Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:06 PM GMT

PDB ID	:	1S00
Title	:	PHOTOSYNTHETIC REACTION CENTER DOUBLE MUTANT FROM RHODOBACTER SPHAEROIDES WITH ASP L213 REPLACED WITH ASN AND ARG M233 REPLACED WITH CYS IN THE CHARGE-SEPARATED D+QAQB- STATE
Authors	:	Xu, Q.; Axelrod, H.L.; Abresch, E.C.; Paddock, M.L.; Okamura, M.Y.; Feher, G.
Deposited on	:	2003-12-29
Resolution	:	2.60 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 (1)) were used in the production of this report:

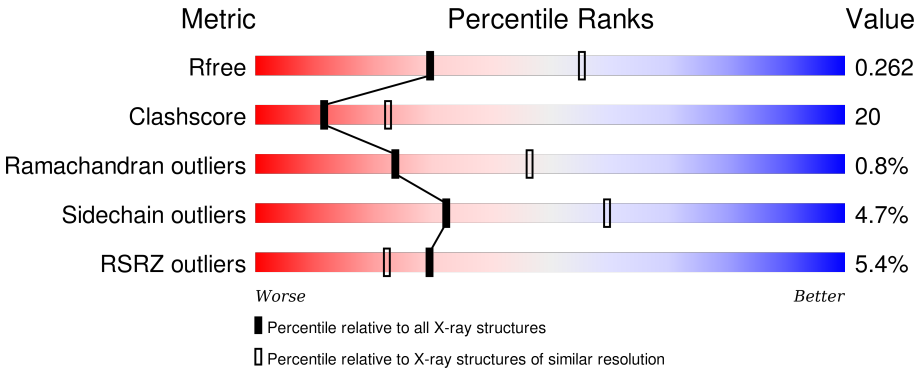
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	L	281	% 63% 34% ·
1	R	281	9% 55% 42% ·
2	M	307	4% 71% 23% · ·
2	S	307	4% 62% 32% · ·
3	H	260	3% 65% 28% · 5%

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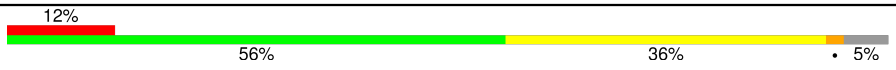
Mol	Chain	Length	Quality of chain
3	T	260	

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
4	BCL	S	2001	-	-	-	X
4	BCL	S	2003	-	-	-	X
5	BPH	L	1006	X	-	-	-
5	BPH	M	1005	X	-	-	-
5	BPH	R	2006	X	-	-	-
6	U10	L	1009[A]	-	-	-	X
6	U10	L	1009[B]	-	-	-	X
6	U10	M	1008	-	-	-	X
6	U10	R	2009[A]	-	-	-	X
6	U10	R	2009[B]	-	-	-	X
8	SPO	M	1010	-	-	-	X
8	SPO	S	2010	-	-	-	X
9	LDA	M	1011	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 14144 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	356	361	8			
1	R	281	Total	C	N	O	S	0	0	0
			2232	1507	356	361	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	213	ASN	ASP	ENGINEERED	UNP P02954
R	213	ASN	ASP	ENGINEERED	UNP P02954

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	301	Total	C	N	O	S	0	0	0
			2399	1602	390	396	11			
2	S	299	Total	C	N	O	S	0	0	0
			2385	1594	388	392	11			

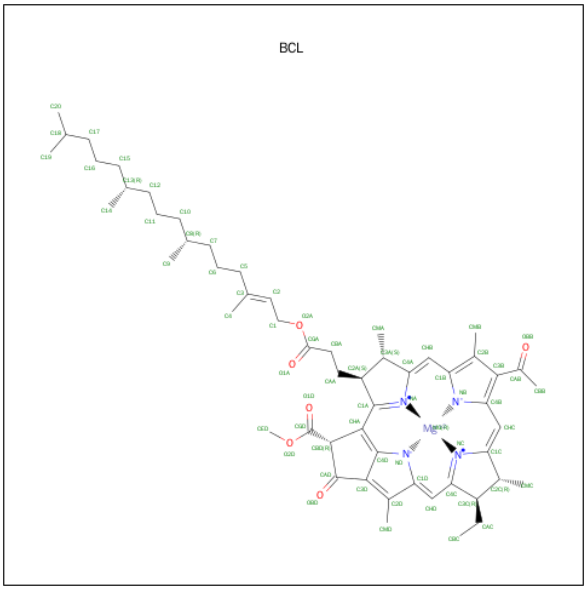
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	233	CYS	ARG	ENGINEERED	UNP P02953
S	233	CYS	ARG	ENGINEERED	UNP P02953

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

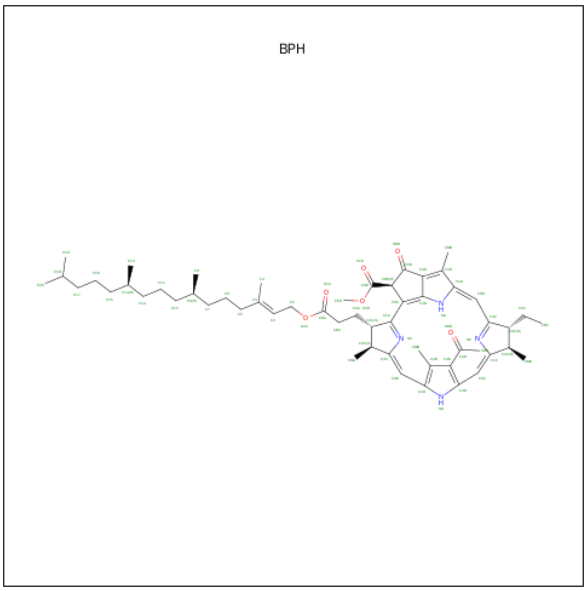
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	246	Total	C	N	O	S	0	0	0
			1869	1196	320	343	10			
3	T	246	Total	C	N	O	S	0	0	0
			1869	1196	320	343	10			

- Molecule 4 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



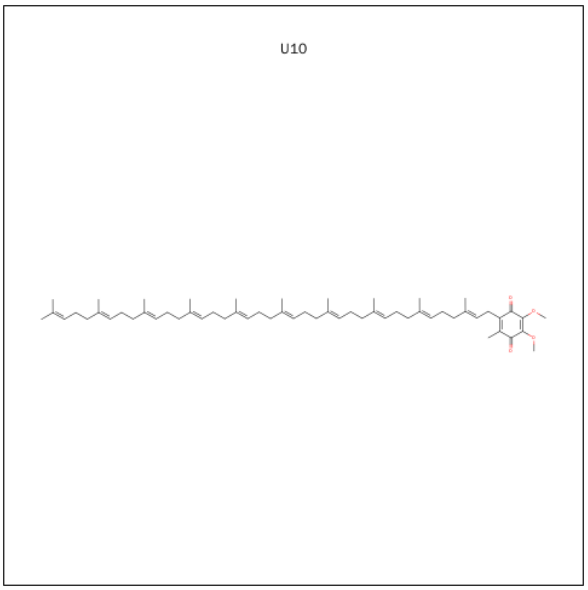
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	R	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	S	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
4	S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

- Molecule 5 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	M	1	Total	C	N	O	0	0
			55	45	4	6		
5	R	1	Total	C	N	O	0	0
			65	55	4	6		
5	S	1	Total	C	N	O	0	0
			51	41	4	6		

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

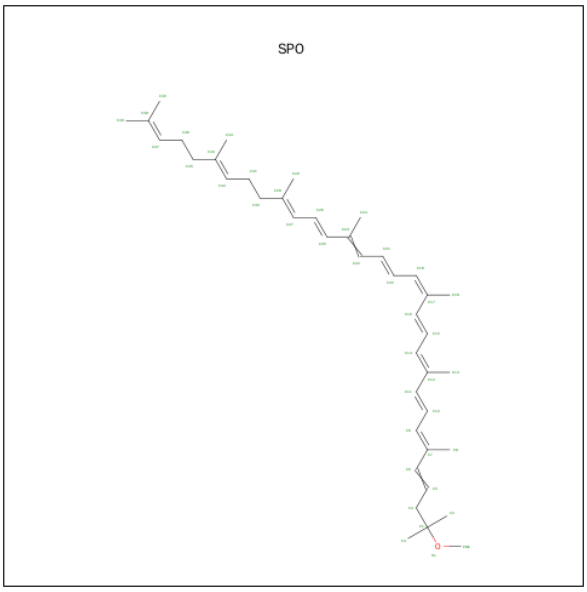


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	1	Total C O 60 52 8	0	1
6	M	1	Total C O 38 34 4	0	0
6	R	1	Total C O 36 28 8	0	1
6	S	1	Total C O 32 28 4	0	0

- Molecule 7 is FE (II) ION (three-letter code: FE2) (formula: Fe).

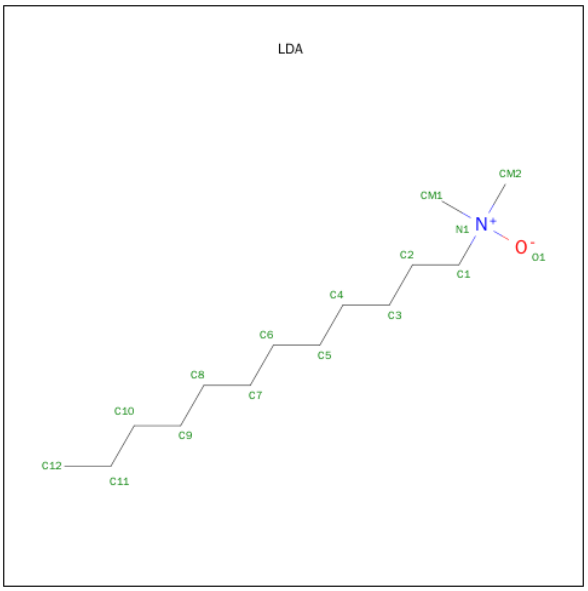
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	S	1	Total Fe 1 1	0	0
7	M	1	Total Fe 1 1	0	0

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



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

- Molecule 9 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



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

- Molecule 10 is water.

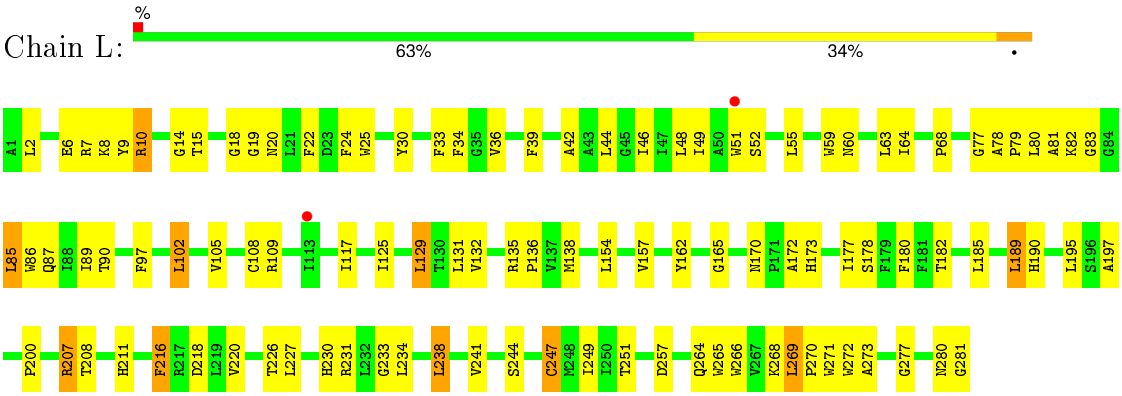
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	L	26	Total O 26 26	0	0
10	M	42	Total O 42 42	0	0
10	H	39	Total O 39 39	0	0
10	R	13	Total O 13 13	0	0
10	S	24	Total O 24 24	0	0
10	T	12	Total O 12 12	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

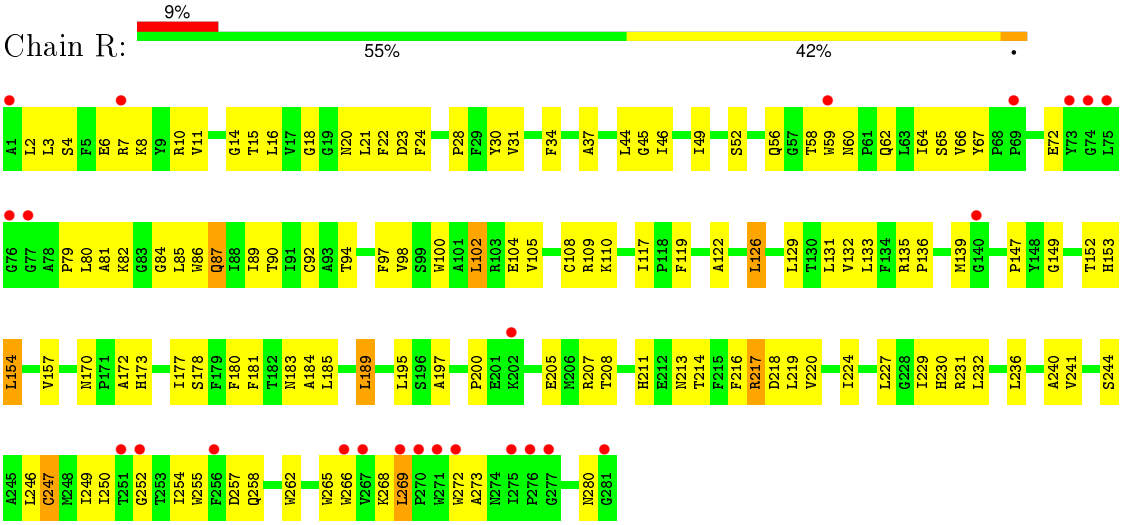
• Molecule 1: Reaction center protein L chain

Chain L:



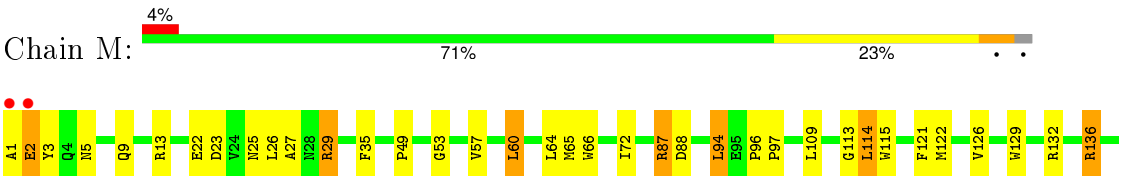
• Molecule 1: Reaction center protein L chain

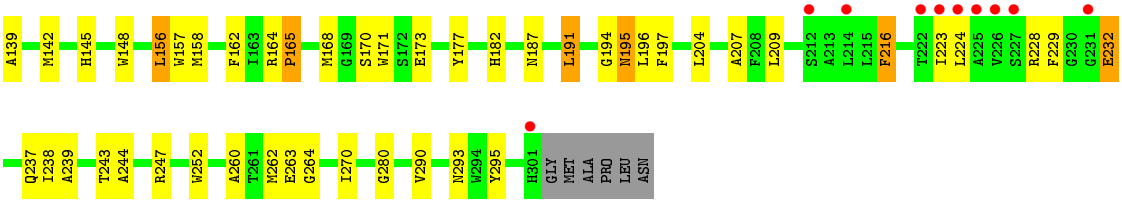
Chain R:



