



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:03 PM GMT

PDB ID : 1DS8
Title : PHOTOSYNTHETIC REACTION CENTER FROM RHODOBACTER SPHAEROIDES IN THE CHARGE-NEUTRAL DQAQB STATE WITH THE PROTON TRANSFER INHIBITOR CD2+
Authors : Axelrod, H.L.; Abresch, E.C.; Paddock, M.L.; Okamura, M.Y.; Feher, G.
Deposited on : 2000-01-07
Resolution : 2.50 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 ⓘ](#)) 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

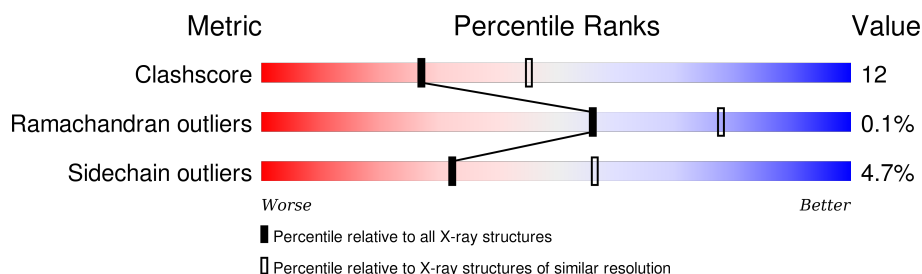
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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 $\leq 5\%$. 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	
1	R	281	
2	M	307	
2	S	307	
3	H	260	
3	T	260	

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 14529 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
			2232	1507	355	362	8			
1	R	281	Total	C	N	O	S	0	0	0
			2232	1507	355	362	8			

- Molecule 2 is a protein called REACTION CENTER PROTEIN M CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	299	Total	C	N	O	S	0	0	0
			2390	1597	391	392	10			
2	S	299	Total	C	N	O	S	0	0	0
			2390	1597	391	392	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	307	ALA	ASN	CONFLICT	UNP P02953
S	307	ALA	ASN	CONFLICT	UNP P02953

- Molecule 3 is a protein called REACTION CENTER PROTEIN H CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	246	Total	C	N	O	S	0	0	0
			1869	1196	320	343	10			
3	T	246	Total	C	N	O	S	0	0	0
			1869	1196	320	343	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	8	GLN	GLY	CONFLICT	UNP P11846
T	8	GLN	GLY	CONFLICT	UNP P11846

- Molecule 4 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

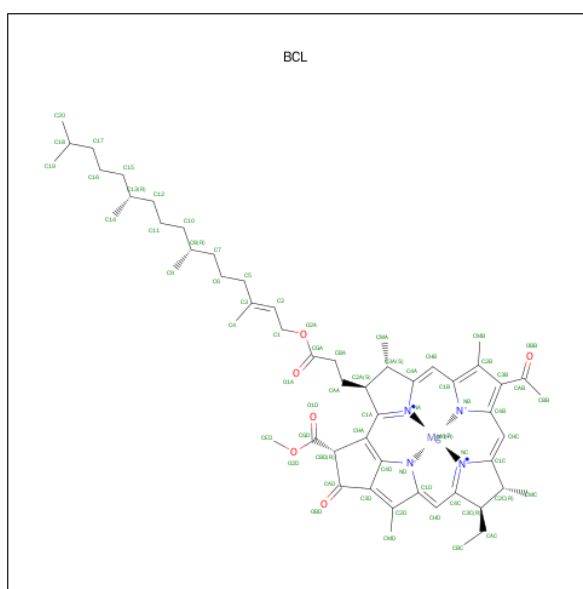
- Molecule 5 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	1	Total Cd 1 1	0	0
5	T	1	Total Cd 1 1	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

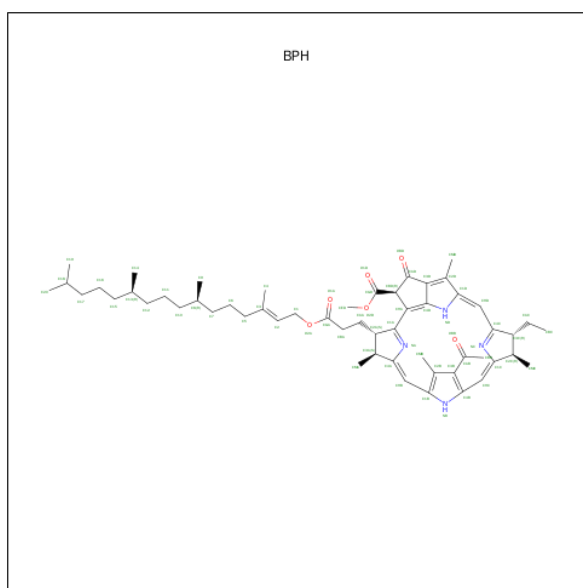
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	S	1	Total Cl 1 1	0	0
6	M	1	Total Cl 1 1	0	0

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



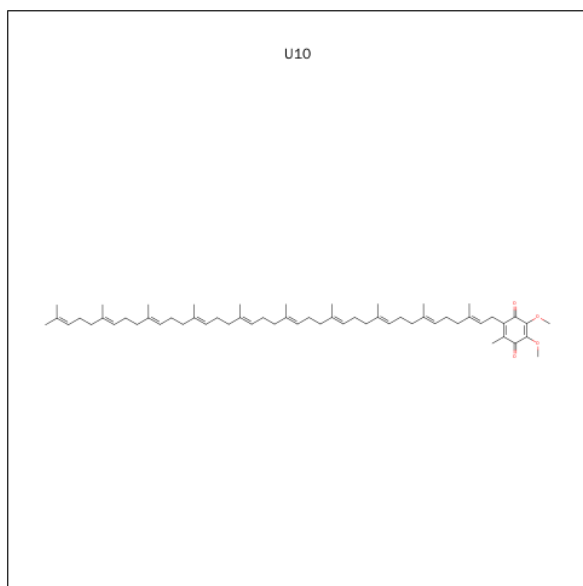
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	L	1	Total 51	C 40	Mg 1	N 4	O 6	0	0
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	R	1	Total 51	C 40	Mg 1	N 4	O 6	0	0
7	R	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	S	1	Total 66	C 55	Mg 1	N 4	O 6	0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

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



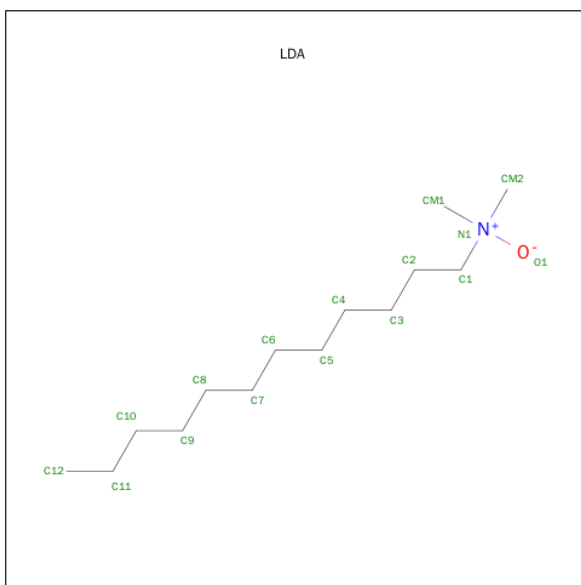
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	M	1	Total	C	N	O	0	0
			51	41	4	6		
8	L	1	Total	C	N	O	0	0
			65	55	4	6		
8	S	1	Total	C	N	O	0	0
			52	42	4	6		
8	R	1	Total	C	N	O	0	0
			65	55	4	6		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	M	1	Total	C	O	0	0
			38	34	4		
9	L	1	Total	C	O	0	0
			44	40	4		
9	S	1	Total	C	O	0	0
			32	28	4		
9	R	1	Total	C	O	0	0
			18	14	4		

- 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	0	0
			16	14	1	1		
10	M	1	Total	C	N	O	0	0
			16	14	1	1		
10	M	1	Total	C	N	O	0	0
			16	14	1	1		
10	S	1	Total	C	N	O	0	0
			16	14	1	1		
10	S	1	Total	C	N	O	0	0
			16	14	1	1		
10	S	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 11 is water.

