65	111.00
3	H	56	PHE	CB-CG-CD1	5.48	124.64	120.80
1	L	259	TRP	CG-CD2-CE3	5.48	138.83	133.90
2	M	29	ARG	CA-C-N	-5.47	105.17	117.20
2	M	294	TRP	CG-CD1-NE1	-5.44	104.66	110.10
1	L	142	TRP	CG-CD1-NE1	-5.43	104.67	110.10
1	L	255	TRP	CG-CD2-CE3	5.42	138.78	133.90
1	L	86	TRP	CG-CD1-NE1	-5.41	104.69	110.10
2	M	66	TRP	CG-CD1-NE1	-5.38	104.72	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	148	TRP	CE2-CD2-CG	-5.35	103.02	107.30
2	M	75	TRP	CB-CG-CD1	-5.34	120.05	127.00
3	H	46	ASP	CA-C-N	-5.34	105.51	116.20
1	L	169	TYR	CB-CG-CD2	-5.30	117.82	121.00
2	M	268	TRP	CB-CG-CD1	-5.29	120.12	127.00
2	M	254	TRP	CG-CD2-CE3	5.28	138.65	133.90
2	M	41	TRP	CG-CD1-NE1	-5.27	104.83	110.10
2	M	261	THR	CA-CB-OG1	-5.26	97.95	109.00
3	H	159	GLU	N-CA-C	5.25	125.16	111.00
3	H	168	TRP	CG-CD1-NE1	-5.25	104.86	110.10
2	M	171	TRP	CG-CD1-NE1	-5.24	104.86	110.10
1	L	262	TRP	CG-CD1-NE1	-5.23	104.87	110.10
1	L	156	TRP	CB-CG-CD1	-5.20	120.24	127.00
3	H	210	SER	N-CA-C	-5.18	97.00	111.00
1	L	92	CYS	CA-CB-SG	-5.12	104.78	114.00
2	M	130	TRP	CG-CD2-CE3	5.12	138.51	133.90
2	M	252	TRP	CB-CG-CD1	-5.10	120.38	127.00
3	H	21	TRP	CG-CD1-NE1	-5.08	105.02	110.10
3	H	105	MET	CA-CB-CG	-5.08	104.67	113.30
2	M	185	TRP	CG-CD2-CE3	5.07	138.46	133.90
2	M	13	ARG	CD-NE-CZ	5.06	130.68	123.60
1	L	59	TRP	CB-CG-CD1	-5.06	120.43	127.00
2	M	185	TRP	CB-CG-CD1	-5.05	120.43	127.00
2	M	263	GLU	CA-CB-CG	5.05	124.50	113.40
2	M	226	VAL	CB-CA-C	5.04	120.98	111.40
3	H	237	VAL	CG1-CB-CG2	-5.03	102.85	110.90
2	M	247	ARG	NE-CZ-NH2	-5.03	117.78	120.30
3	H	70	ARG	NE-CZ-NH1	5.03	122.81	120.30
3	H	114	TRP	CG-CD1-NE1	-5.03	105.07	110.10
2	M	109	LEU	N-CA-C	-5.02	97.45	111.00
1	L	25	TRP	CG-CD1-NE1	-5.01	105.09	110.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	245	ALA	Peptide
3	H	83	ARG	Peptide
1	L	269	LEU	Peptide
2	M	96	PRO	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	2121	0	2077	59	0
2	M	2362	0	2281	74	0
3	H	1807	0	1814	66	0
4	M	1	0	0	0	0
5	L	66	0	74	16	0
5	M	168	0	156	18	0
6	L	65	0	76	5	0
6	M	65	0	76	3	0
7	L	41	0	52	3	0
7	M	51	0	68	8	0
8	M	42	0	57	1	0
All	All	6789	0	6731	200	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 15.