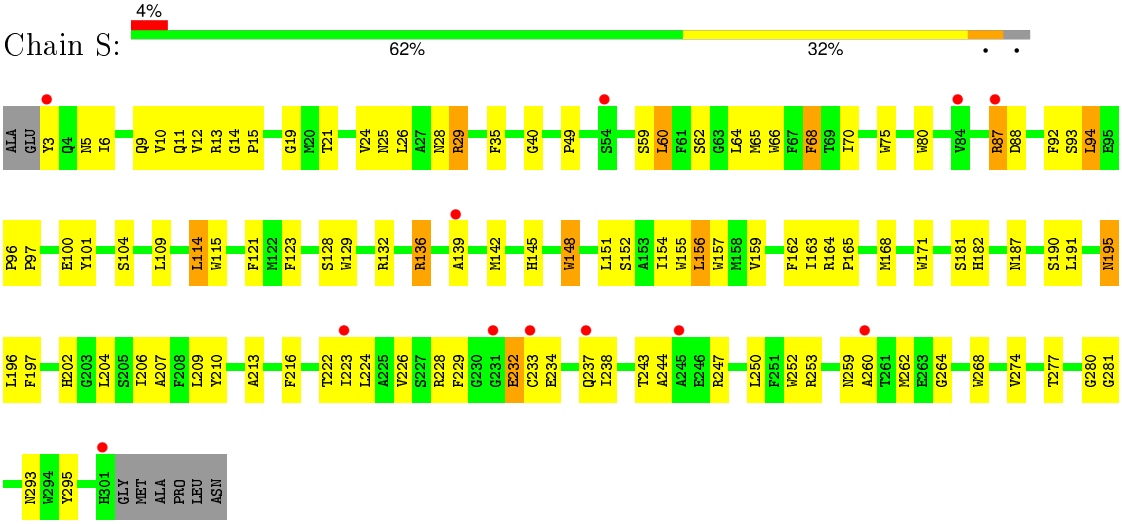
• Molecule 2: Reaction center protein M chain

Chain M:

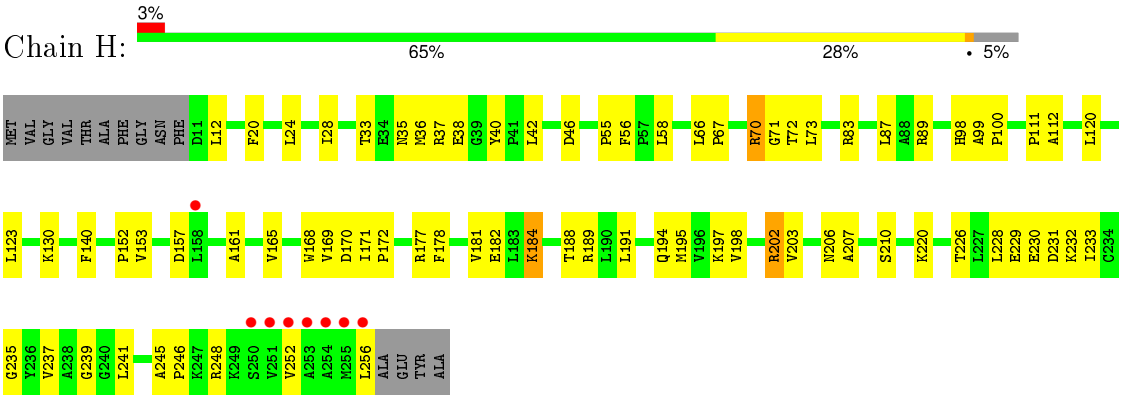




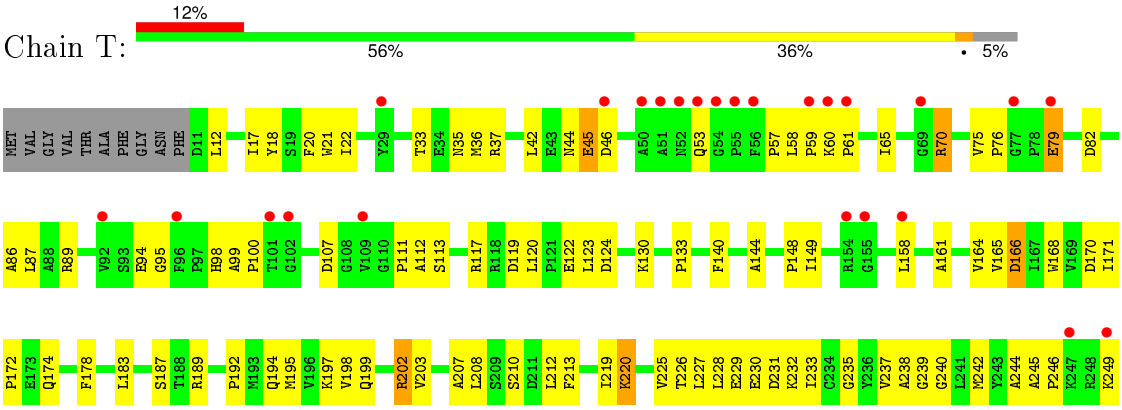
• Molecule 2: Reaction center protein M chain

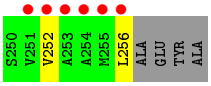


• Molecule 3: Reaction center protein H chain



• Molecule 3: Reaction center protein H chain




S250
V251
V252
A253
A254
M255
L256
ALA
GLU
TYR
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	137.73Å 137.73Å 277.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.84 – 2.60 39.84 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.8 (39.84-2.60) 94.9 (39.84-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.226 , 0.268 0.223 , 0.262	Depositor DCC
R_{free} test set	3965 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	51.1	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 56.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 78308 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	14144	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, LDA, BPH, FE2, 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	0.43	0/2320	0.60	0/3175
1	R	0.38	0/2320	0.58	0/3175
2	M	0.42	0/2491	0.59	0/3402
2	S	0.39	0/2477	0.55	0/3383
3	H	0.39	0/1917	0.64	0/2608
3	T	0.33	0/1917	0.60	0/2608
All	All	0.39	0/13442	0.59	0/18351

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

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	2189	103	0
1	R	2232	0	2189	120	0
2	M	2399	0	2310	83	0
2	S	2385	0	2296	114	0
3	H	1869	0	1884	74	0
3	T	1869	0	1884	99	0
4	L	183	0	189	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	M	66	0	74	19	0
4	R	66	0	74	11	0
4	S	183	0	189	29	0
5	L	65	0	74	5	0
5	M	55	0	53	0	0
5	R	65	0	74	8	0
5	S	51	0	45	7	0
6	L	60	0	70	3	0
6	M	38	0	47	0	0
6	R	36	0	30	3	0
6	S	32	0	39	0	0
7	M	1	0	0	0	0
7	S	1	0	0	0	0
8	M	42	0	60	6	0
8	S	42	0	60	2	0
9	M	16	0	31	2	0
10	H	39	0	0	2	0
10	L	26	0	0	4	0
10	M	42	0	0	1	0
10	R	13	0	0	0	0
10	S	24	0	0	2	0
10	T	12	0	0	1	0
All	All	14144	0	13861	565	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 20.

