Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:05 PM GMT

PDB ID	:	1RZZ
Title	:	PHOTOSYNTHETIC REACTION CENTER DOUBLE MUTANT FROM RHODOBACTER SPHAEROIDES WITH ASP L213 REPLACED WITH ASN AND ARG M233 REPLACED WITH CYS IN THE CHARGE-NEUTRAL DQAQB STATE (TETRAGONAL FORM)
Authors	:	Xu, Q.; Axelrod, H.L.; Abresch, E.C.; Paddock, M.L.; Okamura, M.Y.; Feher, G.
Deposited on	:	2003-12-29
Resolution	:	2.40 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:

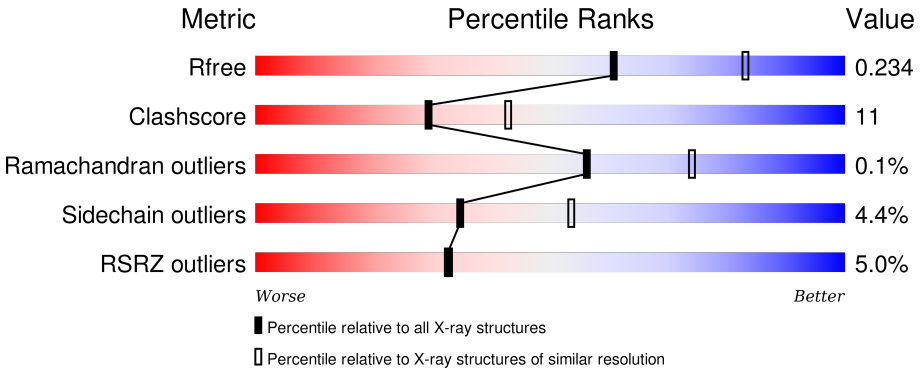
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	L	281	2% 77% 21%
1	R	281	6% 75% 22%
2	M	307	5% 78% 18%
2	S	307	3% 78% 18%
3	H	260	4% 79% 15% 5%

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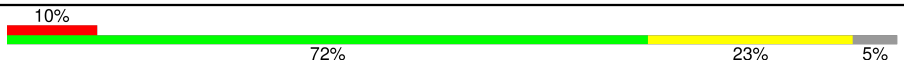
Mol	Chain	Length	Quality of chain
3	T	260	

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	L	1002	-	-	-	X
4	BCL	R	2002	-	-	-	X
4	BCL	S	2001	-	-	-	X
4	BCL	S	2003	-	-	-	X
5	U10	L	1009	-	-	-	X
5	U10	R	2009	-	-	-	X
5	U10	S	2008	-	-	-	X
7	BPH	M	1005	X	-	-	-
7	BPH	M	1006	X	-	-	-
7	BPH	R	2006	X	-	-	-
7	BPH	S	2005	X	-	-	-
8	SPO	M	1010	-	-	-	X
8	SPO	S	2010	-	-	-	X
9	LDA	M	1011	-	-	-	X
9	LDA	M	1012	-	-	-	X
9	LDA	M	1013	-	-	-	X
9	LDA	M	1014	-	-	-	X
9	LDA	S	2011	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 14481 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	299	Total	C	N	O	S	0	0	0
			2385	1594	388	392	11			
2	S	299	Total	C	N	O	S	0	0	0
			2385	1594	388	392	11			

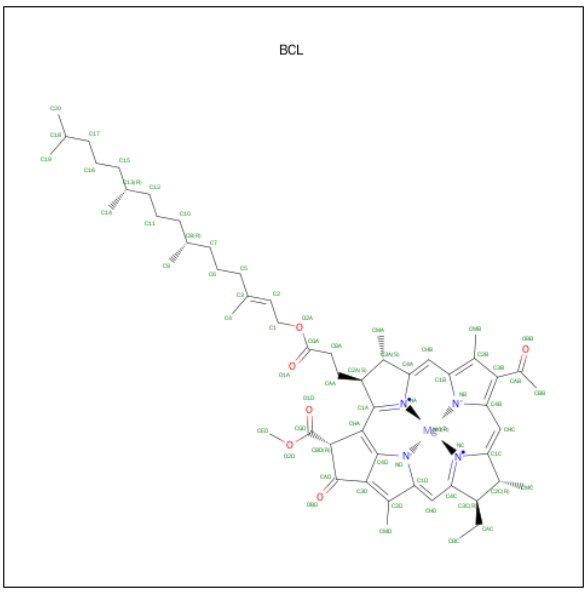
There are 2 discrepancies between the modelled and reference sequences:

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.

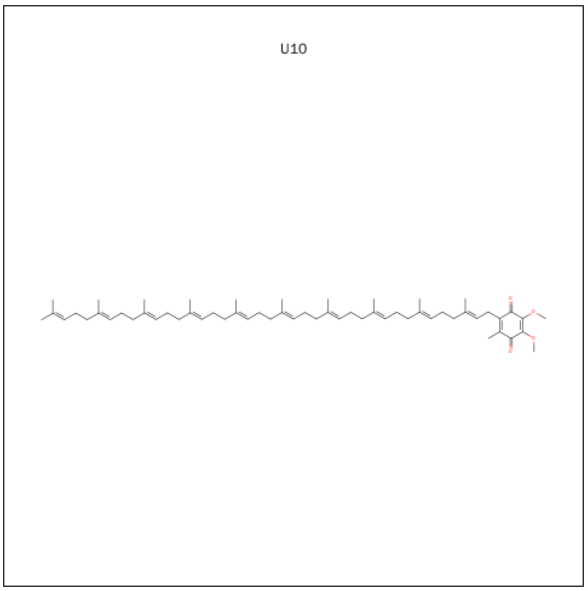
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	246	Total	C	N	O	S	0	0	0
			1869	1196	320	343	10			
3	T	246	Total	C	N	O	S	0	0	0
			1869	1196	320	343	10			

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

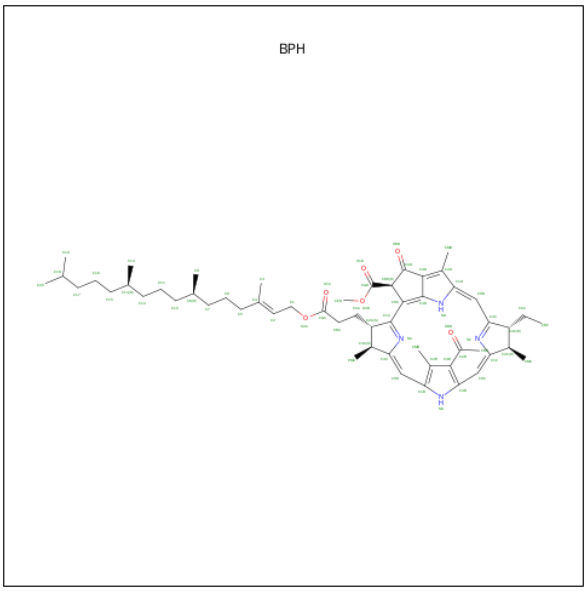


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	1	Total C O 44 40 4	0	0
5	M	1	Total C O 38 34 4	0	0
5	R	1	Total C O 18 14 4	0	0
5	S	1	Total C O 32 28 4	0	0

- Molecule 6 is FE (II) ION (three-letter code: FE2) (formula: Fe).

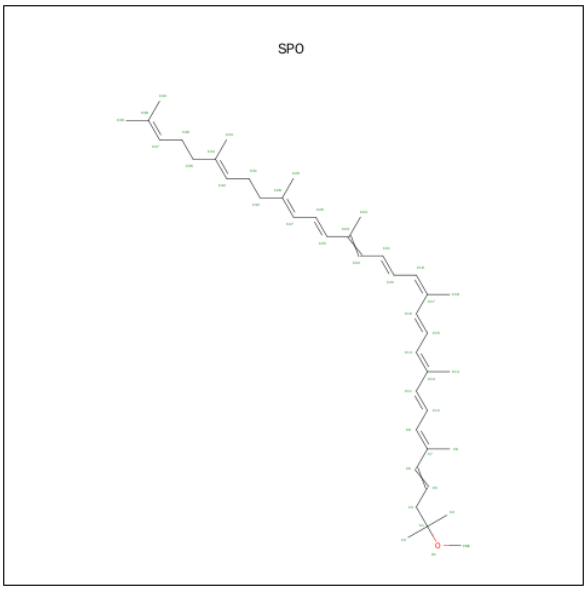
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	S	1	Total Fe 1 1	0	0
6	M	1	Total Fe 1 1	0	0