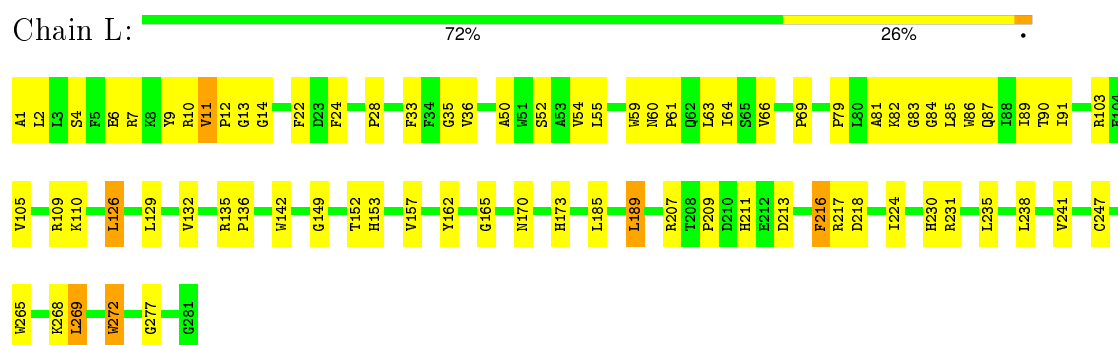
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	H	122	Total	O	0	0
			122	122		
11	L	88	Total	O	0	0
			88	88		
11	M	133	Total	O	0	0
			133	133		
11	R	62	Total	O	0	0
			62	62		
11	S	92	Total	O	0	0
			92	92		
11	T	85	Total	O	0	0
			85	85		

3 Residue-property plots

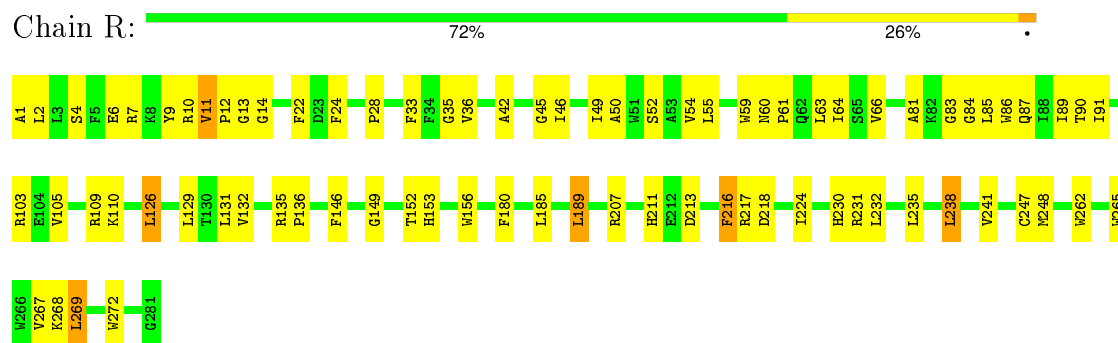
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

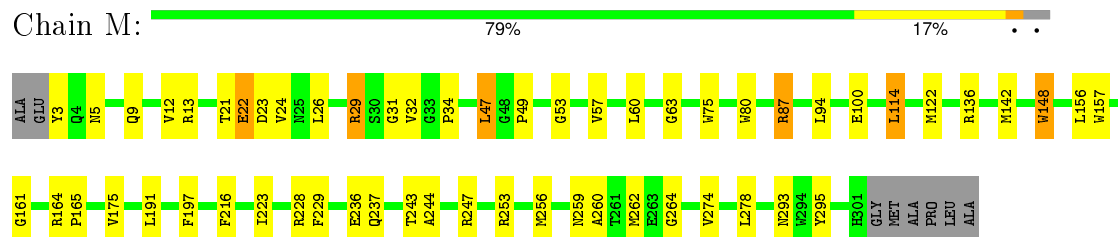
• Molecule 1: REACTION CENTER PROTEIN L CHAIN




• Molecule 1: REACTION CENTER PROTEIN L CHAIN

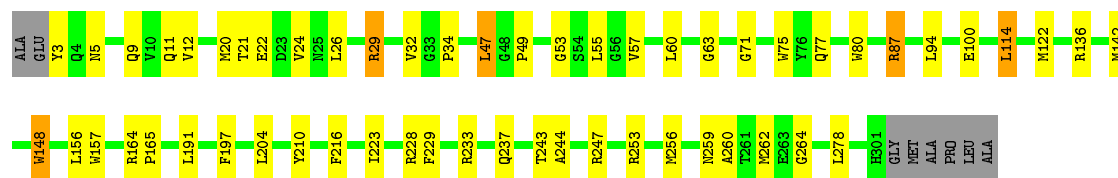


• Molecule 2: REACTION CENTER PROTEIN M CHAIN



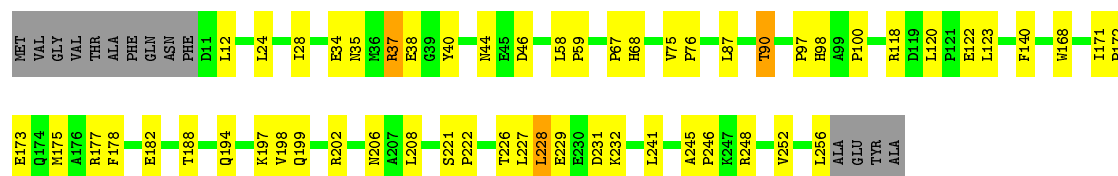
• Molecule 2: REACTION CENTER PROTEIN M CHAIN

Chain S:  79% 17% • •



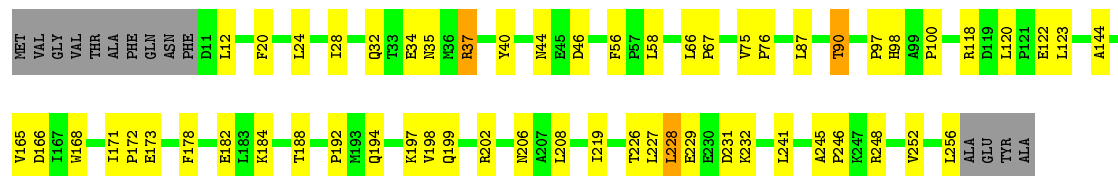
• Molecule 3: REACTION CENTER PROTEIN H CHAIN

Chain H:  73% 20% • 5%



• Molecule 3: REACTION CENTER PROTEIN H CHAIN

Chain T:  72% 21% • 5%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	139.59Å 139.59Å 272.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50	Depositor
% Data completeness (in resolution range)	99.8 (50.00-2.50)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.227 , 0.256	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14529	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, LDA, CL, BPH, CD, FE2, 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	0.39	0/2320	0.55	0/3175
1	R	0.40	0/2320	0.55	0/3175
2	M	0.41	0/2482	0.54	0/3389
2	S	0.40	0/2482	0.54	0/3389
3	H	0.35	0/1917	0.60	0/2608
3	T	0.35	0/1917	0.60	0/2608
All	All	0.39	0/13438	0.56	0/18344

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	59	0
1	R	2232	0	2187	63	0
2	M	2390	0	2304	53	0
2	S	2390	0	2304	49	0
3	H	1869	0	1884	49	0
3	T	1869	0	1884	45	0
4	M	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	S	1	0	0	0	0
5	H	1	0	0	0	0
5	T	1	0	0	0	0
6	M	1	0	0	0	0
6	S	1	0	0	0	0
7	L	183	0	189	17	0
7	M	66	0	73	8	0
7	R	183	0	189	17	0
7	S	66	0	74	6	0
8	L	65	0	76	5	0
8	M	51	0	45	5	0
8	R	65	0	76	14	0
8	S	52	0	47	4	0
9	L	44	0	57	2	0
9	M	38	0	47	2	0
9	R	18	0	15	3	0
9	S	32	0	39	2	0
10	M	48	0	93	7	0
10	S	48	0	93	5	0
11	H	122	0	0	6	0
11	L	88	0	0	7	0
11	M	133	0	0	2	0
11	R	62	0	0	2	0
11	S	92	0	0	3	0
11	T	85	0	0	3	0
All	All	14529	0	13863	333	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 12.