All (565) 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:R:200:PRO:HB3	1:R:207:ARG:HD3	1.42	1.02
2:S:157:TRP:HB2	4:S:2003:BCL:H62	1.44	0.99
1:R:219:LEU:HD13	1:R:220:VAL:HG23	1.48	0.95
3:T:226:THR:OG1	3:T:229:GLU:HG3	1.68	0.93
1:R:208:THR:H	1:R:211:HIS:HD2	1.18	0.92
1:R:189:LEU:HG	1:R:216:PHE:HZ	1.37	0.90
1:L:241:VAL:HG21	5:L:1006:BPH:HAC1	1.53	0.89
2:M:157:TRP:HB2	4:M:1003:BCL:H62	1.57	0.86
1:R:208:THR:H	1:R:211:HIS:CD2	1.94	0.86
2:M:239:ALA:HB1	3:H:66:LEU:HD11	1.60	0.83
1:L:55:LEU:HD13	1:L:81:ALA:HB2	1.59	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:77:GLY:HA2	1:L:87:GLN:HE22	1.44	0.82
2:S:21:THR:HG23	2:S:26:LEU:HD21	1.59	0.82
3:T:194:GLN:H	3:T:194:GLN:NE2	1.78	0.81
1:R:153:HIS:O	1:R:157:VAL:HG23	1.81	0.81
2:S:243:THR:O	2:S:247:ARG:HG3	1.81	0.81
2:M:13:ARG:HD2	2:M:35:PHE:CD2	2.16	0.80
1:L:52:SER:HB2	1:L:85:LEU:HD23	1.63	0.80
1:L:189:LEU:HG	1:L:216:PHE:HZ	1.46	0.79
3:H:70:ARG:HH11	3:H:70:ARG:HG2	1.47	0.79
3:H:228:LEU:HD11	3:H:232:LYS:HE3	1.63	0.78
2:S:197:PHE:HZ	4:S:2003:BCL:HBB2	1.47	0.78
1:L:79:PRO:HG2	1:L:82:LYS:HB2	1.66	0.77
1:L:227:LEU:HD13	2:M:232:GLU:HG2	1.65	0.77
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.66	0.77
1:L:257:ASP:HB3	10:L:1010:HOH:O	1.83	0.77
1:L:157:VAL:HG11	4:M:1003:BCL:HBB1	1.67	0.76
1:R:227:LEU:HD13	2:S:232:GLU:HG2	1.66	0.76
3:H:178:PHE:HZ	3:H:230:GLU:HG2	1.51	0.75
2:S:13:ARG:HD2	2:S:35:PHE:CD2	2.21	0.74
2:M:197:PHE:HZ	4:M:1003:BCL:HBB2	1.53	0.74
2:S:228:ARG:HA	3:T:194:GLN:CG	2.17	0.74
2:S:268:TRP:HE1	3:T:35:ASN:ND2	1.85	0.74
1:R:189:LEU:HG	1:R:216:PHE:CZ	2.24	0.72
3:H:171:ILE:HB	3:H:172:PRO:HD3	1.72	0.72
3:T:252:VAL:O	3:T:256:LEU:HD13	1.89	0.72
1:R:241:VAL:HG21	5:R:2006:BPH:HAC1	1.70	0.72
2:S:11:GLN:HB2	3:T:144:ALA:HB3	1.70	0.72
5:R:2006:BPH:H7C2	4:S:2004:BCL:H201	1.71	0.72
1:R:200:PRO:CB	1:R:207:ARG:HD3	2.18	0.72
4:R:2002:BCL:HBD	4:S:2004:BCL:HBC1	1.70	0.72
1:L:190:HIS:HA	6:L:1009[B]:U10:O2	1.89	0.72
1:R:79:PRO:HG2	1:R:82:LYS:HB2	1.72	0.71
2:S:101:TYR:O	2:S:104:SER:HB3	1.91	0.70
2:S:229:PHE:HB2	2:S:244:ALA:HB2	1.73	0.70
2:M:197:PHE:CZ	4:M:1003:BCL:HBB2	2.26	0.70
1:R:105:VAL:O	1:R:109:ARG:HG3	1.90	0.70
3:T:42:LEU:N	3:T:53:GLN:HE22	1.89	0.70
1:R:195:LEU:HB3	2:S:145:HIS:CD2	2.26	0.70
2:S:136:ARG:NE	2:S:136:ARG:HA	2.06	0.70
3:T:133:PRO:HG3	3:T:168:TRP:CE2	2.27	0.69
4:L:1002:BCL:HBD	4:L:1004:BCL:CBC	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:207:ARG:HG3	2:S:142:MET:HG2	1.74	0.69
2:M:157:TRP:HB2	4:M:1003:BCL:C6	2.21	0.69
1:R:66:VAL:HG11	1:R:89:ILE:HD12	1.72	0.69
3:T:171:ILE:HB	3:T:172:PRO:HD3	1.75	0.68
1:R:4:SER:HB2	3:T:79:GLU:CG	2.24	0.68
2:S:207:ALA:HA	4:S:2004:BCL:O1A	1.93	0.68
2:M:97:PRO:HG2	2:M:171:TRP:HB2	1.76	0.68
3:T:119:ASP:O	3:T:120:LEU:HD23	1.92	0.68
3:T:112:ALA:HA	3:T:235:GLY:O	1.94	0.68
3:T:87:LEU:HD23	3:T:100:PRO:HA	1.75	0.68
2:S:152:SER:HB2	2:S:274:VAL:HG13	1.75	0.67
3:T:194:GLN:H	3:T:194:GLN:CD	1.96	0.67
4:L:1004:BCL:HMA1	4:L:1004:BCL:H121	1.77	0.67
2:S:9:GLN:NE2	3:T:198:VAL:H	1.94	0.66
1:R:60:ASN:O	1:R:64:ILE:HG13	1.96	0.66
1:L:208:THR:H	1:L:211:HIS:CD2	2.13	0.66
1:R:52:SER:HB2	1:R:85:LEU:HD23	1.76	0.66
2:S:237:GLN:HB2	2:S:262:MET:HG2	1.78	0.66
2:M:243:THR:O	2:M:247:ARG:HG3	1.96	0.66
2:M:228:ARG:HA	3:H:194:GLN:CG	2.26	0.66
4:R:2002:BCL:HBD	4:S:2004:BCL:CBC	2.25	0.66
1:R:2:LEU:HB3	1:R:6:GLU:HB3	1.77	0.66
3:T:189:ARG:HH11	3:T:189:ARG:HG2	1.60	0.65
2:M:9:GLN:NE2	3:H:198:VAL:H	1.95	0.65
3:H:202:ARG:HG2	3:H:203:VAL:N	2.10	0.65
1:L:14:GLY:O	1:L:109:ARG:HD3	1.97	0.65
3:H:37:ARG:O	3:H:38:GLU:HG2	1.97	0.65
1:R:85:LEU:O	1:R:89:ILE:HG13	1.96	0.65
3:T:165:VAL:O	3:T:166:ASP:HB2	1.94	0.65
2:M:2:GLU:O	2:M:3:TYR:HB3	1.98	0.64
1:L:265:TRP:O	1:L:269:LEU:HD13	1.97	0.64
2:M:156:LEU:HD13	4:M:1003:BCL:H43	1.79	0.64
1:R:4:SER:HB2	3:T:79:GLU:HG2	1.79	0.64
3:H:226:THR:OG1	3:H:229:GLU:HG3	1.97	0.64
3:H:170:ASP:HB2	3:H:177:ARG:HG3	1.79	0.63
1:L:218:ASP:OD1	2:M:29:ARG:HD2	1.98	0.63
2:M:53:GLY:O	2:M:57:VAL:HG23	1.97	0.63
2:M:228:ARG:HA	3:H:194:GLN:HG2	1.81	0.63
2:M:9:GLN:HE22	3:H:197:LYS:HA	1.62	0.63
1:L:195:LEU:HB3	2:M:145:HIS:CD2	2.33	0.63
2:S:25:ASN:HD22	2:S:28:ASN:ND2	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:112:ALA:HB2	3:H:239:GLY:HA3	1.80	0.63
4:L:1001:BCL:HBB3	4:M:1003:BCL:H41	1.79	0.63
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.33	0.62
4:L:1001:BCL:HBC1	4:M:1003:BCL:CBD	2.29	0.62
1:R:205:GLU:HG2	3:T:65:ILE:HG22	1.82	0.62
3:T:130:LYS:HE3	3:T:170:ASP:OD2	1.99	0.62
3:H:220:LYS:HB2	3:H:220:LYS:NZ	2.15	0.62
1:R:8:LYS:HD2	3:T:113:SER:HB3	1.82	0.62
3:H:130:LYS:HE3	3:H:170:ASP:OD2	1.99	0.62
1:L:7:ARG:HH12	3:H:87:LEU:HB2	1.65	0.62
2:S:109:LEU:HD22	2:S:114:LEU:HD13	1.81	0.61
2:S:60:LEU:O	2:S:64:LEU:HG	2.00	0.61
4:L:1002:BCL:HBD	4:L:1004:BCL:HBC1	1.81	0.61
1:R:20:ASN:HA	1:R:23:ASP:HB2	1.82	0.61
1:L:189:LEU:HG	1:L:216:PHE:CZ	2.33	0.61
3:H:87:LEU:HD23	3:H:100:PRO:HA	1.81	0.61
2:S:97:PRO:HG2	2:S:171:TRP:HB2	1.80	0.61
2:S:229:PHE:CE2	2:S:247:ARG:HD2	2.36	0.61
1:L:208:THR:H	1:L:211:HIS:HD2	1.47	0.61
4:S:2001:BCL:HBC1	4:S:2003:BCL:CAD	2.30	0.61
2:M:109:LEU:HD22	2:M:114:LEU:HD13	1.83	0.61
1:L:207:ARG:HG2	2:M:142:MET:HG2	1.83	0.60
3:H:70:ARG:HG2	3:H:70:ARG:NH1	2.14	0.60
2:M:260:ALA:HB1	3:H:35:ASN:OD1	2.01	0.60
3:H:229:GLU:O	3:H:233:ILE:HG13	2.01	0.60
1:L:200:PRO:HB3	1:L:207:ARG:HD3	1.83	0.60
2:M:280:GLY:HA2	4:M:1003:BCL:HED2	1.84	0.60
2:S:9:GLN:HE22	3:T:198:VAL:H	1.50	0.60
3:H:161:ALA:HB2	3:H:210:SER:HA	1.82	0.60
1:L:33:PHE:O	1:L:36:VAL:HG22	2.02	0.60
3:T:60:LYS:HG2	3:T:61:PRO:HD2	1.83	0.60
1:R:86:TRP:CZ2	1:R:132:VAL:HG13	2.37	0.59
3:H:112:ALA:HA	3:H:235:GLY:O	2.03	0.59
2:M:136:ARG:NE	2:M:136:ARG:HA	2.16	0.59
2:M:1:ALA:O	2:M:2:GLU:HB2	2.02	0.59
1:R:135:ARG:HB3	1:R:136:PRO:HD3	1.85	0.59
2:M:164:ARG:HB3	2:M:165:PRO:HD3	1.82	0.59
3:T:33:THR:HA	3:T:36:MET:CG	2.32	0.59
2:M:168:MET:CB	2:M:173:GLU:HG3	2.32	0.59
3:T:202:ARG:HG2	3:T:203:VAL:N	2.16	0.59
1:R:265:TRP:O	1:R:269:LEU:HD13	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:1001:BCL:HBC1	4:M:1003:BCL:HBD	1.85	0.59
3:H:66:LEU:HB2	3:H:71:GLY:O	2.03	0.58
3:H:152:PRO:HG2	3:H:202:ARG:HB2	1.85	0.58
2:S:62:SER:O	2:S:121:PHE:HB3	2.03	0.58
2:S:3:TYR:CZ	2:S:5:ASN:HA	2.39	0.58
2:S:25:ASN:ND2	2:S:28:ASN:ND2	2.51	0.58
3:T:42:LEU:H	3:T:53:GLN:HE22	1.51	0.58
2:M:162:PHE:HB2	8:M:1010:SPO:H291	1.85	0.58
2:S:268:TRP:NE1	3:T:35:ASN:ND2	2.52	0.58
3:H:248:ARG:HB2	3:H:248:ARG:NH1	2.18	0.58
3:T:183:LEU:HD21	3:T:213:PHE:HB3	1.86	0.58
2:S:88:ASP:HB2	2:S:92:PHE:CZ	2.39	0.58
1:R:207:ARG:N	1:R:207:ARG:HD2	2.18	0.58
2:S:228:ARG:HA	3:T:194:GLN:HG2	1.84	0.58
3:H:194:GLN:H	3:H:194:GLN:NE2	2.01	0.58
1:L:34:PHE:CE1	1:L:102:LEU:HD23	2.38	0.58
1:R:178:SER:HA	4:S:2001:BCL:HBA2	1.86	0.57
2:S:264:GLY:HA3	3:T:35:ASN:OD1	2.04	0.57
2:M:9:GLN:HE22	3:H:198:VAL:H	1.52	0.57
2:S:152:SER:CB	2:S:274:VAL:HG13	2.33	0.57
1:L:241:VAL:CG2	5:L:1006:BPH:HAC1	2.30	0.57
1:L:230:HIS:CD2	2:M:223:ILE:HG13	2.39	0.57
1:R:157:VAL:HG11	4:S:2003:BCL:HBB1	1.86	0.57
2:S:9:GLN:HE22	3:T:197:LYS:HA	1.69	0.57
3:H:194:GLN:H	3:H:194:GLN:CD	2.08	0.57
1:L:277:GLY:O	1:L:281:GLY:HA3	2.05	0.57
2:S:197:PHE:CZ	4:S:2003:BCL:HBB2	2.36	0.57
10:L:1032:HOH:O	2:M:49:PRO:HG2	2.03	0.57
3:H:245:ALA:HB3	3:H:246:PRO:HD3	1.85	0.57
1:L:49:ILE:CG1	1:L:89:ILE:HD13	2.35	0.57
1:L:51:TRP:CE3	1:L:85:LEU:HD11	2.40	0.56
1:R:18:GLY:O	1:R:21:LEU:HG	2.04	0.56
1:L:44:LEU:O	1:L:48:LEU:HG	2.04	0.56
2:S:49:PRO:HG2	10:S:2019:HOH:O	2.05	0.56
3:T:44:ASN:O	3:T:46:ASP:N	2.38	0.56
3:T:44:ASN:C	3:T:46:ASP:H	2.07	0.56
2:M:182:HIS:CG	8:M:1010:SPO:H181	2.40	0.56
2:M:157:TRP:CE3	2:M:158:MET:HG2	2.40	0.56
4:L:1002:BCL:HBD	4:L:1004:BCL:HBC3	1.86	0.56
2:S:209:LEU:HD22	4:S:2003:BCL:H3A	1.88	0.56
1:R:230:HIS:CD2	2:S:223:ILE:HG13	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:90:THR:HG23	1:L:132:VAL:HG11	1.88	0.56
3:T:12:LEU:N	3:T:12:LEU:HD22	2.21	0.56
3:T:133:PRO:HG3	3:T:168:TRP:CZ2	2.41	0.56
3:T:168:TRP:HB2	3:T:178:PHE:HB2	1.88	0.56
4:S:2001:BCL:HBB3	4:S:2003:BCL:H61	1.89	0.55
2:S:66:TRP:NE1	2:S:70:ILE:HD11	2.21	0.55
2:S:228:ARG:HA	3:T:194:GLN:HG3	1.88	0.55
2:M:195:ASN:HD22	2:M:195:ASN:C	2.10	0.55
2:M:195:ASN:ND2	2:M:197:PHE:H	2.04	0.55
3:H:33:THR:HA	3:H:36:MET:HE1	1.89	0.55
2:S:274:VAL:HA	5:S:2005:BPH:HBC1	1.88	0.55
1:L:49:ILE:HG13	1:L:89:ILE:HD13	1.88	0.55
4:L:1002:BCL:H122	5:L:1006:BPH:H3A	1.88	0.55
2:S:24:VAL:HG22	2:S:139:ALA:HB1	1.89	0.55
2:M:290:VAL:HG11	3:H:12:LEU:HB2	1.90	0.54
2:S:210:TYR:HB2	4:S:2004:BCL:O1A	2.08	0.54
4:R:2002:BCL:H122	5:R:2006:BPH:H3A	1.89	0.54
2:S:202:HIS:CE1	2:S:206:ILE:HD11	2.42	0.54
1:R:139:MET:HE3	1:R:252:GLY:O	2.07	0.54
3:T:189:ARG:HG2	3:T:189:ARG:NH1	2.23	0.54
1:L:189:LEU:HB3	6:L:1009[A]:U10:H4M3	1.88	0.54
2:M:94:LEU:HD22	2:M:115:TRP:HB2	1.89	0.54
1:R:46:ILE:HG12	4:S:2004:BCL:H202	1.90	0.54
1:R:86:TRP:CH2	1:R:132:VAL:HG13	2.43	0.54
1:L:180:PHE:HE2	4:L:1002:BCL:HMA2	1.72	0.54
1:L:182:THR:HG21	6:L:1009[B]:U10:H18	1.90	0.54
2:M:66:TRP:CD1	2:M:122:MET:HB2	2.43	0.54
3:H:182:GLU:HA	3:H:188:THR:HG22	1.89	0.53
1:L:197:ALA:HA	1:L:207:ARG:HB2	1.90	0.53
3:T:229:GLU:O	3:T:233:ILE:HG13	2.08	0.53
2:M:168:MET:HB2	2:M:173:GLU:HG3	1.89	0.53
2:S:70:ILE:HA	2:S:94:LEU:HD12	1.91	0.53
1:L:80:LEU:H	1:L:80:LEU:CD2	2.22	0.53
2:S:164:ARG:HB3	2:S:165:PRO:HD3	1.91	0.53
3:T:33:THR:HA	3:T:36:MET:HG3	1.91	0.52
3:H:40:TYR:HB3	3:H:58:LEU:HD21	1.90	0.52
1:R:11:VAL:O	1:R:110:LYS:NZ	2.35	0.52
1:R:185:LEU:HD13	5:S:2005:BPH:ND	2.24	0.52
2:S:65:MET:HB3	2:S:121:PHE:CD2	2.44	0.52
1:R:131:LEU:HD11	4:S:2004:BCL:HBC2	1.91	0.52
3:T:33:THR:HA	3:T:36:MET:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:228:LEU:O	3:T:232:LYS:HG3	2.09	0.52
3:T:86:ALA:HB3	3:T:107:ASP:HB3	1.92	0.52
2:S:10:VAL:HG21	3:T:148:PRO:HD3	1.90	0.52
4:S:2001:BCL:H11	5:S:2005:BPH:HMB2	1.91	0.52
3:T:178:PHE:HZ	3:T:230:GLU:HG3	1.73	0.52
3:T:44:ASN:HB2	3:T:46:ASP:OD1	2.10	0.52
3:T:164:VAL:HG21	3:T:203:VAL:HG21	1.92	0.52
2:M:237:GLN:HB2	2:M:262:MET:HG2	1.90	0.52
1:R:219:LEU:HD22	1:R:219:LEU:O	2.09	0.52
1:R:22:PHE:HA	1:R:24:PHE:CE2	2.45	0.52
5:R:2006:BPH:H152	4:S:2004:BCL:HBB3	1.93	0.51
1:L:15:THR:HG22	1:L:30:TYR:OH	2.10	0.51
2:M:232:GLU:OE1	2:M:232:GLU:N	2.39	0.51
2:S:204:LEU:HD13	3:T:20:PHE:CE2	2.45	0.51
1:L:170:ASN:HB3	1:L:173:HIS:HB2	1.91	0.51
2:S:280:GLY:HA2	4:S:2003:BCL:HED2	1.93	0.51
1:R:100:TRP:O	1:R:104:GLU:HG3	2.10	0.51
1:R:246:LEU:O	1:R:250:ILE:HG12	2.10	0.51
4:L:1002:BCL:HAA2	4:L:1004:BCL:HBC1	1.93	0.51
1:L:80:LEU:H	1:L:80:LEU:HD22	1.76	0.51
2:M:60:LEU:CD2	2:M:64:LEU:HG	2.41	0.51
4:L:1001:BCL:HBB2	8:M:1010:SPO:H243	1.92	0.51
2:S:233:CYS:O	2:S:237:GLN:HG2	2.10	0.51
2:M:72:ILE:HD12	8:M:1010:SPO:HM11	1.93	0.51
1:L:117:ILE:HD13	2:M:252:TRP:CZ2	2.46	0.51
1:R:244:SER:HB3	4:R:2002:BCL:O1A	2.10	0.51
1:L:211:HIS:HE1	2:M:22:GLU:OE1	1.93	0.51
3:T:36:MET:HB2	3:T:59:PRO:HD3	1.92	0.50
1:R:200:PRO:HG3	1:R:205:GLU:O	2.10	0.50
1:L:135:ARG:NH1	1:L:251:THR:O	2.45	0.50
2:S:148:TRP:HA	2:S:148:TRP:CE3	2.46	0.50
2:S:148:TRP:HA	2:S:148:TRP:HE3	1.76	0.50
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.92	0.50
2:S:64:LEU:O	2:S:68:PHE:HB2	2.11	0.50
2:S:232:GLU:O	2:S:234:GLU:HG3	2.12	0.50
2:M:65:MET:HB3	2:M:121:PHE:CD2	2.47	0.50
3:T:122:GLU:OE1	3:T:227:LEU:HD11	2.12	0.50
2:M:209:LEU:HD22	4:M:1003:BCL:H3A	1.94	0.50
3:H:165:VAL:HG11	3:H:182:GLU:HB2	1.94	0.50
1:R:45:GLY:O	1:R:49:ILE:HG13	2.11	0.50
1:L:233:GLY:HA3	2:M:216:PHE:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:66:VAL:HG12	1:R:86:TRP:HB2	1.93	0.49
2:S:25:ASN:HD22	2:S:28:ASN:HD21	1.58	0.49
3:H:87:LEU:HA	3:H:99:ALA:O	2.13	0.49
3:H:252:VAL:O	3:H:256:LEU:HD13	2.12	0.49
1:R:122:ALA:O	1:R:126:LEU:HD22	2.11	0.49
2:S:21:THR:CG2	2:S:26:LEU:HD21	2.37	0.49
2:S:24:VAL:HG22	2:S:139:ALA:CB	2.41	0.49
1:R:255:TRP:HZ2	1:R:258:GLN:O	1.96	0.49
1:L:226:THR:HG23	1:L:227:LEU:N	2.27	0.49
2:S:3:TYR:CE1	2:S:9:GLN:HG3	2.47	0.49
3:T:18:TYR:O	3:T:22:ILE:HG12	2.13	0.49
1:L:162:TYR:HA	1:L:165:GLY:O	2.13	0.49
3:T:220:LYS:HG3	3:T:229:GLU:OE2	2.13	0.49
2:M:177:TYR:HE1	8:M:1010:SPO:H22	1.77	0.49
3:T:59:PRO:HG2	3:T:76:PRO:HD3	1.95	0.49
2:S:293:ASN:OD1	2:S:295:TYR:HB3	2.12	0.49
1:L:86:TRP:CH2	1:L:132:VAL:HG13	2.48	0.49
3:T:12:LEU:HD22	3:T:12:LEU:H	1.75	0.48
2:S:222:THR:O	2:S:226:VAL:HG22	2.13	0.48
4:L:1001:BCL:HBC1	4:M:1003:BCL:CAD	2.43	0.48
1:L:105:VAL:O	1:L:109:ARG:HG3	2.14	0.48
3:H:220:LYS:HB2	3:H:220:LYS:HZ2	1.77	0.48
3:H:55:PRO:HG2	3:H:56:PHE:CD2	2.48	0.48
4:L:1004:BCL:O1A	2:M:207:ALA:HA	2.14	0.48
3:T:207:ALA:HB1	3:T:237:VAL:O	2.12	0.48
2:S:123:PHE:HA	2:S:157:TRP:HH2	1.79	0.48
3:T:45:GLU:HG3	3:T:94:GLU:OE1	2.13	0.48
1:R:241:VAL:CG2	5:R:2006:BPH:HAC1	2.43	0.48