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



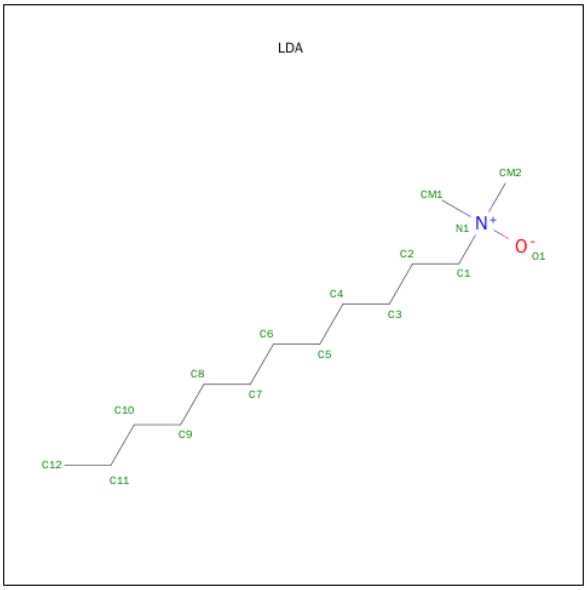
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	M	1	Total C N O 55 45 4 6	0	0
7	M	1	Total C N O 65 55 4 6	0	0
7	R	1	Total C N O 65 55 4 6	0	0
7	S	1	Total C N O 55 45 4 6	0	0

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

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	L	72	Total O 72 72	0	0
10	M	107	Total O 107 107	0	0

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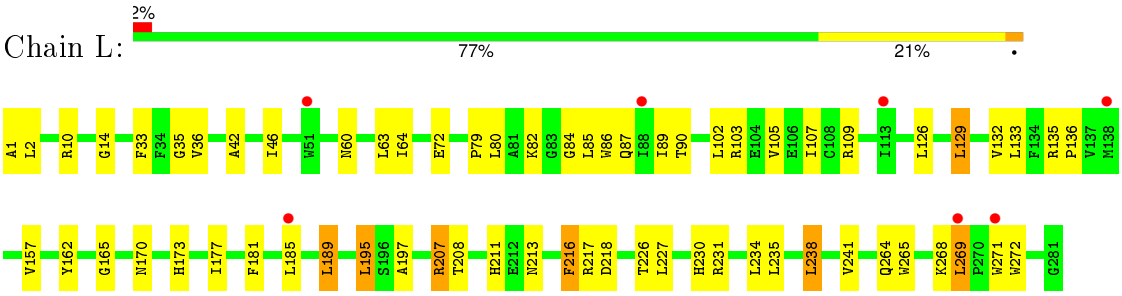
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	H	109	Total O 109 109	0	0
10	R	47	Total O 47 47	0	0
10	S	75	Total O 75 75	0	0
10	T	63	Total O 63 63	0	0

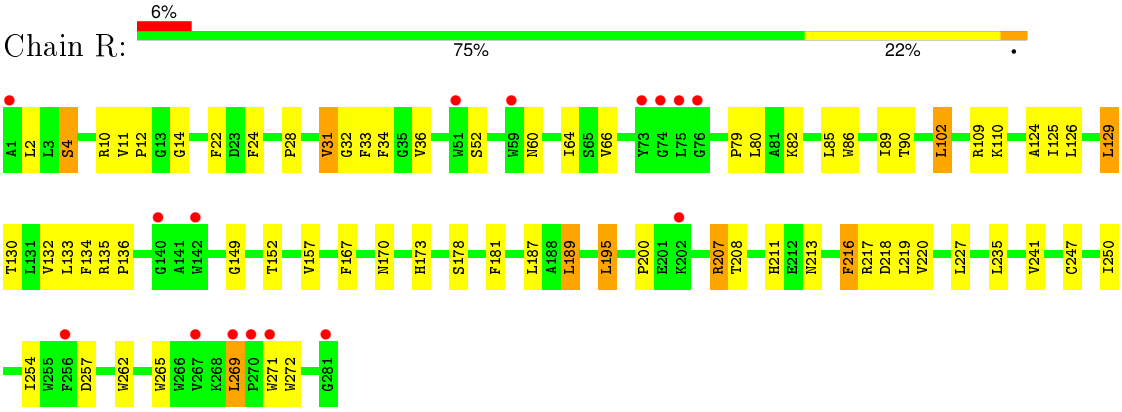
3 Residue-property plots

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.

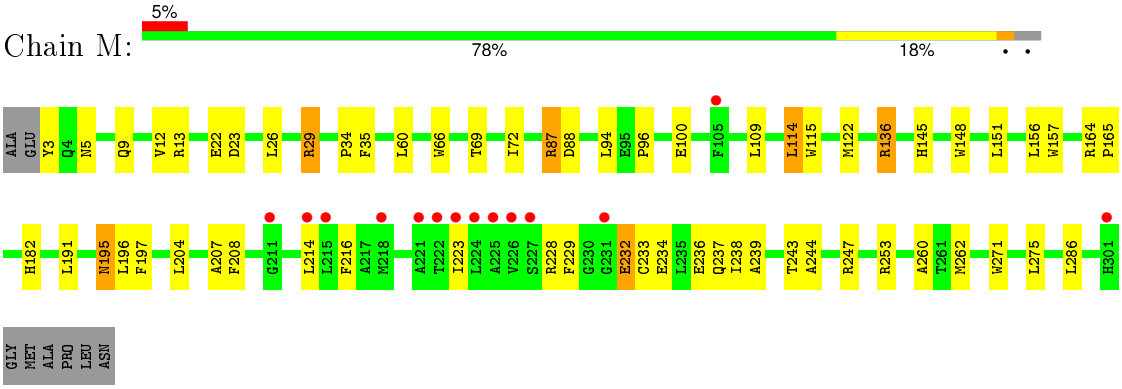
- Molecule 1: Reaction center protein L chain



- Molecule 1: Reaction center protein L chain

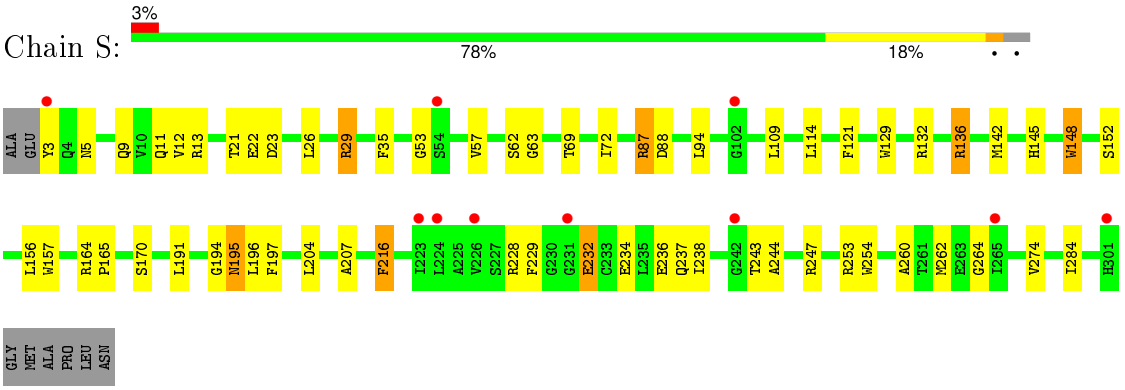


- Molecule 2: Reaction center protein M chain



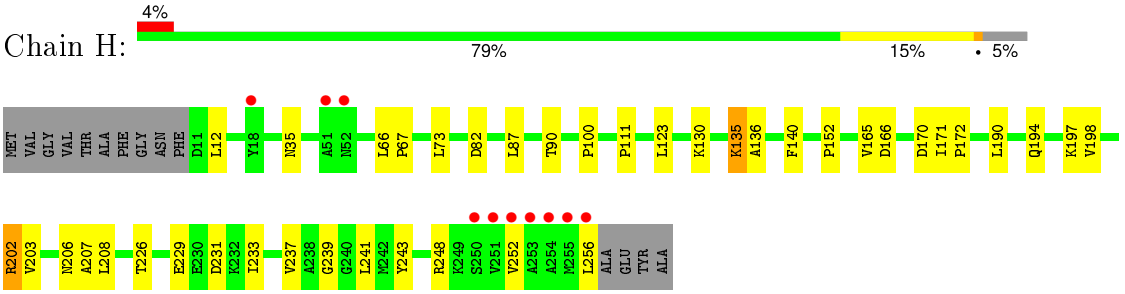
- Molecule 2: Reaction center protein M chain

Chain S:



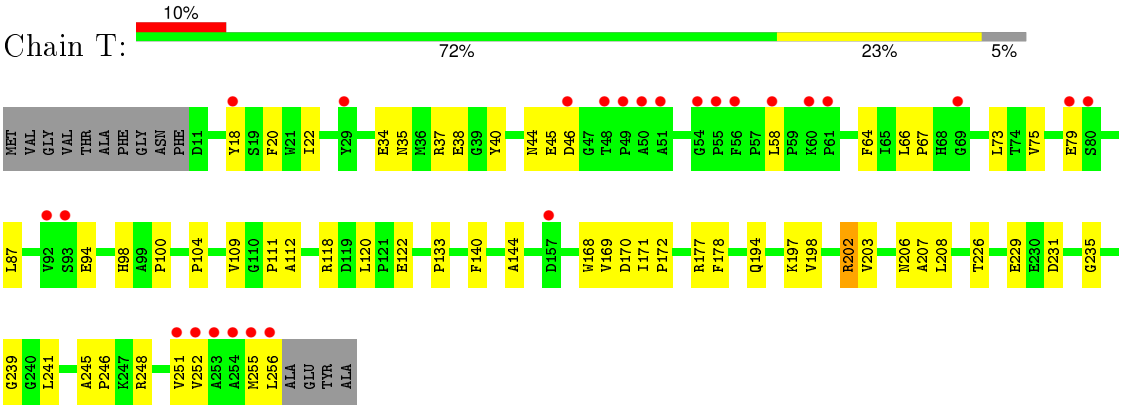
- Molecule 3: Reaction center protein H chain