All (200) 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)
1:L:111:LEU:HD21	2:M:250:LEU:HD12	1.44	0.99
2:M:264:GLY:HA2	2:M:267:ARG:HG3	1.63	0.80
3:H:204:HIS:HB3	3:H:206:ASN:OD1	1.86	0.76
3:H:87:LEU:HG	3:H:98:HIS:HB3	1.68	0.75
3:H:61:PRO:HA	3:H:76:PRO:HG2	1.72	0.72
3:H:154:ARG:HA	3:H:160:ILE:HA	1.75	0.69
2:M:165:PRO:HG3	2:M:173:GLU:HB2	1.73	0.69
2:M:13:ARG:HB2	3:H:143:SER:OG	1.95	0.67
1:L:97:PHE:CE1	5:L:2:BCL:H121	2.30	0.66
3:H:189:ARG:HD3	3:H:216:ILE:HB	1.77	0.66
3:H:148:PRO:HD2	3:H:167:ILE:HD11	1.78	0.66
5:L:2:BCL:H171	6:L:271:BPH:H4C3	1.77	0.65
5:M:1:BCL:HHC	5:M:1:BCL:HBB2	1.79	0.65
2:M:260:ALA:HB2	7:M:303:U10:H103	1.79	0.65
2:M:35:PHE:HB2	2:M:47:LEU:HD11	1.80	0.63
5:M:3:BCL:HBB2	5:M:3:BCL:HHC	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:96:PRO:HA	2:M:115:TRP:CG	2.35	0.61
3:H:118:ARG:HH11	3:H:118:ARG:HB2	1.65	0.61
2:M:190:SER:HB2	5:M:3:BCL:H3C	1.81	0.61
1:L:168:HIS:HB3	2:M:183:LEU:HD13	1.81	0.61
1:L:6:GLU:HA	1:L:9:TYR:HD2	1.66	0.61
3:H:29:TYR:HB3	3:H:30:TYR:HD1	1.65	0.60
3:H:42:LEU:HD23	3:H:58:LEU:HG	1.82	0.60
3:H:198:VAL:HA	3:H:203:VAL:HG23	1.85	0.58
2:M:130:TRP:HZ3	2:M:147:ALA:O	1.87	0.58
1:L:13:GLY:HA3	1:L:110:LYS:HG2	1.86	0.58
3:H:133:PRO:HA	3:H:168:TRP:HA	1.84	0.58
2:M:125:ALA:HB1	6:M:5:BPH:H4C2	1.84	0.58
3:H:29:TYR:HB3	3:H:30:TYR:CD1	2.39	0.57
3:H:111:PRO:HG3	3:H:242:MET:SD	2.44	0.57
2:M:228:ARG:HA	3:H:194:GLN:HG3	1.85	0.57
5:L:2:BCL:H112	5:M:4:BCL:HBB2	1.86	0.57
2:M:215:LEU:HD11	2:M:265:ILE:HD11	1.87	0.57
5:M:1:BCL:HBC1	5:M:3:BCL:HAA2	1.85	0.56
2:M:280:GLY:HA2	5:M:3:BCL:HED3	1.87	0.56
3:H:142:VAL:HG21	3:H:147:ASN:OD1	2.05	0.56
1:L:170:ASN:OD1	1:L:247:CYS:HB2	2.05	0.56
1:L:48:LEU:HD23	1:L:89:ILE:HG13	1.87	0.56
2:M:20:MET:SD	2:M:22:GLU:HB2	2.46	0.56
2:M:235:LEU:HA	2:M:238:ILE:HD12	1.87	0.56
3:H:29:TYR:CE2	3:H:55:PRO:HA	2.41	0.55
3:H:148:PRO:HA	3:H:151:LEU:HD12	1.88	0.55
2:M:209:LEU:HD23	2:M:276:VAL:HG11	1.88	0.55
5:L:2:BCL:HAA2	5:M:4:BCL:HBC1	1.88	0.55
3:H:178:PHE:HZ	3:H:230:GLU:HG2	1.70	0.55
3:H:154:ARG:HG3	3:H:202:ARG:HE	1.72	0.55
1:L:141:ALA:HB3	1:L:144:TYR:CE2	2.42	0.54
5:L:2:BCL:H122	6:L:271:BPH:HBA1	1.89	0.54
3:H:76:PRO:O	3:H:78:PRO:HD3	2.08	0.53
1:L:197:ALA:HB1	2:M:235:LEU:HD21	1.90	0.53
1:L:44:LEU:O	1:L:48:LEU:HB2	2.09	0.53
3:H:226:THR:HB	3:H:229:GLU:HG3	1.90	0.53
1:L:38:THR:HG21	1:L:100:TRP:HE3	1.73	0.53
3:H:213:PHE:O	3:H:216:ILE:HG13	2.08	0.53
2:M:193:HIS:HA	2:M:292:ASP:O	2.09	0.53
1:L:177:ILE:HD13	5:M:1:BCL:HMD1	1.91	0.53
5:L:2:BCL:HBB2	5:M:3:BCL:NB	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:123:LEU:HD23	3:H:128:HIS:H	1.73	0.53
3:H:68:HIS:HB3	3:H:123:LEU:HD22	1.91	0.52
1:L:128:TYR:HB2	5:L:2:BCL:H51	1.91	0.52
5:L:2:BCL:HBB3	5:L:2:BCL:HMB1	1.90	0.52
1:L:266:TRP:NE1	2:M:87:ARG:HA	2.24	0.52
5:M:3:BCL:CBB	5:M:3:BCL:HHC	2.39	0.52
1:L:79:PRO:HG2	1:L:82:LYS:HB2	1.89	0.52
3:H:129:ASN:HD21	3:H:224:GLU:HG3	1.75	0.52
3:H:108:GLY:HA3	3:H:114:TRP:CZ3	2.45	0.52
2:M:84:VAL:O	2:M:87:ARG:HG2	2.10	0.52