1:R:241:VAL:HG21	5:R:2006:BPH:CAC	2.42	0.48
1:L:170:ASN:HB3	1:L:173:HIS:CB	2.43	0.48
3:T:75:VAL:HA	3:T:76:PRO:C	2.33	0.48
1:L:60:ASN:ND2	1:L:63:LEU:HD23	2.28	0.48
1:L:138:MET:SD	1:L:249:ILE:HD11	2.54	0.48
4:L:1004:BCL:H202	5:L:1006:BPH:H7C2	1.96	0.48
1:R:44:LEU:HD23	1:R:92:CYS:SG	2.53	0.48
2:S:59:SER:HB2	2:S:128:SER:OG	2.14	0.48
4:S:2001:BCL:HBC1	4:S:2003:BCL:CBD	2.44	0.48
4:L:1001:BCL:HHC	4:L:1001:BCL:HBB2	1.96	0.48
3:H:228:LEU:CD1	3:H:232:LYS:HE3	2.39	0.48
1:R:268:LYS:HA	1:R:273:ALA:HB2	1.94	0.48
1:L:42:ALA:O	1:L:46:ILE:HG13	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:218:ASP:OD1	2:S:29:ARG:HD2	2.13	0.47
1:R:119:PHE:O	1:R:122:ALA:HB3	2.14	0.47
4:R:2002:BCL:NC	4:S:2003:BCL:HBB3	2.29	0.47
2:M:122:MET:O	2:M:126:VAL:HG23	2.14	0.47
1:L:172:ALA:HB3	1:L:247:CYS:HA	1.95	0.47
3:T:208:LEU:HD12	3:T:240:GLY:HA3	1.96	0.47
1:L:97:PHE:CE1	4:L:1002:BCL:H121	2.49	0.47
3:H:170:ASP:HB2	3:H:177:ARG:CG	2.44	0.47
2:S:164:ARG:O	2:S:168:MET:HG2	2.14	0.47
1:R:246:LEU:HA	1:R:249:ILE:HG22	1.96	0.47
1:L:234:LEU:O	1:L:238:LEU:HB2	2.15	0.47
3:H:195:MET:CE	3:H:207:ALA:HB2	2.44	0.47
2:S:60:LEU:HD22	2:S:60:LEU:O	2.15	0.47
2:S:65:MET:HB3	2:S:121:PHE:CE2	2.50	0.47
3:T:12:LEU:H	3:T:12:LEU:CD2	2.28	0.47
1:R:183:ASN:ND2	2:S:213:ALA:HA	2.30	0.47
1:R:157:VAL:CG1	4:S:2003:BCL:HBB1	2.45	0.47
1:L:55:LEU:CD1	1:L:81:ALA:HB2	2.38	0.47
1:R:250:ILE:HB	1:R:254:ILE:HD11	1.97	0.47
2:M:25:ASN:OD1	2:M:27:ALA:HB3	2.15	0.47
1:R:213:ASN:O	1:R:217:ARG:HB2	2.14	0.47
1:L:22:PHE:HA	1:L:24:PHE:CE2	2.50	0.47
3:T:79:GLU:HA	3:T:79:GLU:OE1	2.15	0.47
1:R:3:LEU:HD12	2:S:250:LEU:HD21	1.96	0.47
2:S:60:LEU:HA	5:S:2005:BPH:H4C2	1.97	0.47
2:S:87:ARG:HG3	2:S:88:ASP:N	2.30	0.47
1:L:86:TRP:CZ2	1:L:132:VAL:HG13	2.50	0.47
1:L:125:ILE:O	1:L:129:LEU:HB2	2.14	0.47
1:L:227:LEU:HD11	2:M:5:ASN:HD21	1.79	0.46
3:H:33:THR:HA	3:H:36:MET:CE	2.45	0.46
1:L:220:VAL:O	1:L:220:VAL:CG1	2.62	0.46
4:R:2002:BCL:H2C	4:S:2003:BCL:H2C	1.96	0.46
3:H:111:PRO:HB2	3:H:239:GLY:HA2	1.96	0.46
5:R:2006:BPH:CMC	2:S:213:ALA:HB3	2.46	0.46
2:M:194:GLY:O	2:M:195:ASN:HB3	2.16	0.46
1:L:8:LYS:HE2	1:L:9:TYR:CZ	2.50	0.46
1:L:80:LEU:HD22	1:L:80:LEU:N	2.30	0.46
2:S:75:TRP:HB3	2:S:80:TRP:CE3	2.49	0.46
1:L:59:TRP:HA	1:L:59:TRP:CE3	2.51	0.46
1:L:241:VAL:HG21	5:L:1006:BPH:H2C	1.97	0.46
4:L:1001:BCL:HBB3	4:M:1003:BCL:C4	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:22:GLU:HB3	2:M:139:ALA:O	2.15	0.46
2:S:157:TRP:HB2	4:S:2003:BCL:C6	2.32	0.46
2:M:229:PHE:CB	2:M:244:ALA:HB2	2.40	0.46
3:T:70:ARG:NH2	3:T:123:LEU:HD13	2.31	0.46
1:R:177:ILE:HG12	4:R:2002:BCL:HMB3	1.97	0.46
1:R:129:LEU:O	1:R:133:LEU:HB3	2.16	0.46
1:L:280:ASN:ND2	2:M:88:ASP:OD1	2.40	0.46
1:R:97:PHE:CE1	4:R:2002:BCL:H121	2.51	0.46
1:L:178:SER:HA	4:L:1001:BCL:O1A	2.16	0.46
2:M:195:ASN:HD22	2:M:196:LEU:N	2.14	0.46
3:T:42:LEU:H	3:T:53:GLN:NE2	2.14	0.46
3:T:170:ASP:O	3:T:174:GLN:N	2.48	0.46
1:L:207:ARG:HD2	1:L:207:ARG:HA	1.67	0.46
3:H:206:ASN:ND2	3:H:248:ARG:HD3	2.30	0.46
1:L:266:TRP:HE1	2:M:87:ARG:HA	1.80	0.46
3:H:153:VAL:HG21	3:H:181:VAL:HG22	1.98	0.46
1:R:181:PHE:CE1	4:S:2003:BCL:O1A	2.68	0.46
1:R:15:THR:HG22	1:R:30:TYR:OH	2.16	0.46
3:H:37:ARG:C	3:H:38:GLU:HG2	2.36	0.46
1:R:2:LEU:N	1:R:2:LEU:HD12	2.30	0.45
1:R:207:ARG:HB3	1:R:211:HIS:CG	2.51	0.45
2:M:13:ARG:O	3:H:140:PHE:HA	2.15	0.45
4:R:2002:BCL:H52	5:R:2006:BPH:HBB2	1.97	0.45
2:S:274:VAL:HA	5:S:2005:BPH:CBC	2.47	0.45
3:T:45:GLU:CD	3:T:95:GLY:H	2.20	0.45
1:R:67:TYR:CD2	1:R:147:PRO:HB3	2.52	0.45
4:L:1001:BCL:CBC	4:M:1003:BCL:CAD	2.94	0.45
2:S:3:TYR:CE2	3:T:194:GLN:HA	2.52	0.45
1:R:265:TRP:CG	1:R:266:TRP:N	2.85	0.45
3:T:37:ARG:HH11	3:T:37:ARG:HG2	1.81	0.45
2:M:3:TYR:CE1	2:M:9:GLN:HG3	2.52	0.45
2:S:156:LEU:HD12	2:S:277:THR:HG22	1.97	0.45
1:R:197:ALA:HA	1:R:207:ARG:HG2	1.99	0.45
3:T:199:GLN:HB2	3:T:202:ARG:O	2.16	0.45
1:R:214:THR:O	1:R:218:ASP:HB2	2.16	0.45
1:R:56:GLN:NE2	1:R:58:THR:HG21	2.30	0.45
3:H:24:LEU:O	3:H:28:ILE:HG13	2.16	0.45
3:T:161:ALA:HB2	3:T:210:SER:HA	1.99	0.45
1:L:157:VAL:CG1	4:M:1003:BCL:HBB1	2.43	0.45
3:T:245:ALA:HB3	3:T:246:PRO:HD3	1.99	0.45
3:H:46:ASP:HB3	10:H:266:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:66:LEU:HA	3:H:67:PRO:HD3	1.79	0.45
3:H:140:PHE:CD2	3:H:169:VAL:HG11	2.52	0.45
3:H:70:ARG:CG	3:H:70:ARG:NH1	2.80	0.45
1:R:14:GLY:O	1:R:109:ARG:HD3	2.17	0.45
1:R:6:GLU:OE2	1:R:10:ARG:NH1	2.50	0.45
1:L:68:PRO:HB3	1:L:86:TRP:CD2	2.52	0.45
2:S:155:TRP:NE1	2:S:281:GLY:HA3	2.32	0.45
1:R:180:PHE:CE2	4:R:2002:BCL:HMA2	2.52	0.44
1:R:3:LEU:HB2	1:R:6:GLU:HB2	1.99	0.44
1:L:7:ARG:HH11	1:L:7:ARG:HG2	1.81	0.44
3:H:40:TYR:CE2	3:H:42:LEU:HD21	2.53	0.44
1:R:224:ILE:HG22	6:R:2009[A]:U10:H3M3	1.99	0.44
3:H:184:LYS:HD3	3:H:184:LYS:N	2.33	0.44
1:L:18:GLY:O	1:L:19:GLY:C	2.55	0.44
1:R:170:ASN:HB3	1:R:173:HIS:CB	2.48	0.44
2:S:3:TYR:CD2	3:T:194:GLN:HA	2.52	0.44
1:L:49:ILE:HG12	1:L:89:ILE:HD13	1.99	0.44
3:T:183:LEU:HD12	3:T:189:ARG:NH1	2.33	0.44
2:S:94:LEU:HD22	2:S:115:TRP:HB2	1.99	0.44
3:T:207:ALA:O	3:T:240:GLY:HA3	2.17	0.44
1:R:232:LEU:O	1:R:236:LEU:HG	2.18	0.44
1:R:72:GLU:CD	1:R:72:GLU:H	2.21	0.44
1:R:94:THR:O	1:R:98:VAL:HG23	2.17	0.44
2:M:238:ILE:HD13	2:M:263:GLU:HB2	1.99	0.44
1:L:80:LEU:HD12	1:L:85:LEU:CD1	2.48	0.44
1:L:105:VAL:O	1:L:108:CYS:HB2	2.17	0.44
1:L:60:ASN:O	1:L:64:ILE:HG13	2.18	0.44
1:R:224:ILE:N	6:R:2009[B]:U10:O5	2.51	0.44
2:S:100:GLU:CD	2:S:100:GLU:H	2.20	0.44
1:L:90:THR:CG2	1:L:132:VAL:HG11	2.48	0.44
2:M:148:TRP:HA	2:M:148:TRP:CE3	2.53	0.44
2:S:129:TRP:O	2:S:132:ARG:HB3	2.17	0.44
1:R:173:HIS:CE1	1:R:177:ILE:HD11	2.52	0.44
3:T:187:SER:HB2	10:T:269:HOH:O	2.17	0.44
3:T:111:PRO:HG2	3:T:242:MET:SD	2.58	0.44
1:R:22:PHE:HA	1:R:24:PHE:HE2	1.82	0.43
2:S:187:ASN:HA	4:S:2003:BCL:CBC	2.49	0.43
1:L:231:ARG:HD2	2:M:5:ASN:O	2.17	0.43
1:R:213:ASN:HB3	1:R:217:ARG:NH2	2.33	0.43
3:H:153:VAL:HG21	3:H:181:VAL:CG2	2.47	0.43
2:S:253:ARG:HB2	2:S:259:ASN:OD1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:11:GLN:OE1	2:S:40:GLY:HA3	2.17	0.43
1:R:105:VAL:O	1:R:108:CYS:HB2	2.18	0.43
3:T:87:LEU:HD22	3:T:98:HIS:O	2.18	0.43
2:M:87:ARG:HG3	2:M:88:ASP:N	2.33	0.43
3:T:111:PRO:HB2	3:T:239:GLY:HA2	2.00	0.43
2:S:10:VAL:HG21	3:T:148:PRO:CD	2.47	0.43
2:M:148:TRP:HA	2:M:148:TRP:HE3	1.83	0.43
2:M:129:TRP:O	2:M:132:ARG:HB3	2.19	0.43
1:R:184:ALA:HB3	5:S:2005:BPH:CMC	2.49	0.43
3:H:40:TYR:CZ	3:H:42:LEU:HD21	2.54	0.43
4:L:1002:BCL:NC	4:M:1003:BCL:HBB3	2.34	0.43
1:L:226:THR:CG2	1:L:227:LEU:N	2.81	0.43
3:T:117:ARG:O	3:T:228:LEU:HB2	2.18	0.43
1:L:2:LEU:HB3	1:L:6:GLU:HB3	2.01	0.43
2:M:204:LEU:HD13	3:H:20:PHE:CE2	2.54	0.43
1:R:231:ARG:NE	2:S:6:ILE:O	2.52	0.43
1:L:244:SER:HB3	4:L:1002:BCL:O1A	2.18	0.43
4:L:1002:BCL:H2C	4:M:1003:BCL:H2C	2.00	0.43
3:T:36:MET:HE2	3:T:57:PRO:O	2.19	0.43
3:H:178:PHE:CZ	3:H:230:GLU:HG2	2.40	0.43
1:R:219:LEU:CD1	1:R:220:VAL:HG23	2.33	0.43
3:H:189:ARG:HG2	3:H:189:ARG:HH11	1.83	0.43
1:L:268:LYS:HD3	1:L:268:LYS:HA	1.71	0.43
2:S:157:TRP:HD1	4:S:2001:BCL:HBB1	1.84	0.42
4:L:1004:BCL:H71	4:L:1004:BCL:C2	2.48	0.42
1:R:85:LEU:HD12	1:R:85:LEU:HA	1.89	0.42
3:T:36:MET:HB3	3:T:58:LEU:HD23	2.01	0.42
1:R:102:LEU:O	1:R:105:VAL:HB	2.18	0.42
1:R:7:ARG:HH12	3:T:87:LEU:HB2	1.84	0.42
3:H:241:LEU:HB2	10:H:276:HOH:O	2.19	0.42
6:R:2009[B]:U10:H3M1	10:S:2023:HOH:O	2.18	0.42
1:R:65:SER:CB	1:R:152:THR:HG21	2.49	0.42
1:R:97:PHE:HE1	4:R:2002:BCL:H121	1.85	0.42
2:S:15:PRO:HD2	3:T:140:PHE:CE1	2.54	0.42
3:T:58:LEU:HA	3:T:58:LEU:HD23	1.90	0.42
3:H:40:TYR:CB	3:H:58:LEU:HD21	2.49	0.42
2:M:191:LEU:HD12	2:M:191:LEU:HA	1.89	0.42
2:S:159:VAL:HA	2:S:163:ILE:HB	2.00	0.42
1:R:172:ALA:HB3	1:R:247:CYS:HA	2.01	0.42
4:L:1001:BCL:H2C	4:L:1001:BCL:HBC2	1.79	0.42
8:M:1010:SPO:H42	8:M:1010:SPO:HM12	1.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:2:GLU:O	2:M:3:TYR:CB	2.64	0.42
1:L:269:LEU:HG	1:L:271:TRP:CH2	2.54	0.42
2:S:96:PRO:HA	2:S:115:TRP:CG	2.55	0.42
2:M:96:PRO:HB3	2:M:115:TRP:CE2	2.55	0.42
1:R:84:GLY:HA2	1:R:87:GLN:HE21	1.84	0.42
3:H:157:ASP:N	3:H:157:ASP:OD1	2.53	0.42
3:H:168:TRP:HB2	3:H:178:PHE:HB2	2.01	0.42
1:R:16:LEU:HD11	1:R:105:VAL:HG11	2.02	0.42
1:L:60:ASN:CG	1:L:63:LEU:HD23	2.39	0.42
2:S:196:LEU:HD12	2:S:196:LEU:HA	1.87	0.42
3:H:89:ARG:HG2	3:H:98:HIS:CE1	2.54	0.42
1:R:60:ASN:OD1	1:R:62:GLN:N	2.53	0.42
2:S:97:PRO:CG	2:S:171:TRP:HB2	2.46	0.42
3:T:44:ASN:C	3:T:46:ASP:N	2.72	0.42
3:T:37:ARG:HG2	3:T:37:ARG:NH1	2.35	0.42
1:L:131:LEU:HD11	4:L:1004:BCL:HBC2	2.01	0.42
2:S:13:ARG:O	3:T:140:PHE:HA	2.19	0.42
2:S:260:ALA:HA	3:T:35:ASN:HB3	2.00	0.42
2:S:190:SER:HB2	4:S:2003:BCL:H3C	2.00	0.42
1:L:10:ARG:NH2	1:L:25:TRP:HB2	2.35	0.42
1:R:220:VAL:HG21	5:S:2005:BPH:HED3	2.00	0.42
2:S:14:GLY:HA3	3:T:140:PHE:CZ	2.55	0.42
1:R:280:ASN:HB2	2:S:88:ASP:OD1	2.20	0.42
1:L:185:LEU:CD1	1:L:189:LEU:HD22	2.49	0.42
2:S:232:GLU:O	2:S:234:GLU:N	2.52	0.42
1:R:79:PRO:O	1:R:81:ALA:N	2.53	0.42
1:R:149:GLY:HA3	1:R:152:THR:OG1	2.20	0.42
2:S:224:LEU:HD23	2:S:224:LEU:HA	1.89	0.42
3:T:219:ILE:CG2	3:T:225:VAL:HG23	2.50	0.42
1:L:208:THR:OG1	1:L:211:HIS:HD2	2.03	0.41
1:R:28:PRO:HB3	2:S:253:ARG:HH11	1.85	0.41
3:H:36:MET:HB2	3:H:36:MET:HE2	1.92	0.41
1:L:280:ASN:HB2	2:M:87:ARG:HE	1.84	0.41
1:R:90:THR:HG23	1:R:132:VAL:HG11	2.02	0.41
3:H:248:ARG:CZ	3:H:248:ARG:HB2	2.49	0.41
3:H:241:LEU:O	3:H:248:ARG:NH2	2.53	0.41
1:L:264:GLN:OE1	1:L:268:LYS:HE2	2.20	0.41
3:T:17:ILE:O	3:T:21:TRP:CD1	2.73	0.41
3:T:158:LEU:HG	3:T:249:LYS:HG3	2.02	0.41
1:R:180:PHE:CD2	1:R:240:ALA:HB1	2.54	0.41
1:R:189:LEU:HD12	1:R:189:LEU:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:234:GLU:O	2:S:238:ILE:HG13	2.20	0.41
1:R:16:LEU:HD11	1:R:105:VAL:CG1	2.50	0.41
1:R:7:ARG:NH2	3:T:98:HIS:HD2	2.19	0.41
2:S:162:PHE:C	2:S:165:PRO:HD2	2.40	0.41
1:R:268:LYS:HA	1:R:273:ALA:CB	2.49	0.41
3:H:66:LEU:HD23	3:H:72:THR:HA	2.02	0.41
2:M:5:ASN:HD22	2:M:224:LEU:HD22	1.84	0.41
1:L:268:LYS:C	1:L:273:ALA:HB2	2.41	0.41
1:R:34:PHE:HA	1:R:37:ALA:HB3	2.02	0.41
3:T:99:ALA:HA	3:T:100:PRO:HD3	1.84	0.41
2:M:22:GLU:HB3	2:M:23:ASP:H	1.65	0.41
2:M:109:LEU:HA	2:M:113:GLY:HA3	2.01	0.41
2:M:264:GLY:HA3	3:H:35:ASN:OD1	2.21	0.41
1:R:246:LEU:O	1:R:249:ILE:HG22	2.21	0.41
2:M:293:ASN:OD1	2:M:295:TYR:HB3	2.21	0.41
3:T:195:MET:HE2	3:T:238:ALA:HA	2.03	0.41
1:R:117:ILE:HD13	2:S:252:TRP:CZ2	2.55	0.41
4:S:2001:BCL:HHC	4:S:2001:BCL:HBB2	2.01	0.41
1:L:85:LEU:O	1:L:89:ILE:HG13	2.21	0.41
1:L:102:LEU:HD12	1:L:102:LEU:HA	1.84	0.41
3:H:165:VAL:CG1	3:H:182:GLU:HB2	2.50	0.41
3:T:212:LEU:CD1	3:T:244:ALA:HB2	2.51	0.41
4:S:2001:BCL:HBB2	8:S:2010:SPO:H243	2.03	0.41
1:L:51:TRP:CZ3	1:L:85:LEU:HD11	2.55	0.41
3:T:199:GLN:OE1	3:T:202:ARG:HD2	2.21	0.41
1:R:280:ASN:HB2	2:S:87:ARG:HE	1.86	0.41
2:S:151:LEU:O	2:S:155:TRP:N	2.49	0.41
2:S:182:HIS:CG	8:S:2010:SPO:H181	2.56	0.41
4:M:1003:BCL:H62	4:M:1003:BCL:H92	1.93	0.41
2:S:21:THR:HG23	2:S:26:LEU:CD2	2.42	0.41
3:T:149:ILE:CD1	3:T:166:ASP:HA	2.51	0.41
3:H:120:LEU:N	3:H:226:THR:HB	2.36	0.41
10:L:1032:HOH:O	2:M:29:ARG:HD2	2.21	0.41
2:S:93:SER:HB2	2:S:181:SER:HB3	2.03	0.41
1:L:83:GLY:O	1:L:87:GLN:HG3	2.21	0.41
1:L:78:ALA:HB1	1:L:79:PRO:HD2	2.02	0.41
2:S:151:LEU:HA	2:S:154:ILE:HB	2.02	0.41
2:M:170:SER:HB2	10:M:1041:HOH:O	2.21	0.41
2:M:9:GLN:HE22	3:H:198:VAL:N	2.17	0.40
1:L:20:ASN:HB3	10:L:1018:HOH:O	2.21	0.40
1:L:80:LEU:HB3	1:L:85:LEU:HD13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:3:LEU:HD12	2:S:250:LEU:CD2	2.51	0.40
2:M:145:HIS:CE1	9:M:1011:LDA:HM13	2.56	0.40
1:L:60:ASN:HB3	1:L:63:LEU:HB2	2.03	0.40
3:T:60:LYS:CG	3:T:61:PRO:HD2	2.50	0.40
3:H:207:ALA:HB1	3:H:237:VAL:O	2.22	0.40
1:L:129:LEU:HD12	1:L:129:LEU:HA	1.89	0.40
2:S:75:TRP:HB3	2:S:80:TRP:CZ3	2.56	0.40
1:R:59:TRP:HA	1:R:59:TRP:CE3	2.57	0.40
4:L:1001:BCL:CBB	4:L:1001:BCL:HHC	2.50	0.40
4:L:1004:BCL:H161	4:L:1004:BCL:H141	1.90	0.40
2:M:187:ASN:HA	4:M:1003:BCL:CBC	2.52	0.40
1:R:6:GLU:HG3	2:S:250:LEU:HD22	2.02	0.40
1:R:262:TRP:O	1:R:265:TRP:HD1	2.05	0.40
1:R:269:LEU:HA	1:R:269:LEU:HD12	1.91	0.40
1:R:230:HIS:NE2	2:S:223:ILE:HG13	2.37	0.40
1:R:154:LEU:O	1:R:157:VAL:HB	2.21	0.40
2:S:123:PHE:HA	2:S:157:TRP:CH2	2.57	0.40
1:L:180:PHE:CE2	4:L:1002:BCL:HMA2	2.54	0.40
3:T:192:PRO:CB	3:T:194:GLN:HE21	2.35	0.40
2:M:270:ILE:HD13	9:M:1011:LDA:H32	2.04	0.40
1:L:39:PHE:C	1:L:39:PHE:CD1	2.95	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%)	262 (94%)	16 (6%)	1 (0%)	39 65
1	R	279/281 (99%)	264 (95%)	12 (4%)	3 (1%)	17 36
2	M	299/307 (97%)	280 (94%)	18 (6%)	1 (0%)	46 72
2	S	297/307 (97%)	284 (96%)	11 (4%)	2 (1%)	26 51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	H	244/260 (94%)	233 (96%)	11 (4%)	0	100 100
3	T	244/260 (94%)	223 (91%)	15 (6%)	6 (2%)	7 12
All	All	1642/1696 (97%)	1546 (94%)	83 (5%)	13 (1%)	24 46

