Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:30 PM GMT

PDB ID	:	1PCR
Title	:	STRUCTURE OF THE PHOTOSYNTHETIC REACTION CENTRE FROM RHODOBACTER SPHAEROIDES AT 2.65 ANGSTROMS RESOLUTION: COFACTORS AND PROTEIN-COFACTOR INTERACTIONS
Authors	:	Ermler, U.; Fritzsch, G.; Michel, H.
Deposited on	:	1994-11-10
Resolution	:	2.65 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:

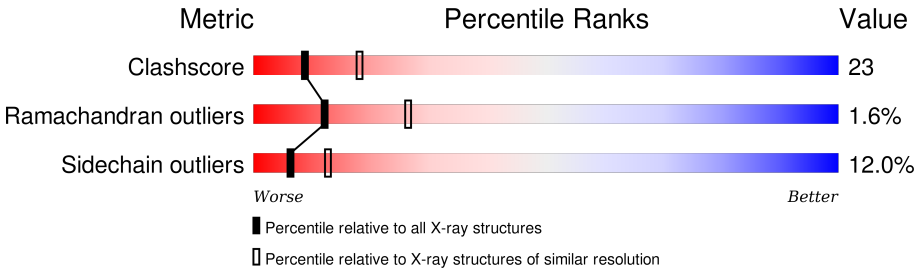
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.65 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	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)

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	281	57% 36% 7%
2	M	307	54% 38% 6%
3	H	260	53% 35% 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
6	BCL	L	301	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	BCL	L	304	X	-	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7311 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	281	Total	C	N	O	S	0	0	0
			2232	1507	355	362	8			

- Molecule 2 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	302	Total	C	N	O	S	0	0	0
			2408	1607	394	397	10			

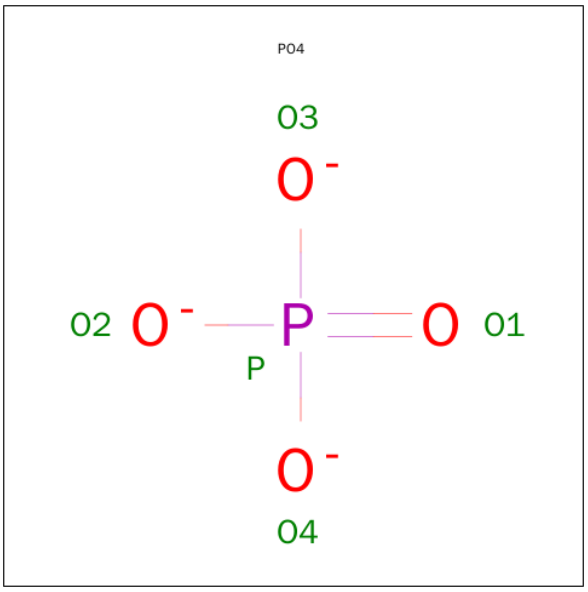
- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	240	Total	C	N	O	S	0	0	0
			1829	1169	314	337	9			

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

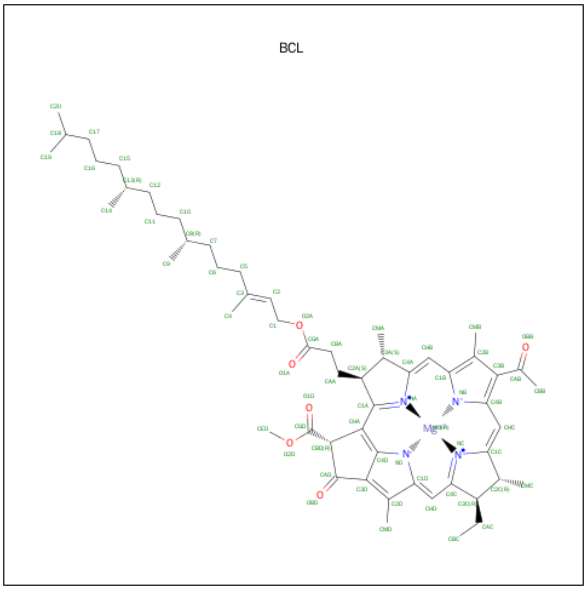
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	1	Total	Fe	0	0
			1	1		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 6 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



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

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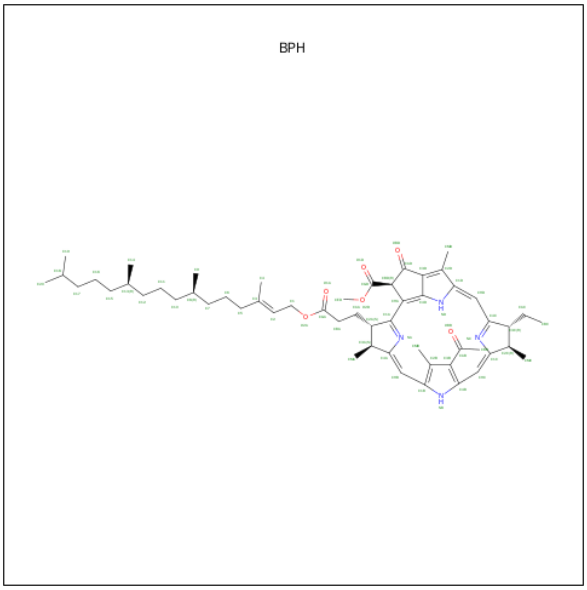
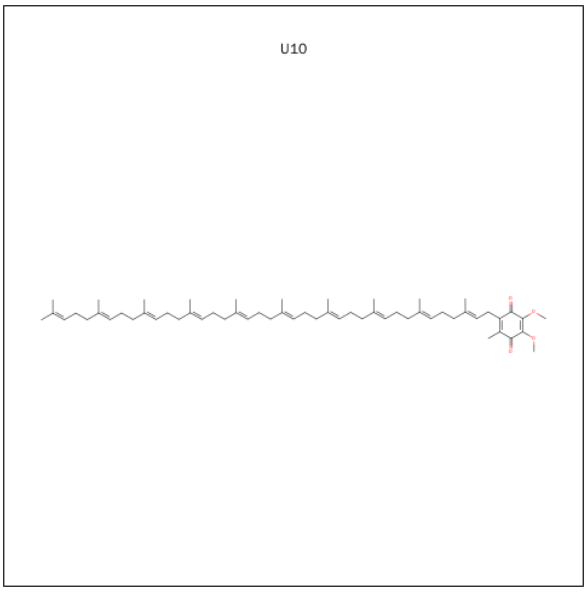
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 7 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



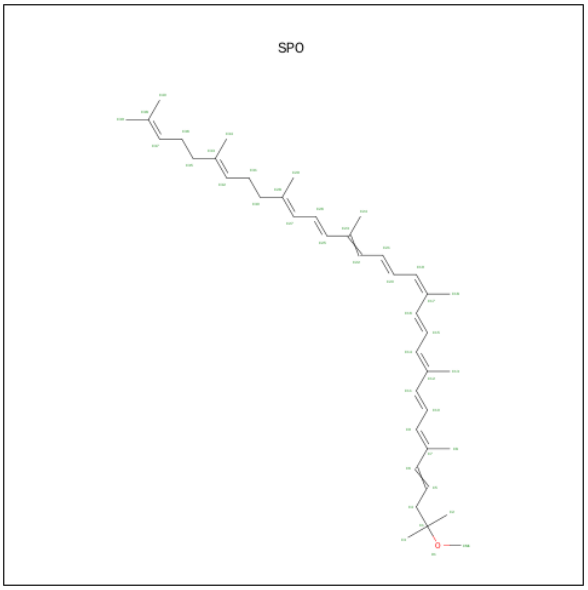
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	M	1	Total	C	N	O	0	0
			65	55	4	6		
7	L	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 8 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



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

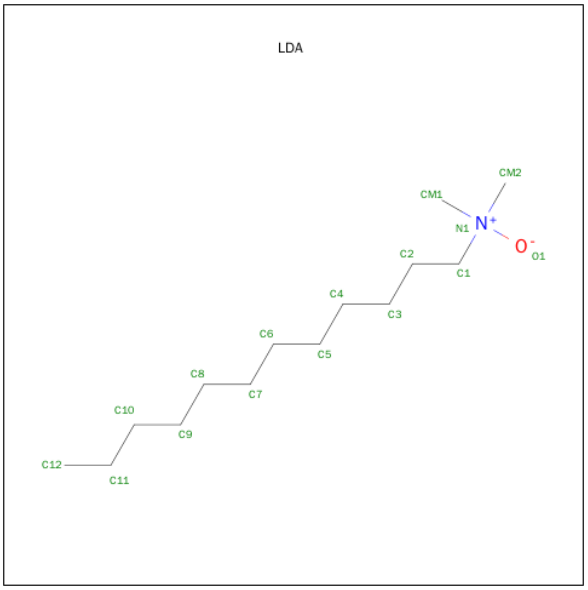
- Molecule 9 is SPHEROIDENE (three-letter code: SPO) (formula: $C_{41}H_{60}O$).