3:H:24:LEU:O	3:H:28:ILE:HG12	2.09	0.52
2:M:206:ILE:HG23	5:M:3:BCL:HMB3	1.91	0.52
2:M:164:ARG:HB3	2:M:165:PRO:HD3	1.92	0.52
3:H:233:ILE:O	3:H:237:VAL:HG23	2.10	0.52
1:L:195:LEU:HB3	2:M:145:HIS:CE1	2.45	0.51
3:H:154:ARG:HD3	3:H:160:ILE:HG13	1.91	0.51
3:H:43:GLU:HB3	3:H:49:PRO:O	2.11	0.51
2:M:202:HIS:CE1	2:M:206:ILE:HD11	2.45	0.51
3:H:44:ASN:O	3:H:49:PRO:HA	2.11	0.51
3:H:29:TYR:HE2	3:H:55:PRO:HA	1.76	0.50
1:L:120:ALA:HA	1:L:238:LEU:HD21	1.93	0.50
2:M:200:PRO:HB2	3:H:17:ILE:HD12	1.93	0.50
3:H:40:TYR:O	3:H:42:LEU:HD12	2.11	0.50
1:L:7:ARG:NH1	3:H:85:ILE:HB	2.27	0.50
1:L:231:ARG:HG2	2:M:224:LEU:HD11	1.93	0.50
1:L:161:GLY:HA3	5:L:2:BCL:HAC1	1.93	0.50
2:M:22:GLU:HG2	2:M:139:ALA:O	2.12	0.49
3:H:104:PRO:HA	3:H:107:ASP:HB2	1.94	0.49
1:L:131:LEU:HD21	5:L:2:BCL:HED2	1.95	0.49
1:L:196:SER:HB2	2:M:142:MET:HB3	1.95	0.49
2:M:108:PRO:HB2	2:M:110:LYS:O	2.12	0.49
2:M:293:ASN:OD1	2:M:295:TYR:HB3	2.13	0.49
1:L:7:ARG:HH12	3:H:85:ILE:HB	1.78	0.48
2:M:197:PHE:HZ	5:M:3:BCL:HBB2	1.78	0.48
2:M:110:LYS:HD3	2:M:114:LEU:HD13	1.94	0.48
3:H:85:ILE:HG22	3:H:87:LEU:HB2	1.95	0.48
3:H:154:ARG:HB3	3:H:202:ARG:HH21	1.78	0.48
1:L:154:LEU:HD12	2:M:197:PHE:HB3	1.95	0.48
7:M:303:U10:H1M1	7:M:303:U10:H71	1.67	0.48
3:H:119:ASP:HA	3:H:226:THR:HG23	1.95	0.48
1:L:207:ARG:HG3	1:L:211:HIS:CG	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:63:THR:HA	3:H:73:LEU:O	2.14	0.47
1:L:190:HIS:HA	7:L:272:U10:O2	2.13	0.47
2:M:59:SER:OG	2:M:128:SER:HB2	2.14	0.47
1:L:154:LEU:O	1:L:157:VAL:HB	2.14	0.47
2:M:249:ALA:HA	7:M:303:U10:H4M2	1.96	0.47
1:L:8:LYS:NZ	3:H:113:SER:HB3	2.30	0.47
1:L:177:ILE:HG23	5:L:2:BCL:HMB3	1.97	0.47
7:M:303:U10:O5	7:M:303:U10:H8	2.15	0.47
2:M:144:LYS:HE3	2:M:148:TRP:HB2	1.97	0.46
1:L:109:ARG:HH22	1:L:115:TYR:HB3	1.80	0.46
2:M:260:ALA:HB1	3:H:36:MET:SD	2.55	0.46
1:L:177:ILE:HG12	5:L:2:BCL:HMB3	1.98	0.46
2:M:190:SER:HA	2:M:196:LEU:HD23	1.98	0.46
5:M:4:BCL:CBB	5:M:4:BCL:HMB1	2.45	0.46
1:L:13:GLY:CA	1:L:110:LYS:HG2	2.45	0.46
1:L:193:LEU:HD11	1:L:212:GLU:HA	1.96	0.46
1:L:9:TYR:CD2	2:M:250:LEU:HD11	2.50	0.46
3:H:62:LYS:O	3:H:75:VAL:HG23	2.15	0.46
2:M:204:LEU:HD21	3:H:20:PHE:CD2	2.50	0.46
1:L:36:VAL:HG12	7:M:303:U10:H403	1.98	0.46
7:M:303:U10:H162	7:M:303:U10:H121	1.81	0.46
6:L:271:BPH:HBB2	2:M:210:TYR:HB3	1.97	0.46
1:L:80:LEU:HB3	1:L:85:LEU:HD22	1.98	0.46
2:M:110:LYS:H	2:M:114:LEU:HD22	1.81	0.45
3:H:38:GLU:O	3:H:42:LEU:HD11	2.17	0.45
3:H:108:GLY:HA3	3:H:114:TRP:HZ3	1.81	0.45
1:L:6:GLU:HG2	1:L:10:ARG:HD3	1.98	0.45
2:M:20:MET:SD	2:M:22:GLU:OE1	2.75	0.45
2:M:37:THR:HG22	2:M:38:LEU:HG	1.98	0.45
2:M:105:PHE:HD1	2:M:106:ALA:H	1.63	0.45
2:M:73:TRP:CH2	2:M:109:LEU:HB3	2.52	0.45
2:M:63:GLY:HA3	6:M:5:BPH:H5C2	1.98	0.45
3:H:154:ARG:HG3	3:H:202:ARG:HB3	1.99	0.45
2:M:237:GLN:NE2	2:M:244:ALA:HB3	2.32	0.45
1:L:158:SER:HA	5:L:2:BCL:HBC1	1.98	0.44
2:M:144:LYS:NZ	2:M:148:TRP:HA	2.32	0.44
2:M:69:THR:O	2:M:72:ILE:HG13	2.16	0.44
3:H:241:LEU:O	3:H:242:MET:HB3	2.17	0.44
3:H:61:PRO:HA	3:H:76:PRO:CG	2.44	0.44