All (333) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:197:PHE:HZ	7:M:1003:BCL:HBB2	1.34	0.91
2:M:197:PHE:CZ	7:M:1003:BCL:HBB2	2.11	0.86
1:L:217:ARG:HD2	11:M:1108:HOH:O	1.77	0.85
2:M:161:GLY:HA3	10:M:1014:LDA:HM12	1.62	0.82
1:R:131:LEU:HD21	7:R:2002:BCL:HED2	1.64	0.80
8:R:2006:BPH:HBB3	8:R:2006:BPH:HHC	1.68	0.76
2:S:197:PHE:HZ	7:S:2003:BCL:HBB2	1.51	0.75
7:R:2001:BCL:HHC	7:R:2001:BCL:HBB3	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:228:ARG:HA	3:T:194:GLN:CG	2.18	0.73
2:M:9:GLN:NE2	3:H:198:VAL:H	1.86	0.73
2:M:9:GLN:HE22	3:H:197:LYS:HA	1.54	0.72
2:S:243:THR:O	2:S:247:ARG:HG3	1.90	0.71
11:L:1019:HOH:O	2:M:253:ARG:HD3	1.90	0.71
2:M:161:GLY:CA	10:M:1014:LDA:HM12	2.20	0.71
2:M:122:MET:CE	2:M:157:TRP:HE1	2.04	0.70
2:S:228:ARG:HA	3:T:194:GLN:HG2	1.73	0.70
1:R:217:ARG:HD2	11:S:2024:HOH:O	1.91	0.70
1:L:224:ILE:HG22	9:L:1009:U10:H3M3	1.72	0.69
2:S:63:GLY:HA3	8:S:2005:BPH:H5C2	1.73	0.69
3:T:90:THR:HB	3:T:97:PRO:O	1.92	0.69
2:S:122:MET:CE	2:S:157:TRP:HE1	2.06	0.69
1:R:224:ILE:HG22	9:R:2009:U10:H3M3	1.74	0.69
1:L:105:VAL:O	1:L:109:ARG:HG3	1.93	0.68
7:R:2001:BCL:CBB	7:R:2001:BCL:HHC	2.23	0.67
3:H:90:THR:HB	3:H:97:PRO:O	1.94	0.67
2:S:197:PHE:CZ	7:S:2003:BCL:HBB2	2.29	0.67
3:H:173:GLU:HG3	11:H:1088:HOH:O	1.94	0.67
8:R:2006:BPH:HBB2	2:S:210:TYR:HB3	1.76	0.67
1:R:189:LEU:HB3	9:R:2009:U10:H4M3	1.75	0.67
2:S:21:THR:O	2:S:24:VAL:HG13	1.93	0.67
1:R:105:VAL:O	1:R:109:ARG:HG3	1.94	0.67
1:L:55:LEU:HD13	1:L:81:ALA:HB2	1.75	0.67
1:R:55:LEU:HD13	1:R:81:ALA:HB2	1.77	0.66
1:R:218:ASP:OD1	2:S:29:ARG:HD2	1.97	0.65
3:H:175:MET:HE1	11:H:1028:HOH:O	1.97	0.65
3:T:87:LEU:HD23	3:T:100:PRO:HA	1.80	0.64
2:M:21:THR:O	2:M:24:VAL:HG13	1.96	0.64
3:H:87:LEU:HD23	3:H:100:PRO:HA	1.79	0.64
1:R:231:ARG:HD2	2:S:5:ASN:O	1.98	0.63
2:M:243:THR:O	2:M:247:ARG:HG3	1.99	0.63
7:L:1004:BCL:HBB2	7:L:1004:BCL:HMB1	1.81	0.63
7:R:2004:BCL:HBB2	7:R:2004:BCL:HMB1	1.80	0.62
7:L:1002:BCL:HMB1	7:L:1002:BCL:CBB	2.30	0.62
1:R:265:TRP:O	1:R:269:LEU:HD13	2.00	0.62
7:M:1003:BCL:CBB	7:M:1003:BCL:HHC	2.29	0.62
8:R:2006:BPH:CBB	8:R:2006:BPH:HHC	2.29	0.61
2:S:77:GLN:HG2	11:S:2029:HOH:O	2.00	0.61
3:T:194:GLN:H	3:T:194:GLN:CD	2.03	0.61
3:H:194:GLN:H	3:H:194:GLN:CD	2.04	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:252:VAL:O	3:H:256:LEU:HD13	2.02	0.60
1:L:60:ASN:HB3	1:L:63:LEU:HD23	1.84	0.60
2:M:9:GLN:HE22	3:H:198:VAL:H	1.49	0.60
2:M:161:GLY:HA3	10:M:1014:LDA:HM23	1.83	0.60
1:L:265:TRP:O	1:L:269:LEU:HD13	2.00	0.60
1:L:60:ASN:O	1:L:64:ILE:HG13	2.02	0.60
11:S:2020:HOH:O	3:T:173:GLU:HG2	2.01	0.59
1:L:218:ASP:OD1	2:M:29:ARG:HD2	2.02	0.59
1:R:238:LEU:HD12	8:R:2006:BPH:CBC	2.33	0.59
3:T:226:THR:OG1	3:T:229:GLU:HG3	2.03	0.59
1:R:28:PRO:HB3	2:S:253:ARG:NH1	2.18	0.59
7:L:1001:BCL:CBB	7:L:1001:BCL:HHC	2.33	0.58
1:R:60:ASN:HB3	1:R:63:LEU:HD23	1.84	0.58
2:M:63:GLY:HA3	8:M:1005:BPH:H5C2	1.84	0.58
3:T:252:VAL:O	3:T:256:LEU:HD13	2.03	0.58
1:R:60:ASN:O	1:R:64:ILE:HG13	2.02	0.58
9:M:1008:U10:H4M2	9:M:1008:U10:H3M3	1.83	0.58
1:R:86:TRP:CH2	1:R:132:VAL:HG13	2.39	0.58
1:L:86:TRP:CH2	1:L:132:VAL:HG13	2.38	0.58
3:T:118:ARG:HD3	3:T:120:LEU:HD12	1.86	0.58
1:L:272:TRP:CD2	2:M:87:ARG:HB3	2.38	0.58
7:S:2003:BCL:CBB	7:S:2003:BCL:HHC	2.34	0.58
1:R:13:GLY:O	1:R:110:LYS:HE2	2.04	0.57
1:R:189:LEU:HD13	8:S:2005:BPH:HMD2	1.86	0.57
1:L:13:GLY:O	1:L:110:LYS:HE2	2.04	0.57
2:S:256:MET:CE	9:S:2008:U10:H102	2.35	0.57
7:R:2004:BCL:CBB	7:R:2004:BCL:HMB1	2.35	0.57
1:R:248:MET:HG3	7:R:2002:BCL:HED2	1.85	0.57
3:H:118:ARG:HD3	3:H:120:LEU:HD12	1.86	0.57
7:R:2002:BCL:CBB	7:R:2002:BCL:HMB1	2.35	0.57
2:S:148:TRP:HD1	10:S:2013:LDA:H12	1.70	0.56
9:L:1009:U10:H311	2:M:31:GLY:O	2.06	0.56
2:S:122:MET:HE3	2:S:157:TRP:HE1	1.68	0.56
2:S:20:MET:HA	11:T:2085:HOH:O	2.04	0.56
2:M:122:MET:HE1	2:M:157:TRP:HE1	1.69	0.55
1:L:189:LEU:HG	1:L:216:PHE:HZ	1.72	0.55
1:R:135:ARG:HB3	1:R:136:PRO:HD3	1.89	0.55
1:L:28:PRO:HB3	2:M:253:ARG:NH1	2.22	0.55
7:R:2002:BCL:H192	8:R:2006:BPH:HMA1	1.88	0.54
1:R:267:VAL:HG13	2:S:87:ARG:HD2	1.90	0.54
2:S:9:GLN:HE22	3:T:198:VAL:H	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:228:ARG:HA	3:H:194:GLN:HG2	1.88	0.54
7:L:1004:BCL:HMB1	7:L:1004:BCL:CBB	2.38	0.54
7:L:1004:BCL:O1D	10:M:1013:LDA:H21	2.08	0.54
7:L:1001:BCL:HBB3	7:M:1003:BCL:H41	1.90	0.54
1:L:231:ARG:HD2	2:M:5:ASN:O	2.08	0.54
1:R:189:LEU:HG	1:R:216:PHE:HZ	1.72	0.54
7:L:1002:BCL:HBB3	7:L:1002:BCL:HMB1	1.89	0.54
2:S:164:ARG:HB3	2:S:165:PRO:HD3	1.90	0.53
1:R:230:HIS:CD2	2:S:223:ILE:HG13	2.44	0.53
2:M:13:ARG:O	3:H:140:PHE:HA	2.07	0.53
1:R:54:VAL:HA	11:R:2068:HOH:O	2.09	0.53
1:L:14:GLY:O	1:L:109:ARG:HD3	2.08	0.53
1:R:14:GLY:O	1:R:109:ARG:HD3	2.08	0.53
3:T:199:GLN:HE22	3:T:202:ARG:NH1	2.07	0.53
1:R:87:GLN:O	1:R:91:ILE:HG12	2.08	0.53
11:L:1054:HOH:O	3:H:67:PRO:HG2	2.08	0.53
3:H:199:GLN:HE22	3:H:202:ARG:NH1	2.08	0.52
1:L:241:VAL:HG21	8:L:1006:BPH:HAC1	1.91	0.52
3:T:34:GLU:O	3:T:37:ARG:HD3	2.09	0.52
7:S:2003:BCL:HBB2	7:S:2003:BCL:HHC	1.91	0.52
11:R:2018:HOH:O	2:S:233:ARG:HA	2.10	0.52
2:M:164:ARG:HB3	2:M:165:PRO:HD3	1.90	0.52
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.91	0.52
3:H:37:ARG:HH11	3:H:76:PRO:HD3	1.75	0.51
7:R:2002:BCL:H122	8:R:2006:BPH:H3A	1.93	0.51
2:M:122:MET:HE3	2:M:157:TRP:HE1	1.76	0.51
3:H:34:GLU:O	3:H:37:ARG:HD3	2.09	0.51
1:L:83:GLY:O	1:L:87:GLN:HG3	2.10	0.51
1:L:52:SER:HB2	1:L:85:LEU:HD23	1.91	0.51
1:R:6:GLU:OE2	1:R:10:ARG:HD3	2.10	0.51
1:L:28:PRO:HB3	2:M:253:ARG:HH11	1.75	0.51
1:L:272:TRP:CE2	2:M:87:ARG:HB3	2.45	0.51
1:R:42:ALA:HA	8:R:2006:BPH:H9C2	1.93	0.51
2:S:9:GLN:NE2	3:T:198:VAL:H	2.07	0.51
3:H:226:THR:OG1	3:H:229:GLU:HG3	2.11	0.51
3:T:87:LEU:HD22	3:T:98:HIS:O	2.11	0.51
2:M:228:ARG:HA	3:H:194:GLN:CG	2.41	0.51
2:M:32:VAL:HG22	2:M:49:PRO:HD3	1.92	0.51
1:R:45:GLY:HA3	8:R:2006:BPH:H9C1	1.93	0.50
3:T:37:ARG:HH11	3:T:76:PRO:HD3	1.75	0.50
2:M:148:TRP:HA	2:M:148:TRP:CE3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:3:TYR:CE1	2:M:9:GLN:HG3	2.47	0.50
1:R:232:LEU:HD21	9:R:2009:U10:H8	1.92	0.50
1:L:87:GLN:O	1:L:91:ILE:HG12	2.11	0.50
1:R:83:GLY:O	1:R:87:GLN:HG3	2.12	0.50
2:M:148:TRP:HA	2:M:148:TRP:HE3	1.77	0.50
3:T:199:GLN:NE2	3:T:202:ARG:NH1	2.60	0.50
2:S:148:TRP:HA	2:S:148:TRP:CE3	2.47	0.50
1:R:28:PRO:HB3	2:S:253:ARG:HH11	1.76	0.49
2:S:32:VAL:HG22	2:S:49:PRO:HD3	1.94	0.49
2:S:148:TRP:HA	2:S:148:TRP:HE3	1.77	0.49
3:H:199:GLN:NE2	3:H:202:ARG:NH1	2.60	0.49
1:R:50:ALA:O	1:R:54:VAL:HG23	2.12	0.49
7:R:2004:BCL:HED1	10:S:2014:LDA:H11	1.94	0.49
1:R:52:SER:HB2	1:R:85:LEU:HD23	1.94	0.49
2:S:100:GLU:CD	2:S:100:GLU:H	2.15	0.49
1:L:277:GLY:HA3	11:L:1085:HOH:O	2.12	0.49
7:L:1002:BCL:H122	8:L:1006:BPH:H3A	1.95	0.49
1:L:189:LEU:HD13	8:M:1005:BPH:HMD2	1.95	0.49
2:M:274:VAL:HG11	10:M:1012:LDA:H61	1.95	0.49
1:L:50:ALA:O	1:L:54:VAL:HG23	2.13	0.49
3:H:228:LEU:CD2	3:H:232:LYS:HE3	2.43	0.48
2:S:3:TYR:CE1	2:S:9:GLN:HG3	2.47	0.48
3:T:168:TRP:HB2	3:T:178:PHE:HB2	1.95	0.48
3:H:87:LEU:HD22	3:H:98:HIS:O	2.13	0.48
3:H:199:GLN:NE2	3:H:202:ARG:HH11	2.12	0.48
2:M:136:ARG:CZ	2:M:136:ARG:HA	2.44	0.48
2:M:100:GLU:H	2:M:100:GLU:CD	2.17	0.48
2:M:236:GLU:HB3	11:H:1012:HOH:O	2.13	0.48
3:T:122:GLU:HB2	3:T:227:LEU:HD21	1.95	0.48
3:T:241:LEU:O	3:T:248:ARG:NH2	2.46	0.48
2:M:136:ARG:NE	2:M:136:ARG:HA	2.28	0.48
1:L:209:PRO:HG3	11:M:1113:HOH:O	2.14	0.48
3:T:228:LEU:CD2	3:T:232:LYS:HE3	2.43	0.48
3:H:241:LEU:O	3:H:248:ARG:NH2	2.47	0.48
1:L:6:GLU:OE2	1:L:10:ARG:HD3	2.13	0.48
2:S:71:GLY:HA2	10:S:2012:LDA:HM11	1.95	0.47
3:H:168:TRP:HB2	3:H:178:PHE:HB2	1.96	0.47
3:T:184:LYS:HG3	11:T:2090:HOH:O	2.14	0.47
1:R:35:GLY:HA2	1:R:103:ARG:HD2	1.97	0.47
3:H:24:LEU:O	3:H:28:ILE:HG13	2.15	0.47