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

- Molecule 10 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:

$C_{14}H_{31}NO$).



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

- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	H	70	Total O 70 70	0	0
11	L	40	Total O 40 40	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	M	50	Total	O	0	0
			50	50		

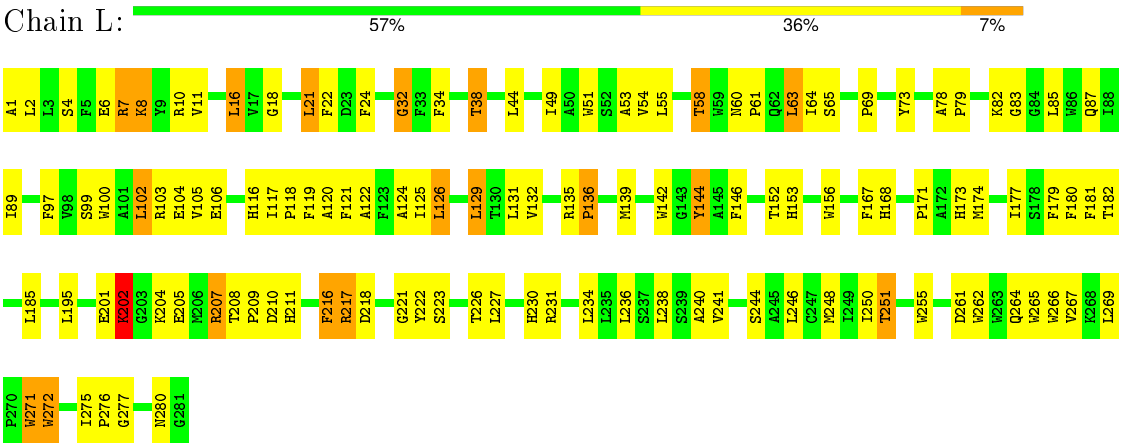
3 Residue-property plots (i)

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.

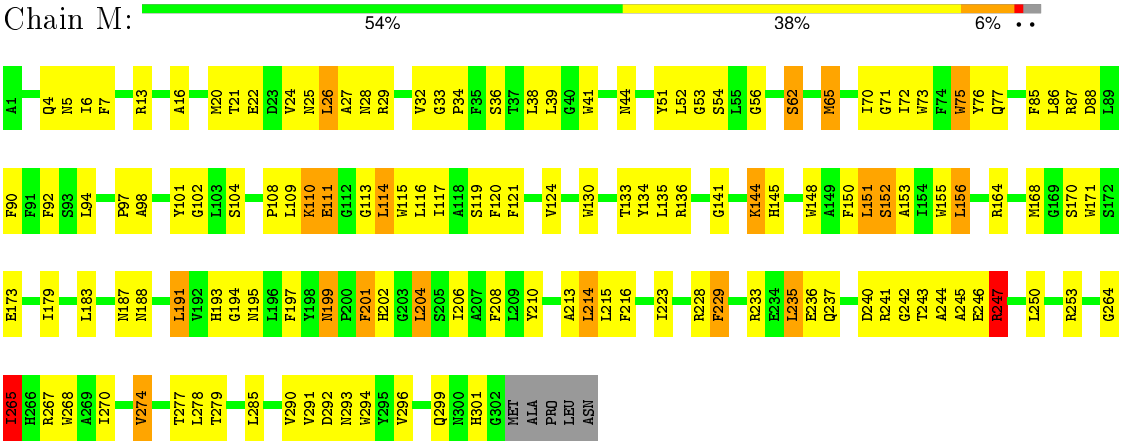
• Molecule 1: PHOTOSYNTHETIC REACTION CENTER

Chain L:



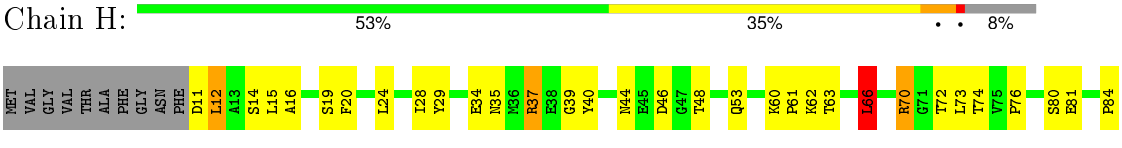
• Molecule 2: PHOTOSYNTHETIC REACTION CENTER

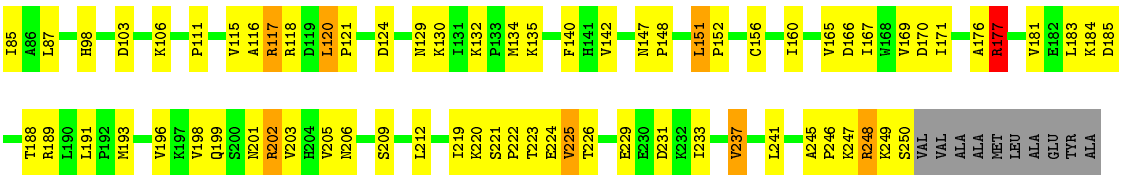
Chain M:



• Molecule 3: PHOTOSYNTHETIC REACTION CENTER

Chain H:




I85
A86
L87
H98
D103
K106
P111
V115
A116
R117
R118
D119
L120
P121
D124
N129
K130
I131
K132
P133
M134
K135
F140
H141
V142
N147
P148
L151
P152
C156
I160
V165
D166
I167
W168
V169
D170
I171
A176
R177
V181
E182
L183
K184
D185
T188
R189
L190
L191
P192
M193
V196
K197
V198
Q199
S200
N201
R202
V203
E204
V205
N206
S209
L212
I219
K220
S221
P222
T223
E224
V225
T226
E229
E230
D231
K232
I233
V237
L241
A245
P246
K247
R248
K249
S250
VAL
VAL
ALA
ALA
MET
LEU
ALA
GLU
TYR
ALA

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 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	141.30Å 141.30Å 187.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.65	Depositor
% Data completeness (in resolution range)	88.9 (10.00-2.65)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.186 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7311	wwPDB-VP
Average B, all atoms (Å^2)	34.0	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, LDA, BPH, PO4, FE, SPO, 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	0.64	0/2320	0.71	0/3175
2	M	0.61	0/2500	0.69	1/3413 (0.0%)
3	H	0.63	0/1877	0.74	0/2553
All	All	0.63	0/6697	0.71	1/9141 (0.0%)

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	6
2	M	0	4
3	H	0	4
All	All	0	14

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	156	LEU	CA-CB-CG	5.59	128.16	115.30

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	177	ARG	Sidechain
3	H	29	TYR	Sidechain
3	H	37	ARG	Sidechain

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Mol	Chain	Res	Type	Group
3	H	66	LEU	Peptide
1	L	103	ARG	Sidechain
1	L	144	TYR	Sidechain
1	L	167	PHE	Sidechain
1	L	216	PHE	Sidechain
1	L	32	GLY	Peptide
1	L	73	TYR	Sidechain
2	M	201	PHE	Sidechain
2	M	247	ARG	Sidechain
2	M	265	ILE	Mainchain
2	M	76	TYR	Sidechain

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	2232	0	2187	105	0
2	M	2408	0	2321	142	0
3	H	1829	0	1836	73	0
4	M	1	0	0	0	0
5	M	5	0	0	0	0
6	L	198	0	222	21	0
6	M	66	0	74	14	0
7	L	65	0	76	12	0
7	M	65	0	76	8	0
8	L	48	0	63	8	0
8	M	48	0	63	8	0
9	M	42	0	60	7	0
10	L	48	0	93	2	0
10	M	96	0	186	25	0
11	H	70	0	0	7	0
11	L	40	0	0	2	0
11	M	50	0	0	3	0
All	All	7311	0	7257	338	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 23.