2:M:82:PRO:HA	2:M:85:PHE:HB3	2.00	0.44
1:L:168:HIS:NE2	5:L:2:BCL:OBB	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:262:TRP:O	1:L:265:TRP:HD1	2.00	0.44
6:L:271:BPH:HBB1	2:M:210:TYR:CD2	2.51	0.44
1:L:107:ILE:O	1:L:111:LEU:HB2	2.18	0.44
2:M:20:MET:SD	2:M:22:GLU:HA	2.58	0.44
2:M:113:GLY:O	2:M:117:ILE:HG12	2.17	0.44
2:M:103:LEU:HA	2:M:171:TRP:CD1	2.52	0.44
6:M:5:BPH:H3A	6:M:5:BPH:HBA1	1.80	0.44
1:L:135:ARG:HB3	1:L:136:PRO:HD3	2.00	0.44
3:H:184:LYS:HD2	3:H:184:LYS:HA	1.88	0.44
1:L:49:ILE:HG13	1:L:89:ILE:HD13	2.00	0.43
3:H:56:PHE:O	3:H:58:LEU:N	2.51	0.43
3:H:207:ALA:O	3:H:240:GLY:HA3	2.18	0.43
1:L:157:VAL:HG11	5:M:3:BCL:HBB1	2.00	0.43
1:L:266:TRP:HE1	2:M:87:ARG:HA	1.83	0.43
2:M:66:TRP:CD1	2:M:122:MET:HB2	2.54	0.43
1:L:9:TYR:CE2	2:M:246:GLU:HG2	2.53	0.43
3:H:154:ARG:O	3:H:204:HIS:CE1	2.72	0.43
5:M:3:BCL:HBC2	5:M:3:BCL:H2C	1.83	0.43
2:M:236:GLU:HB3	3:H:117:ARG:HH22	1.81	0.43
3:H:54:GLY:HA2	3:H:55:PRO:HD2	1.83	0.43
2:M:74:PHE:HB3	2:M:85:PHE:HE1	1.84	0.43
3:H:204:HIS:CG	3:H:205:VAL:N	2.87	0.43
3:H:87:LEU:CG	3:H:98:HIS:HB3	2.44	0.43
6:L:271:BPH:HHC	6:L:271:BPH:HBB3	2.00	0.43
2:M:94:LEU:HD21	2:M:114:LEU:HG	2.01	0.43
7:L:272:U10:H171	7:L:272:U10:H151	1.90	0.43
1:L:12:PRO:HG3	3:H:97:PRO:HB3	2.01	0.43
1:L:109:ARG:NH2	1:L:115:TYR:H	2.17	0.42
1:L:9:TYR:CG	2:M:250:LEU:HD11	2.54	0.42
1:L:207:ARG:HG3	1:L:211:HIS:ND1	2.33	0.42
7:L:272:U10:H71	7:L:272:U10:H1M1	1.66	0.42
2:M:211:GLY:O	2:M:214:LEU:HB3	2.19	0.42
1:L:174:MET:HB3	5:M:1:BCL:O1D	2.20	0.42
5:L:2:BCL:NC	5:M:3:BCL:HBB3	2.34	0.42
1:L:255:TRP:HE1	1:L:259:TRP:HA	1.84	0.42
1:L:66:VAL:HB	1:L:148:TYR:HB2	2.01	0.42
3:H:147:ASN:HA	3:H:148:PRO:HD3	1.87	0.42
2:M:66:TRP:HD1	2:M:118:ALA:O	2.02	0.42
8:M:304:CRT:H26	8:M:304:CRT:H241	1.83	0.42
1:L:52:SER:OG	1:L:85:LEU:HD23	2.20	0.42
2:M:164:ARG:NH1	2:M:168:MET:SD	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:35:PHE:HB2	2:M:47:LEU:CD1	2.49	0.41
1:L:85:LEU:HD12	1:L:85:LEU:HA	1.90	0.41
1:L:153:HIS:CE1	1:L:154:LEU:HD23	2.55	0.41
2:M:103:LEU:HD21	2:M:165:PRO:O	2.20	0.41
2:M:130:TRP:CZ3	2:M:147:ALA:HB1	2.55	0.41
2:M:130:TRP:CZ3	2:M:151:LEU:HG	2.56	0.41
2:M:152:SER:O	2:M:155:TRP:HB3	2.21	0.41
1:L:189:LEU:HD12	2:M:146:THR:HG23	2.02	0.41
2:M:110:LYS:HD3	2:M:114:LEU:CD1	2.51	0.41
3:H:226:THR:CG2	3:H:229:GLU:HG3	2.51	0.41
1:L:269:LEU:H	1:L:270:PRO:C	2.24	0.41
7:M:303:U10:H271	7:M:303:U10:H251	1.83	0.41
3:H:119:ASP:HA	3:H:226:THR:CG2	2.51	0.41
2:M:107:ALA:HB1	2:M:111:GLU:O	2.21	0.41
3:H:192:PRO:HG2	3:H:195:MET:HB2	2.02	0.41
1:L:131:LEU:HD22	1:L:156:TRP:HH2	1.86	0.40
3:H:99:ALA:HA	3:H:100:PRO:HD3	1.93	0.40
5:L:2:BCL:H142	5:M:4:BCL:HMB1	2.02	0.40
7:M:303:U10:H222	7:M:303:U10:H201	1.93	0.40
3:H:121:PRO:HB3	3:H:225:VAL:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	L	264/266 (99%)	236 (89%)	21 (8%)	7 (3%)	6 32
2	M	294/296 (99%)	245 (83%)	32 (11%)	17 (6%)	2 12
3	H	235/237 (99%)	173 (74%)	37 (16%)	25 (11%)	0 3
All	All	793/799 (99%)	654 (82%)	90 (11%)	49 (6%)	2 10