Chain H:



- Molecule 3: Reaction center protein H chain

Chain T:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	139.58Å 139.58Å 274.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.76 – 2.40 39.76 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.2 (39.76-2.40) 98.3 (39.76-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.216 , 0.238 0.212 , 0.234	Depositor DCC
R_{free} test set	5283 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	36.9	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 56.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Outliers	1 of 104640 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	14481	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% 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	0.42	0/2320	0.57	0/3175
1	R	0.37	0/2320	0.55	0/3175
2	M	0.41	0/2477	0.56	0/3383
2	S	0.39	0/2477	0.53	0/3383
3	H	0.35	0/1917	0.60	0/2608
3	T	0.31	0/1917	0.56	0/2608
All	All	0.38	0/13428	0.56	0/18332

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	57	0
1	R	2232	0	2189	60	0
2	M	2385	0	2296	51	0
2	S	2385	0	2296	63	0
3	H	1869	0	1884	36	0
3	T	1869	0	1884	52	0
4	L	183	0	189	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	M	66	0	74	13	0
4	R	66	0	74	5	0
4	S	183	0	189	21	0
5	L	44	0	56	3	0
5	M	38	0	47	4	0
5	R	18	0	15	0	0
5	S	32	0	39	1	0
6	M	1	0	0	0	0
6	S	1	0	0	0	0
7	M	120	0	127	6	0
7	R	65	0	74	5	0
7	S	55	0	53	2	0
8	M	42	0	60	4	0
8	S	42	0	60	3	0
9	M	64	0	124	3	0
9	S	16	0	31	0	0
10	H	109	0	0	1	0
10	L	72	0	0	1	0
10	M	107	0	0	2	0
10	R	47	0	0	2	0
10	S	75	0	0	3	0
10	T	63	0	0	1	0
All	All	14481	0	13950	317	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 11.