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	2	GLU
3	T	45	GLU
3	T	220	LYS
1	R	80	LEU
1	R	257	ASP
2	S	195	ASN
3	T	70	ARG
3	T	124	ASP
1	L	270	PRO
3	T	89	ARG
3	T	166	ASP
1	R	31	VAL
2	S	19	GLY

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%)	208 (94%)	12 (6%)	27 51
1	R	220/220 (100%)	210 (96%)	10 (4%)	34 62
2	M	236/240 (98%)	223 (94%)	13 (6%)	27 51
2	S	235/240 (98%)	221 (94%)	14 (6%)	24 47
3	H	199/208 (96%)	191 (96%)	8 (4%)	38 67
3	T	199/208 (96%)	195 (98%)	4 (2%)	63 85
All	All	1309/1336 (98%)	1248 (95%)	61 (5%)	32 59

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	10	ARG
1	L	85	LEU
1	L	102	LEU
1	L	129	LEU
1	L	154	LEU
1	L	189	LEU
1	L	207	ARG
1	L	216	PHE
1	L	238	LEU
1	L	247	CYS
1	L	269	LEU
1	L	272	TRP
2	M	26	LEU
2	M	29	ARG
2	M	60	LEU
2	M	87	ARG
2	M	94	LEU
2	M	114	LEU
2	M	136	ARG
2	M	156	LEU
2	M	165	PRO
2	M	191	LEU
2	M	195	ASN
2	M	216	PHE
2	M	232	GLU
3	H	70	ARG
3	H	73	LEU
3	H	83	ARG
3	H	123	LEU
3	H	184	LYS
3	H	191	LEU
3	H	202	ARG
3	H	231	ASP
1	R	87	GLN
1	R	102	LEU
1	R	126	LEU
1	R	154	LEU
1	R	189	LEU
1	R	217	ARG
1	R	229	ILE
1	R	247	CYS
1	R	269	LEU

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Mol	Chain	Res	Type
1	R	272	TRP
2	S	12	VAL
2	S	29	ARG
2	S	60	LEU
2	S	68	PHE
2	S	87	ARG
2	S	94	LEU
2	S	114	LEU
2	S	136	ARG
2	S	148	TRP
2	S	156	LEU
2	S	191	LEU
2	S	195	ASN
2	S	216	PHE
2	S	232	GLU
3	T	79	GLU
3	T	82	ASP
3	T	202	ARG
3	T	231	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	87	GLN
1	L	211	HIS
1	L	274	ASN
2	M	5	ASN
2	M	9	GLN
2	M	195	ASN
3	H	194	GLN
3	H	206	ASN
1	R	87	GLN
1	R	211	HIS
1	R	274	ASN
2	S	5	ASN
2	S	9	GLN
2	S	28	ASN
2	S	44	ASN
2	S	195	ASN
3	T	53	GLN
3	T	128	HIS
3	T	174	GLN

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Mol	Chain	Res	Type
3	T	194	GLN