1:L:59:TRP:CE3	1:L:59:TRP:HA	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:189:LEU:HG	1:R:216:PHE:CZ	2.50	0.47
8:M:1005:BPH:HBC3	8:M:1005:BPH:HHB	1.96	0.47
2:S:136:ARG:NE	2:S:136:ARG:HA	2.30	0.47
1:R:11:VAL:HG13	1:R:12:PRO:HD2	1.97	0.47
2:M:34:PRO:O	2:M:47:LEU:HB2	2.15	0.47
1:L:35:GLY:HA2	1:L:103:ARG:HD2	1.97	0.47
1:R:59:TRP:CE3	1:R:59:TRP:HA	2.50	0.47
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.97	0.47
3:H:122:GLU:HB2	3:H:227:LEU:HD21	1.97	0.46
1:L:189:LEU:HG	1:L:216:PHE:CZ	2.50	0.46
3:T:199:GLN:NE2	3:T:202:ARG:HH11	2.12	0.46
2:M:175:VAL:HB	10:M:1014:LDA:H11	1.97	0.46
3:H:206:ASN:O	3:H:248:ARG:NH1	2.49	0.46
1:R:42:ALA:O	1:R:46:ILE:HG13	2.16	0.46
3:T:206:ASN:O	3:T:248:ARG:NH1	2.49	0.46
2:S:204:LEU:HD13	3:T:20:PHE:CE2	2.51	0.46
8:R:2006:BPH:H192	8:R:2006:BPH:H151	1.97	0.46
3:T:87:LEU:HD23	3:T:100:PRO:CA	2.44	0.46
7:L:1002:BCL:HAA2	7:L:1002:BCL:HBD	1.97	0.46
2:M:3:TYR:CZ	2:M:5:ASN:HA	2.51	0.46
3:H:75:VAL:HA	3:H:76:PRO:C	2.36	0.46
3:T:171:ILE:HB	3:T:172:PRO:HD3	1.98	0.46
7:R:2004:BCL:H193	8:R:2006:BPH:H102	1.97	0.46
2:S:53:GLY:O	2:S:57:VAL:HG23	2.16	0.46
2:S:3:TYR:CZ	2:S:5:ASN:HA	2.51	0.45
7:R:2002:BCL:CGA	7:R:2004:BCL:HBC1	2.47	0.45
2:S:122:MET:HE1	2:S:157:TRP:HE1	1.80	0.45
3:T:228:LEU:HD22	3:T:232:LYS:HE3	1.98	0.45
1:L:207:ARG:HG2	2:M:142:MET:HG2	1.98	0.45
1:L:2:LEU:HB3	1:L:6:GLU:HB3	1.98	0.45
2:S:136:ARG:HA	2:S:136:ARG:CZ	2.46	0.45
7:L:1001:BCL:HBB2	7:L:1001:BCL:HHC	1.99	0.45
3:T:40:TYR:HB3	3:T:58:LEU:HD21	1.99	0.45
1:R:85:LEU:O	1:R:89:ILE:HG13	2.16	0.45
11:L:1028:HOH:O	3:H:173:GLU:HG2	2.16	0.45
8:M:1005:BPH:CMB	8:M:1005:BPH:HBB3	2.47	0.45
1:L:11:VAL:HG13	1:L:12:PRO:HD2	1.99	0.45
7:L:1002:BCL:CGA	7:L:1004:BCL:HBC1	2.47	0.45
2:M:256:MET:CE	9:M:1008:U10:H102	2.46	0.45
1:R:149:GLY:HA3	1:R:152:THR:OG1	2.17	0.45
1:R:90:THR:HG23	1:R:132:VAL:HG11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:171:ILE:HB	3:H:172:PRO:HD3	1.99	0.44
3:T:24:LEU:O	3:T:28:ILE:HG13	2.17	0.44
1:R:153:HIS:CE1	8:R:2006:BPH:H201	2.53	0.44
1:R:238:LEU:HD12	8:R:2006:BPH:HBC3	1.99	0.44
2:M:278:LEU:HD12	2:M:278:LEU:HA	1.88	0.44
2:S:34:PRO:O	2:S:47:LEU:HB2	2.18	0.44
3:H:87:LEU:HD23	3:H:100:PRO:CA	2.44	0.44
2:M:260:ALA:HB1	3:H:35:ASN:OD1	2.18	0.44
2:M:264:GLY:HA3	3:H:35:ASN:OD1	2.16	0.44
7:R:2004:BCL:HED1	10:S:2014:LDA:O1	2.18	0.44
3:T:194:GLN:H	3:T:194:GLN:NE2	2.15	0.44
3:H:44:ASN:HB2	3:H:46:ASP:OD1	2.18	0.44
1:L:90:THR:HG23	1:L:132:VAL:HG11	2.00	0.44
3:H:40:TYR:HB3	3:H:58:LEU:HD21	2.00	0.44
3:T:75:VAL:HA	3:T:76:PRO:C	2.37	0.44
2:S:264:GLY:HA3	3:T:35:ASN:OD1	2.18	0.44
3:T:182:GLU:HA	3:T:188:THR:HG22	2.00	0.43
1:L:9:TYR:O	1:L:11:VAL:N	2.50	0.43
3:T:44:ASN:HB2	3:T:46:ASP:OD1	2.19	0.43
3:H:194:GLN:H	3:H:194:GLN:NE2	2.16	0.43
3:H:206:ASN:HD21	3:H:248:ARG:HD2	1.83	0.43
3:T:219:ILE:HG12	11:T:2062:HOH:O	2.19	0.43
1:R:213:ASP:O	1:R:217:ARG:HB2	2.18	0.43
1:L:66:VAL:HG12	1:L:86:TRP:HB2	2.00	0.43
1:R:268:LYS:HA	1:R:268:LYS:HD3	1.83	0.43
7:L:1002:BCL:HBD	7:L:1004:BCL:HAC1	2.00	0.43
1:R:2:LEU:HB3	1:R:6:GLU:HB3	1.99	0.43
1:L:213:ASP:O	1:L:217:ARG:HB2	2.19	0.43
7:R:2002:BCL:HBB3	7:R:2002:BCL:HMB1	2.01	0.43
7:S:2003:BCL:HBC2	7:S:2003:BCL:H2C	1.88	0.43
1:L:185:LEU:HD13	8:M:1005:BPH:ND	2.32	0.43
1:L:84:GLY:HA2	1:L:87:GLN:HE21	1.83	0.43
3:H:177:ARG:NH1	3:H:177:ARG:HG2	2.33	0.43
2:S:55:LEU:HD12	2:S:55:LEU:HA	1.89	0.43
8:S:2005:BPH:HBB3	8:S:2005:BPH:CMB	2.49	0.43
2:S:253:ARG:HB2	2:S:259:ASN:OD1	2.19	0.43
1:R:22:PHE:HA	1:R:24:PHE:CE2	2.54	0.43
2:S:11:GLN:HB2	3:T:144:ALA:HB3	2.01	0.43
1:L:33:PHE:O	1:L:36:VAL:HG22	2.19	0.43
1:R:60:ASN:HA	1:R:61:PRO:HD3	1.85	0.43
1:R:84:GLY:HA2	1:R:87:GLN:HE21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:9:TYR:O	1:R:11:VAL:N	2.49	0.43
1:R:207:ARG:HG3	1:R:211:HIS:CG	2.54	0.43
1:L:185:LEU:HD12	1:L:189:LEU:HD22	2.01	0.42
1:L:162:TYR:HA	1:L:165:GLY:O	2.19	0.42
1:R:238:LEU:HD12	8:R:2006:BPH:HBC1	2.00	0.42
1:R:45:GLY:O	1:R:49:ILE:HG13	2.20	0.42
2:S:260:ALA:HB1	3:T:35:ASN:OD1	2.19	0.42
1:R:33:PHE:O	1:R:36:VAL:HG22	2.18	0.42
3:T:245:ALA:N	3:T:246:PRO:CD	2.82	0.42
2:S:237:GLN:HB2	2:S:262:MET:HG2	2.02	0.42
2:M:253:ARG:HB2	2:M:259:ASN:OD1	2.20	0.42
7:L:1001:BCL:HBC1	7:M:1003:BCL:HAA2	2.02	0.42
7:L:1002:BCL:CBA	7:L:1004:BCL:HBC1	2.50	0.42
3:T:37:ARG:NH1	3:T:76:PRO:HD3	2.35	0.42
3:H:228:LEU:HD22	3:H:232:LYS:HE3	2.00	0.42
2:M:237:GLN:HB2	2:M:262:MET:HG2	2.02	0.42
7:M:1003:BCL:HBB2	7:M:1003:BCL:HHC	2.00	0.42
7:L:1002:BCL:H192	8:L:1006:BPH:HMA1	2.02	0.42
3:H:34:GLU:HG3	11:H:1021:HOH:O	2.20	0.42
1:L:85:LEU:O	1:L:89:ILE:HG13	2.19	0.42
2:M:53:GLY:O	2:M:57:VAL:HG23	2.19	0.42
3:H:245:ALA:N	3:H:246:PRO:CD	2.82	0.42
7:M:1003:BCL:HMB1	7:M:1003:BCL:OBB	2.20	0.42
1:R:241:VAL:HG21	8:R:2006:BPH:HAC2	2.01	0.42
1:L:1:ALA:C	1:L:2:LEU:HD12	2.40	0.42
1:L:11:VAL:HG13	11:L:1086:HOH:O	2.19	0.42
2:M:293:ASN:OD1	2:M:295:TYR:HB3	2.20	0.42
1:L:149:GLY:HA3	1:L:152:THR:OG1	2.19	0.42
3:H:221:SER:HA	3:H:222:PRO:HD3	1.84	0.42
7:M:1003:BCL:HHC	7:M:1003:BCL:HBB3	2.02	0.42
1:R:185:LEU:HD12	1:R:189:LEU:HD22	2.01	0.42
1:L:241:VAL:HG21	8:L:1006:BPH:CAC	2.50	0.42
1:R:66:VAL:HG12	1:R:86:TRP:HB2	2.01	0.42
1:R:1:ALA:C	1:R:2:LEU:HD12	2.40	0.42
3:H:182:GLU:HA	3:H:188:THR:HG22	2.01	0.42
10:M:1014:LDA:HM11	10:M:1014:LDA:H22	1.68	0.42
1:R:185:LEU:HD13	8:S:2005:BPH:ND	2.35	0.42
1:L:60:ASN:HA	1:L:61:PRO:HD3	1.84	0.41
3:H:175:MET:CE	11:H:1028:HOH:O	2.61	0.41
1:L:152:THR:HG23	11:L:1081:HOH:O	2.20	0.41
11:L:1069:HOH:O	2:M:29:ARG:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:268:LYS:HA	1:L:268:LYS:HD3	1.81	0.41
2:M:114:LEU:HD12	2:M:114:LEU:HA	1.92	0.41
7:L:1002:BCL:OBB	7:L:1002:BCL:HHC	2.20	0.41
1:R:262:TRP:O	1:R:265:TRP:HD1	2.03	0.41
2:S:278:LEU:HA	2:S:278:LEU:HD12	1.86	0.41
1:L:126:LEU:HA	1:L:126:LEU:HD12	1.87	0.41
3:H:68:HIS:HD2	11:H:1030:HOH:O	2.04	0.41
3:T:206:ASN:HD21	3:T:248:ARG:HD2	1.85	0.41
7:R:2001:BCL:HBB2	10:S:2012:LDA:H123	2.03	0.41
2:S:114:LEU:HA	2:S:114:LEU:HD12	1.91	0.41
3:T:66:LEU:HA	3:T:67:PRO:HD3	1.77	0.41
2:S:229:PHE:HB2	2:S:244:ALA:HB2	2.02	0.41
1:R:180:PHE:HE2	7:R:2002:BCL:HMA2	1.85	0.41
1:L:60:ASN:CB	1:L:63:LEU:HD23	2.49	0.41
3:H:37:ARG:C	3:H:38:GLU:HG2	2.41	0.41
3:H:177:ARG:HH11	3:H:177:ARG:HG2	1.86	0.41
1:L:69:PRO:HD2	1:L:142:TRP:HB2	2.03	0.41
7:R:2002:BCL:H203	9:S:2008:U10:H252	2.03	0.41
1:R:207:ARG:HG2	2:S:142:MET:HG2	2.03	0.41
2:S:75:TRP:HB3	2:S:80:TRP:CE3	2.56	0.41
3:H:37:ARG:NH1	3:H:76:PRO:HD3	2.36	0.40
1:L:79:PRO:HB2	1:L:82:LYS:HB2	2.02	0.40
1:L:153:HIS:O	1:L:157:VAL:HG23	2.21	0.40
1:R:126:LEU:HA	1:R:126:LEU:HD12	1.87	0.40
1:L:170:ASN:HB3	1:L:173:HIS:CB	2.51	0.40
2:S:9:GLN:HE22	3:T:197:LYS:HA	1.87	0.40
7:L:1004:BCL:H193	8:L:1006:BPH:H102	2.02	0.40
1:L:22:PHE:HA	1:L:24:PHE:CE2	2.55	0.40
3:T:192:PRO:HB3	3:T:194:GLN:HE21	1.87	0.40
1:L:207:ARG:HG3	1:L:211:HIS:CG	2.56	0.40
3:T:32:GLN:HG2	3:T:56:PHE:CD2	2.57	0.40
2:M:75:TRP:HB3	2:M:80:TRP:CE3	2.56	0.40
3:H:37:ARG:HD2	3:H:59:PRO:HG3	2.03	0.40
3:T:165:VAL:O	3:T:166:ASP:HB2	2.20	0.40
7:S:2003:BCL:OBB	7:S:2003:BCL:HMB1	2.22	0.40
1:R:146:PHE:HB3	1:R:156:TRP:CD2	2.56	0.40
2:M:22:GLU:HB3	2:M:23:ASP:H	1.69	0.40
1:L:230:HIS:CD2	2:M:223:ILE:HG13	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	279/281 (99%)	266 (95%)	12 (4%)	1 (0%)	39	61
1	R	279/281 (99%)	266 (95%)	12 (4%)	1 (0%)	39	61
2	M	297/307 (97%)	288 (97%)	9 (3%)	0	100	100
2	S	297/307 (97%)	289 (97%)	8 (3%)	0	100	100
3	H	244/260 (94%)	236 (97%)	8 (3%)	0	100	100
3	T	244/260 (94%)	234 (96%)	10 (4%)	0	100	100
All	All	1640/1696 (97%)	1579 (96%)	59 (4%)	2 (0%)	56	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	R	4	SER
1	L	4	SER