All (317) 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:241:VAL:HG21	7:R:2006:BPH:HAC1	1.40	1.03
1:L:241:VAL:HG21	7:M:1006:BPH:HAC2	1.38	1.01
2:M:109:LEU:HD12	2:M:114:LEU:HD13	1.56	0.86
2:S:157:TRP:HB2	4:S:2003:BCL:H62	1.58	0.84
4:S:2001:BCL:HBC1	4:S:2003:BCL:CAD	2.09	0.82
1:R:79:PRO:HG2	1:R:82:LYS:HB2	1.61	0.82
1:R:208:THR:H	1:R:211:HIS:HD2	1.28	0.81
2:S:207:ALA:HA	4:S:2004:BCL:O1A	1.81	0.80
2:S:21:THR:HG23	2:S:26:LEU:HD11	1.63	0.80
1:R:227:LEU:HD13	2:S:232:GLU:HG2	1.64	0.80
2:S:13:ARG:HD2	2:S:35:PHE:CD2	2.18	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:208:THR:H	1:R:211:HIS:CD2	2.01	0.78
2:M:157:TRP:HB2	4:M:1003:BCL:H62	1.65	0.77
1:R:52:SER:HB2	1:R:85:LEU:HD23	1.66	0.77
1:L:189:LEU:HG	1:L:216:PHE:HZ	1.50	0.76
1:L:217:ARG:HD2	10:M:1043:HOH:O	1.85	0.75
5:M:1008:U10:H202	9:M:1012:LDA:H123	1.68	0.75
2:S:197:PHE:HZ	4:S:2003:BCL:HBB2	1.50	0.75
1:L:79:PRO:HG2	1:L:82:LYS:HB2	1.69	0.74
1:R:189:LEU:HG	1:R:216:PHE:HZ	1.53	0.73
1:R:2:LEU:HG	1:R:10:ARG:NH1	2.04	0.73
2:M:197:PHE:HZ	4:M:1003:BCL:HBB2	1.54	0.72
4:L:1001:BCL:HBB3	4:M:1003:BCL:H41	1.72	0.71
3:H:202:ARG:HG2	3:H:203:VAL:N	2.06	0.71
4:R:2002:BCL:HBD	4:S:2004:BCL:HBC1	1.73	0.70
1:R:217:ARG:HD2	10:S:2014:HOH:O	1.92	0.70
2:S:63:GLY:HA3	7:S:2005:BPH:H5C2	1.74	0.70
2:M:253:ARG:HD3	10:M:1016:HOH:O	1.91	0.69
4:L:1002:BCL:HBD	4:L:1004:BCL:CBC	2.21	0.69
2:S:136:ARG:NE	2:S:136:ARG:HA	2.07	0.69
3:H:252:VAL:O	3:H:256:LEU:HD13	1.92	0.68
3:H:171:ILE:HB	3:H:172:PRO:HD3	1.75	0.68
4:L:1004:BCL:HMA1	4:L:1004:BCL:H121	1.76	0.68
3:T:226:THR:OG1	3:T:229:GLU:HG3	1.94	0.68
3:T:44:ASN:HB2	3:T:46:ASP:OD1	1.94	0.67
3:T:202:ARG:HG2	3:T:203:VAL:N	2.09	0.67
10:R:2021:HOH:O	2:S:253:ARG:HD3	1.94	0.67
1:L:105:VAL:O	1:L:109:ARG:HG3	1.94	0.67
2:S:228:ARG:HA	3:T:194:GLN:CG	2.25	0.66
2:S:243:THR:O	2:S:247:ARG:HG3	1.94	0.66
3:T:73:LEU:HD11	3:T:75:VAL:HG13	1.77	0.66
1:R:135:ARG:HB3	1:R:136:PRO:HD3	1.77	0.66
2:S:9:GLN:NE2	3:T:198:VAL:H	1.94	0.66
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.77	0.66
2:M:9:GLN:NE2	3:H:198:VAL:H	1.93	0.65
3:H:87:LEU:HD23	3:H:100:PRO:HA	1.78	0.65
3:T:252:VAL:O	3:T:256:LEU:HD13	1.97	0.65
4:R:2002:BCL:HBD	4:S:2004:BCL:CBC	2.27	0.65
2:M:197:PHE:CZ	4:M:1003:BCL:HBB2	2.32	0.65
2:M:136:ARG:NE	2:M:136:ARG:HA	2.10	0.64
1:L:86:TRP:CH2	1:L:132:VAL:HG13	2.33	0.64
1:L:80:LEU:H	1:L:80:LEU:HD22	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:14:GLY:O	1:R:109:ARG:HD3	1.97	0.64
2:M:13:ARG:HD2	2:M:35:PHE:CD2	2.33	0.63
1:L:208:THR:H	1:L:211:HIS:CD2	2.16	0.63
4:S:2001:BCL:HBB3	4:S:2003:BCL:H41	1.79	0.63
1:L:185:LEU:HD23	4:L:1001:BCL:H42	1.80	0.63
2:S:109:LEU:HD12	2:S:114:LEU:HD13	1.80	0.63
1:L:33:PHE:O	1:L:36:VAL:HG22	1.98	0.62
4:L:1004:BCL:O1A	2:M:207:ALA:HA	1.99	0.62
4:L:1001:BCL:HBC1	4:M:1003:BCL:CBD	2.29	0.62
3:T:118:ARG:HD3	3:T:120:LEU:HD12	1.80	0.62
2:M:9:GLN:HE22	3:H:197:LYS:HA	1.64	0.61
1:L:189:LEU:HB3	5:L:1009:U10:H4M3	1.81	0.61
2:S:69:THR:O	2:S:72:ILE:HG22	2.00	0.61
2:S:195:ASN:ND2	2:S:197:PHE:H	1.98	0.61
4:L:1002:BCL:HBD	4:L:1004:BCL:HBC1	1.82	0.61
1:L:84:GLY:HA2	1:L:87:GLN:HE21	1.64	0.60
2:M:208:PHE:HE1	9:M:1014:LDA:H101	1.65	0.60
4:L:1004:BCL:H61	5:M:1008:U10:H203	1.84	0.60
1:L:86:TRP:CZ2	1:L:132:VAL:HG13	2.36	0.60
1:L:208:THR:H	1:L:211:HIS:HD2	1.48	0.60
2:S:236:GLU:HG3	3:T:122:GLU:OE2	2.01	0.60
1:L:60:ASN:CG	1:L:63:LEU:HD23	2.22	0.59
2:M:243:THR:O	2:M:247:ARG:HG3	2.03	0.59
2:S:9:GLN:HE22	3:T:198:VAL:H	1.50	0.59
2:M:228:ARG:HA	3:H:194:GLN:HG2	1.85	0.59
1:L:265:TRP:O	1:L:269:LEU:HD13	2.02	0.59
3:T:87:LEU:HD23	3:T:100:PRO:HA	1.84	0.58
2:M:260:ALA:HB1	3:H:35:ASN:OD1	2.05	0.57
1:L:14:GLY:O	1:L:109:ARG:HD3	2.05	0.57
3:T:194:GLN:CD	3:T:194:GLN:H	2.07	0.57
1:R:178:SER:HA	4:S:2001:BCL:O1A	2.05	0.57
2:S:157:TRP:HB2	4:S:2003:BCL:C6	2.30	0.56
2:M:69:THR:O	2:M:72:ILE:HG22	2.04	0.56
1:R:28:PRO:HB3	2:S:253:ARG:NH1	2.20	0.56
4:L:1002:BCL:HBD	4:L:1004:BCL:HBC3	1.85	0.56
3:H:135:LYS:HB3	3:H:135:LYS:NZ	2.20	0.56
3:T:133:PRO:HG3	3:T:168:TRP:CZ2	2.40	0.56
3:T:37:ARG:O	3:T:38:GLU:HG2	2.06	0.56
4:L:1001:BCL:HBC1	4:M:1003:BCL:HBD	1.88	0.56
2:S:228:ARG:HA	3:T:194:GLN:HG3	1.86	0.56
4:L:1001:BCL:HBC1	4:M:1003:BCL:CAD	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:197:PHE:CZ	4:S:2003:BCL:HBB2	2.35	0.56
1:L:218:ASP:OD1	2:M:29:ARG:HD2	2.05	0.56
3:T:133:PRO:HG3	3:T:168:TRP:CE2	2.41	0.56
2:M:157:TRP:HB2	4:M:1003:BCL:C6	2.35	0.56
1:L:60:ASN:O	1:L:64:ILE:HG13	2.06	0.56
1:L:157:VAL:HG11	4:M:1003:BCL:HBB1	1.87	0.55
3:T:45:GLU:HG3	3:T:94:GLU:OE1	2.06	0.55
2:S:264:GLY:HA3	3:T:35:ASN:OD1	2.06	0.55
3:H:206:ASN:HD21	3:H:248:ARG:HD2	1.71	0.55
3:T:73:LEU:CD1	3:T:75:VAL:HG13	2.35	0.55
1:L:60:ASN:ND2	1:L:63:LEU:HD23	2.22	0.55
1:R:218:ASP:OD1	2:S:29:ARG:HD2	2.07	0.55
2:S:12:VAL:HG21	3:T:169:VAL:HG21	1.89	0.54
2:S:195:ASN:HD22	2:S:195:ASN:C	2.09	0.54
1:R:170:ASN:HB3	1:R:173:HIS:CB	2.38	0.54
1:R:265:TRP:O	1:R:269:LEU:HD13	2.08	0.54
2:S:152:SER:HB2	2:S:274:VAL:HG13	1.89	0.54
1:L:269:LEU:HD23	1:L:271:TRP:CZ2	2.44	0.53
3:T:241:LEU:O	3:T:248:ARG:NH2	2.41	0.53
1:L:264:GLN:OE1	1:L:268:LYS:HE2	2.08	0.53
1:L:103:ARG:O	1:L:107:ILE:HG13	2.07	0.53
3:H:130:LYS:HE3	3:H:170:ASP:OD2	2.08	0.53
2:S:9:GLN:HE22	3:T:197:LYS:HA	1.73	0.53
3:T:37:ARG:HH11	3:T:37:ARG:HG2	1.73	0.53
1:R:213:ASN:O	1:R:217:ARG:HB2	2.08	0.53
3:T:251:VAL:O	3:T:255:MET:HG3	2.09	0.53
1:L:80:LEU:H	1:L:80:LEU:CD2	2.22	0.53
1:R:189:LEU:HG	1:R:216:PHE:CZ	2.41	0.52
1:R:157:VAL:HG11	4:S:2003:BCL:HBB1	1.91	0.52
2:S:157:TRP:HD1	4:S:2001:BCL:HBB1	1.73	0.52
4:L:1002:BCL:H122	7:M:1006:BPH:H3A	1.92	0.52
3:H:152:PRO:HG2	3:H:202:ARG:HB2	1.91	0.52
3:T:168:TRP:HB2	3:T:178:PHE:HB2	1.90	0.52
2:S:152:SER:CB	2:S:274:VAL:HG13	2.40	0.52
3:T:171:ILE:HB	3:T:172:PRO:HD3	1.92	0.52
3:H:66:LEU:HD22	3:H:66:LEU:N	2.25	0.52
1:L:238:LEU:HD12	7:M:1006:BPH:CBC	2.41	0.51
1:L:213:ASN:O	1:L:217:ARG:HB2	2.10	0.51
1:R:269:LEU:HD23	1:R:271:TRP:CZ2	2.45	0.51
1:R:33:PHE:O	1:R:36:VAL:HG22	2.10	0.51
2:M:271:TRP:O	2:M:275:LEU:HG	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:241:LEU:O	3:H:248:ARG:NH2	2.44	0.51
1:R:22:PHE:HA	1:R:24:PHE:CE2	2.45	0.51
1:R:257:ASP:HB3	10:R:2056:HOH:O	2.10	0.51
3:H:207:ALA:O	3:H:208:LEU:HD12	2.11	0.51
2:S:164:ARG:HB3	2:S:165:PRO:HD3	1.94	0.50
2:S:284:ILE:HG12	4:S:2003:BCL:HED3	1.93	0.50
2:S:13:ARG:O	3:T:140:PHE:HA	2.11	0.50
1:L:85:LEU:O	1:L:89:ILE:HG13	2.10	0.50
1:L:216:PHE:CE1	5:L:1009:U10:H4M2	2.46	0.50
3:H:194:GLN:H	3:H:194:GLN:CD	2.14	0.50
2:M:9:GLN:HE22	3:H:198:VAL:H	1.57	0.50
4:R:2002:BCL:H122	7:R:2006:BPH:H3A	1.93	0.50
4:S:2004:BCL:HMA1	4:S:2004:BCL:H121	1.93	0.50
1:L:189:LEU:HG	1:L:216:PHE:CZ	2.40	0.50
1:R:85:LEU:O	1:R:89:ILE:HG13	2.12	0.50
2:S:21:THR:HG23	2:S:26:LEU:CD1	2.38	0.50
1:R:80:LEU:HB3	1:R:85:LEU:HD13	1.92	0.50
4:L:1001:BCL:HBB2	8:M:1010:SPO:H243	1.94	0.49
3:H:135:LYS:NZ	3:H:135:LYS:CB	2.75	0.49
1:L:72:GLU:HG3	10:L:1062:HOH:O	2.11	0.49
2:M:195:ASN:ND2	2:M:197:PHE:H	2.10	0.49
1:L:231:ARG:HD2	2:M:5:ASN:O	2.13	0.49
3:H:82:ASP:N	3:H:82:ASP:OD1	2.45	0.49
1:R:28:PRO:HB3	2:S:253:ARG:HH11	1.75	0.49
4:R:2002:BCL:H52	7:R:2006:BPH:HBB2	1.94	0.49
2:S:3:TYR:CE1	2:S:9:GLN:HG3	2.47	0.49
3:T:37:ARG:HG2	3:T:37:ARG:NH1	2.28	0.49
3:H:66:LEU:HD22	3:H:66:LEU:H	1.77	0.49