All (338) 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:M:801:BCL:HBB3	6:M:801:BCL:HHC	1.35	1.09
1:L:272:TRP:HA	1:L:275:ILE:HD13	1.39	1.01
2:M:119:SER:HB2	9:M:600:SPO:H342	1.47	0.93
3:H:44:ASN:HD22	3:H:48:THR:HB	1.36	0.89
1:L:182:THR:HG22	1:L:236:LEU:HD13	1.54	0.88
1:L:32:GLY:HA3	11:L:712:HOH:O	1.74	0.87
8:M:501:U10:H202	10:M:703:LDA:H112	1.58	0.86
3:H:148:PRO:HA	3:H:151:LEU:HD22	1.56	0.86
2:M:204:LEU:HB3	2:M:279:THR:HG21	1.57	0.86
6:L:301:BCL:HHC	6:L:301:BCL:HBB2	1.55	0.85
2:M:242:GLY:HA2	3:H:117:ARG:HD2	1.60	0.83
6:L:302:BCL:HBB2	6:M:801:BCL:NB	1.93	0.82
1:L:34:PHE:O	1:L:38:THR:HG23	1.80	0.80
7:L:402:BPH:HBB3	7:L:402:BPH:HHC	1.64	0.80
2:M:97:PRO:HG2	2:M:171:TRP:HB2	1.62	0.79
11:L:718:HOH:O	2:M:253:ARG:HD3	1.82	0.78
3:H:198:VAL:HA	3:H:203:VAL:HG22	1.64	0.77
6:L:301:BCL:HBB3	6:M:801:BCL:H41	1.67	0.76
1:L:179:PHE:CE1	8:L:502:U10:H18	2.21	0.76
2:M:197:PHE:CZ	6:M:801:BCL:HBB2	2.20	0.76
6:M:801:BCL:HHC	6:M:801:BCL:CBB	2.14	0.76
1:L:7:ARG:HH11	3:H:98:HIS:CD2	2.06	0.74
3:H:61:PRO:HA	3:H:76:PRO:HD2	1.69	0.74
2:M:108:PRO:HG2	2:M:111:GLU:HB2	1.69	0.73
6:L:301:BCL:HHC	6:L:301:BCL:CBB	2.18	0.73
1:L:69:PRO:HG2	1:L:142:TRP:HB2	1.70	0.72
10:M:706:LDA:H71	10:M:706:LDA:HM21	1.71	0.72
1:L:231:ARG:HD3	2:M:5:ASN:O	1.90	0.71
2:M:197:PHE:HZ	6:M:801:BCL:HBB2	1.53	0.71
2:M:72:ILE:HG13	2:M:73:TRP:N	2.05	0.70
2:M:153:ALA:HB2	7:M:401:BPH:HAC1	1.73	0.70
3:H:103:ASP:HB3	3:H:106:LYS:HB2	1.73	0.69
1:L:8:LYS:HA	3:H:87:LEU:HD11	1.73	0.69
3:H:169:VAL:HG23	3:H:171:ILE:HD12	1.73	0.69
10:M:706:LDA:HM21	10:M:706:LDA:H52	1.73	0.69
7:L:402:BPH:HBB2	2:M:210:TYR:HB3	1.75	0.69
2:M:243:THR:O	2:M:247:ARG:HG2	1.92	0.69
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.75	0.67
3:H:156:CYS:SG	3:H:248:ARG:HA	2.34	0.67
2:M:130:TRP:HD1	2:M:150:PHE:CD2	2.12	0.67
2:M:197:PHE:HZ	6:M:801:BCL:CBB	2.07	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:62:SER:HA	2:M:65:MET:HB2	1.77	0.66
6:L:301:BCL:HMD2	6:L:302:BCL:OBB	1.95	0.66
1:L:182:THR:HG22	1:L:236:LEU:CD1	2.26	0.65
1:L:51:TRP:O	1:L:54:VAL:HG22	1.97	0.65
2:M:13:ARG:O	3:H:140:PHE:HA	1.98	0.64
9:M:600:SPO:H5	9:M:600:SPO:HM13	1.79	0.64
1:L:38:THR:HG22	1:L:99:SER:HB3	1.79	0.63
2:M:193:HIS:O	2:M:293:ASN:HA	1.97	0.63
1:L:22:PHE:HA	1:L:24:PHE:CE2	2.34	0.63
3:H:196:VAL:HG12	3:H:205:VAL:HG22	1.81	0.63
1:L:208:THR:HB	1:L:209:PRO:HD2	1.80	0.63
7:L:402:BPH:CBB	2:M:210:TYR:HB3	2.29	0.62
1:L:7:ARG:NH1	3:H:98:HIS:CD2	2.66	0.62
1:L:69:PRO:HB3	1:L:78:ALA:HB2	1.80	0.62
2:M:90:PHE:HD1	2:M:179:ILE:HD13	1.65	0.62
2:M:130:TRP:HD1	2:M:150:PHE:HD2	1.46	0.62
3:H:233:ILE:O	3:H:237:VAL:HG13	1.99	0.62
2:M:102:GLY:HA2	2:M:170:SER:CB	2.30	0.62
1:L:230:HIS:CD2	2:M:223:ILE:HG13	2.35	0.62
1:L:265:TRP:CH2	1:L:266:TRP:HE3	2.18	0.61
1:L:201:GLU:O	1:L:202:LYS:HB2	2.00	0.61
1:L:181:PHE:CD2	7:M:401:BPH:HBB1	2.35	0.61
1:L:269:LEU:HB2	1:L:272:TRP:NE1	2.15	0.61
1:L:168:HIS:HB3	2:M:183:LEU:HD13	1.80	0.61
1:L:244:SER:OG	6:L:302:BCL:HMA2	2.01	0.60
2:M:253:ARG:NH2	10:M:703:LDA:HM12	2.15	0.60
2:M:119:SER:HB3	9:M:600:SPO:H311	1.84	0.60
1:L:135:ARG:NH1	1:L:251:THR:HG22	2.17	0.59
2:M:120:PHE:O	2:M:124:VAL:HG13	2.03	0.59
1:L:38:THR:HG22	1:L:99:SER:CB	2.32	0.59
10:L:708:LDA:H92	10:L:708:LDA:H51	1.85	0.59
3:H:156:CYS:HB3	3:H:206:ASN:O	2.02	0.58
2:M:208:PHE:HE1	10:M:701:LDA:H91	1.68	0.58
2:M:242:GLY:CA	3:H:117:ARG:HD2	2.31	0.58
1:L:202:LYS:C	1:L:204:LYS:H	2.05	0.58
2:M:152:SER:O	2:M:155:TRP:HB3	2.04	0.58
1:L:116:HIS:O	1:L:119:PHE:HB3	2.04	0.58
3:H:129:ASN:ND2	3:H:224:GLU:HG3	2.19	0.58
1:L:8:LYS:HA	3:H:87:LEU:CD1	2.33	0.57
3:H:132:LYS:HB2	3:H:171:ILE:HD11	1.86	0.57
2:M:270:ILE:O	2:M:274:VAL:HB	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:269:LEU:HD12	1:L:272:TRP:CZ2	2.39	0.57
2:M:114:LEU:HD21	10:M:706:LDA:HM13	1.86	0.57
2:M:301:HIS:N	2:M:301:HIS:CD2	2.73	0.57
3:H:70:ARG:NH2	3:H:121:PRO:O	2.37	0.57
1:L:231:ARG:HD2	2:M:6:ILE:O	2.05	0.57
3:H:66:LEU:HD12	3:H:118:ARG:NH2	2.20	0.56
7:M:401:BPH:HBB3	7:M:401:BPH:HHC	1.85	0.56
2:M:90:PHE:CD1	2:M:179:ILE:HD13	2.40	0.56
1:L:180:PHE:CE2	1:L:240:ALA:HB1	2.40	0.56
1:L:241:VAL:HG21	7:L:402:BPH:HAC2	1.87	0.56
10:M:706:LDA:H72	10:M:706:LDA:HM11	1.87	0.56
6:L:301:BCL:H51	7:M:401:BPH:HMB2	1.88	0.56
3:H:202:ARG:HG2	3:H:203:VAL:N	2.19	0.56
2:M:164:ARG:NH1	2:M:173:GLU:HG3	2.20	0.56
1:L:85:LEU:O	1:L:89:ILE:HG13	2.06	0.56
2:M:130:TRP:CD1	2:M:150:PHE:HD2	2.23	0.55
3:H:66:LEU:N	3:H:66:LEU:HD23	2.21	0.55
10:M:703:LDA:HM12	3:H:40:TYR:OH	2.06	0.55
2:M:24:VAL:HG11	2:M:29:ARG:NH1	2.21	0.55
8:M:501:U10:H202	10:M:703:LDA:C11	2.33	0.54
2:M:65:MET:HB3	2:M:121:PHE:CD2	2.42	0.54
7:L:402:BPH:HMC3	2:M:213:ALA:HB3	1.90	0.54
1:L:181:PHE:HB3	7:M:401:BPH:CBB	2.38	0.54
6:L:301:BCL:H72	6:M:801:BCL:H203	1.89	0.54
3:H:118:ARG:HD2	11:H:311:HOH:O	2.07	0.54
3:H:148:PRO:HA	3:H:151:LEU:CD2	2.34	0.53
10:M:706:LDA:H12	10:M:706:LDA:H52	1.90	0.53
3:H:11:ASP:HB2	11:H:323:HOH:O	2.08	0.53
2:M:24:VAL:HG21	2:M:29:ARG:HH12	1.74	0.53
6:L:302:BCL:H203	6:L:304:BCL:H102	1.91	0.53
7:L:402:BPH:HBB3	7:L:402:BPH:CHC	2.36	0.53