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 23 ligands modelled in this entry, 2 are monoatomic - leaving 21 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	BCL	L	1001	-	38,59,74	1.35	4 (10%)	40,97,115	2.13	14 (35%)
4	BCL	L	1002	-	53,74,74	1.04	3 (5%)	57,115,115	1.88	17 (29%)
4	BCL	L	1004	-	53,74,74	1.15	4 (7%)	57,115,115	1.68	15 (26%)
5	BPH	L	1006	-	64,70,70	1.48	8 (12%)	73,101,101	2.18	16 (21%)
6	U10	L	1009[A]	-	30,30,63	2.14	11 (36%)	36,39,79	2.09	13 (36%)
6	U10	L	1009[B]	-	30,30,63	2.05	9 (30%)	36,39,79	2.04	11 (30%)
4	BCL	M	1003	-	53,74,74	1.01	3 (5%)	57,115,115	1.96	21 (36%)
5	BPH	M	1005	-	54,60,70	1.36	7 (12%)	61,89,101	2.32	16 (26%)
6	U10	M	1008	-	38,38,63	2.08	11 (28%)	46,49,79	1.79	9 (19%)
8	SPO	M	1010	-	40,41,41	3.29	22 (55%)	45,50,50	2.54	14 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	LDA	M	1011	-	15,15,15	3.66	2 (13%)	16,17,17	2.68	4 (25%)
4	BCL	R	2002	-	53,74,74	1.06	2 (3%)	57,115,115	1.87	18 (31%)
5	BPH	R	2006	-	64,70,70	1.44	8 (12%)	73,101,101	2.20	18 (24%)
6	U10	R	2009[A]	-	18,18,63	2.00	6 (33%)	22,25,79	2.09	5 (22%)
6	U10	R	2009[B]	-	18,18,63	1.98	6 (33%)	22,25,79	2.05	4 (18%)
4	BCL	S	2001	-	38,59,74	1.33	6 (15%)	40,97,115	2.01	14 (35%)
4	BCL	S	2003	-	53,74,74	1.02	1 (1%)	57,115,115	1.95	20 (35%)
4	BCL	S	2004	-	53,74,74	1.12	4 (7%)	57,115,115	1.82	15 (26%)
5	BPH	S	2005	-	50,56,70	1.49	9 (18%)	56,84,101	2.37	15 (26%)
6	U10	S	2008	-	32,32,63	1.98	10 (31%)	38,41,79	1.91	9 (23%)
8	SPO	S	2010	-	40,41,41	3.31	24 (60%)	45,50,50	2.58	12 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BCL	L	1001	-	-	0/19/119/137	0/0/9/9
4	BCL	L	1002	-	-	0/37/137/137	0/0/9/9
4	BCL	L	1004	-	-	0/37/137/137	0/0/9/9
5	BPH	L	1006	-	2/2/18/22	0/54/105/105	0/1/6/6
6	U10	L	1009[A]	-	-	0/24/48/87	0/1/1/1
6	U10	L	1009[B]	-	-	0/24/48/87	0/1/1/1
4	BCL	M	1003	-	-	0/37/137/137	0/0/9/9
5	BPH	M	1005	-	1/1/16/22	0/42/93/105	0/1/6/6
6	U10	M	1008	-	-	0/33/57/87	0/1/1/1
8	SPO	M	1010	-	-	0/47/47/47	0/0/0/0
9	LDA	M	1011	-	-	0/13/13/13	0/0/0/0
4	BCL	R	2002	-	-	0/37/137/137	0/0/9/9
5	BPH	R	2006	-	2/2/18/22	0/54/105/105	0/1/6/6
6	U10	R	2009[A]	-	-	0/9/33/87	0/1/1/1
6	U10	R	2009[B]	-	-	0/9/33/87	0/1/1/1
4	BCL	S	2001	-	-	0/19/119/137	0/0/9/9
4	BCL	S	2003	-	-	0/37/137/137	0/0/9/9
4	BCL	S	2004	-	-	0/37/137/137	0/0/9/9
5	BPH	S	2005	-	-	0/38/89/105	0/1/6/6
6	U10	S	2008	-	-	0/26/50/87	0/1/1/1
8	SPO	S	2010	-	-	0/47/47/47	0/0/0/0

All (160) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	1011	LDA	O1-N1	-13.39	1.26	1.39
5	L	1006	BPH	C11-C10	-5.08	1.28	1.52
5	R	2006	BPH	C11-C10	-5.00	1.29	1.52
4	L	1001	BCL	C3C-C4C	-4.22	1.46	1.51
6	M	1008	U10	C7-C8	-3.84	1.44	1.50
9	M	1011	LDA	CM2-N1	-3.79	1.43	1.49
4	S	2001	BCL	C3C-C4C	-3.50	1.47	1.51
6	R	2009[A]	U10	C7-C8	-3.33	1.45	1.50
6	S	2008	U10	C7-C8	-3.15	1.45	1.50
6	R	2009[B]	U10	O3-C3M	-3.14	1.37	1.45
6	L	1009[B]	U10	O3-C3M	-3.13	1.37	1.45
4	L	1004	BCL	C3C-C4C	-3.11	1.47	1.51
6	R	2009[B]	U10	C7-C8	-3.06	1.46	1.50
8	M	1010	SPO	C6-C7	-2.94	1.39	1.45
8	S	2010	SPO	C11-C12	-2.87	1.39	1.45
6	L	1009[B]	U10	C7-C8	-2.86	1.46	1.50
6	L	1009[A]	U10	O3-C3M	-2.84	1.38	1.45
6	S	2008	U10	O3-C3M	-2.84	1.38	1.45
8	S	2010	SPO	C25-C23	-2.83	1.39	1.45
6	L	1009[A]	U10	C7-C8	-2.83	1.46	1.50
6	R	2009[A]	U10	O3-C3M	-2.76	1.38	1.45
4	S	2004	BCL	C3C-C4C	-2.76	1.48	1.51
8	M	1010	SPO	C25-C23	-2.74	1.39	1.45
5	R	2006	BPH	O2D-CED	-2.72	1.38	1.45
6	M	1008	U10	O3-C3M	-2.72	1.38	1.45
8	M	1010	SPO	C11-C12	-2.70	1.39	1.45
6	M	1008	U10	C27-C28	-2.64	1.43	1.50
5	L	1006	BPH	O2D-CED	-2.57	1.39	1.45
8	S	2010	SPO	C6-C7	-2.57	1.40	1.45
5	M	1005	BPH	O2D-CED	-2.55	1.39	1.45
5	S	2005	BPH	O2D-CED	-2.47	1.39	1.45
4	L	1002	BCL	C3C-C4C	-2.41	1.48	1.51
4	M	1003	BCL	C3C-C4C	-2.31	1.48	1.51
4	M	1003	BCL	C2-C3	-2.28	1.28	1.33
4	S	2001	BCL	OBD-CAD	-2.28	1.18	1.22
4	L	1004	BCL	C3D-CAD	-2.20	1.39	1.45
4	L	1001	BCL	C3D-CAD	-2.17	1.39	1.45
4	M	1003	BCL	C3D-CAD	-2.12	1.39	1.45
5	M	1005	BPH	C2C-C3C	-2.06	1.48	1.54
5	S	2005	BPH	C2C-C3C	-2.01	1.48	1.54
5	R	2006	BPH	CHA-C1A	2.01	1.41	1.37
5	L	1006	BPH	O1D-CGD	2.02	1.26	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	S	2005	BPH	O1D-CGD	2.03	1.26	1.21
6	M	1008	U10	C20-C19	2.03	1.55	1.50
4	S	2001	BCL	CAA-CBA	2.03	1.59	1.52
4	S	2001	BCL	C1-C2	2.05	1.55	1.49
4	L	1002	BCL	CBB-CAB	2.05	1.55	1.49
4	S	2001	BCL	CBB-CAB	2.05	1.55	1.49
6	L	1009[B]	U10	C6-C1	2.10	1.40	1.35
8	S	2010	SPO	C15-C14	2.11	1.50	1.43
6	S	2008	U10	C6-C1	2.11	1.40	1.35
6	L	1009[A]	U10	C20-C19	2.12	1.55	1.50
8	S	2010	SPO	C24-C23	2.14	1.55	1.50
6	S	2008	U10	C20-C19	2.16	1.56	1.50
8	S	2010	SPO	C35-C33	2.16	1.56	1.51
4	L	1004	BCL	C4-C3	2.17	1.56	1.50
4	S	2003	BCL	C4-C3	2.19	1.56	1.50
4	S	2004	BCL	CAA-CBA	2.19	1.60	1.52
4	L	1004	BCL	C6-C5	2.19	1.60	1.52
4	R	2002	BCL	C4-C3	2.21	1.56	1.50
6	S	2008	U10	C15-C14	2.21	1.56	1.50
5	S	2005	BPH	C2A-C1A	2.21	1.55	1.51
5	L	1006	BPH	CAA-C2A	2.23	1.58	1.54
4	L	1001	BCL	CAA-CBA	2.24	1.60	1.52
4	L	1001	BCL	CAA-C2A	2.25	1.58	1.54
8	S	2010	SPO	C13-C12	2.25	1.55	1.50
8	S	2010	SPO	C22-C23	2.26	1.38	1.35
8	M	1010	SPO	C24-C23	2.29	1.55	1.50
5	M	1005	BPH	CMB-C2B	2.30	1.55	1.50
4	L	1002	BCL	C4-C3	2.30	1.56	1.50
6	R	2009[B]	U10	C6-C1	2.31	1.40	1.35
5	R	2006	BPH	CAA-C2A	2.32	1.58	1.54
8	M	1010	SPO	C15-C14	2.35	1.51	1.43
6	L	1009[B]	U10	C15-C14	2.38	1.56	1.50
5	R	2006	BPH	C2A-C1A	2.39	1.55	1.51
6	M	1008	U10	C15-C14	2.42	1.56	1.50
8	S	2010	SPO	C8-C7	2.42	1.56	1.50
4	R	2002	BCL	CBB-CAB	2.44	1.57	1.49
8	M	1010	SPO	C13-C12	2.45	1.56	1.50
6	L	1009[A]	U10	C15-C14	2.45	1.56	1.50
6	R	2009[A]	U10	C6-C1	2.46	1.41	1.35
8	M	1010	SPO	C26-C27	2.49	1.51	1.43
6	R	2009[A]	U10	C8-C9	2.49	1.39	1.32
4	S	2004	BCL	C4-C3	2.51	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	S	2001	BCL	CAA-C2A	2.52	1.59	1.54
8	S	2010	SPO	C26-C27	2.52	1.51	1.43
5	S	2005	BPH	CHC-C1C	2.52	1.41	1.36
8	M	1010	SPO	C8-C7	2.55	1.56	1.50
6	L	1009[A]	U10	C7-C6	2.55	1.56	1.51
6	M	1008	U10	O3-C3	2.62	1.43	1.37
6	L	1009[A]	U10	C6-C1	2.65	1.41	1.35
4	S	2004	BCL	CAA-C2A	2.67	1.59	1.54
8	S	2010	SPO	C10-C9	2.68	1.52	1.43
5	S	2005	BPH	CAA-C2A	2.72	1.59	1.54
8	S	2010	SPO	C9-C7	2.72	1.39	1.35
6	R	2009[B]	U10	C8-C9	2.73	1.40	1.32
5	L	1006	BPH	CHC-C1C	2.73	1.41	1.36
6	L	1009[B]	U10	O3-C3	2.75	1.44	1.37
6	S	2008	U10	O3-C3	2.75	1.44	1.37
8	M	1010	SPO	C10-C9	2.83	1.52	1.43
6	M	1008	U10	C8-C9	2.83	1.38	1.33
8	M	1010	SPO	C37-C38	2.84	1.41	1.32
6	R	2009[B]	U10	O3-C3	2.91	1.44	1.37
5	M	1005	BPH	CAA-C2A	3.07	1.60	1.54
8	M	1010	SPO	C9-C7	3.08	1.39	1.35
6	L	1009[A]	U10	O3-C3	3.10	1.45	1.37
6	R	2009[A]	U10	O3-C3	3.14	1.45	1.37
8	S	2010	SPO	C37-C38	3.20	1.42	1.32
5	M	1005	BPH	O2A-CGA	3.24	1.43	1.33
5	S	2005	BPH	C2-C3	3.27	1.39	1.33
5	M	1005	BPH	C2-C3	3.27	1.39	1.33
6	L	1009[A]	U10	C18-C19	3.32	1.39	1.33
8	S	2010	SPO	C32-C33	3.35	1.39	1.33
6	S	2008	U10	C8-C9	3.38	1.39	1.33
6	L	1009[B]	U10	C18-C19	3.40	1.39	1.33
8	M	1010	SPO	C32-C33	3.43	1.39	1.33
8	S	2010	SPO	C4-C1	3.43	1.58	1.53
6	S	2008	U10	C18-C19	3.45	1.39	1.33
5	R	2006	BPH	C2-C3	3.52	1.39	1.33
5	R	2006	BPH	O2D-CGD	3.58	1.42	1.33
5	M	1005	BPH	O2D-CGD	3.59	1.42	1.33
8	M	1010	SPO	C19-C17	3.60	1.40	1.35
5	S	2005	BPH	O2D-CGD	3.65	1.42	1.33
6	M	1008	U10	C18-C19	3.67	1.40	1.33
5	L	1006	BPH	C2-C3	3.72	1.40	1.33
8	S	2010	SPO	C14-C12	3.75	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	1006	BPH	O2A-CGA	3.82	1.44	1.33
6	L	1009[B]	U10	C8-C9	3.84	1.40	1.33
8	M	1010	SPO	C4-C1	3.85	1.58	1.53
5	R	2006	BPH	O2A-CGA	4.03	1.45	1.33
8	S	2010	SPO	C19-C17	4.06	1.41	1.35
5	L	1006	BPH	O2D-CGD	4.10	1.43	1.33
6	M	1008	U10	C23-C24	4.14	1.41	1.33
8	M	1010	SPO	O1-CM1	4.15	1.56	1.43
8	M	1010	SPO	C27-C28	4.16	1.38	1.34
8	M	1010	SPO	C14-C12	4.16	1.41	1.35
5	S	2005	BPH	O2A-CGA	4.16	1.45	1.33
6	L	1009[B]	U10	O4-C4	4.20	1.48	1.37
6	L	1009[A]	U10	C8-C9	4.22	1.41	1.33
6	R	2009[B]	U10	O4-C4	4.29	1.48	1.37
6	L	1009[A]	U10	O4-C4	4.30	1.48	1.37
8	S	2010	SPO	O1-CM1	4.30	1.56	1.43
6	R	2009[A]	U10	O4-C4	4.35	1.48	1.37
6	M	1008	U10	C13-C14	4.38	1.41	1.33
6	S	2008	U10	O4-C4	4.53	1.48	1.37
6	S	2008	U10	C13-C14	4.67	1.42	1.33
8	M	1010	SPO	C26-C25	4.84	1.47	1.34
8	S	2010	SPO	C26-C25	4.86	1.47	1.34
6	M	1008	U10	O4-C4	5.01	1.50	1.37
8	S	2010	SPO	C21-C20	5.02	1.49	1.35
6	L	1009[B]	U10	C13-C14	5.03	1.42	1.33
8	M	1010	SPO	C21-C20	5.15	1.49	1.35
6	L	1009[A]	U10	C13-C14	5.16	1.43	1.33
8	S	2010	SPO	C27-C28	5.37	1.40	1.34
8	S	2010	SPO	C15-C16	7.40	1.53	1.34
8	M	1010	SPO	C10-C11	7.64	1.54	1.34
8	M	1010	SPO	C6-C5	7.75	1.53	1.31
8	S	2010	SPO	C10-C11	7.78	1.54	1.34
8	S	2010	SPO	C6-C5	7.93	1.54	1.31
8	M	1010	SPO	C15-C16	8.01	1.55	1.34