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	115	TYR
1	L	269	LEU
2	M	21	THR
2	M	24	VAL
2	M	34	PRO
2	M	96	PRO
2	M	99	PRO
2	M	105	PHE
2	M	111	GLU
2	M	144	LYS
2	M	234	GLU
2	M	244	ALA
3	H	13	ALA
3	H	70	ARG
3	H	128	HIS
3	H	138	ALA
3	H	142	VAL
3	H	185	ASP
3	H	210	SER
1	L	71	LEU
2	M	100	GLU
3	H	129	ASN
3	H	207	ALA
1	L	31	VAL
1	L	78	ALA
1	L	145	ALA
2	M	104	SER
2	M	195	ASN
3	H	68	HIS
3	H	194	GLN
3	H	242	MET
3	H	247	LYS
1	L	12	PRO
2	M	80	TRP
2	M	110	LYS
3	H	50	ALA
3	H	91	ALA
3	H	203	VAL
2	M	97	PRO
3	H	40	TYR
3	H	57	PRO
3	H	200	SER

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Mol	Chain	Res	Type
3	H	201	ASN
3	H	245	ALA
2	M	98	ALA
3	H	43	GLU
3	H	154	ARG
3	H	209	SER
3	H	76	PRO

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	210/210 (100%)	185 (88%)	25 (12%)	6 26
2	M	232/232 (100%)	203 (88%)	29 (12%)	6 24
3	H	192/192 (100%)	144 (75%)	48 (25%)	1 3
All	All	634/634 (100%)	532 (84%)	102 (16%)	3 14

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	20	ASN
1	L	21	LEU
1	L	54	VAL
1	L	64	ILE
1	L	82	LYS
1	L	85	LEU
1	L	109	ARG
1	L	132	VAL
1	L	136	PRO
1	L	138	MET
1	L	158	SER
1	L	159	ASN
1	L	185	LEU
1	L	193	LEU
1	L	195	LEU

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Mol	Chain	Res	Type
1	L	202	LYS
1	L	204	LYS
1	L	208	THR
1	L	216	PHE
1	L	220	VAL
1	L	229	ILE
1	L	235	LEU
1	L	253	THR
1	L	264	GLN
1	L	269	LEU
2	M	13	ARG
2	M	18	LEU
2	M	21	THR
2	M	23	ASP
2	M	24	VAL
2	M	29	ARG
2	M	34	PRO
2	M	35	PHE
2	M	58	LEU
2	M	74	PHE
2	M	80	TRP
2	M	96	PRO
2	M	97	PRO
2	M	99	PRO
2	M	101	TYR
2	M	122	MET
2	M	130	TRP
2	M	138	GLN
2	M	148	TRP
2	M	156	LEU
2	M	182	HIS
2	M	216	PHE
2	M	226	VAL
2	M	240	ASP
2	M	243	THR
2	M	258	PHE
2	M	259	ASN
2	M	263	GLU
2	M	271	TRP
3	H	34	GLU
3	H	35	ASN
3	H	40	TYR

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Mol	Chain	Res	Type
3	H	48	THR
3	H	56	PHE
3	H	58	LEU
3	H	60	LYS
3	H	61	PRO
3	H	70	ARG
3	H	72	THR
3	H	73	LEU
3	H	75	VAL
3	H	78	PRO
3	H	83	ARG
3	H	89	ARG
3	H	94	GLU
3	H	96	PHE
3	H	97	PRO
3	H	98	HIS
3	H	105	MET
3	H	106	LYS
3	H	109	VAL
3	H	118	ARG
3	H	120	LEU
3	H	128	HIS
3	H	130	LYS
3	H	146	LYS
3	H	153	VAL
3	H	157	ASP
3	H	158	LEU
3	H	163	LYS
3	H	175	MET
3	H	188	THR
3	H	189	ARG
3	H	193	MET
3	H	194	GLN
3	H	195	MET
3	H	196	VAL
3	H	211	ASP
3	H	212	LEU
3	H	213	PHE
3	H	217	PRO
3	H	218	THR
3	H	225	VAL
3	H	226	THR

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Mol	Chain	Res	Type
3	H	227	LEU
3	H	246	PRO
3	H	247	LYS

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

Mol	Chain	Res	Type
1	L	211	HIS
2	M	193	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	$\#\|Z\| > 2$
5	BCL	L	2	1	53,74,74	1.06	5 (9%)	57,115,115	1.43	10 (17%)
6	BPH	L	271	-	64,70,70	1.14	7 (10%)	73,101,101	1.78	16 (21%)
7	U10	L	272	-	41,41,63	1.85	10 (24%)	49,52,79	2.32	15 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	BCL	M	1	2	38,59,74	1.25	6 (15%)	40,97,115	1.98	5 (12%)
5	BCL	M	3	2	53,74,74	1.03	5 (9%)	57,115,115	1.59	12 (21%)
7	U10	M	303	-	51,51,63	1.74	15 (29%)	61,64,79	2.05	22 (36%)
8	CRT	M	304	-	40,41,43	4.04	24 (60%)	44,50,54	2.62	18 (40%)
5	BCL	M	4	1	38,59,74	1.28	5 (13%)	40,97,115	1.80	8 (20%)
6	BPH	M	5	-	64,70,70	1.20	7 (10%)	73,101,101	1.85	13 (17%)

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
5	BCL	L	2	1	-	0/37/137/137	0/0/9/9
6	BPH	L	271	-	1/1/18/22	0/54/105/105	0/1/6/6
7	U10	L	272	-	-	0/37/61/87	0/1/1/1
5	BCL	M	1	2	-	0/19/119/137	0/0/9/9
5	BCL	M	3	2	2/2/21/25	0/37/137/137	0/0/9/9
7	U10	M	303	-	-	0/49/73/87	0/1/1/1
8	CRT	M	304	-	-	1/47/47/51	0/0/0/0
5	BCL	M	4	1	-	0/19/119/137	0/0/9/9
6	BPH	M	5	-	-	2/54/105/105	0/1/6/6