2:M:85:PHE:HD2	2:M:86:LEU:HD12	1.74	0.53
1:L:269:LEU:HD12	1:L:272:TRP:HZ2	1.74	0.52
1:L:250:ILE:HD12	8:L:502:U10:H402	1.91	0.52
1:L:4:SER:OG	3:H:39:GLY:HA2	2.09	0.52
3:H:20:PHE:HE2	3:H:24:LEU:HD22	1.74	0.52
2:M:102:GLY:HA2	2:M:170:SER:HB2	1.91	0.52
10:M:701:LDA:H101	10:M:703:LDA:C12	2.39	0.52
3:H:226:THR:OG1	3:H:229:GLU:HG3	2.09	0.52
6:L:301:BCL:H72	6:M:801:BCL:C20	2.40	0.52
2:M:108:PRO:HG2	2:M:111:GLU:CB	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:148:TRP:HA	2:M:148:TRP:CE3	2.44	0.52
1:L:195:LEU:HB3	2:M:145:HIS:CD2	2.45	0.52
2:M:32:VAL:HG12	2:M:33:GLY:O	2.10	0.52
1:L:201:GLU:HG3	2:M:141:GLY:C	2.30	0.52
1:L:202:LYS:C	1:L:204:LYS:N	2.63	0.52
3:H:245:ALA:N	3:H:246:PRO:HD2	2.25	0.52
8:L:502:U10:H122	10:M:702:LDA:H92	1.92	0.52
6:L:301:BCL:HBB3	6:M:801:BCL:C4	2.38	0.51
2:M:152:SER:HB2	2:M:274:VAL:HG22	1.91	0.51
2:M:77:GLN:NE2	2:M:92:PHE:CD1	2.77	0.51
1:L:267:VAL:HG23	2:M:87:ARG:HG2	1.92	0.51
2:M:21:THR:HG23	2:M:26:LEU:CD1	2.40	0.51
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.45	0.51
2:M:25:ASN:OD1	2:M:27:ALA:HB3	2.10	0.51
2:M:41:TRP:CB	10:M:702:LDA:HM21	2.39	0.51
1:L:271:TRP:CD1	1:L:271:TRP:N	2.79	0.51
2:M:202:HIS:CE1	2:M:206:ILE:HD11	2.46	0.51
2:M:134:TYR:CE2	2:M:144:LYS:HG2	2.46	0.51
3:H:63:THR:HA	3:H:73:LEU:O	2.10	0.51
2:M:119:SER:CB	9:M:600:SPO:H342	2.31	0.50
1:L:135:ARG:NH1	1:L:251:THR:O	2.45	0.50
2:M:237:GLN:HE22	2:M:242:GLY:HA3	1.77	0.50
2:M:199:ASN:HD22	2:M:199:ASN:C	2.15	0.50
7:L:402:BPH:HMC3	2:M:213:ALA:CB	2.42	0.50
2:M:241:ARG:HD3	2:M:246:GLU:HG2	1.94	0.49
2:M:301:HIS:H	2:M:301:HIS:CD2	2.30	0.49
2:M:236:GLU:HB3	11:H:270:HOH:O	2.11	0.49
1:L:16:LEU:N	1:L:106:GLU:OE2	2.44	0.49
2:M:247:ARG:NH2	3:H:111:PRO:O	2.46	0.49
2:M:197:PHE:CZ	6:M:801:BCL:CBB	2.89	0.49
2:M:75:TRP:HZ3	9:M:600:SPO:O1	1.95	0.49
6:L:302:BCL:HAA2	6:L:304:BCL:HAC1	1.93	0.49
2:M:113:GLY:HA2	2:M:116:LEU:HD23	1.95	0.49
2:M:253:ARG:HH22	10:M:703:LDA:HM12	1.78	0.49
2:M:77:GLN:HE22	2:M:92:PHE:HA	1.76	0.49
1:L:280:ASN:HD22	2:M:88:ASP:CG	2.16	0.49
1:L:264:GLN:O	1:L:267:VAL:HG12	2.13	0.49
1:L:102:LEU:O	1:L:105:VAL:HB	2.13	0.48
3:H:44:ASN:HB2	3:H:46:ASP:OD1	2.12	0.48
2:M:88:ASP:HB2	2:M:92:PHE:CZ	2.48	0.48
1:L:227:LEU:O	1:L:231:ARG:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:135:ARG:HB3	1:L:136:PRO:CD	2.41	0.48
3:H:170:ASP:OD2	3:H:177:ARG:NH1	2.46	0.48
1:L:234:LEU:O	1:L:238:LEU:HG	2.13	0.48
1:L:201:GLU:O	1:L:202:LYS:CB	2.62	0.48
8:M:501:U10:H322	8:M:501:U10:H28	1.64	0.48
2:M:164:ARG:NH1	2:M:173:GLU:CG	2.77	0.48
2:M:241:ARG:HD3	2:M:246:GLU:CG	2.43	0.48
2:M:264:GLY:HA3	3:H:35:ASN:OD1	2.14	0.48
2:M:278:LEU:HD13	10:M:705:LDA:H102	1.96	0.48
2:M:21:THR:HG23	2:M:26:LEU:HD11	1.95	0.48
8:L:502:U10:H122	10:M:702:LDA:C9	2.44	0.48
3:H:206:ASN:O	3:H:248:ARG:NH1	2.47	0.48
1:L:277:GLY:O	2:M:87:ARG:NH2	2.47	0.47
3:H:20:PHE:CE2	3:H:24:LEU:HD22	2.48	0.47
6:L:302:BCL:HBB2	6:M:801:BCL:C1B	2.43	0.47
7:L:402:BPH:H6C2	7:L:402:BPH:H2	1.66	0.47
3:H:199:GLN:OE1	3:H:202:ARG:HD2	2.14	0.47
3:H:177:ARG:O	3:H:193:MET:HB2	2.14	0.47
1:L:171:PRO:HA	1:L:174:MET:HG3	1.96	0.47
1:L:87:GLN:NE2	1:L:142:TRP:CD1	2.82	0.47
2:M:21:THR:HG22	2:M:21:THR:O	2.13	0.47
1:L:65:SER:CB	1:L:152:THR:HG21	2.44	0.47
7:L:402:BPH:CMC	2:M:213:ALA:HB3	2.45	0.47
6:L:304:BCL:HMD1	2:M:206:ILE:HD13	1.96	0.47
2:M:75:TRP:CZ3	9:M:600:SPO:O1	2.67	0.47
2:M:268:TRP:CD1	8:M:501:U10:H111	2.50	0.47
10:M:701:LDA:H101	10:M:703:LDA:H121	1.97	0.47
3:H:117:ARG:HA	11:H:290:HOH:O	2.13	0.47
1:L:6:GLU:OE2	1:L:10:ARG:NH1	2.44	0.47
2:M:20:MET:O	2:M:29:ARG:NH2	2.48	0.47
2:M:265:ILE:HG21	8:M:501:U10:H3M3	1.97	0.46
2:M:187:ASN:HA	6:M:801:BCL:CBC	2.45	0.46
3:H:70:ARG:NH2	3:H:120:LEU:CB	2.79	0.46
1:L:146:PHE:HA	1:L:156:TRP:CD1	2.50	0.46
2:M:44:ASN:HB3	11:M:812:HOH:O	2.14	0.46
1:L:58:THR:HG21	1:L:63:LEU:HD23	1.97	0.46
3:H:183:LEU:HD11	3:H:189:ARG:HG2	1.98	0.46
2:M:70:ILE:O	2:M:73:TRP:HB3	2.15	0.46
2:M:242:GLY:HA2	3:H:117:ARG:CD	2.38	0.46
2:M:267:ARG:HD2	3:H:34:GLU:HG2	1.98	0.46
1:L:60:ASN:HA	1:L:61:PRO:HD3	1.75	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:53:ALA:HB2	1:L:64:ILE:HD13	1.97	0.46
3:H:148:PRO:HG2	3:H:167:ILE:HD11	1.98	0.46
1:L:124:ALA:HB2	7:L:402:BPH:HAC1	1.97	0.46
3:H:241:LEU:O	3:H:248:ARG:NH2	2.49	0.46
1:L:22:PHE:HA	1:L:24:PHE:HE2	1.80	0.46
2:M:199:ASN:HD22	2:M:201:PHE:H	1.62	0.46
3:H:142:VAL:HG21	3:H:147:ASN:ND2	2.31	0.46
3:H:16:ALA:O	3:H:19:SER:HB2	2.16	0.46
2:M:194:GLY:O	2:M:195:ASN:HB3	2.14	0.46
2:M:130:TRP:NE1	2:M:151:LEU:HD22	2.30	0.46
1:L:177:ILE:HG23	6:L:302:BCL:HMB3	1.98	0.45
7:L:402:BPH:HMC2	2:M:214:LEU:N	2.30	0.45
1:L:11:VAL:HB	11:H:286:HOH:O	2.16	0.45
2:M:114:LEU:HD23	2:M:117:ILE:HD12	1.97	0.45
2:M:240:ASP:O	3:H:117:ARG:NH1	2.50	0.45
2:M:29:ARG:HA	2:M:51:TYR:HA	1.98	0.45
3:H:219:ILE:HG21	3:H:225:VAL:HG13	1.99	0.45
1:L:100:TRP:CH2	8:M:501:U10:H251	2.52	0.45
8:L:502:U10:H372	8:L:502:U10:H351	1.70	0.45
1:L:79:PRO:HD2	1:L:82:LYS:HB2	1.97	0.45
1:L:222:TYR:CG	1:L:223:SER:N	2.84	0.45
1:L:8:LYS:NZ	3:H:81:GLU:OE1	2.47	0.45
1:L:217:ARG:O	1:L:221:GLY:HA2	2.17	0.45
7:M:401:BPH:HBB3	7:M:401:BPH:CHC	2.47	0.45