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	220/220 (100%)	209 (95%)	11 (5%)	30	53
1	R	220/220 (100%)	209 (95%)	11 (5%)	30	53
2	M	235/239 (98%)	222 (94%)	13 (6%)	27	48
2	S	235/239 (98%)	222 (94%)	13 (6%)	27	48
3	H	199/209 (95%)	192 (96%)	7 (4%)	43	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	T	199/209 (95%)	192 (96%)	7 (4%)	43 70
All	All	1308/1336 (98%)	1246 (95%)	62 (5%)	32 56

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	7	ARG
1	L	11	VAL
1	L	126	LEU
1	L	129	LEU
1	L	189	LEU
1	L	216	PHE
1	L	235	LEU
1	L	238	LEU
1	L	247	CYS
1	L	269	LEU
1	L	272	TRP
2	M	12	VAL
2	M	22	GLU
2	M	26	LEU
2	M	29	ARG
2	M	47	LEU
2	M	60	LEU
2	M	87	ARG
2	M	94	LEU
2	M	114	LEU
2	M	148	TRP
2	M	156	LEU
2	M	191	LEU
2	M	216	PHE
3	H	12	LEU
3	H	37	ARG
3	H	90	THR
3	H	123	LEU
3	H	208	LEU
3	H	228	LEU
3	H	231	ASP
1	R	7	ARG
1	R	11	VAL
1	R	126	LEU
1	R	129	LEU
1	R	189	LEU