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	304	CRT	C37-C38	-5.11	1.37	1.54
7	L	272	U10	C7-C8	-3.95	1.44	1.50
6	M	5	BPH	C3D-CAD	-3.90	1.38	1.46
7	M	303	U10	C3-C2	-3.90	1.37	1.48
8	M	304	CRT	C30-C28	-3.87	1.37	1.45
6	L	271	BPH	C3D-CAD	-3.71	1.39	1.46
8	M	304	CRT	C6-C7	-3.66	1.37	1.45
5	L	2	BCL	O2D-CGD	-3.65	1.23	1.33
5	M	4	BCL	O2D-CGD	-3.64	1.23	1.33
8	M	304	CRT	C25-C23	-3.47	1.38	1.45
6	L	271	BPH	O2D-CGD	-3.45	1.24	1.33
5	M	1	BCL	O2D-CGD	-3.43	1.24	1.33
6	M	5	BPH	O2D-CGD	-3.41	1.24	1.33
5	M	1	BCL	C3B-CAB	-3.39	1.39	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	304	CRT	C11-C12	-3.36	1.38	1.45
6	M	5	BPH	O2A-CGA	-3.33	1.23	1.33
5	M	1	BCL	O2A-CGA	-3.28	1.23	1.33
6	L	271	BPH	C1B-C2B	-3.23	1.38	1.45
5	M	3	BCL	O2A-CGA	-3.19	1.23	1.33
7	M	303	U10	C4-C5	-3.18	1.39	1.48
5	M	3	BCL	O2D-CGD	-3.18	1.25	1.33
6	L	271	BPH	O2A-CGA	-3.17	1.23	1.33
6	M	5	BPH	C1B-C2B	-3.15	1.38	1.45
8	M	304	CRT	C16-C17	-3.08	1.39	1.45
5	M	4	BCL	O2A-CGA	-3.08	1.24	1.33
5	M	3	BCL	C3B-CAB	-2.98	1.40	1.49
5	L	2	BCL	C3B-CAB	-2.82	1.41	1.49
5	L	2	BCL	O2A-CGA	-2.79	1.24	1.33
7	M	303	U10	C22-C23	-2.78	1.42	1.50
7	L	272	U10	C3-C2	-2.75	1.41	1.48
5	M	4	BCL	C3D-CAD	-2.68	1.38	1.45
5	M	4	BCL	C3B-CAB	-2.48	1.42	1.49
7	M	303	U10	O4-C4M	-2.47	1.39	1.45
6	L	271	BPH	C3B-CAB	-2.43	1.39	1.46
5	M	3	BCL	C3D-CAD	-2.41	1.39	1.45
5	L	2	BCL	C3D-CAD	-2.36	1.39	1.45
5	M	1	BCL	C3A-C2A	-2.21	1.47	1.54
5	M	1	BCL	C3D-CAD	-2.20	1.39	1.45
6	M	5	BPH	C3A-C2A	-2.17	1.48	1.54
6	L	271	BPH	C3A-C2A	-2.15	1.48	1.54
7	L	272	U10	C4-C5	-2.13	1.42	1.48
6	M	5	BPH	C3B-CAB	-2.12	1.40	1.46
7	M	303	U10	C12-C13	-2.11	1.44	1.50
8	M	304	CRT	C19-C17	2.05	1.38	1.35
7	M	303	U10	C7-C6	2.07	1.55	1.51
5	M	4	BCL	C2-C3	2.08	1.38	1.32
5	M	1	BCL	C2-C3	2.08	1.38	1.32
8	M	304	CRT	C8-C7	2.12	1.55	1.50
7	L	272	U10	C6-C1	2.29	1.40	1.35
7	M	303	U10	C23-C24	2.37	1.37	1.33
7	M	303	U10	C6-C1	2.45	1.41	1.35
7	M	303	U10	C13-C14	2.48	1.37	1.33
7	M	303	U10	C44-C43	2.53	1.46	1.28
6	M	5	BPH	C2-C3	2.53	1.37	1.33
7	L	272	U10	C34-C33	2.65	1.47	1.28
8	M	304	CRT	C9-C7	2.66	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	3	BCL	C2-C3	2.81	1.38	1.33
8	M	304	CRT	C15-C14	2.86	1.52	1.43
7	M	303	U10	C18-C19	2.88	1.38	1.33
7	M	303	U10	C8-C9	2.88	1.38	1.33
8	M	304	CRT	C21-C22	2.89	1.52	1.43
5	L	2	BCL	C2-C3	2.90	1.38	1.33
8	M	304	CRT	C26-C27	3.02	1.53	1.43
6	L	271	BPH	C2-C3	3.02	1.38	1.33
7	M	303	U10	C28-C29	3.19	1.39	1.33
7	M	303	U10	C33-C34	3.21	1.39	1.33
7	L	272	U10	C23-C24	3.22	1.39	1.33
7	L	272	U10	C8-C9	3.24	1.39	1.33
7	L	272	U10	C28-C29	3.24	1.39	1.33
8	M	304	CRT	C10-C9	3.25	1.53	1.43
8	M	304	CRT	C20-C19	3.32	1.54	1.43
7	L	272	U10	C13-C14	3.66	1.40	1.33
7	M	303	U10	C38-C39	3.68	1.40	1.33
8	M	304	CRT	C35-C33	3.84	1.54	1.45
8	M	304	CRT	C31-C32	3.90	1.55	1.43
8	M	304	CRT	C4-C5	3.91	1.55	1.50
7	L	272	U10	C18-C19	3.96	1.40	1.33
8	M	304	CRT	C21-C20	6.57	1.53	1.35
8	M	304	CRT	C31-C30	7.32	1.53	1.34
8	M	304	CRT	C10-C11	7.75	1.54	1.34
8	M	304	CRT	C15-C16	7.95	1.55	1.34
8	M	304	CRT	C35-C36	7.98	1.54	1.31
8	M	304	CRT	C6-C5	8.19	1.54	1.31
8	M	304	CRT	C26-C25	8.42	1.56	1.34