1:L:135:ARG:HH12	1:L:251:THR:HG22	1.80	0.45
2:M:24:VAL:HG13	2:M:51:TYR:CD2	2.51	0.45
7:L:402:BPH:HBB1	2:M:210:TYR:CD2	2.52	0.45
2:M:4:GLN:HB3	2:M:6:ILE:CD1	2.47	0.45
1:L:129:LEU:HD12	1:L:129:LEU:HA	1.67	0.45
3:H:241:LEU:HA	3:H:248:ARG:NH2	2.33	0.44
1:L:218:ASP:OD1	2:M:29:ARG:HD3	2.17	0.44
3:H:62:LYS:O	3:H:74:THR:HA	2.17	0.44
1:L:2:LEU:N	1:L:2:LEU:HD23	2.32	0.44
2:M:151:LEU:HA	2:M:151:LEU:HD13	1.65	0.44
1:L:54:VAL:HG23	1:L:55:LEU:N	2.33	0.44
2:M:152:SER:CB	2:M:274:VAL:HG22	2.47	0.44
2:M:24:VAL:HG11	2:M:29:ARG:CZ	2.47	0.44
3:H:70:ARG:NH2	3:H:120:LEU:HB2	2.32	0.44
8:L:502:U10:H271	8:L:502:U10:H251	1.79	0.44
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.99	0.44
2:M:41:TRP:CD1	10:M:702:LDA:HM11	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:49:ILE:CG1	1:L:89:ILE:HD13	2.48	0.44
2:M:228:ARG:HG3	2:M:229:PHE:CE1	2.53	0.44
2:M:98:ALA:HB3	2:M:101:TYR:CE1	2.52	0.44
3:H:181:VAL:O	3:H:188:THR:HA	2.17	0.44
2:M:148:TRP:HB3	10:M:705:LDA:H61	2.00	0.44
2:M:53:GLY:O	2:M:56:GLY:N	2.51	0.44
2:M:41:TRP:CE3	2:M:41:TRP:HA	2.53	0.43
3:H:209:SER:OG	3:H:212:LEU:HD12	2.17	0.43
2:M:135:LEU:HD23	2:M:135:LEU:HA	1.83	0.43
2:M:134:TYR:CD1	2:M:134:TYR:C	2.91	0.43
1:L:131:LEU:HD21	1:L:248:MET:HG3	2.00	0.43
1:L:122:ALA:O	1:L:126:LEU:HB2	2.18	0.43
3:H:176:ALA:O	3:H:193:MET:HG2	2.18	0.43
3:H:148:PRO:CG	3:H:167:ILE:HD11	2.48	0.43
2:M:4:GLN:HB3	2:M:6:ILE:HD12	1.99	0.43
10:M:705:LDA:H31	10:M:705:LDA:H61	1.83	0.43
1:L:131:LEU:HB2	1:L:146:PHE:HE1	1.83	0.43
2:M:164:ARG:O	2:M:168:MET:HG2	2.18	0.43
2:M:235:LEU:HD12	2:M:235:LEU:HA	1.62	0.43
3:H:130:LYS:HD2	11:H:284:HOH:O	2.18	0.43
2:M:245:ALA:HB1	11:M:807:HOH:O	2.18	0.43
1:L:117:ILE:HB	1:L:118:PRO:HD3	2.01	0.43
3:H:60:LYS:HA	3:H:61:PRO:HD3	1.78	0.43
1:L:261:ASP:O	1:L:264:GLN:HB2	2.19	0.43
1:L:264:GLN:HA	1:L:267:VAL:HG12	2.00	0.43
2:M:94:LEU:HD21	2:M:115:TRP:HA	2.00	0.43
2:M:197:PHE:CE1	6:M:801:BCL:HBB2	2.53	0.43
2:M:130:TRP:CZ2	2:M:151:LEU:HD21	2.53	0.43
2:M:265:ILE:HG21	8:M:501:U10:C3M	2.49	0.42
1:L:223:SER:OG	8:L:502:U10:H3M1	2.19	0.42
1:L:85:LEU:HA	1:L:85:LEU:HD23	1.89	0.42
2:M:130:TRP:HE1	2:M:151:LEU:HD22	1.84	0.42
10:L:707:LDA:H42	10:L:707:LDA:H71	1.88	0.42
2:M:110:LYS:HE3	2:M:110:LYS:HB2	1.69	0.42
3:H:84:PRO:C	3:H:85:ILE:HD13	2.39	0.42
2:M:191:LEU:HD13	2:M:191:LEU:HA	1.59	0.42
3:H:152:PRO:HB2	3:H:160:ILE:HD13	2.00	0.42
1:L:223:SER:O	2:M:44:ASN:HB2	2.20	0.42
3:H:37:ARG:HH21	3:H:61:PRO:HA	1.84	0.42
1:L:121:PHE:CE2	1:L:125:ILE:HD11	2.55	0.42
6:L:302:BCL:H162	6:L:302:BCL:H141	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:41:TRP:HB3	10:M:702:LDA:HM21	2.02	0.42
2:M:16:ALA:HB1	2:M:32:VAL:HG21	2.02	0.42
2:M:134:TYR:CD2	2:M:144:LYS:HG2	2.55	0.42
1:L:132:VAL:HG13	1:L:146:PHE:CE1	2.55	0.42
3:H:248:ARG:CZ	3:H:248:ARG:HB2	2.49	0.42
1:L:265:TRP:CE3	1:L:266:TRP:HA	2.54	0.42
1:L:49:ILE:HG12	1:L:89:ILE:HD13	2.02	0.42
1:L:255:TRP:CZ2	1:L:262:TRP:HB2	2.55	0.42
2:M:71:GLY:HA3	9:M:600:SPO:C6	2.50	0.41
3:H:134:MET:HB2	3:H:167:ILE:O	2.19	0.41
1:L:97:PHE:CE1	6:L:302:BCL:H121	2.55	0.41
10:M:703:LDA:HM11	10:M:703:LDA:H22	1.80	0.41
6:L:301:BCL:CHC	6:L:301:BCL:CBB	2.92	0.41
2:M:7:PHE:CE1	10:M:702:LDA:HM22	2.55	0.41
3:H:98:HIS:HE1	11:H:276:HOH:O	2.03	0.41
2:M:25:ASN:OD1	2:M:25:ASN:C	2.58	0.41
1:L:1:ALA:C	1:L:2:LEU:HD23	2.41	0.41
2:M:36:SER:OG	2:M:38:LEU:HB3	2.20	0.41
3:H:148:PRO:HD2	3:H:167:ILE:HD11	2.02	0.41
2:M:77:GLN:NE2	2:M:92:PHE:HB3	2.35	0.41
1:L:120:ALA:HB1	1:L:238:LEU:HD21	2.01	0.41
2:M:101:TYR:HB3	2:M:104:SER:HB3	2.03	0.41
2:M:265:ILE:HG12	8:M:501:U10:C2	2.51	0.41
3:H:165:VAL:O	3:H:166:ASP:HB2	2.21	0.41
2:M:296:VAL:O	2:M:299:GLN:HB2	2.20	0.41
6:L:304:BCL:H122	6:L:304:BCL:H161	1.80	0.41
3:H:103:ASP:OD2	3:H:106:LYS:HD3	2.21	0.41
1:L:18:GLY:O	1:L:21:LEU:HB2	2.21	0.41
3:H:12:LEU:HD13	3:H:15:LEU:HD23	2.02	0.41
1:L:204:LYS:HE3	1:L:204:LYS:HB2	1.79	0.41
10:M:705:LDA:HM13	11:M:803:HOH:O	2.21	0.41
2:M:291:VAL:HG11	2:M:294:TRP:CD2	2.56	0.41
6:L:304:BCL:H162	6:L:304:BCL:H202	1.85	0.41
1:L:97:PHE:CZ	6:L:302:BCL:H121	2.56	0.41
1:L:69:PRO:HD3	1:L:83:GLY:O	2.21	0.40
1:L:139:MET:HB3	1:L:144:TYR:CD2	2.56	0.40
2:M:208:PHE:CE1	10:M:701:LDA:H91	2.53	0.40
1:L:21:LEU:HD13	1:L:22:PHE:CE1	2.56	0.40
1:L:208:THR:O	1:L:211:HIS:HB2	2.21	0.40
1:L:65:SER:HB2	1:L:152:THR:HG21	2.03	0.40
2:M:98:ALA:HB3	2:M:101:TYR:HE1	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:104:GLU:HB3	1:L:118:PRO:HG3	2.03	0.40
1:L:216:PHE:CE1	8:L:502:U10:H4M2	2.56	0.40
7:M:401:BPH:H6C2	7:M:401:BPH:H102	1.96	0.40
2:M:164:ARG:HH12	2:M:173:GLU:CG	2.34	0.40
1:L:217:ARG:HD3	1:L:217:ARG:HH11	1.76	0.40
2:M:36:SER:HB3	2:M:39:LEU:HB2	2.03	0.40
2:M:277:THR:CG2	7:M:401:BPH:HAC2	2.52	0.40
3:H:84:PRO:O	3:H:85:ILE:HD13	2.21	0.40
3:H:247:LYS:O	3:H:249:LYS:N	2.55	0.40
2:M:28:ASN:HB3	2:M:52:LEU: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	279/281 (99%)	261 (94%)	15 (5%)	3 (1%)	17 38
2	M	300/307 (98%)	278 (93%)	18 (6%)	4 (1%)	15 33
3	H	238/260 (92%)	215 (90%)	17 (7%)	6 (2%)	7 15
All	All	817/848 (96%)	754 (92%)	50 (6%)	13 (2%)	12 26