1:L:1:ALA:C	1:L:2:LEU:HD12	2.34	0.49
4:L:1001:BCL:HBB2	4:L:1001:BCL:HHC	1.95	0.48
2:M:208:PHE:CE1	9:M:1014:LDA:H101	2.46	0.48
1:R:80:LEU:O	1:R:85:LEU:HB2	2.12	0.48
2:M:3:TYR:CE1	2:M:9:GLN:HG3	2.47	0.48
1:R:195:LEU:HB3	2:S:145:HIS:CD2	2.47	0.48
1:R:80:LEU:H	1:R:80:LEU:HD22	1.78	0.48
1:L:162:TYR:HA	1:L:165:GLY:O	2.13	0.48
3:T:170:ASP:HB2	3:T:177:ARG:HG3	1.96	0.48
4:S:2001:BCL:HBB2	8:S:2010:SPO:H243	1.95	0.48
3:T:118:ARG:HG2	3:T:120:LEU:HB2	1.96	0.48
1:R:133:LEU:C	1:R:133:LEU:HD23	2.34	0.48
2:M:164:ARG:HB3	2:M:165:PRO:HD3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:90:THR:CG2	1:L:132:VAL:HG11	2.44	0.48
2:M:195:ASN:HD22	2:M:195:ASN:C	2.17	0.48
3:T:206:ASN:HD21	3:T:248:ARG:HD2	1.79	0.47
2:M:114:LEU:HD12	2:M:114:LEU:HA	1.73	0.47
4:L:1002:BCL:HAA2	4:L:1004:BCL:HBC1	1.97	0.47
1:R:125:ILE:HG22	1:R:129:LEU:HD22	1.96	0.47
3:T:34:GLU:HA	3:T:34:GLU:OE1	2.13	0.47
2:M:66:TRP:CD1	2:M:122:MET:HB2	2.50	0.47
2:M:237:GLN:HB2	2:M:262:MET:HG2	1.96	0.47
1:R:181:PHE:CZ	4:S:2003:BCL:O1A	2.68	0.47
1:R:241:VAL:CG2	7:R:2006:BPH:HAC1	2.30	0.47
4:R:2002:BCL:NC	4:S:2003:BCL:HBB3	2.30	0.47
1:R:170:ASN:HB3	1:R:173:HIS:HB2	1.96	0.47
1:L:170:ASN:HB3	1:L:173:HIS:CB	2.45	0.46
1:R:66:VAL:HG11	1:R:89:ILE:HD12	1.97	0.46
1:L:227:LEU:HD13	2:M:232:GLU:HG2	1.98	0.46
1:R:60:ASN:O	1:R:64:ILE:HG13	2.15	0.46
4:L:1001:BCL:CBC	4:M:1003:BCL:CAD	2.93	0.46
2:S:228:ARG:HA	3:T:194:GLN:HG2	1.96	0.46
2:M:234:GLU:O	2:M:238:ILE:HG13	2.14	0.46
3:T:111:PRO:HB2	3:T:239:GLY:HA2	1.98	0.46
4:S:2001:BCL:HBB3	4:S:2003:BCL:H61	1.97	0.46
3:H:111:PRO:HB2	3:H:239:GLY:HA2	1.97	0.46
2:S:3:TYR:CZ	2:S:5:ASN:HA	2.51	0.46
1:R:11:VAL:HB	1:R:12:PRO:HD2	1.98	0.46
1:R:80:LEU:H	1:R:80:LEU:CD2	2.29	0.46
3:T:87:LEU:HD22	3:T:98:HIS:O	2.15	0.46
2:S:204:LEU:HD13	3:T:20:PHE:CE2	2.51	0.46
3:H:233:ILE:O	3:H:237:VAL:HG23	2.16	0.46
1:L:35:GLY:HA2	1:L:103:ARG:HD2	1.98	0.46
4:L:1001:BCL:H41	5:L:1009:U10:H112	1.97	0.45
1:L:80:LEU:HD22	1:L:80:LEU:N	2.28	0.45
4:S:2001:BCL:HHC	4:S:2001:BCL:HBB2	1.99	0.45
3:H:135:LYS:HB3	3:H:135:LYS:HZ3	1.82	0.45
3:H:111:PRO:HD2	3:H:243:TYR:CE2	2.52	0.45
3:H:165:VAL:O	3:H:166:ASP:HB2	2.17	0.45
2:M:228:ARG:HA	3:H:194:GLN:CG	2.45	0.45
2:S:237:GLN:HB2	2:S:262:MET:HG2	1.98	0.45
3:H:226:THR:OG1	3:H:229:GLU:HG3	2.16	0.45
2:S:194:GLY:O	2:S:195:ASN:HB3	2.17	0.45
3:T:40:TYR:HB3	3:T:58:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:1004:BCL:HBB3	7:M:1006:BPH:H152	1.99	0.45
1:L:185:LEU:HD13	7:M:1005:BPH:ND	2.32	0.45
1:R:170:ASN:HB3	1:R:173:HIS:HB3	1.97	0.44
2:M:286:LEU:CD2	3:H:12:LEU:HD12	2.48	0.44
4:S:2001:BCL:CBB	8:S:2010:SPO:H243	2.47	0.44
1:R:149:GLY:HA3	1:R:152:THR:OG1	2.17	0.44
1:R:211:HIS:HE1	2:S:22:GLU:OE1	2.00	0.44
2:M:195:ASN:HD22	2:M:197:PHE:H	1.64	0.44
1:R:34:PHE:CE1	1:R:102:LEU:HD23	2.52	0.44
3:T:207:ALA:HA	3:T:241:LEU:HD23	2.00	0.44
1:R:129:LEU:HB3	1:R:134:PHE:CE2	2.52	0.44
2:S:148:TRP:HA	2:S:148:TRP:CE3	2.53	0.44
1:L:207:ARG:HD2	1:L:207:ARG:HA	1.57	0.44
1:R:207:ARG:HG3	2:S:142:MET:HG2	1.99	0.44
1:L:226:THR:HG23	1:L:227:LEU:N	2.33	0.44
2:S:229:PHE:HB2	2:S:244:ALA:HB2	2.00	0.44
3:H:90:THR:HG22	10:H:290:HOH:O	2.16	0.44
1:R:262:TRP:O	1:R:265:TRP:HD1	2.01	0.44
3:H:66:LEU:HA	3:H:67:PRO:HD3	1.85	0.44
3:T:64:PHE:HD2	3:T:73:LEU:HD12	1.82	0.44
3:H:12:LEU:C	3:H:12:LEU:HD13	2.38	0.44
2:M:196:LEU:HA	2:M:196:LEU:HD12	1.85	0.44
3:T:18:TYR:O	3:T:22:ILE:HG12	2.18	0.44
2:S:148:TRP:HE3	2:S:148:TRP:HA	1.82	0.43
2:S:87:ARG:HG3	2:S:88:ASP:N	2.33	0.43
4:L:1001:BCL:HMB2	7:M:1005:BPH:HMB3	2.00	0.43
2:S:53:GLY:O	2:S:57:VAL:HG23	2.18	0.43
2:S:129:TRP:O	2:S:132:ARG:HB3	2.17	0.43
2:M:96:PRO:HB3	2:M:115:TRP:CE2	2.53	0.43
2:S:11:GLN:HB2	3:T:144:ALA:HB3	2.00	0.43
1:L:177:ILE:HG12	4:L:1002:BCL:HMB3	2.00	0.43
2:S:236:GLU:OE1	3:T:122:GLU:HG2	2.18	0.43
2:S:62:SER:HB3	2:S:121:PHE:O	2.18	0.43
3:T:112:ALA:HA	3:T:235:GLY:O	2.19	0.43
2:S:63:GLY:CA	7:S:2005:BPH:H5C2	2.47	0.43
2:M:13:ARG:O	3:H:140:PHE:HA	2.19	0.43
1:R:90:THR:HG23	1:R:132:VAL:HG11	2.01	0.43
1:L:80:LEU:HD12	1:L:85:LEU:HD13	2.00	0.43
2:M:22:GLU:HB3	2:M:23:ASP:H	1.67	0.43
1:R:86:TRP:CH2	1:R:132:VAL:HG13	2.54	0.42
2:S:234:GLU:O	2:S:238:ILE:HG13	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:87:ARG:HG3	2:M:88:ASP:N	2.34	0.42
1:R:227:LEU:HD13	2:S:232:GLU:CG	2.43	0.42
3:T:66:LEU:HA	3:T:67:PRO:HD3	1.84	0.42
1:R:130:THR:HA	1:R:134:PHE:HD2	1.84	0.42
1:L:197:ALA:HA	1:L:207:ARG:HB2	2.01	0.42
1:L:230:HIS:CD2	2:M:223:ILE:HG13	2.54	0.42
4:L:1004:BCL:HBA2	4:L:1004:BCL:H3A	1.73	0.42
1:L:170:ASN:HB3	1:L:173:HIS:HB3	2.01	0.42
2:M:214:LEU:HD21	5:M:1008:U10:H172	2.00	0.42
2:S:22:GLU:HB3	2:S:23:ASP:H	1.61	0.42
3:T:104:PRO:HA	3:T:109:VAL:HG22	2.01	0.42
4:M:1003:BCL:CBB	4:M:1003:BCL:HHC	2.49	0.42
2:M:182:HIS:CG	8:M:1010:SPO:H181	2.54	0.42
1:L:185:LEU:HD12	1:L:185:LEU:O	2.19	0.42
2:M:13:ARG:HD2	2:M:35:PHE:CE2	2.54	0.42
3:T:206:ASN:ND2	10:T:312:HOH:O	2.48	0.42
1:R:133:LEU:HD22	1:R:134:PHE:CD1	2.54	0.42
1:L:129:LEU:HD12	1:L:129:LEU:HA	1.86	0.42
2:S:114:LEU:HA	2:S:114:LEU:HD12	1.94	0.42
3:H:194:GLN:H	3:H:194:GLN:NE2	2.18	0.42
1:L:211:HIS:HE1	2:M:22:GLU:OE1	2.02	0.42
2:M:239:ALA:HB1	3:H:66:LEU:HD11	2.02	0.42
1:R:219:LEU:HG	1:R:220:VAL:HG13	2.01	0.42
2:S:170:SER:HB2	10:S:2022:HOH:O	2.20	0.42
1:L:42:ALA:O	1:L:46:ILE:HG13	2.19	0.42
5:M:1008:U10:H4M2	5:M:1008:U10:H3M3	2.02	0.41
2:S:260:ALA:HB1	3:T:35:ASN:OD1	2.19	0.41
1:R:250:ILE:HB	1:R:254:ILE:HD11	2.03	0.41
1:L:195:LEU:HB3	2:M:145:HIS:CD2	2.55	0.41
2:S:195:ASN:HD22	2:S:196:LEU:N	2.18	0.41
8:S:2010:SPO:H131	8:S:2010:SPO:H15	1.85	0.41
3:H:190:LEU:HB2	3:H:233:ILE:HD13	2.00	0.41
1:R:187:LEU:HD13	2:S:216:PHE:CG	2.55	0.41
1:R:4:SER:O	3:T:79:GLU:HG2	2.20	0.41
1:R:110:LYS:HD2	2:S:254:TRP:CZ3	2.55	0.41
10:S:2032:HOH:O	3:T:194:GLN:HB3	2.20	0.41
1:R:2:LEU:HG	1:R:10:ARG:HH12	1.83	0.41
3:T:73:LEU:C	3:T:73:LEU:HD13	2.41	0.41
2:M:148:TRP:HA	2:M:148:TRP:HE3	1.85	0.41
3:T:73:LEU:HD11	3:T:75:VAL:CG1	2.47	0.41
3:H:135:LYS:HG2	3:H:136:ALA:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:234:LEU:O	1:L:238:LEU:HB2	2.21	0.41
1:L:90:THR:HG23	1:L:132:VAL:HG11	2.01	0.41
2:M:233:CYS:O	2:M:236:GLU:HB3	2.21	0.41
2:M:204:LEU:O	2:M:207:ALA:HB3	2.20	0.41
8:M:1010:SPO:H131	8:M:1010:SPO:H15	1.88	0.41
1:L:135:ARG:N	1:L:136:PRO:CD	2.84	0.41
1:R:31:VAL:HG12	1:R:32:GLY:N	2.36	0.41
2:M:100:GLU:H	2:M:100:GLU:CD	2.25	0.41
3:T:245:ALA:N	3:T:246:PRO:CD	2.84	0.41
2:S:195:ASN:ND2	2:S:195:ASN:C	2.73	0.41
4:M:1003:BCL:H62	4:M:1003:BCL:H92	1.94	0.40
1:R:200:PRO:HB3	1:R:207:ARG:HD3	2.04	0.40
1:R:124:ALA:HB2	7:R:2006:BPH:HBC3	2.03	0.40
1:L:181:PHE:CZ	4:M:1003:BCL:O1A	2.74	0.40
2:M:148:TRP:HA	2:M:148:TRP:CE3	2.56	0.40
4:L:1001:BCL:CBB	8:M:1010:SPO:H243	2.51	0.40
4:S:2004:BCL:H61	5:S:2008:U10:H203	2.03	0.40
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.56	0.40
1:R:66:VAL:HG12	1:R:86:TRP:HB2	2.02	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%)	269 (96%)	10 (4%)	0	100	100
1	R	279/281 (99%)	263 (94%)	14 (5%)	2 (1%)	26	38
2	M	297/307 (97%)	285 (96%)	12 (4%)	0	100	100
2	S	297/307 (97%)	287 (97%)	10 (3%)	0	100	100
3	H	244/260 (94%)	236 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	T	244/260 (94%)	235 (96%)	9 (4%)	0	100 100
All	All	1640/1696 (97%)	1575 (96%)	63 (4%)	2 (0%)	56 74