All (280) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	M	1011	LDA	CM2-N1-CM1	-8.11	99.68	108.83
8	M	1010	SPO	O1-C1-C4	-7.97	86.37	105.87
8	S	2010	SPO	O1-C1-C4	-7.85	86.66	105.87
8	S	2010	SPO	C15-C14-C12	-6.38	117.98	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	S	2010	SPO	C20-C21-C22	-5.79	110.59	123.39
8	M	1010	SPO	C20-C21-C22	-5.55	111.12	123.39
8	M	1010	SPO	C15-C14-C12	-5.54	119.19	127.20
4	L	1001	BCL	CBC-CAC-C3C	-5.27	100.68	113.57
5	L	1006	BPH	O1D-CGD-CBD	-5.25	117.10	124.62
5	S	2005	BPH	O1D-CGD-CBD	-5.22	117.15	124.62
5	R	2006	BPH	O1D-CGD-CBD	-5.16	117.22	124.62
5	M	1005	BPH	O1D-CGD-CBD	-5.15	117.24	124.62
4	L	1001	BCL	C1-C2-C3	-5.11	118.34	126.71
8	S	2010	SPO	C25-C23-C22	-4.93	111.03	118.98
4	S	2001	BCL	CBC-CAC-C3C	-4.90	101.59	113.57
8	M	1010	SPO	C25-C23-C22	-4.87	111.14	118.98
4	S	2003	BCL	OBD-CAD-CBD	-4.77	118.74	125.94
4	L	1002	BCL	O2D-CGD-CBD	-4.22	105.50	111.30
4	M	1003	BCL	C11-C12-C13	-4.13	101.78	115.49
4	S	2003	BCL	C11-C12-C13	-4.10	101.91	115.49
4	M	1003	BCL	OBD-CAD-CBD	-4.07	119.80	125.94
8	S	2010	SPO	C4-C5-C6	-3.92	119.09	124.67
6	R	2009[A]	U10	O5-C5-C6	-3.80	114.53	121.68
4	L	1001	BCL	CAC-C3C-C4C	-3.78	104.20	112.58
6	L	1009[A]	U10	O5-C5-C6	-3.77	114.59	121.68
4	L	1002	BCL	OBD-CAD-CBD	-3.76	120.27	125.94
6	S	2008	U10	O5-C5-C6	-3.68	114.76	121.68
5	S	2005	BPH	O2D-CGD-O1D	-3.67	116.21	123.79
6	R	2009[B]	U10	O5-C5-C6	-3.64	114.83	121.68
8	S	2010	SPO	C6-C7-C9	-3.62	113.14	118.98
8	M	1010	SPO	C18-C17-C19	-3.62	117.55	122.90
4	L	1004	BCL	CAC-C3C-C4C	-3.58	104.63	112.58
5	R	2006	BPH	O2D-CGD-O1D	-3.57	116.43	123.79
6	L	1009[B]	U10	O5-C5-C6	-3.56	114.99	121.68
4	S	2001	BCL	OBD-CAD-CBD	-3.56	120.57	125.94
6	M	1008	U10	O5-C5-C6	-3.55	115.00	121.68
4	R	2002	BCL	C7-C6-C5	-3.55	102.57	113.06
6	L	1009[B]	U10	O2-C2-C3	-3.54	113.11	120.79
4	S	2003	BCL	OBB-CAB-CBB	-3.54	111.64	120.13
6	M	1008	U10	C20-C19-C21	-3.54	110.00	115.41
4	R	2002	BCL	OBD-CAD-CBD	-3.54	120.60	125.94
4	S	2004	BCL	C11-C12-C13	-3.53	103.77	115.49
4	L	1004	BCL	OBB-CAB-CBB	-3.53	111.67	120.13
4	M	1003	BCL	CAA-CBA-CGA	-3.53	103.00	113.32
4	S	2004	BCL	OBD-CAD-CBD	-3.51	120.64	125.94
8	S	2010	SPO	C15-C16-C17	-3.44	116.18	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	1003	BCL	OBB-CAB-CBB	-3.43	111.90	120.13
4	L	1002	BCL	C7-C6-C5	-3.43	102.93	113.06
4	L	1001	BCL	OBB-CAB-CBB	-3.42	111.93	120.13
4	S	2004	BCL	OBB-CAB-CBB	-3.37	112.05	120.13
4	R	2002	BCL	O2D-CGD-CBD	-3.34	106.71	111.30
6	L	1009[B]	U10	C20-C19-C21	-3.34	110.31	115.41
8	M	1010	SPO	C15-C16-C17	-3.33	116.52	126.32
5	M	1005	BPH	O2D-CGD-O1D	-3.31	116.96	123.79
5	L	1006	BPH	O2D-CGD-O1D	-3.27	117.04	123.79
4	R	2002	BCL	C11-C12-C13	-3.26	104.67	115.49
6	L	1009[A]	U10	C20-C19-C21	-3.24	110.46	115.41
4	R	2002	BCL	OBB-CAB-CBB	-3.22	112.41	120.13
8	M	1010	SPO	C4-C5-C6	-3.22	120.08	124.67
6	R	2009[B]	U10	O2-C2-C3	-3.21	113.84	120.79
6	L	1009[A]	U10	C1-C6-C5	-3.20	116.47	120.12
4	S	2004	BCL	CBC-CAC-C3C	-3.20	105.75	113.57
6	R	2009[A]	U10	O2-C2-C3	-3.18	113.89	120.79
4	L	1001	BCL	CAA-C2A-C3A	-3.17	104.11	113.22
6	L	1009[A]	U10	O2-C2-C3	-3.17	113.94	120.79
4	S	2004	BCL	CAA-C2A-C3A	-3.15	104.16	113.22
8	S	2010	SPO	C18-C17-C19	-3.15	118.25	122.90
8	M	1010	SPO	C6-C7-C9	-3.14	113.92	118.98
4	L	1004	BCL	OBD-CAD-CBD	-3.13	121.22	125.94
6	S	2008	U10	C20-C19-C21	-3.12	110.64	115.41
4	L	1002	BCL	OBB-CAB-CBB	-3.12	112.66	120.13
4	S	2004	BCL	CAC-C3C-C4C	-3.10	105.69	112.58
4	S	2001	BCL	CAA-C2A-C3A	-3.09	104.32	113.22
4	L	1001	BCL	OBD-CAD-CBD	-3.09	121.27	125.94
4	S	2001	BCL	OBB-CAB-CBB	-3.08	112.74	120.13
6	L	1009[B]	U10	C1-C6-C5	-3.07	116.61	120.12
4	L	1004	BCL	CBC-CAC-C3C	-3.03	106.16	113.57
4	S	2004	BCL	C16-C15-C13	-2.99	105.57	115.49
6	S	2008	U10	O2-C2-C3	-2.96	114.37	120.79
6	M	1008	U10	O2-C2-C3	-2.94	114.43	120.79
4	L	1004	BCL	C11-C12-C13	-2.91	105.83	115.49
6	R	2009[A]	U10	C1-C6-C5	-2.90	116.81	120.12
4	S	2003	BCL	CAA-CBA-CGA	-2.89	104.85	113.32
6	R	2009[B]	U10	C1-C6-C5	-2.87	116.85	120.12
4	R	2002	BCL	CAC-C3C-C4C	-2.84	106.27	112.58
8	S	2010	SPO	C20-C19-C17	-2.81	123.14	127.20
4	R	2002	BCL	CAA-C2A-C3A	-2.77	105.25	113.22
6	S	2008	U10	C1-C6-C5	-2.76	116.97	120.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	M	1010	SPO	C10-C9-C7	-2.74	123.24	127.20
4	L	1002	BCL	C16-C15-C13	-2.73	106.44	115.49
4	L	1002	BCL	CAC-C3C-C4C	-2.72	106.54	112.58
4	L	1004	BCL	CAC-C3C-C2C	-2.69	107.38	114.13
4	S	2004	BCL	CHA-C1A-NA	-2.68	119.47	126.06
4	M	1003	BCL	CHA-C1A-NA	-2.64	119.56	126.06
5	M	1005	BPH	CAA-C2A-C3A	-2.62	105.68	113.22
6	M	1008	U10	C1-C6-C5	-2.58	117.17	120.12
5	L	1006	BPH	C7-C6-C5	-2.58	105.45	113.06
6	L	1009[A]	U10	C7-C6-C5	-2.56	115.55	118.56
4	L	1002	BCL	C11-C12-C13	-2.56	107.01	115.49
5	L	1006	BPH	OBD-CAD-CBD	-2.55	122.09	125.94
4	L	1002	BCL	CAA-C2A-C3A	-2.54	105.92	113.22
4	S	2003	BCL	CHA-C1A-NA	-2.51	119.89	126.06
4	R	2002	BCL	CMB-C2B-C1B	-2.50	124.22	128.36
5	S	2005	BPH	CAA-C2A-C3A	-2.50	106.03	113.22
5	M	1005	BPH	O2A-CGA-O1A	-2.50	117.04	123.49
4	S	2003	BCL	CMB-C2B-C1B	-2.49	124.25	128.36
4	L	1001	BCL	CHA-C1A-NA	-2.48	119.95	126.06
4	S	2004	BCL	CAC-C3C-C2C	-2.47	107.91	114.13
4	R	2002	BCL	CHA-C1A-NA	-2.47	119.98	126.06
5	R	2006	BPH	O2A-CGA-O1A	-2.47	117.12	123.49
4	M	1003	BCL	CBC-CAC-C3C	-2.46	107.56	113.57
4	M	1003	BCL	CGD-CBD-CAD	-2.45	102.31	110.62
5	L	1006	BPH	O2A-CGA-O1A	-2.45	117.18	123.49
5	M	1005	BPH	OBD-CAD-CBD	-2.43	122.28	125.94
4	S	2001	BCL	CAC-C3C-C4C	-2.42	107.21	112.58
4	L	1002	BCL	CHA-C1A-NA	-2.42	120.10	126.06
4	S	2001	BCL	CHA-C1A-NA	-2.40	120.15	126.06
4	L	1002	BCL	CMB-C2B-C1B	-2.37	124.44	128.36
5	M	1005	BPH	C2A-C1A-NA	-2.36	109.05	112.08
8	M	1010	SPO	C20-C19-C17	-2.35	123.80	127.20
4	S	2003	BCL	CBC-CAC-C3C	-2.34	107.83	113.57
5	L	1006	BPH	CAA-C2A-C3A	-2.33	106.51	113.22
5	R	2006	BPH	C5-C3-C2	-2.32	116.65	121.05
5	R	2006	BPH	CAA-C2A-C1A	-2.30	106.81	112.86
4	S	2001	BCL	C1-C2-C3	-2.30	122.94	126.71
4	L	1004	BCL	CHA-C1A-NA	-2.29	120.42	126.06
4	R	2002	BCL	C16-C15-C13	-2.27	107.95	115.49
6	L	1009[A]	U10	C10-C9-C11	-2.26	111.95	115.41
5	S	2005	BPH	OBD-CAD-CBD	-2.26	122.53	125.94
4	S	2003	BCL	CAA-C2A-C3A	-2.26	106.73	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	1003	BCL	C11-C10-C8	-2.25	108.02	115.49
5	R	2006	BPH	CAA-C2A-C3A	-2.22	106.84	113.22
4	S	2003	BCL	CAC-C3C-C4C	-2.19	107.73	112.58
5	S	2005	BPH	C2A-C1A-NA	-2.19	109.28	112.08
4	S	2003	BCL	CGD-CBD-CAD	-2.19	103.21	110.62
4	M	1003	BCL	CAC-C3C-C4C	-2.18	107.75	112.58
6	R	2009[A]	U10	C7-C6-C5	-2.18	116.00	118.56
4	S	2004	BCL	C7-C6-C5	-2.18	106.64	113.06
5	R	2006	BPH	C7-C6-C5	-2.17	106.65	113.06
5	L	1006	BPH	CMA-C3A-C2A	-2.17	104.75	114.35
5	L	1006	BPH	CAA-C2A-C1A	-2.16	107.17	112.86
5	M	1005	BPH	CAC-C3C-C2C	-2.16	108.70	114.13
5	R	2006	BPH	CBB-CAB-C3B	-2.16	115.72	120.52
5	S	2005	BPH	C5-C3-C2	-2.15	115.95	120.74
4	L	1004	BCL	CMB-C2B-C1B	-2.13	124.84	128.36
4	M	1003	BCL	CAA-C2A-C3A	-2.12	107.13	113.22
5	S	2005	BPH	O2A-CGA-O1A	-2.11	118.04	123.49
4	R	2002	BCL	CBC-CAC-C3C	-2.10	108.43	113.57
9	M	1011	LDA	C9-C8-C7	-2.09	103.72	114.53
5	M	1005	BPH	C3A-C4A-NA	-2.09	109.91	113.57
4	M	1003	BCL	O2A-CGA-O1A	-2.09	118.11	123.49
4	L	1002	BCL	C12-C11-C10	-2.08	102.65	112.99
5	R	2006	BPH	C3A-C4A-NA	-2.07	109.95	113.57
4	L	1002	BCL	CMA-C3A-C2A	-2.06	105.22	114.35
4	S	2003	BCL	CAC-C3C-C2C	-2.06	108.96	114.13
5	L	1006	BPH	C3A-C4A-NA	-2.05	109.98	113.57
5	M	1005	BPH	CMA-C3A-C2A	-2.04	105.31	114.35
8	M	1010	SPO	C5-C6-C7	-2.04	122.63	125.75
5	R	2006	BPH	OBD-CAD-CBD	-2.04	122.86	125.94
4	M	1003	BCL	CMB-C2B-C1B	-2.04	124.99	128.36
4	S	2003	BCL	C11-C10-C8	-2.04	108.73	115.49
4	L	1004	BCL	C12-C11-C10	-2.02	102.95	112.99
9	M	1011	LDA	CM1-N1-C1	-2.02	103.26	109.77
4	M	1003	BCL	C2C-C3C-C4C	2.02	104.92	101.50
4	M	1003	BCL	O2A-CGA-CBA	2.03	118.07	111.90
6	S	2008	U10	C17-C16-C14	2.03	119.32	112.71
4	L	1002	BCL	C2C-C3C-C4C	2.04	104.96	101.50
4	L	1004	BCL	CBA-CAA-C2A	2.05	119.50	113.73
5	S	2005	BPH	C6-C5-C3	2.05	123.57	112.89
5	R	2006	BPH	CMD-C2D-C3D	2.06	129.12	125.09
4	L	1001	BCL	CHD-C4C-NC	2.07	127.46	125.06
4	L	1004	BCL	C3D-CAD-CBD	2.07	110.53	107.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	S	2003	BCL	C2C-C3C-C4C	2.08	105.02	101.50
6	L	1009[A]	U10	C17-C16-C14	2.10	119.57	112.71
4	R	2002	BCL	C6-C5-C3	2.11	117.12	112.48
6	L	1009[B]	U10	C7-C8-C9	2.11	130.28	126.70
6	L	1009[A]	U10	C22-C21-C19	2.12	117.96	114.43
6	L	1009[B]	U10	C17-C16-C14	2.12	119.63	112.71
6	M	1008	U10	C17-C18-C19	2.13	132.39	127.76
5	S	2005	BPH	CMD-C2D-C3D	2.18	129.35	125.09
4	L	1001	BCL	C3D-CAD-CBD	2.20	110.70	107.60
4	R	2002	BCL	C3D-CAD-CBD	2.20	110.70	107.60
6	L	1009[B]	U10	C22-C21-C19	2.20	118.10	114.43
4	S	2001	BCL	CBB-CAB-C3B	2.21	126.89	120.33
5	M	1005	BPH	C2C-C3C-C4C	2.22	105.25	101.50
6	L	1009[A]	U10	C8-C7-C6	2.27	118.45	111.64
4	S	2003	BCL	CBA-CAA-C2A	2.27	120.13	113.73
4	L	1002	BCL	CBB-CAB-C3B	2.28	127.08	120.33
4	L	1001	BCL	CMB-C2B-C3B	2.28	129.55	125.09
4	L	1001	BCL	CBB-CAB-C3B	2.29	127.12	120.33
5	M	1005	BPH	CMD-C2D-C3D	2.34	129.67	125.09
4	R	2002	BCL	CBB-CAB-C3B	2.35	127.31	120.33
4	S	2004	BCL	C3D-CAD-CBD	2.35	110.92	107.60
4	S	2001	BCL	CMB-C2B-C3B	2.37	129.72	125.09
5	R	2006	BPH	C2C-C3C-C4C	2.37	105.52	101.50
4	M	1003	BCL	CMB-C2B-C3B	2.38	129.74	125.09
6	L	1009[A]	U10	C21-C19-C18	2.38	125.56	121.05
4	L	1001	BCL	O1D-CGD-CBD	2.38	128.04	124.62
6	L	1009[B]	U10	C21-C19-C18	2.39	125.58	121.05
4	R	2002	BCL	C4-C3-C5	2.39	119.06	115.41
4	S	2004	BCL	CMB-C2B-C3B	2.45	129.89	125.09
6	S	2008	U10	C21-C19-C18	2.46	125.72	121.05
5	L	1006	BPH	C2C-C3C-C4C	2.48	105.70	101.50
4	S	2003	BCL	CBB-CAB-C3B	2.48	127.68	120.33
6	L	1009[A]	U10	C17-C18-C19	2.49	133.17	127.76
4	L	1004	BCL	CMB-C2B-C3B	2.49	129.97	125.09
4	S	2001	BCL	C3D-CAD-CBD	2.50	111.12	107.60
4	S	2001	BCL	O1D-CGD-CBD	2.50	128.21	124.62
6	M	1008	U10	C21-C19-C18	2.51	125.81	121.05
5	S	2005	BPH	C2C-C3C-C4C	2.52	105.78	101.50
4	M	1003	BCL	C3D-CAD-CBD	2.56	111.21	107.60
4	S	2004	BCL	C2C-C3C-C4C	2.59	105.90	101.50
6	M	1008	U10	C16-C14-C13	2.59	125.97	121.05
4	L	1004	BCL	CBB-CAB-C3B	2.60	128.03	120.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	S	2008	U10	C17-C18-C19	2.61	133.44	127.76
4	M	1003	BCL	CBB-CAB-C3B	2.63	128.14	120.33
4	L	1004	BCL	C2C-C3C-C4C	2.65	106.00	101.50
4	S	2004	BCL	CBB-CAB-C3B	2.66	128.21	120.33
4	S	2003	BCL	CMB-C2B-C3B	2.69	130.34	125.09
4	S	2003	BCL	O1D-CGD-CBD	2.73	128.53	124.62
4	L	1002	BCL	CMB-C2B-C3B	2.75	130.46	125.09
6	L	1009[B]	U10	C17-C18-C19	2.76	133.76	127.76
4	S	2001	BCL	C2C-C3C-C4C	2.78	106.20	101.50
4	R	2002	BCL	CMB-C2B-C3B	2.83	130.62	125.09
4	M	1003	BCL	O1D-CGD-CBD	2.86	128.73	124.62
4	S	2003	BCL	C3D-CAD-CBD	2.88	111.67	107.60
4	L	1001	BCL	C2C-C3C-C4C	2.89	106.39	101.50
4	S	2001	BCL	CBA-CAA-C2A	2.95	122.06	113.73
6	S	2008	U10	C16-C14-C13	2.96	126.66	121.05
8	S	2010	SPO	C8-C7-C6	3.05	123.17	118.10
8	M	1010	SPO	C8-C7-C6	3.06	123.19	118.10
5	S	2005	BPH	CBC-CAC-C3C	3.07	121.08	113.57
4	M	1003	BCL	CMD-C2D-C3D	3.10	131.15	125.09
4	M	1003	BCL	CBA-CAA-C2A	3.17	122.69	113.73
6	L	1009[A]	U10	C16-C14-C13	3.20	127.12	121.05
6	L	1009[B]	U10	C16-C14-C13	3.22	127.15	121.05
8	S	2010	SPO	C3-C1-C2	3.28	116.84	110.22
4	R	2002	BCL	CMD-C2D-C3D	3.50	131.94	125.09
8	M	1010	SPO	C3-C1-C2	3.50	117.29	110.22
4	S	2003	BCL	CMD-C2D-C3D	3.52	131.96	125.09
4	R	2002	BCL	O1D-CGD-CBD	3.54	129.69	124.62
4	S	2003	BCL	C4-C3-C5	3.55	120.83	115.41
5	L	1006	BPH	C11-C10-C8	3.69	127.72	115.49
5	S	2005	BPH	C4-C3-C5	3.70	119.87	115.68
8	S	2010	SPO	C24-C23-C25	3.74	124.33	118.10
4	S	2001	BCL	CMD-C2D-C3D	3.77	132.45	125.09
4	L	1002	BCL	CMD-C2D-C3D	3.78	132.49	125.09
5	R	2006	BPH	CED-O2D-CGD	3.82	124.95	115.99
5	M	1005	BPH	CBC-CAC-C3C	3.83	122.93	113.57
4	M	1003	BCL	C4-C3-C5	3.83	121.26	115.41
4	L	1004	BCL	CMD-C2D-C3D	3.84	132.60	125.09
5	L	1006	BPH	C4A-NA-C1A	3.88	111.68	108.21
5	S	2005	BPH	CED-O2D-CGD	3.89	125.11	115.99
5	R	2006	BPH	C11-C10-C8	3.91	128.46	115.49
8	M	1010	SPO	C24-C23-C25	3.91	124.61	118.10
4	L	1001	BCL	CMD-C2D-C3D	3.93	132.78	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	S	2005	BPH	C4A-NA-C1A	3.96	111.74	108.21
6	M	1008	U10	C27-C28-C29	3.98	143.06	127.73
4	S	2004	BCL	CMD-C2D-C3D	4.00	132.91	125.09
4	L	1002	BCL	O1D-CGD-CBD	4.02	130.38	124.62
5	M	1005	BPH	CED-O2D-CGD	4.22	125.90	115.99
5	M	1005	BPH	C4A-NA-C1A	4.26	112.01	108.21
5	L	1006	BPH	CED-O2D-CGD	4.30	126.07	115.99
5	R	2006	BPH	CBC-CAC-C3C	4.38	124.27	113.57
5	L	1006	BPH	CBC-CAC-C3C	4.53	124.65	113.57
5	R	2006	BPH	C4A-NA-C1A	4.58	112.30	108.21
5	M	1005	BPH	C6-C5-C3	4.73	122.87	112.48
5	R	2006	BPH	C6-C5-C3	4.95	123.35	112.48
9	M	1011	LDA	O1-N1-C1	5.27	116.20	110.27
5	L	1006	BPH	C6-C5-C3	5.49	124.53	112.48
6	M	1008	U10	C3M-O3-C3	5.74	137.03	116.61
6	L	1009[B]	U10	C3M-O3-C3	5.97	137.85	116.61
6	S	2008	U10	C3M-O3-C3	6.09	138.27	116.61
6	R	2009[B]	U10	C3M-O3-C3	6.26	138.86	116.61
6	R	2009[A]	U10	C3M-O3-C3	6.37	139.25	116.61
6	L	1009[A]	U10	C3M-O3-C3	6.39	139.32	116.61
5	M	1005	BPH	O2D-CGD-CBD	10.56	125.80	111.30
5	L	1006	BPH	O2D-CGD-CBD	10.59	125.83	111.30
5	R	2006	BPH	O2D-CGD-CBD	10.93	126.30	111.30
5	S	2005	BPH	O2D-CGD-CBD	11.18	126.64	111.30