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	202	LYS
2	M	54	SER
3	H	116	ALA
1	L	207	ARG
3	H	124	ASP
3	H	185	ASP
3	H	248	ARG

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Mol	Chain	Res	Type
2	M	22	GLU
3	H	201	ASN
2	M	290	VAL
1	L	276	PRO
3	H	222	PRO
2	M	34	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	220/220 (100%)	196 (89%)	24 (11%)	8	16
2	M	236/240 (98%)	206 (87%)	30 (13%)	5	11
3	H	195/208 (94%)	171 (88%)	24 (12%)	6	12
All	All	651/668 (98%)	573 (88%)	78 (12%)	6	13

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	7	ARG
1	L	8	LYS
1	L	16	LEU
1	L	21	LEU
1	L	38	THR
1	L	44	LEU
1	L	58	THR
1	L	63	LEU
1	L	102	LEU
1	L	126	LEU
1	L	129	LEU
1	L	136	PRO
1	L	153	HIS
1	L	185	LEU
1	L	202	LYS
1	L	205	GLU

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Mol	Chain	Res	Type
1	L	207	ARG
1	L	210	ASP
1	L	217	ARG
1	L	226	THR
1	L	246	LEU
1	L	251	THR
1	L	271	TRP
1	L	272	TRP
2	M	26	LEU
2	M	62	SER
2	M	65	MET
2	M	75	TRP
2	M	109	LEU
2	M	110	LYS
2	M	111	GLU
2	M	114	LEU
2	M	133	THR
2	M	136	ARG
2	M	144	LYS
2	M	151	LEU
2	M	152	SER
2	M	156	LEU
2	M	188	ASN
2	M	191	LEU
2	M	199	ASN
2	M	204	LEU
2	M	214	LEU
2	M	215	LEU
2	M	216	PHE
2	M	229	PHE
2	M	233	ARG
2	M	235	LEU
2	M	247	ARG
2	M	250	LEU
2	M	265	ILE
2	M	274	VAL
2	M	285	LEU
2	M	292	ASP
3	H	12	LEU
3	H	14	SER
3	H	28	ILE
3	H	53	GLN

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Mol	Chain	Res	Type
3	H	66	LEU
3	H	70	ARG
3	H	72	THR
3	H	80	SER
3	H	115	VAL
3	H	117	ARG
3	H	120	LEU
3	H	135	LYS
3	H	151	LEU
3	H	177	ARG
3	H	184	LYS
3	H	191	LEU
3	H	202	ARG
3	H	220	LYS
3	H	221	SER
3	H	223	THR
3	H	225	VAL
3	H	231	ASP
3	H	237	VAL
3	H	250	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	159	ASN
1	L	183	ASN
1	L	280	ASN
2	M	44	ASN
2	M	77	GLN
2	M	193	HIS
2	M	199	ASN
2	M	301	HIS
3	H	44	ASN
3	H	68	HIS
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 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	BCL	L	301	2	53,74,74	1.25	4 (7%)	57,115,115	1.89	9 (15%)
6	BCL	L	302	1,6	53,74,74	1.37	7 (13%)	57,115,115	1.88	10 (17%)
6	BCL	L	304	1	53,74,74	1.17	5 (9%)	57,115,115	2.62	12 (21%)
7	BPH	L	402	-	64,70,70	1.18	5 (7%)	73,101,101	1.71	8 (10%)
8	U10	L	502	-	48,48,63	2.24	21 (43%)	58,61,79	1.05	4 (6%)
10	LDA	L	707	-	15,15,15	4.40	2 (13%)	16,17,17	0.58	0
10	LDA	L	708	-	15,15,15	4.13	1 (6%)	16,17,17	0.61	0
10	LDA	L	709	-	15,15,15	4.62	2 (13%)	16,17,17	0.59	0
7	BPH	M	401	-	64,70,70	1.25	8 (12%)	73,101,101	1.84	11 (15%)
8	U10	M	501	-	48,48,63	2.61	21 (43%)	58,61,79	1.40	10 (17%)
9	SPO	M	600	-	40,41,41	3.40	22 (55%)	45,50,50	2.11	14 (31%)
10	LDA	M	701	-	15,15,15	4.89	2 (13%)	16,17,17	0.52	0
10	LDA	M	702	-	15,15,15	4.85	1 (6%)	16,17,17	1.04	1 (6%)
10	LDA	M	703	-	15,15,15	4.78	4 (26%)	16,17,17	0.85	0
10	LDA	M	704	-	15,15,15	3.75	1 (6%)	16,17,17	0.60	0
10	LDA	M	705	-	15,15,15	4.28	4 (26%)	16,17,17	0.57	0
10	LDA	M	706	-	15,15,15	4.52	2 (13%)	16,17,17	0.61	0
5	PO4	M	800	-	4,4,4	1.33	0	6,6,6	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	BCL	M	801	2,6	53,74,74	0.96	3 (5%)	57,115,115	1.76	8 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BCL	L	301	2	2/2/21/25	0/37/137/137	0/0/9/9
6	BCL	L	302	1,6	-	0/37/137/137	0/0/9/9
6	BCL	L	304	1	1/1/21/25	0/37/137/137	0/0/9/9
7	BPH	L	402	-	-	0/54/105/105	0/1/6/6
8	U10	L	502	-	-	0/45/69/87	0/1/1/1
10	LDA	L	707	-	-	0/13/13/13	0/0/0/0
10	LDA	L	708	-	-	0/13/13/13	0/0/0/0
10	LDA	L	709	-	-	0/13/13/13	0/0/0/0
7	BPH	M	401	-	-	0/54/105/105	0/1/6/6
8	U10	M	501	-	-	0/45/69/87	0/1/1/1
9	SPO	M	600	-	-	0/47/47/47	0/0/0/0
10	LDA	M	701	-	-	0/13/13/13	0/0/0/0
10	LDA	M	702	-	-	0/13/13/13	0/0/0/0
10	LDA	M	703	-	-	0/13/13/13	0/0/0/0
10	LDA	M	704	-	-	0/13/13/13	0/0/0/0
10	LDA	M	705	-	-	0/13/13/13	0/0/0/0
10	LDA	M	706	-	-	0/13/13/13	0/0/0/0
5	PO4	M	800	-	-	0/0/0/0	0/0/0/0
6	BCL	M	801	2,6	-	0/37/137/137	0/0/9/9