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	R	4	SER
1	R	31	VAL

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%)	207 (94%)	13 (6%)	24 38
1	R	220/220 (100%)	208 (94%)	12 (6%)	27 42
2	M	235/240 (98%)	220 (94%)	15 (6%)	22 34
2	S	235/240 (98%)	225 (96%)	10 (4%)	35 55
3	H	199/208 (96%)	194 (98%)	5 (2%)	55 76
3	T	199/208 (96%)	196 (98%)	3 (2%)	72 87
All	All	1308/1336 (98%)	1250 (96%)	58 (4%)	35 53

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	10	ARG
1	L	102	LEU
1	L	126	LEU
1	L	129	LEU
1	L	133	LEU
1	L	189	LEU
1	L	195	LEU
1	L	207	ARG
1	L	216	PHE

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Mol	Chain	Res	Type
1	L	235	LEU
1	L	238	LEU
1	L	269	LEU
1	L	272	TRP
2	M	12	VAL
2	M	26	LEU
2	M	29	ARG
2	M	34	PRO
2	M	60	LEU
2	M	87	ARG
2	M	94	LEU
2	M	114	LEU
2	M	136	ARG
2	M	151	LEU
2	M	156	LEU
2	M	191	LEU
2	M	195	ASN
2	M	216	PHE
2	M	232	GLU
3	H	73	LEU
3	H	123	LEU
3	H	135	LYS
3	H	202	ARG
3	H	231	ASP
1	R	102	LEU
1	R	126	LEU
1	R	129	LEU
1	R	167	PHE
1	R	189	LEU
1	R	195	LEU
1	R	207	ARG
1	R	216	PHE
1	R	235	LEU
1	R	247	CYS
1	R	269	LEU
1	R	272	TRP
2	S	29	ARG
2	S	87	ARG
2	S	94	LEU
2	S	136	ARG
2	S	148	TRP
2	S	156	LEU

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Mol	Chain	Res	Type
2	S	191	LEU
2	S	195	ASN
2	S	216	PHE
2	S	232	GLU
3	T	202	ARG
3	T	208	LEU
3	T	231	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	87	GLN
1	L	183	ASN
1	L	211	HIS
2	M	9	GLN
2	M	44	ASN
2	M	195	ASN
3	H	206	ASN
1	R	87	GLN
1	R	159	ASN
1	R	183	ASN
1	R	211	HIS
2	S	9	GLN
2	S	195	ASN
3	T	98	HIS
3	T	128	HIS
3	T	194	GLN
3	T	206	ASN

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 (i)

Of 25 ligands modelled in this entry, 2 are monoatomic - leaving 23 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	1.42	3 (7%)	40,97,115	2.00	12 (30%)
4	BCL	L	1002	-	53,74,74	0.97	2 (3%)	57,115,115	1.83	16 (28%)
4	BCL	L	1004	-	53,74,74	1.18	4 (7%)	57,115,115	1.73	16 (28%)
5	U10	L	1009	-	44,44,63	2.20	18 (40%)	53,56,79	3.16	16 (30%)
4	BCL	M	1003	-	53,74,74	1.05	3 (5%)	57,115,115	1.90	18 (31%)
7	BPH	M	1005	-	54,60,70	1.43	6 (11%)	61,89,101	2.28	13 (21%)
7	BPH	M	1006	-	64,70,70	1.44	9 (14%)	73,101,101	2.19	17 (23%)
5	U10	M	1008	-	38,38,63	2.04	11 (28%)	46,49,79	1.89	9 (19%)
8	SPO	M	1010	-	40,41,41	3.48	21 (52%)	45,50,50	2.44	13 (28%)
9	LDA	M	1011	-	15,15,15	3.65	2 (13%)	16,17,17	2.64	4 (25%)
9	LDA	M	1012	-	15,15,15	3.93	2 (13%)	16,17,17	2.58	4 (25%)
9	LDA	M	1013	-	15,15,15	3.86	2 (13%)	16,17,17	2.57	4 (25%)
9	LDA	M	1014	-	15,15,15	3.93	2 (13%)	16,17,17	2.65	5 (31%)
4	BCL	R	2002	-	53,74,74	1.04	2 (3%)	57,115,115	1.91	17 (29%)
7	BPH	R	2006	-	64,70,70	1.53	9 (14%)	73,101,101	2.23	16 (21%)
5	U10	R	2009	-	18,18,63	2.07	7 (38%)	22,25,79	2.15	6 (27%)
4	BCL	S	2001	-	38,59,74	1.28	2 (5%)	40,97,115	1.99	12 (30%)
4	BCL	S	2003	-	53,74,74	1.01	1 (1%)	57,115,115	2.00	23 (40%)
4	BCL	S	2004	-	53,74,74	1.16	5 (9%)	57,115,115	1.77	16 (28%)
7	BPH	S	2005	-	54,60,70	1.43	9 (16%)	61,89,101	2.44	17 (27%)
5	U10	S	2008	-	32,32,63	2.01	9 (28%)	38,41,79	1.93	9 (23%)
8	SPO	S	2010	-	40,41,41	3.35	25 (62%)	45,50,50	2.50	13 (28%)
9	LDA	S	2011	-	15,15,15	3.83	2 (13%)	16,17,17	2.62	4 (25%)