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	L	1006	BPH	C8
5	L	1006	BPH	C13
5	R	2006	BPH	C8
5	R	2006	BPH	C13
5	M	1005	BPH	C8

There are no torsion outliers.

There are no ring outliers.

18 monomers are involved in 102 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	1001	BCL	11	0
4	L	1002	BCL	11	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	1004	BCL	10	0
5	L	1006	BPH	5	0
6	L	1009[A]	U10	1	0
6	L	1009[B]	U10	2	0
4	M	1003	BCL	19	0
8	M	1010	SPO	6	0
9	M	1011	LDA	2	0
4	R	2002	BCL	11	0
5	R	2006	BPH	8	0
6	R	2009[A]	U10	1	0
6	R	2009[B]	U10	2	0
4	S	2001	BCL	8	0
4	S	2003	BCL	16	0
4	S	2004	BCL	8	0
5	S	2005	BPH	7	0
8	S	2010	SPO	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	L	281/281 (100%)	0.17	2 (0%) 89 87	23, 42, 61, 77	0
1	R	281/281 (100%)	0.46	24 (8%) 13 9	35, 56, 73, 82	0
2	M	301/307 (98%)	0.14	12 (3%) 42 34	26, 38, 53, 85	0
2	S	299/307 (97%)	0.18	12 (4%) 42 34	37, 50, 59, 89	0
3	H	246/260 (94%)	0.06	8 (3%) 50 43	28, 44, 65, 97	0
3	T	246/260 (94%)	0.54	31 (12%) 5 3	47, 62, 84, 99	0
All	All	1654/1696 (97%)	0.26	89 (5%) 29 22	23, 49, 74, 99	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	1	ALA	6.1
3	T	55	PRO	5.7
3	H	252	VAL	5.0
3	T	252	VAL	4.5
3	T	158	LEU	4.2
3	T	51	ALA	4.1
3	H	255	MET	4.0
3	T	54	GLY	4.0
3	T	69	GLY	3.9
3	H	251	VAL	3.9
3	T	46	ASP	3.7
1	R	252	GLY	3.7
3	T	254	ALA	3.7
1	R	75	LEU	3.7
3	T	92	VAL	3.5
2	M	301	HIS	3.4
3	T	253	ALA	3.4
2	S	233	CYS	3.3
2	S	223	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
3	T	29	TYR	3.3
3	T	52	ASN	3.3
2	M	1	ALA	3.2
1	R	74	GLY	3.1
1	R	202	LYS	3.1
1	R	276	PRO	3.0
1	R	275	ILE	3.0
3	T	255	MET	3.0
2	M	226	VAL	2.9
1	R	272	TRP	2.9
1	L	51	TRP	2.9
1	R	7	ARG	2.9
2	M	224	LEU	2.9
3	T	77	GLY	2.9
3	H	253	ALA	2.8
3	T	155	GLY	2.8
3	H	254	ALA	2.8
3	T	102	GLY	2.7
1	R	77	GLY	2.7
1	R	140	GLY	2.7
1	R	277	GLY	2.7
2	S	84	VAL	2.7
2	M	223	ILE	2.6
2	M	227	SER	2.6
1	R	69	PRO	2.6
1	R	267	VAL	2.6
2	S	87	ARG	2.5
3	T	154	ARG	2.5
1	R	251	THR	2.5
1	R	73	TYR	2.5
3	T	247	LYS	2.5
3	T	101	THR	2.5
3	T	53	GLN	2.4
2	M	225	ALA	2.4
3	T	251	VAL	2.4
3	T	56	PHE	2.4
1	R	59	TRP	2.4
2	S	245	ALA	2.4
1	R	76	GLY	2.4
2	S	3	TYR	2.4
3	T	109	VAL	2.4
2	S	139	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
2	S	301	HIS	2.4
3	T	256	LEU	2.3
3	T	96	PHE	2.3
1	R	271	TRP	2.3
2	S	260	ALA	2.3
3	H	256	LEU	2.2
1	L	113	ILE	2.2
3	T	50	ALA	2.2
2	M	231	GLY	2.2
3	T	60	LYS	2.2
2	S	231	GLY	2.1
3	T	249	LYS	2.1
2	S	237	GLN	2.1
2	M	214	LEU	2.1
2	S	54	SER	2.1
1	R	266	TRP	2.1
3	H	158	LEU	2.1
3	T	79	GLU	2.1
3	H	250	SER	2.1
3	T	59	PRO	2.1
3	T	61	PRO	2.1
1	R	281	GLY	2.1
1	R	269	LEU	2.0
2	M	222	THR	2.0
1	R	256	PHE	2.0
2	M	2	GLU	2.0
2	M	212	SER	2.0
1	R	270	PRO	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	U10	L	1009[B]	30/63	0.67	0.64	9.67	44,54,65,66	30
6	U10	R	2009[B]	18/63	0.65	0.53	8.87	95,96,97,97	18
6	U10	L	1009[A]	30/63	0.67	0.64	8.09	54,67,69,70	30
6	U10	R	2009[A]	18/63	0.65	0.53	7.63	94,96,97,98	18
9	LDA	M	1011	16/16	0.74	0.34	7.30	49,61,78,78	0
8	SPO	S	2010	42/42	0.90	0.24	2.37	38,49,64,66	0
4	BCL	S	2001	51/66	0.90	0.23	2.32	38,45,58,61	0
6	U10	M	1008	38/63	0.91	0.36	2.25	36,42,63,64	0
8	SPO	M	1010	42/42	0.90	0.24	2.24	31,36,59,61	0
4	BCL	S	2003	66/66	0.92	0.23	2.01	44,49,62,71	0
6	U10	S	2008	32/63	0.96	0.38	1.97	56,58,64,66	0
5	BPH	L	1006	65/65	0.92	0.29	1.79	24,35,41,43	0
4	BCL	L	1002	66/66	0.90	0.24	1.78	31,36,44,52	0
4	BCL	L	1004	66/66	0.93	0.32	1.76	28,34,57,59	0
4	BCL	S	2004	66/66	0.91	0.23	1.74	44,52,74,75	0
5	BPH	R	2006	65/65	0.90	0.24	1.69	47,56,61,62	0
4	BCL	R	2002	66/66	0.89	0.21	1.30	42,53,56,56	0
4	BCL	L	1001	51/66	0.93	0.23	1.21	26,32,45,48	0
4	BCL	M	1003	66/66	0.93	0.22	1.09	24,38,47,49	0
5	BPH	S	2005	51/65	0.94	0.20	0.85	35,42,51,52	0
5	BPH	M	1005	55/65	0.94	0.21	0.65	26,32,43,46	0
7	FE2	S	2007	1/1	0.98	0.14	-1.79	51,51,51,51	0
7	FE2	M	1007	1/1	0.99	0.15	-2.22	33,33,33,33	0

6.5 Other polymers (i)

There are no such residues in this entry.