All (115) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	701	LDA	O1-N1	-18.73	1.21	1.39
10	M	702	LDA	O1-N1	-18.56	1.21	1.39
10	M	703	LDA	O1-N1	-17.68	1.22	1.39
10	L	709	LDA	O1-N1	-17.65	1.22	1.39
10	M	706	LDA	O1-N1	-17.22	1.23	1.39
10	L	707	LDA	O1-N1	-16.81	1.23	1.39
10	M	705	LDA	O1-N1	-16.03	1.24	1.39
10	L	708	LDA	O1-N1	-15.78	1.24	1.39
10	M	704	LDA	O1-N1	-14.44	1.25	1.39
8	M	501	U10	C27-C28	-8.47	1.26	1.50
6	L	302	BCL	O2D-CED	-4.99	1.33	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	501	U10	C17-C18	-4.47	1.38	1.50
7	M	401	BPH	O2D-CED	-3.95	1.35	1.45
6	L	302	BCL	C1-C2	-3.84	1.36	1.49
8	M	501	U10	C37-C38	-3.80	1.39	1.50
8	M	501	U10	C22-C23	-3.80	1.39	1.50
8	L	502	U10	C17-C18	-3.64	1.40	1.50
10	M	703	LDA	CM1-N1	-3.61	1.43	1.49
9	M	600	SPO	C4-C5	-3.58	1.45	1.50
9	M	600	SPO	C31-C32	-3.56	1.40	1.50
6	L	301	BCL	O2D-CED	-3.31	1.37	1.45
10	M	703	LDA	C1-N1	-3.26	1.45	1.51
9	M	600	SPO	C11-C12	-3.20	1.38	1.45
9	M	600	SPO	C6-C7	-3.14	1.39	1.45
7	L	402	BPH	O2D-CED	-3.03	1.37	1.45
8	L	502	U10	O4-C4M	-2.83	1.38	1.45
9	M	600	SPO	C25-C23	-2.70	1.39	1.45
6	L	304	BCL	CMB-C2B	-2.56	1.46	1.51
10	M	705	LDA	CM1-N1	-2.56	1.45	1.49
8	M	501	U10	O4-C4M	-2.40	1.39	1.45
10	M	703	LDA	CM2-N1	-2.33	1.45	1.49
10	M	706	LDA	CM1-N1	-2.32	1.45	1.49
8	L	502	U10	C7-C8	-2.30	1.47	1.50
10	M	705	LDA	C1-N1	-2.27	1.47	1.51
6	M	801	BCL	O2D-CED	-2.24	1.39	1.45
8	M	501	U10	O3-C3M	-2.22	1.39	1.45
8	M	501	U10	C7-C8	-2.21	1.47	1.50
10	L	707	LDA	C1-N1	-2.21	1.47	1.51
10	M	701	LDA	CM2-N1	-2.19	1.46	1.49
10	M	705	LDA	CM2-N1	-2.15	1.46	1.49
9	M	600	SPO	C16-C17	-2.14	1.41	1.45
10	L	709	LDA	CM2-N1	-2.12	1.46	1.49
6	L	301	BCL	C3D-C2D	-2.09	1.35	1.40
7	M	401	BPH	C3A-C2A	-2.03	1.48	1.54
6	L	302	BCL	CMC-C2C	-2.01	1.48	1.53
6	L	304	BCL	C3D-C2D	-2.00	1.35	1.40
7	M	401	BPH	C3D-C4D	2.00	1.43	1.41
6	L	302	BCL	O2D-CGD	2.03	1.38	1.33
7	M	401	BPH	C5-C3	2.04	1.55	1.51
7	L	402	BPH	C4-C3	2.05	1.55	1.50
6	M	801	BCL	O2A-CGA	2.06	1.39	1.33
8	L	502	U10	C16-C14	2.09	1.56	1.51
8	L	502	U10	C25-C24	2.09	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	501	U10	O2-C2	2.19	1.28	1.23
8	M	501	U10	C28-C29	2.23	1.37	1.33
7	M	401	BPH	CHA-C1A	2.25	1.42	1.37
6	L	302	BCL	C2-C3	2.28	1.37	1.33
8	L	502	U10	C35-C34	2.28	1.56	1.50
6	L	302	BCL	C4-C3	2.30	1.56	1.50
9	M	600	SPO	C35-C33	2.39	1.56	1.51
8	L	502	U10	C15-C14	2.40	1.56	1.50
8	L	502	U10	C10-C9	2.40	1.56	1.50
6	L	304	BCL	O2A-CGA	2.45	1.40	1.33
8	M	501	U10	C15-C14	2.49	1.56	1.50
8	M	501	U10	C38-C39	2.51	1.40	1.32
8	M	501	U10	C30-C29	2.54	1.56	1.50
7	L	402	BPH	O2A-CGA	2.55	1.41	1.33
8	L	502	U10	C21-C19	2.55	1.57	1.51
9	M	600	SPO	C37-C38	2.65	1.40	1.32
9	M	600	SPO	C19-C17	2.66	1.39	1.35
9	M	600	SPO	C9-C7	2.69	1.39	1.35
8	L	502	U10	C31-C29	2.72	1.57	1.51
8	L	502	U10	C38-C39	2.78	1.40	1.32
7	M	401	BPH	O2A-CGA	2.84	1.41	1.33
8	L	502	U10	C18-C19	2.96	1.38	1.33
8	M	501	U10	C18-C19	2.97	1.38	1.33
8	L	502	U10	C36-C34	2.98	1.58	1.51
7	L	402	BPH	O2D-CGD	2.99	1.40	1.33
9	M	600	SPO	O1-CM1	3.02	1.52	1.43
8	M	501	U10	C13-C14	3.07	1.39	1.33
9	M	600	SPO	C13-C12	3.11	1.57	1.50
8	M	501	U10	C36-C34	3.21	1.58	1.51
6	L	304	BCL	C2-C3	3.23	1.39	1.33
7	M	401	BPH	C2-C3	3.25	1.39	1.33
7	M	401	BPH	O2D-CGD	3.25	1.41	1.33
8	M	501	U10	O4-C4	3.30	1.45	1.37
6	M	801	BCL	C2-C3	3.34	1.39	1.33
8	M	501	U10	C23-C24	3.35	1.39	1.33
7	L	402	BPH	C2-C3	3.38	1.39	1.33
9	M	600	SPO	C32-C33	3.38	1.39	1.33
8	M	501	U10	C35-C34	3.39	1.58	1.50
6	L	301	BCL	C2-C3	3.44	1.39	1.33
8	M	501	U10	C8-C9	3.49	1.39	1.33
8	L	502	U10	C7-C6	3.51	1.57	1.51
9	M	600	SPO	C10-C9	3.54	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	502	U10	O4-C4	3.62	1.46	1.37
8	L	502	U10	C13-C14	3.65	1.40	1.33
8	L	502	U10	C8-C9	3.69	1.40	1.33
8	M	501	U10	C33-C34	3.79	1.40	1.33
8	L	502	U10	C23-C24	3.87	1.40	1.33
6	L	302	BCL	O2A-CGA	4.06	1.45	1.33
8	L	502	U10	C28-C29	4.13	1.41	1.33
8	L	502	U10	O3-C3	4.15	1.47	1.37
8	L	502	U10	C33-C34	4.17	1.41	1.33
9	M	600	SPO	C27-C28	4.20	1.38	1.34
6	L	304	BCL	O2D-CGD	4.43	1.44	1.33
9	M	600	SPO	C15-C14	4.48	1.57	1.43
9	M	600	SPO	C14-C12	4.48	1.41	1.35
6	L	301	BCL	O2A-CGA	4.89	1.48	1.33
9	M	600	SPO	C26-C25	5.27	1.48	1.34
9	M	600	SPO	C21-C20	5.90	1.51	1.35
8	M	501	U10	O3-C3	6.67	1.54	1.37
9	M	600	SPO	C6-C5	6.97	1.51	1.31
9	M	600	SPO	C10-C11	7.10	1.53	1.34
9	M	600	SPO	C15-C16	9.38	1.59	1.34