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	U10	L	1009	-	-	1/41/65/87	0/1/1/1
4	BCL	M	1003	-	-	0/37/137/137	0/0/9/9
7	BPH	M	1005	-	1/1/16/22	0/42/93/105	0/1/6/6
7	BPH	M	1006	-	2/2/18/22	1/54/105/105	0/1/6/6
5	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
9	LDA	M	1012	-	-	0/13/13/13	0/0/0/0
9	LDA	M	1013	-	-	0/13/13/13	0/0/0/0
9	LDA	M	1014	-	-	0/13/13/13	0/0/0/0
4	BCL	R	2002	-	-	0/37/137/137	0/0/9/9
7	BPH	R	2006	-	2/2/18/22	0/54/105/105	0/1/6/6
5	U10	R	2009	-	-	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
7	BPH	S	2005	-	1/1/16/22	0/42/93/105	0/1/6/6
5	U10	S	2008	-	-	0/26/50/87	0/1/1/1
8	SPO	S	2010	-	-	0/47/47/47	0/0/0/0
9	LDA	S	2011	-	-	0/13/13/13	0/0/0/0

All (156) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	1012	LDA	O1-N1	-14.56	1.25	1.39
9	M	1014	LDA	O1-N1	-14.47	1.25	1.39
9	M	1013	LDA	O1-N1	-14.29	1.26	1.39
9	S	2011	LDA	O1-N1	-14.12	1.26	1.39
9	M	1011	LDA	O1-N1	-13.41	1.26	1.39
7	M	1006	BPH	C11-C10	-4.95	1.29	1.52
7	R	2006	BPH	C11-C10	-4.93	1.29	1.52
4	L	1001	BCL	C3C-C4C	-4.92	1.45	1.51
5	M	1008	U10	C7-C8	-4.32	1.44	1.50
4	S	2001	BCL	C3C-C4C	-3.99	1.46	1.51
9	M	1014	LDA	CM2-N1	-3.86	1.43	1.49
9	S	2011	LDA	CM2-N1	-3.83	1.43	1.49
9	M	1012	LDA	CM2-N1	-3.80	1.43	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	1011	LDA	CM2-N1	-3.71	1.43	1.49
9	M	1013	LDA	CM2-N1	-3.70	1.43	1.49
5	S	2008	U10	C7-C8	-3.26	1.45	1.50
5	M	1008	U10	O3-C3M	-3.14	1.37	1.45
4	L	1004	BCL	C3C-C4C	-2.99	1.47	1.51
8	M	1010	SPO	C25-C23	-2.85	1.39	1.45
5	R	2009	U10	O3-C3M	-2.84	1.38	1.45
7	M	1005	BPH	O2D-CED	-2.83	1.38	1.45
5	R	2009	U10	C7-C8	-2.82	1.46	1.50
8	S	2010	SPO	C25-C23	-2.82	1.39	1.45
5	S	2008	U10	O3-C3M	-2.81	1.38	1.45
4	S	2004	BCL	C3C-C4C	-2.81	1.48	1.51
7	M	1006	BPH	O2D-CED	-2.78	1.38	1.45
5	L	1009	U10	C7-C8	-2.78	1.46	1.50
5	L	1009	U10	C32-C33	-2.73	1.42	1.50
5	L	1009	U10	O3-C3M	-2.66	1.38	1.45
8	M	1010	SPO	C11-C12	-2.63	1.40	1.45
5	M	1008	U10	C27-C28	-2.60	1.43	1.50
8	S	2010	SPO	C11-C12	-2.59	1.40	1.45
7	R	2006	BPH	O2D-CED	-2.48	1.39	1.45
8	S	2010	SPO	C6-C7	-2.34	1.40	1.45
7	S	2005	BPH	O2D-CED	-2.31	1.39	1.45
5	L	1009	U10	C27-C28	-2.25	1.44	1.50
7	S	2005	BPH	C2C-C3C	-2.19	1.48	1.54
4	M	1003	BCL	C3C-C4C	-2.11	1.48	1.51
8	S	2010	SPO	C31-C32	-2.05	1.44	1.50
4	M	1003	BCL	CMD-C2D	2.00	1.55	1.51
4	S	2001	BCL	CAA-CBA	2.05	1.59	1.52
4	L	1001	BCL	CAA-C2A	2.05	1.58	1.54
7	S	2005	BPH	C2A-C1A	2.06	1.55	1.51
8	S	2010	SPO	C35-C33	2.09	1.56	1.51
8	M	1010	SPO	C26-C27	2.11	1.50	1.43
4	L	1002	BCL	CBB-CAB	2.13	1.56	1.49
4	S	2004	BCL	CBB-CAB	2.16	1.56	1.49
8	M	1010	SPO	C8-C7	2.18	1.55	1.50
7	S	2005	BPH	CHA-C1A	2.18	1.42	1.37
8	S	2010	SPO	C22-C23	2.18	1.38	1.35
4	L	1002	BCL	C4-C3	2.20	1.56	1.50
4	L	1001	BCL	CAA-CBA	2.21	1.60	1.52
4	L	1004	BCL	CBB-CAB	2.23	1.56	1.49
4	L	1004	BCL	C4-C3	2.24	1.56	1.50
4	S	2004	BCL	CAA-CBA	2.26	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	S	2008	U10	C15-C14	2.26	1.56	1.50
8	M	1010	SPO	C13-C12	2.27	1.55	1.50
7	S	2005	BPH	CHC-C1C	2.27	1.40	1.36
7	R	2006	BPH	CHA-C1A	2.27	1.42	1.37
8	S	2010	SPO	C24-C23	2.27	1.55	1.50
7	M	1006	BPH	CHC-C1C	2.29	1.40	1.36
4	L	1004	BCL	C6-C5	2.29	1.60	1.52
8	S	2010	SPO	C15-C14	2.30	1.50	1.43
5	L	1009	U10	C15-C14	2.32	1.56	1.50
7	R	2006	BPH	CAA-C2A	2.33	1.58	1.54
5	L	1009	U10	C30-C29	2.33	1.56	1.50
5	L	1009	U10	C20-C19	2.33	1.56	1.50
7	M	1006	BPH	CHA-C1A	2.33	1.42	1.37
5	S	2008	U10	C6-C1	2.35	1.40	1.35
8	S	2010	SPO	C13-C12	2.35	1.55	1.50
4	R	2002	BCL	C4-C3	2.37	1.56	1.50
7	M	1005	BPH	O1D-CGD	2.38	1.27	1.21
7	M	1006	BPH	C2-C3	2.39	1.37	1.33
8	S	2010	SPO	C26-C27	2.41	1.51	1.43
5	L	1009	U10	C33-C34	2.42	1.37	1.33
4	R	2002	BCL	CBB-CAB	2.42	1.57	1.49
5	M	1008	U10	C15-C14	2.43	1.56	1.50
7	M	1006	BPH	O1D-CGD	2.43	1.27	1.21
4	M	1003	BCL	C4-C3	2.44	1.56	1.50
4	S	2004	BCL	C4-C3	2.45	1.56	1.50
4	S	2004	BCL	CAA-C2A	2.51	1.59	1.54
7	R	2006	BPH	C2A-C1A	2.52	1.55	1.51
5	M	1008	U10	C8-C9	2.54	1.37	1.33
5	L	1009	U10	C31-C29	2.55	1.57	1.51
7	S	2005	BPH	CAA-C2A	2.57	1.59	1.54
5	M	1008	U10	C6-C1	2.58	1.41	1.35
8	S	2010	SPO	C8-C7	2.59	1.56	1.50
5	R	2009	U10	C7-C6	2.62	1.56	1.51
5	L	1009	U10	C6-C1	2.63	1.41	1.35
5	R	2009	U10	C6-C1	2.64	1.41	1.35
5	M	1008	U10	O3-C3	2.66	1.44	1.37
8	S	2010	SPO	C37-C38	2.67	1.40	1.32
5	L	1009	U10	C7-C6	2.70	1.56	1.51
7	R	2006	BPH	CHC-C1C	2.72	1.41	1.36
8	M	1010	SPO	C22-C23	2.74	1.39	1.35
4	S	2003	BCL	C4-C3	2.74	1.57	1.50
8	M	1010	SPO	C15-C14	2.76	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	2009	U10	C8-C9	2.83	1.40	1.32
8	M	1010	SPO	C37-C38	2.89	1.41	1.32
7	M	1006	BPH	CAA-C2A	2.93	1.60	1.54
7	M	1005	BPH	CAA-C2A	2.94	1.60	1.54
8	S	2010	SPO	C10-C9	2.98	1.53	1.43
5	L	1009	U10	C28-C29	3.00	1.38	1.33
5	R	2009	U10	O3-C3	3.01	1.44	1.37
7	S	2005	BPH	C2-C3	3.04	1.38	1.33
5	S	2008	U10	O3-C3	3.06	1.45	1.37
5	L	1009	U10	O3-C3	3.08	1.45	1.37
7	M	1005	BPH	C2-C3	3.13	1.39	1.33
8	M	1010	SPO	C10-C9	3.20	1.53	1.43
8	S	2010	SPO	C32-C33	3.21	1.39	1.33
5	L	1009	U10	C18-C19	3.33	1.39	1.33
8	M	1010	SPO	C32-C33	3.35	1.39	1.33
5	S	2008	U10	C8-C9	3.48	1.39	1.33
8	S	2010	SPO	C9-C7	3.51	1.40	1.35
5	M	1008	U10	C18-C19	3.55	1.39	1.33
7	R	2006	BPH	C2-C3	3.55	1.39	1.33
5	S	2008	U10	C18-C19	3.55	1.39	1.33
8	S	2010	SPO	C19-C17	3.59	1.40	1.35
8	M	1010	SPO	C9-C7	3.66	1.40	1.35
7	M	1006	BPH	O2A-CGA	3.72	1.44	1.33
7	S	2005	BPH	O2D-CGD	3.76	1.42	1.33
8	S	2010	SPO	C4-C1	3.78	1.58	1.53
8	M	1010	SPO	C19-C17	3.79	1.40	1.35
7	M	1005	BPH	O2A-CGA	3.80	1.44	1.33
5	L	1009	U10	C23-C24	3.85	1.40	1.33
5	M	1008	U10	C23-C24	3.87	1.40	1.33
7	R	2006	BPH	O2D-CGD	3.99	1.43	1.33
7	M	1006	BPH	O2D-CGD	4.01	1.43	1.33
7	R	2006	BPH	O2A-CGA	4.10	1.45	1.33
5	M	1008	U10	O4-C4	4.17	1.48	1.37
7	S	2005	BPH	O2A-CGA	4.19	1.45	1.33
8	M	1010	SPO	O1-CM1	4.21	1.56	1.43
8	S	2010	SPO	O1-CM1	4.23	1.56	1.43
7	M	1005	BPH	O2D-CGD	4.26	1.44	1.33
8	M	1010	SPO	C27-C28	4.28	1.38	1.34
8	M	1010	SPO	C26-C25	4.40	1.46	1.34
5	L	1009	U10	O4-C4	4.44	1.48	1.37
5	S	2008	U10	C13-C14	4.45	1.41	1.33
5	L	1009	U10	C8-C9	4.46	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	1008	U10	C13-C14	4.47	1.41	1.33
5	S	2008	U10	O4-C4	4.49	1.48	1.37
5	R	2009	U10	O4-C4	4.50	1.48	1.37
8	S	2010	SPO	C26-C25	4.60	1.46	1.34
8	S	2010	SPO	C27-C28	4.96	1.39	1.34
8	S	2010	SPO	C21-C20	5.11	1.49	1.35
8	S	2010	SPO	C14-C12	5.11	1.42	1.35
8	M	1010	SPO	C14-C12	5.19	1.42	1.35
8	M	1010	SPO	C21-C20	5.30	1.50	1.35
5	L	1009	U10	C13-C14	5.33	1.43	1.33
8	M	1010	SPO	C4-C1	5.44	1.60	1.53
8	S	2010	SPO	C15-C16	7.62	1.54	1.34
8	S	2010	SPO	C10-C11	7.74	1.54	1.34
8	M	1010	SPO	C10-C11	7.77	1.54	1.34
8	S	2010	SPO	C6-C5	8.20	1.54	1.31
8	M	1010	SPO	C15-C16	8.49	1.56	1.34
8	M	1010	SPO	C6-C5	8.61	1.55	1.31