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Mol	Chain	Res	Type
1	R	216	PHE
1	R	235	LEU
1	R	238	LEU
1	R	247	CYS
1	R	269	LEU
1	R	272	TRP
2	S	12	VAL
2	S	22	GLU
2	S	26	LEU
2	S	29	ARG
2	S	47	LEU
2	S	60	LEU
2	S	87	ARG
2	S	94	LEU
2	S	114	LEU
2	S	148	TRP
2	S	156	LEU
2	S	191	LEU
2	S	216	PHE
3	T	12	LEU
3	T	37	ARG
3	T	90	THR
3	T	123	LEU
3	T	208	LEU
3	T	228	LEU
3	T	231	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	87	GLN
1	L	183	ASN
2	M	4	GLN
2	M	9	GLN
2	M	300	ASN
3	H	68	HIS
3	H	194	GLN
3	H	199	GLN
3	H	206	ASN
1	R	87	GLN
2	S	4	GLN
2	S	9	GLN

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Mol	Chain	Res	Type
2	S	300	ASN
3	T	194	GLN
3	T	199	GLN
3	T	206	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 6 are monoatomic - leaving 22 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	$\# Z > 2$
7	BCL	L	1001	2	38,59,74	1.06	4 (10%)	40,97,115	1.65	11 (27%)
7	BCL	L	1002	1	53,74,74	0.93	4 (7%)	57,115,115	1.38	11 (19%)
7	BCL	L	1004	1	53,74,74	0.97	4 (7%)	57,115,115	1.55	11 (19%)
8	BPH	L	1006	-	64,70,70	1.25	8 (12%)	73,101,101	1.56	10 (13%)
9	U10	L	1009	-	44,44,63	1.77	9 (20%)	53,56,79	1.53	10 (18%)
7	BCL	M	1003	2	53,74,74	0.97	5 (9%)	57,115,115	1.44	12 (21%)
8	BPH	M	1005	-	50,56,70	1.17	7 (14%)	56,84,101	1.93	10 (17%)
9	U10	M	1008	-	38,38,63	1.85	11 (28%)	46,49,79	1.30	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	LDA	M	1012	-	15,15,15	4.14	3 (20%)	16,17,17	3.28	3 (18%)
10	LDA	M	1013	-	15,15,15	4.46	3 (20%)	16,17,17	3.13	3 (18%)
10	LDA	M	1014	-	15,15,15	4.54	2 (13%)	16,17,17	2.92	4 (25%)
7	BCL	R	2001	2	38,59,74	1.03	5 (13%)	40,97,115	1.68	7 (17%)
7	BCL	R	2002	1	53,74,74	0.99	3 (5%)	57,115,115	1.34	8 (14%)
7	BCL	R	2004	1	53,74,74	1.00	5 (9%)	57,115,115	1.57	8 (14%)
8	BPH	R	2006	-	64,70,70	1.07	5 (7%)	73,101,101	1.48	9 (12%)
9	U10	R	2009	-	18,18,63	1.80	3 (16%)	22,25,79	1.34	3 (13%)
7	BCL	S	2003	2	53,74,74	0.99	5 (9%)	57,115,115	1.52	11 (19%)
8	BPH	S	2005	-	51,57,70	1.26	5 (9%)	57,85,101	1.74	11 (19%)
9	U10	S	2008	-	32,32,63	1.69	7 (21%)	38,41,79	1.18	4 (10%)
10	LDA	S	2012	-	15,15,15	4.63	3 (20%)	16,17,17	3.29	2 (12%)
10	LDA	S	2013	-	15,15,15	4.39	3 (20%)	16,17,17	3.32	2 (12%)
10	LDA	S	2014	-	15,15,15	4.77	2 (13%)	16,17,17	2.93	3 (18%)

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
7	BCL	L	1001	2	-	0/19/119/137	0/0/9/9
7	BCL	L	1002	1	-	0/37/137/137	0/0/9/9
7	BCL	L	1004	1	-	0/37/137/137	0/0/9/9
8	BPH	L	1006	-	-	0/54/105/105	0/1/6/6
9	U10	L	1009	-	-	0/41/65/87	0/1/1/1
7	BCL	M	1003	2	-	0/37/137/137	0/0/9/9
8	BPH	M	1005	-	-	0/38/89/105	0/1/6/6
9	U10	M	1008	-	-	0/33/57/87	0/1/1/1
10	LDA	M	1012	-	-	0/13/13/13	0/0/0/0
10	LDA	M	1013	-	-	0/13/13/13	0/0/0/0
10	LDA	M	1014	-	-	0/13/13/13	0/0/0/0
7	BCL	R	2001	2	-	0/19/119/137	0/0/9/9
7	BCL	R	2002	1	-	0/37/137/137	0/0/9/9
7	BCL	R	2004	1	-	0/37/137/137	0/0/9/9
8	BPH	R	2006	-	-	0/54/105/105	0/1/6/6
9	U10	R	2009	-	-	0/9/33/87	0/1/1/1
7	BCL	S	2003	2	-	0/37/137/137	0/0/9/9
8	BPH	S	2005	-	-	0/39/90/105	0/1/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	U10	S	2008	-	-	0/26/50/87	0/1/1/1
10	LDA	S	2012	-	-	0/13/13/13	0/0/0/0
10	LDA	S	2013	-	-	0/13/13/13	0/0/0/0
10	LDA	S	2014	-	-	0/13/13/13	0/0/0/0