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L	304	BCL	CBB-CAB-C3B	-8.17	96.08	120.33
6	L	304	BCL	O1D-CGD-CBD	-7.96	113.22	124.62
7	M	401	BPH	O1D-CGD-CBD	-7.18	114.34	124.62
6	L	301	BCL	O1D-CGD-CBD	-6.74	114.96	124.62
7	L	402	BPH	O1D-CGD-CBD	-6.71	115.00	124.62
6	L	302	BCL	CBB-CAB-C3B	-6.50	101.04	120.33
6	M	801	BCL	O1D-CGD-CBD	-5.41	116.86	124.62
9	M	600	SPO	C25-C23-C22	-4.66	111.48	118.98
6	L	301	BCL	CMB-C2B-C1B	-4.36	121.15	128.36
6	L	302	BCL	O1D-CGD-CBD	-4.21	118.59	124.62
6	L	304	BCL	OBB-CAB-CBB	-4.14	110.20	120.13
9	M	600	SPO	C20-C21-C22	-4.12	114.28	123.39
9	M	600	SPO	C15-C14-C12	-4.07	121.32	127.20
8	M	501	U10	C26-C27-C28	-4.01	101.20	111.69
9	M	600	SPO	C20-C19-C17	-3.87	121.61	127.20
9	M	600	SPO	C10-C9-C7	-3.81	121.69	127.20
9	M	600	SPO	C15-C16-C17	-3.80	115.15	126.32
6	L	302	BCL	OBB-CAB-CBB	-3.78	111.06	120.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	M	600	SPO	C18-C17-C19	-3.72	117.40	122.90
7	L	402	BPH	OBD-CAD-CBD	-3.71	120.34	125.94
9	M	600	SPO	C5-C6-C7	-3.67	120.16	125.75
7	M	401	BPH	OBD-CAD-CBD	-3.62	120.48	125.94
9	M	600	SPO	C4-C5-C6	-3.60	119.54	124.67
10	M	702	LDA	CM2-N1-CM1	-3.05	105.39	108.83
6	L	302	BCL	OBD-CAD-CBD	-3.02	121.38	125.94
7	M	401	BPH	C3A-C4A-NA	-2.95	108.42	113.57
8	M	501	U10	C25-C24-C26	-2.78	111.16	115.41
6	L	304	BCL	CMB-C2B-C1B	-2.75	123.81	128.36
6	M	801	BCL	OBD-CAD-CBD	-2.71	121.85	125.94
6	L	301	BCL	OBD-CAD-CBD	-2.58	122.05	125.94
6	L	302	BCL	CMB-C2B-C1B	-2.46	124.29	128.36
6	L	304	BCL	O2A-CGA-O1A	-2.41	117.26	123.49
6	L	304	BCL	CAC-C3C-C4C	-2.38	107.31	112.58
7	L	402	BPH	C3A-C4A-NA	-2.37	109.42	113.57
7	L	402	BPH	CBB-CAB-C3B	-2.31	115.38	120.52
9	M	600	SPO	C21-C22-C23	-2.31	123.86	127.20
7	M	401	BPH	CBB-CAB-C3B	-2.27	115.48	120.52
7	M	401	BPH	C2A-C1A-NA	-2.26	109.19	112.08
8	M	501	U10	C20-C19-C21	-2.25	111.97	115.41
7	M	401	BPH	O2A-CGA-O1A	-2.22	117.76	123.49
6	L	301	BCL	C4-C3-C5	-2.20	112.05	115.41
8	M	501	U10	C31-C29-C28	-2.18	116.91	121.05
9	M	600	SPO	C6-C7-C9	-2.16	115.51	118.98
7	L	402	BPH	C4-C3-C5	-2.13	112.16	115.41
9	M	600	SPO	C10-C11-C12	-2.12	120.07	126.32
7	L	402	BPH	O2A-CGA-O1A	-2.10	118.07	123.49
8	M	501	U10	C10-C9-C11	-2.09	112.22	115.41
9	M	600	SPO	C11-C12-C14	-2.05	115.68	118.98
6	L	304	BCL	OBD-CAD-CBD	-2.03	122.87	125.94
8	L	502	U10	C30-C29-C31	-2.03	112.31	115.41
6	M	801	BCL	CMB-C2B-C1B	-2.02	125.02	128.36
8	M	501	U10	C22-C23-C24	2.02	132.16	127.76
6	L	301	BCL	C5-C3-C2	2.03	124.89	121.05
8	M	501	U10	C25-C24-C23	2.10	127.62	123.50
9	M	600	SPO	C8-C7-C6	2.10	121.59	118.10
8	L	502	U10	C4M-O4-C4	2.12	124.14	116.61
8	M	501	U10	C3M-O3-C3	2.15	124.25	116.61
8	L	502	U10	C3M-O3-C3	2.19	124.41	116.61
6	L	302	BCL	CED-O2D-CGD	2.23	121.22	115.99
8	M	501	U10	C7-C8-C9	2.45	130.85	126.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	401	BPH	C4A-NA-C1A	2.46	110.41	108.21
6	L	304	BCL	CMD-C2D-C3D	2.52	130.02	125.09
7	M	401	BPH	C3A-C4A-CHB	2.55	126.58	121.84
7	M	401	BPH	OBB-CAB-C3B	2.59	125.31	120.31
6	L	301	BCL	C4A-NA-C1A	2.71	109.86	106.36
8	L	502	U10	C7-C8-C9	2.78	131.40	126.70
6	M	801	BCL	CED-O2D-CGD	2.78	122.51	115.99
6	L	301	BCL	CMB-C2B-C3B	2.81	130.59	125.09
6	L	304	BCL	O2A-CGA-CBA	2.88	120.67	111.90
6	M	801	BCL	C4A-NA-C1A	2.94	110.16	106.36
6	L	301	BCL	O2A-CGA-CBA	3.14	121.47	111.90
6	L	302	BCL	C4A-NA-C1A	3.15	110.43	106.36
6	L	304	BCL	C4A-NA-C1A	3.23	110.53	106.36
7	L	402	BPH	O2A-CGA-CBA	3.27	121.85	111.90
6	L	302	BCL	O2A-CGA-CBA	3.27	121.85	111.90
6	L	302	BCL	OBB-CAB-C3B	3.30	125.23	120.00
6	M	801	BCL	OBB-CAB-C3B	3.49	125.53	120.00
6	M	801	BCL	O2A-CGA-CBA	3.52	122.64	111.90
7	M	401	BPH	O2A-CGA-CBA	3.60	122.87	111.90
8	M	501	U10	C27-C28-C29	3.77	135.96	127.76
6	L	302	BCL	O2D-CGD-CBD	6.41	120.09	111.30
6	M	801	BCL	O2D-CGD-CBD	7.28	121.29	111.30
6	L	304	BCL	OBB-CAB-C3B	7.90	132.52	120.00
6	L	301	BCL	O2D-CGD-CBD	8.17	122.51	111.30
7	L	402	BPH	O2D-CGD-CBD	8.22	122.58	111.30
7	M	401	BPH	O2D-CGD-CBD	8.89	123.50	111.30
6	L	304	BCL	O2D-CGD-CBD	10.19	125.28	111.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	L	301	BCL	C8
6	L	301	BCL	C13
6	L	304	BCL	C13

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 94 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	301	BCL	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	302	BCL	10	0
6	L	304	BCL	5	0
7	L	402	BPH	12	0
8	L	502	U10	8	0
10	L	707	LDA	1	0
10	L	708	LDA	1	0
7	M	401	BPH	8	0
8	M	501	U10	8	0
9	M	600	SPO	7	0
10	M	701	LDA	4	0
10	M	702	LDA	6	0
10	M	703	LDA	8	0
10	M	705	LDA	4	0
10	M	706	LDA	5	0
6	M	801	BCL	14	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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.