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	1	BCL	O1D-CGD-CBD	-6.01	116.01	124.62
8	M	304	CRT	C36-C35-C33	-5.87	116.79	125.75
6	M	5	BPH	C4D-C3D-C2D	-5.60	99.85	107.08
6	L	271	BPH	C4D-C3D-C2D	-5.16	100.42	107.08
8	M	304	CRT	C13-C12-C14	-5.13	115.32	122.90
8	M	304	CRT	C37-C36-C35	-5.10	113.97	125.67
6	L	271	BPH	O1D-CGD-CBD	-5.06	117.37	124.62
8	M	304	CRT	C10-C9-C7	-4.93	120.08	127.20
6	M	5	BPH	O1D-CGD-CBD	-4.90	117.59	124.62
7	M	303	U10	C25-C24-C23	-4.55	114.57	123.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	M	304	CRT	C34-C33-C35	-4.43	110.73	118.10
8	M	304	CRT	C24-C23-C22	-4.39	116.42	122.90
8	M	304	CRT	C20-C19-C17	-4.27	121.02	127.20
7	L	272	U10	C7-C8-C9	-4.24	119.51	126.70
7	M	303	U10	C10-C9-C8	-4.12	115.42	123.50
7	M	303	U10	C21-C22-C23	-3.97	101.30	111.69
5	M	4	BCL	CMB-C2B-C1B	-3.88	121.94	128.36
8	M	304	CRT	C10-C11-C12	-3.75	115.28	126.32
7	L	272	U10	C10-C9-C8	-3.65	116.33	123.50
6	L	271	BPH	CBB-CAB-C3B	-3.64	112.44	120.52
5	M	3	BCL	OBD-CAD-CBD	-3.39	120.83	125.94
6	M	5	BPH	OBD-CAD-C3D	-3.32	121.58	128.35
5	M	3	BCL	O1D-CGD-CBD	-3.29	119.91	124.62
7	M	303	U10	C35-C34-C33	-3.29	117.05	123.50
7	M	303	U10	C15-C14-C13	-3.24	117.15	123.50
7	M	303	U10	C30-C29-C28	-3.20	117.22	123.50
7	L	272	U10	C25-C24-C23	-3.10	117.41	123.50
5	M	4	BCL	C1-C2-C3	-3.05	121.70	126.71
7	L	272	U10	C15-C14-C13	-3.04	117.53	123.50
7	M	303	U10	C40-C39-C38	-2.97	117.66	123.50
7	L	272	U10	C30-C29-C28	-2.94	117.73	123.50
7	L	272	U10	C1M-C1-C6	-2.88	117.94	124.10
7	M	303	U10	C1-C6-C5	-2.83	116.89	120.12
5	M	3	BCL	CMB-C2B-C1B	-2.79	123.75	128.36
6	M	5	BPH	CBB-CAB-C3B	-2.79	114.32	120.52
8	M	304	CRT	C30-C28-C27	-2.78	114.51	118.98
7	M	303	U10	C20-C19-C18	-2.76	118.08	123.50
5	L	2	BCL	CAC-C3C-C4C	-2.74	106.50	112.58
8	M	304	CRT	C18-C17-C19	-2.63	119.02	122.90
5	L	2	BCL	CMB-C2B-C1B	-2.62	124.03	128.36
8	M	304	CRT	C26-C25-C23	-2.59	118.70	126.32
5	M	4	BCL	OBD-CAD-C3D	-2.58	123.09	128.35
5	L	2	BCL	OBD-CAD-C3D	-2.58	123.09	128.35
5	L	2	BCL	CBA-CAA-C2A	-2.53	106.58	113.73
7	M	303	U10	C1M-C1-C6	-2.52	118.70	124.10
7	M	303	U10	C27-C28-C29	-2.48	122.37	127.76
6	L	271	BPH	OBD-CAD-C3D	-2.46	123.34	128.35
5	M	4	BCL	CAA-C2A-C3A	-2.42	106.26	113.22
8	M	304	CRT	C26-C27-C28	-2.38	123.76	127.20
7	L	272	U10	C20-C19-C18	-2.38	118.84	123.50
6	L	271	BPH	CAC-C3C-C4C	-2.36	106.61	112.67
5	L	2	BCL	C7-C6-C5	-2.36	106.10	113.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L	271	BPH	C7-C6-C5	-2.28	106.33	113.06
5	M	3	BCL	C4-C3-C2	-2.27	119.04	123.50
6	M	5	BPH	C1C-NC-C4C	-2.27	108.11	110.44
8	M	304	CRT	C4-C5-C6	-2.26	121.45	124.67
5	M	1	BCL	OBD-CAD-C3D	-2.20	123.86	128.35
7	M	303	U10	C12-C13-C14	-2.20	122.98	127.76
6	L	271	BPH	CMC-C2C-C1C	-2.18	105.71	112.33
5	M	3	BCL	CAA-C2A-C3A	-2.14	107.06	113.22
6	M	5	BPH	CAA-C2A-C3A	-2.09	107.21	113.22
5	M	3	BCL	CGD-CBD-CAD	-2.04	103.70	110.62
5	M	3	BCL	CAC-C3C-C4C	-2.04	108.06	112.58