All (106) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	S	2014	LDA	O1-N1	-18.09	1.22	1.39
10	S	2012	LDA	O1-N1	-17.32	1.23	1.39
10	M	1014	LDA	O1-N1	-17.26	1.23	1.39
10	M	1013	LDA	O1-N1	-16.79	1.23	1.39
10	S	2013	LDA	O1-N1	-16.59	1.23	1.39
10	M	1012	LDA	O1-N1	-15.60	1.24	1.39
8	L	1006	BPH	C3D-CAD	-3.62	1.39	1.46
8	S	2005	BPH	C3D-CAD	-3.42	1.39	1.46
8	R	2006	BPH	C3D-CAD	-3.35	1.40	1.46
8	L	1006	BPH	C1B-C2B	-3.30	1.38	1.45
8	R	2006	BPH	C1B-C2B	-3.28	1.38	1.45
7	R	2004	BCL	C3D-CAD	-3.17	1.36	1.45
7	R	2004	BCL	O2D-CGD	-3.14	1.25	1.33
7	L	1001	BCL	O2D-CGD	-3.11	1.25	1.33
7	R	2002	BCL	O2D-CGD	-2.99	1.25	1.33
10	S	2012	LDA	CM1-N1	-2.99	1.44	1.49
8	M	1005	BPH	C3D-CAD	-2.94	1.40	1.46
9	L	1009	U10	C7-C8	-2.93	1.46	1.50
8	R	2006	BPH	O2D-CGD	-2.92	1.25	1.33
7	M	1003	BCL	C3B-CAB	-2.91	1.41	1.49
8	S	2005	BPH	O2D-CGD	-2.90	1.25	1.33
7	S	2003	BCL	O2D-CGD	-2.87	1.25	1.33
7	L	1004	BCL	O2D-CGD	-2.85	1.25	1.33
9	S	2008	U10	C7-C8	-2.83	1.46	1.50
7	M	1003	BCL	C3D-CAD	-2.82	1.37	1.45
7	R	2001	BCL	O2D-CGD	-2.80	1.26	1.33
8	L	1006	BPH	O2A-CGA	-2.77	1.24	1.33
7	L	1001	BCL	O2A-CGA	-2.75	1.25	1.33
8	S	2005	BPH	C1B-C2B	-2.74	1.39	1.45
7	M	1003	BCL	O2D-CGD	-2.71	1.26	1.33
8	M	1005	BPH	O2A-CGA	-2.71	1.25	1.33
7	L	1002	BCL	O2D-CGD	-2.70	1.26	1.33
7	L	1004	BCL	C3D-CAD	-2.68	1.38	1.45
9	M	1008	U10	C7-C8	-2.68	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	1003	BCL	O2A-CGA	-2.62	1.25	1.33
7	R	2002	BCL	O2A-CGA	-2.59	1.25	1.33
10	S	2012	LDA	CM2-N1	-2.58	1.45	1.49
8	S	2005	BPH	O2A-CGA	-2.55	1.25	1.33
8	L	1006	BPH	O2D-CGD	-2.53	1.26	1.33
8	M	1005	BPH	O2D-CGD	-2.52	1.26	1.33
7	S	2003	BCL	O2A-CGA	-2.51	1.25	1.33
7	R	2001	BCL	O2A-CGA	-2.49	1.25	1.33
10	M	1013	LDA	CM2-N1	-2.49	1.45	1.49
7	L	1002	BCL	C3B-CAB	-2.48	1.42	1.49
7	L	1002	BCL	O2A-CGA	-2.45	1.25	1.33
7	S	2003	BCL	C3B-CAB	-2.43	1.42	1.49
7	L	1004	BCL	O2A-CGA	-2.42	1.26	1.33
8	R	2006	BPH	O2A-CGA	-2.42	1.26	1.33
9	S	2008	U10	C4-C5	-2.40	1.42	1.48
9	M	1008	U10	C27-C28	-2.39	1.43	1.50
7	R	2001	BCL	C3B-CAB	-2.38	1.42	1.49
7	S	2003	BCL	C3D-CAD	-2.33	1.39	1.45
7	L	1001	BCL	C3B-CAB	-2.29	1.42	1.49
10	S	2014	LDA	CM2-N1	-2.26	1.46	1.49
7	R	2001	BCL	C3D-CAD	-2.23	1.39	1.45
7	L	1001	BCL	C3D-CAD	-2.22	1.39	1.45
10	S	2013	LDA	CM2-N1	-2.22	1.46	1.49
10	M	1012	LDA	CM2-N1	-2.19	1.46	1.49
7	R	2004	BCL	O2A-CGA	-2.18	1.26	1.33
10	M	1012	LDA	CM1-N1	-2.18	1.46	1.49
8	M	1005	BPH	C1B-C2B	-2.15	1.41	1.45
10	M	1013	LDA	CM1-N1	-2.13	1.46	1.49
9	M	1008	U10	C3-C2	-2.11	1.42	1.48
7	R	2004	BCL	C3B-CAB	-2.10	1.43	1.49
9	L	1009	U10	C17-C18	-2.06	1.44	1.50
10	M	1014	LDA	CM1-N1	-2.05	1.46	1.49
10	S	2013	LDA	CM1-N1	-2.05	1.46	1.49
8	L	1006	BPH	CHA-C1A	2.00	1.41	1.37
9	M	1008	U10	C28-C29	2.05	1.38	1.32
9	M	1008	U10	O3-C3	2.11	1.42	1.37
8	M	1005	BPH	CHC-C1C	2.11	1.40	1.36
8	M	1005	BPH	CMB-C2B	2.15	1.55	1.50
9	S	2008	U10	C4-C3	2.17	1.45	1.35
9	M	1008	U10	C23-C24	2.21	1.37	1.33
7	R	2001	BCL	C2-C3	2.31	1.39	1.32
9	M	1008	U10	C7-C6	2.59	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	1003	BCL	C2-C3	2.64	1.38	1.33
9	S	2008	U10	C13-C14	2.65	1.38	1.33
8	M	1005	BPH	C2-C3	2.68	1.38	1.33
7	L	1004	BCL	C2-C3	2.68	1.38	1.33
9	L	1009	U10	C23-C24	2.71	1.38	1.33
8	L	1006	BPH	CBB-CAB	2.76	1.56	1.50
7	L	1002	BCL	C2-C3	2.92	1.38	1.33
9	M	1008	U10	C8-C9	2.96	1.38	1.33
9	L	1009	U10	C18-C19	3.08	1.39	1.33
9	R	2009	U10	C8-C9	3.11	1.41	1.32
9	L	1009	U10	C13-C14	3.15	1.39	1.33
9	R	2009	U10	C7-C6	3.33	1.57	1.51
8	L	1006	BPH	CHC-C1C	3.37	1.43	1.36
9	S	2008	U10	C8-C9	3.42	1.39	1.33
7	R	2004	BCL	C2-C3	3.46	1.39	1.33
8	R	2006	BPH	C2-C3	3.55	1.39	1.33
9	M	1008	U10	C18-C19	3.60	1.40	1.33
8	S	2005	BPH	C2-C3	3.78	1.40	1.33
9	L	1009	U10	C8-C9	3.81	1.40	1.33
9	L	1009	U10	C33-C34	3.83	1.40	1.33
9	L	1009	U10	C28-C29	3.96	1.40	1.33
9	L	1009	U10	C6-C1	3.99	1.44	1.35
8	L	1006	BPH	C2-C3	4.04	1.40	1.33
9	S	2008	U10	C6-C1	4.06	1.44	1.35
7	R	2002	BCL	C2-C3	4.08	1.41	1.33
9	S	2008	U10	C18-C19	4.08	1.41	1.33
7	S	2003	BCL	C2-C3	4.20	1.41	1.33
9	R	2009	U10	C6-C1	4.37	1.45	1.35
9	M	1008	U10	C13-C14	4.38	1.41	1.33
9	M	1008	U10	C6-C1	5.13	1.47	1.35