6	L	271	BPH	C17-C16-C15	-2.01	102.99	112.99
5	M	4	BCL	C5-C3-C4	2.02	119.60	114.64
7	M	303	U10	C37-C36-C34	2.05	119.38	112.71
5	M	3	BCL	CED-O2D-CGD	2.06	120.81	115.99
6	L	271	BPH	CED-O2D-CGD	2.06	120.81	115.99
5	L	2	BCL	O2A-CGA-CBA	2.06	118.17	111.90
8	M	304	CRT	C9-C10-C11	2.06	129.42	123.13
6	M	5	BPH	C3A-C2A-C1A	2.07	104.46	101.84
6	M	5	BPH	C2B-C1B-NB	2.12	112.90	109.73
6	L	271	BPH	C3A-C2A-C1A	2.14	104.56	101.84
7	L	272	U10	C12-C11-C9	2.17	119.79	112.71
7	M	303	U10	C20-C19-C21	2.19	118.75	115.41
5	L	2	BCL	CED-O2D-CGD	2.26	121.28	115.99
7	M	303	U10	C11-C9-C8	2.27	125.36	121.05
5	L	2	BCL	CBC-CAC-C3C	2.34	119.28	113.57
5	M	3	BCL	C4-C3-C5	2.37	119.03	115.41
7	L	272	U10	C20-C19-C21	2.40	119.08	115.41
7	M	303	U10	C10-C9-C11	2.44	119.14	115.41
7	M	303	U10	C41-C39-C38	2.45	125.70	121.05
5	M	4	BCL	CAA-CBA-CGA	2.46	120.52	113.32
5	L	2	BCL	CMB-C2B-C3B	2.52	130.01	125.09
7	L	272	U10	C25-C24-C26	2.65	119.45	115.41
8	M	304	CRT	C11-C12-C14	2.65	123.26	118.98
5	M	3	BCL	CMB-C2B-C3B	2.67	130.31	125.09
6	L	271	BPH	C2B-C1B-NB	2.69	113.76	109.73
6	M	5	BPH	CBA-CAA-C2A	2.71	121.38	113.73
8	M	304	CRT	C25-C23-C22	2.73	123.39	118.98
6	L	271	BPH	C4-C3-C5	2.84	119.75	115.41
7	L	272	U10	C15-C14-C16	3.13	120.18	115.41
7	L	272	U10	C8-C7-C6	3.18	121.18	111.64
5	M	1	BCL	CBA-CAA-C2A	3.32	123.11	113.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	M	304	CRT	C18-C17-C16	3.33	123.64	118.10
7	M	303	U10	C15-C14-C16	3.36	120.54	115.41
6	L	271	BPH	CBA-CAA-C2A	3.37	123.25	113.73
7	L	272	U10	C30-C29-C31	3.44	120.66	115.41
5	M	3	BCL	C3D-CAD-CBD	3.45	112.48	107.60
6	M	5	BPH	C4-C3-C5	3.47	120.71	115.41
7	M	303	U10	C30-C29-C31	3.60	120.91	115.41
5	M	4	BCL	CMB-C2B-C3B	3.64	132.21	125.09
7	L	272	U10	C10-C9-C11	3.69	121.04	115.41
5	M	1	BCL	C3D-CAD-CBD	3.72	112.86	107.60
7	M	303	U10	C35-C34-C36	3.79	121.19	115.41
7	M	303	U10	C25-C24-C26	3.92	121.39	115.41
6	M	5	BPH	C3D-CAD-CBD	3.92	113.14	107.60
5	L	2	BCL	C3D-CAD-CBD	3.94	113.17	107.60
6	L	271	BPH	C3D-CAD-CBD	4.03	113.29	107.60
6	L	271	BPH	C3C-C4C-NC	4.04	111.98	107.93
5	M	4	BCL	C3D-CAD-CBD	4.38	113.79	107.60
7	M	303	U10	C7-C6-C5	4.42	123.76	118.56
6	L	271	BPH	O2D-CGD-CBD	4.46	117.42	111.30
5	M	3	BCL	O2D-CGD-CBD	4.98	118.13	111.30
6	M	5	BPH	C3C-C4C-NC	5.09	113.03	107.93
8	M	304	CRT	C38-C37-C36	5.38	133.15	113.86
6	M	5	BPH	O2D-CGD-CBD	6.34	120.00	111.30
5	M	1	BCL	O2D-CGD-CBD	6.52	120.24	111.30
7	L	272	U10	C7-C6-C5	9.42	129.64	118.56

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	M	3	BCL	C8
5	M	3	BCL	C13
6	L	271	BPH	C8

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	M	5	BPH	C4B-C3B-CAB-CBB
6	M	5	BPH	OBB-CAB-C3B-C4B
8	M	304	CRT	C22-C21-C20-C19

There are no ring outliers.

9 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	2	BCL	16	0
6	L	271	BPH	5	0
7	L	272	U10	3	0
5	M	1	BCL	4	0
5	M	3	BCL	11	0
7	M	303	U10	8	0
8	M	304	CRT	1	0
5	M	4	BCL	4	0
6	M	5	BPH	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.