All (157) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	S	2012	LDA	CM2-N1-CM1	-11.49	95.87	108.83
10	S	2013	LDA	CM2-N1-CM1	-11.30	96.08	108.83
10	M	1012	LDA	CM2-N1-CM1	-11.27	96.11	108.83
10	M	1013	LDA	CM2-N1-CM1	-10.85	96.59	108.83
10	S	2014	LDA	CM2-N1-CM1	-10.43	97.06	108.83
10	M	1014	LDA	CM2-N1-CM1	-9.94	97.62	108.83
8	S	2005	BPH	C4D-C3D-C2D	-5.44	100.06	107.08
7	R	2004	BCL	OBD-CAD-C3D	-5.33	117.48	128.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	R	2006	BPH	C4D-C3D-C2D	-4.79	100.90	107.08
8	M	1005	BPH	C4D-C3D-C2D	-4.25	101.60	107.08
8	L	1006	BPH	C4D-C3D-C2D	-4.12	101.76	107.08
8	L	1006	BPH	OBD-CAD-C3D	-3.57	121.06	128.35
7	S	2003	BCL	OBD-CAD-CBD	-3.43	120.76	125.94
8	M	1005	BPH	O1D-CGD-CBD	-3.42	119.72	124.62
8	L	1006	BPH	O1D-CGD-CBD	-3.25	119.97	124.62
7	L	1001	BCL	OBD-CAD-C3D	-3.15	121.93	128.35
7	M	1003	BCL	C7-C6-C5	-3.15	103.77	113.06
7	R	2001	BCL	OBD-CAD-C3D	-3.00	122.23	128.35
7	L	1004	BCL	O1D-CGD-CBD	-2.98	120.36	124.62
7	L	1004	BCL	OBD-CAD-CBD	-2.96	121.47	125.94
8	S	2005	BPH	O1D-CGD-CBD	-2.95	120.39	124.62
9	L	1009	U10	C16-C17-C18	-2.94	104.00	111.69
8	R	2006	BPH	O1D-CGD-CBD	-2.90	120.47	124.62
7	R	2001	BCL	O1D-CGD-CBD	-2.86	120.52	124.62
9	M	1008	U10	C17-C18-C19	-2.86	121.55	127.76
9	R	2009	U10	C1-C6-C5	-2.83	116.89	120.12
7	R	2004	BCL	CED-O2D-CGD	-2.82	109.38	115.99
7	S	2003	BCL	CMB-C2B-C1B	-2.76	123.80	128.36
9	M	1008	U10	O5-C5-C6	-2.75	116.50	121.68
7	R	2002	BCL	CMB-C2B-C1B	-2.75	123.81	128.36
7	S	2003	BCL	O1D-CGD-CBD	-2.74	120.70	124.62
7	M	1003	BCL	O1D-CGD-CBD	-2.73	120.71	124.62
9	M	1008	U10	C12-C13-C14	-2.72	121.85	127.76
7	M	1003	BCL	OBD-CAD-C3D	-2.71	122.83	128.35
7	R	2004	BCL	C7-C6-C5	-2.68	105.14	113.06
7	L	1001	BCL	OBB-CAB-CBB	-2.64	113.80	120.13
8	M	1005	BPH	OBD-CAD-CBD	-2.63	121.96	125.94
7	L	1004	BCL	CAC-C3C-C4C	-2.63	106.75	112.58
7	M	1003	BCL	CMB-C2B-C1B	-2.62	124.02	128.36
7	L	1002	BCL	O1D-CGD-CBD	-2.62	120.87	124.62
9	L	1009	U10	C30-C29-C28	-2.60	118.39	123.50
7	L	1004	BCL	OBD-CAD-C3D	-2.55	123.14	128.35
7	S	2003	BCL	CAC-C3C-C4C	-2.55	106.93	112.58
7	R	2004	BCL	CAC-C3C-C4C	-2.54	106.95	112.58
8	L	1006	BPH	C7-C6-C5	-2.45	105.84	113.06
7	L	1001	BCL	O1D-CGD-CBD	-2.40	121.18	124.62
8	S	2005	BPH	OBD-CAD-CBD	-2.37	122.36	125.94
7	L	1002	BCL	CMB-C2B-C1B	-2.34	124.50	128.36
7	M	1003	BCL	CAC-C3C-C4C	-2.33	107.41	112.58
10	M	1014	LDA	C6-C5-C4	-2.33	102.48	114.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	R	2002	BCL	O1D-CGD-CBD	-2.32	121.29	124.62
7	L	1001	BCL	CMB-C2B-C1B	-2.32	124.52	128.36
8	R	2006	BPH	OBD-CAD-C3D	-2.32	123.63	128.35
7	L	1002	BCL	CHA-C1A-NA	-2.30	120.41	126.06
8	R	2006	BPH	C1C-NC-C4C	-2.29	108.09	110.44
7	L	1002	BCL	CAC-C3C-C4C	-2.28	107.52	112.58
7	L	1001	BCL	CHA-C1A-NA	-2.28	120.46	126.06
8	R	2006	BPH	C7-C6-C5	-2.27	106.35	113.06
8	M	1005	BPH	C4-C3-C2	-2.26	119.06	123.50
7	R	2002	BCL	CAC-C3C-C4C	-2.25	107.58	112.58
9	L	1009	U10	C25-C24-C23	-2.22	119.14	123.50
7	S	2003	BCL	CHA-C1A-NA	-2.22	120.61	126.06
10	M	1013	LDA	C6-C5-C4	-2.21	103.09	114.53
7	L	1004	BCL	CMB-C2B-C1B	-2.21	124.71	128.36
10	M	1012	LDA	C6-C5-C4	-2.19	103.24	114.53
7	R	2004	BCL	O1D-CGD-CBD	-2.18	121.50	124.62
9	L	1009	U10	C17-C18-C19	-2.12	123.15	127.76
8	R	2006	BPH	OBD-CAD-CBD	-2.11	122.75	125.94
7	R	2001	BCL	CMB-C2B-C1B	-2.11	124.88	128.36
8	L	1006	BPH	CMA-C3A-C4A	-2.10	106.17	113.01
9	S	2008	U10	C15-C14-C13	-2.09	119.39	123.50
7	L	1004	BCL	CHA-C1A-NA	-2.06	121.00	126.06
8	S	2005	BPH	C1C-NC-C4C	-2.05	108.34	110.44
10	M	1014	LDA	C4-C3-C2	-2.04	103.97	114.53
7	L	1002	BCL	CAA-C2A-C1A	-2.04	105.29	112.47
10	S	2014	LDA	C4-C3-C2	-2.03	104.04	114.53
7	R	2004	BCL	C6-C5-C3	-2.02	108.05	112.48
7	R	2002	BCL	CHA-C1A-NA	-2.01	121.11	126.06
7	L	1001	BCL	CMB-C2B-C3B	2.02	129.04	125.09
7	M	1003	BCL	C4A-NA-C1A	2.02	108.97	106.36
8	S	2005	BPH	CED-O2D-CGD	2.03	120.75	115.99
8	M	1005	BPH	C2B-C1B-NB	2.03	112.77	109.73
7	M	1003	BCL	C2C-C3C-C4C	2.03	104.94	101.50
7	L	1001	BCL	C1-C2-C3	2.04	130.04	126.71
7	L	1004	BCL	CHB-C4A-NA	2.04	127.33	124.51
7	L	1001	BCL	C4A-NA-C1A	2.09	109.06	106.36
7	L	1002	BCL	O2D-CGD-CBD	2.09	114.17	111.30
8	L	1006	BPH	CED-O2D-CGD	2.11	120.95	115.99
9	L	1009	U10	C20-C19-C21	2.13	118.66	115.41
7	S	2003	BCL	C4-C3-C5	2.14	118.67	115.41
9	L	1009	U10	C7-C6-C5	2.14	121.08	118.56
7	R	2002	BCL	C1D-CHD-C4C	2.20	129.43	126.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	1004	BCL	CMB-C2B-C3B	2.23	129.45	125.09
7	L	1002	BCL	CMB-C2B-C3B	2.27	129.52	125.09
8	S	2005	BPH	C3C-C4C-NC	2.28	110.22	107.93
8	S	2005	BPH	C2B-C1B-NB	2.28	113.15	109.73
7	L	1001	BCL	CHB-C4A-NA	2.30	127.69	124.51
9	L	1009	U10	C15-C14-C16	2.39	119.05	115.41
7	S	2003	BCL	O2A-CGA-CBA	2.39	119.17	111.90
9	S	2008	U10	C4M-O4-C4	2.39	125.11	116.61
9	L	1009	U10	C35-C34-C36	2.41	118.41	115.68
7	M	1003	BCL	C15-C13-C12	2.43	126.77	112.27
8	L	1006	BPH	CAC-C3C-C4C	2.46	118.98	112.67
9	R	2009	U10	C8-C7-C6	2.47	119.06	111.64
7	R	2002	BCL	CMB-C2B-C3B	2.49	129.95	125.09
7	M	1003	BCL	CED-O2D-CGD	2.53	121.91	115.99
9	M	1008	U10	C31-C29-C30	2.55	120.92	114.64
7	R	2001	BCL	C1-C2-C3	2.60	130.97	126.71
9	S	2008	U10	C10-C9-C11	2.71	119.55	115.41
7	R	2002	BCL	CED-O2D-CGD	2.72	122.37	115.99
7	M	1003	BCL	CMB-C2B-C3B	2.72	130.41	125.09
7	L	1002	BCL	C3D-CAD-CBD	2.74	111.46	107.60
7	M	1003	BCL	C3D-CAD-CBD	2.74	111.47	107.60
9	R	2009	U10	C3M-O3-C3	2.78	126.49	116.61
9	S	2008	U10	C15-C14-C16	2.78	119.66	115.41
7	R	2001	BCL	CMB-C2B-C3B	2.79	130.54	125.09
7	M	1003	BCL	O2D-CGD-CBD	2.83	115.18	111.30
7	L	1002	BCL	C6-C5-C3	2.85	118.73	112.48
7	L	1004	BCL	C4-C3-C5	2.87	119.79	115.41
7	S	2003	BCL	CMB-C2B-C3B	2.91	130.78	125.09
7	R	2002	BCL	C6-C5-C3	3.10	119.29	112.48
8	S	2005	BPH	C2C-C3C-C4C	3.11	106.78	101.50
7	L	1001	BCL	O2D-CGD-CBD	3.15	115.62	111.30
7	L	1002	BCL	CED-O2D-CGD	3.17	123.41	115.99
7	S	2003	BCL	CED-O2D-CGD	3.18	123.44	115.99
9	L	1009	U10	C30-C29-C31	3.26	120.39	115.41
8	M	1005	BPH	CED-O2D-CGD	3.35	123.85	115.99
7	L	1002	BCL	C4-C3-C5	3.35	120.53	115.41
10	S	2014	LDA	O1-N1-C1	3.41	114.11	110.27
7	R	2004	BCL	O2D-CGD-CBD	3.54	116.15	111.30
7	S	2003	BCL	O2D-CGD-CBD	3.54	116.16	111.30
8	M	1005	BPH	O2D-CGD-CBD	3.65	116.30	111.30
7	L	1001	BCL	C3D-CAD-CBD	3.87	113.07	107.60
8	S	2005	BPH	C3D-CAD-CBD	3.90	113.11	107.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	1004	BCL	O2D-CGD-CBD	4.12	116.96	111.30
8	M	1005	BPH	C3D-CAD-CBD	4.17	113.49	107.60
7	R	2001	BCL	C3D-CAD-CBD	4.23	113.57	107.60
8	R	2006	BPH	C3D-CAD-CBD	4.26	113.62	107.60
8	L	1006	BPH	O2D-CGD-CBD	4.27	117.16	111.30
10	M	1014	LDA	O1-N1-C1	4.37	115.19	110.27
7	R	2004	BCL	C3D-CAD-CBD	4.37	113.78	107.60
8	S	2005	BPH	O2D-CGD-CBD	4.39	117.33	111.30
7	R	2001	BCL	O2D-CGD-CBD	4.40	117.34	111.30
8	R	2006	BPH	C3C-C4C-NC	4.41	112.34	107.93
8	L	1006	BPH	C3D-CAD-CBD	4.53	114.00	107.60
9	L	1009	U10	C25-C24-C26	4.55	122.36	115.41
8	S	2005	BPH	C4-C3-C5	4.56	122.37	115.41
7	S	2003	BCL	C3D-CAD-CBD	4.64	114.15	107.60
8	R	2006	BPH	O2D-CGD-CBD	4.72	117.78	111.30
8	M	1005	BPH	C3C-C4C-NC	4.79	112.72	107.93
10	M	1013	LDA	O1-N1-C1	4.89	115.78	110.27
7	L	1004	BCL	C3D-CAD-CBD	4.90	114.52	107.60
10	S	2012	LDA	O1-N1-C1	5.08	115.99	110.27
10	M	1012	LDA	O1-N1-C1	5.29	116.22	110.27
8	L	1006	BPH	C3C-C4C-NC	5.34	113.28	107.93
10	S	2013	LDA	O1-N1-C1	5.88	116.89	110.27
8	M	1005	BPH	C4-C3-C5	7.14	123.77	115.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

22 monomers are involved in 84 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	L	1001	BCL	4	0
7	L	1002	BCL	9	0
7	L	1004	BCL	7	0
8	L	1006	BPH	5	0
9	L	1009	U10	2	0
7	M	1003	BCL	8	0
8	M	1005	BPH	5	0
9	M	1008	U10	2	0
10	M	1012	LDA	1	0
10	M	1013	LDA	1	0
10	M	1014	LDA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	R	2001	BCL	3	0
7	R	2002	BCL	9	0
7	R	2004	BCL	6	0
8	R	2006	BPH	14	0
9	R	2009	U10	3	0
7	S	2003	BCL	6	0
8	S	2005	BPH	4	0
9	S	2008	U10	2	0
10	S	2012	LDA	2	0
10	S	2013	LDA	1	0
10	S	2014	LDA	2	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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