All (280) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	M	1010	SPO	O1-C1-C4	-8.09	86.08	105.87
9	M	1011	LDA	CM2-N1-CM1	-7.92	99.90	108.83
8	S	2010	SPO	O1-C1-C4	-7.76	86.88	105.87
9	S	2011	LDA	CM2-N1-CM1	-7.73	100.11	108.83
9	M	1014	LDA	CM2-N1-CM1	-7.72	100.12	108.83
9	M	1012	LDA	CM2-N1-CM1	-7.50	100.37	108.83
9	M	1013	LDA	CM2-N1-CM1	-7.45	100.42	108.83
4	S	2001	BCL	CBC-CAC-C3C	-5.90	99.14	113.57
8	S	2010	SPO	C15-C14-C12	-5.68	118.99	127.20
8	M	1010	SPO	C20-C21-C22	-5.55	111.12	123.39
8	S	2010	SPO	C20-C21-C22	-5.46	111.31	123.39
7	S	2005	BPH	O1D-CGD-CBD	-5.45	116.81	124.62
7	M	1005	BPH	O1D-CGD-CBD	-5.29	117.04	124.62
4	L	1001	BCL	CBC-CAC-C3C	-5.24	100.75	113.57
8	M	1010	SPO	C15-C14-C12	-5.23	119.64	127.20
7	R	2006	BPH	O1D-CGD-CBD	-5.08	117.34	124.62
7	M	1006	BPH	O1D-CGD-CBD	-4.99	117.46	124.62
8	S	2010	SPO	C25-C23-C22	-4.86	111.16	118.98
4	S	2003	BCL	OBD-CAD-CBD	-4.72	118.81	125.94
8	M	1010	SPO	C25-C23-C22	-4.54	111.67	118.98
5	M	1008	U10	C20-C19-C21	-4.31	108.82	115.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	M	1010	SPO	C18-C17-C19	-4.14	116.78	122.90
4	S	2003	BCL	C11-C12-C13	-4.14	101.77	115.49
4	M	1003	BCL	OBD-CAD-CBD	-4.05	119.82	125.94
4	R	2002	BCL	O2D-CGD-CBD	-3.93	105.90	111.30
4	M	1003	BCL	C11-C12-C13	-3.91	102.52	115.49
8	S	2010	SPO	C18-C17-C19	-3.90	117.14	122.90
4	R	2002	BCL	OBD-CAD-CBD	-3.83	120.16	125.94
5	L	1009	U10	C20-C19-C21	-3.82	109.58	115.41
4	S	2004	BCL	C11-C12-C13	-3.79	102.93	115.49
5	R	2009	U10	O5-C5-C6	-3.78	114.58	121.68
7	S	2005	BPH	O2D-CGD-O1D	-3.78	115.99	123.79
4	L	1004	BCL	OBD-CAD-CBD	-3.74	120.30	125.94
5	L	1009	U10	O5-C5-C6	-3.72	114.68	121.68
4	S	2001	BCL	C1-C2-C3	-3.70	120.64	126.71
4	L	1002	BCL	OBD-CAD-CBD	-3.69	120.38	125.94
4	L	1001	BCL	CAC-C3C-C4C	-3.65	104.49	112.58
4	L	1004	BCL	CAC-C3C-C4C	-3.63	104.52	112.58
5	S	2008	U10	O5-C5-C6	-3.61	114.90	121.68
5	M	1008	U10	O5-C5-C6	-3.58	114.94	121.68
7	R	2006	BPH	O2D-CGD-O1D	-3.58	116.40	123.79
4	L	1002	BCL	O2D-CGD-CBD	-3.57	106.40	111.30
4	L	1004	BCL	OBB-CAB-CBB	-3.49	111.76	120.13
5	S	2008	U10	C20-C19-C21	-3.48	110.09	115.41
4	L	1001	BCL	OBD-CAD-CBD	-3.46	120.71	125.94
4	S	2001	BCL	OBD-CAD-CBD	-3.44	120.74	125.94
8	S	2010	SPO	C4-C5-C6	-3.42	119.80	124.67
4	R	2002	BCL	C7-C6-C5	-3.41	102.98	113.06
4	S	2004	BCL	OBB-CAB-CBB	-3.41	111.96	120.13
4	S	2003	BCL	OBB-CAB-CBB	-3.41	111.96	120.13
5	L	1009	U10	O2-C2-C3	-3.35	113.54	120.79
7	M	1006	BPH	O2D-CGD-O1D	-3.34	116.89	123.79
5	L	1009	U10	C1-C6-C5	-3.34	116.31	120.12
4	M	1003	BCL	OBB-CAB-CBB	-3.34	112.13	120.13
4	L	1002	BCL	C7-C6-C5	-3.33	103.22	113.06
4	L	1001	BCL	OBB-CAB-CBB	-3.31	112.19	120.13
4	S	2001	BCL	OBB-CAB-CBB	-3.31	112.20	120.13
4	S	2004	BCL	OBD-CAD-CBD	-3.30	120.96	125.94
8	S	2010	SPO	C15-C16-C17	-3.29	116.63	126.32
4	R	2002	BCL	OBB-CAB-CBB	-3.29	112.25	120.13
4	L	1002	BCL	OBB-CAB-CBB	-3.29	112.25	120.13
4	S	2001	BCL	CAA-C2A-C3A	-3.24	103.89	113.22
4	L	1001	BCL	CAA-C2A-C3A	-3.24	103.90	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	S	2010	SPO	C6-C7-C9	-3.23	113.77	118.98
7	M	1005	BPH	O2D-CGD-O1D	-3.23	117.13	123.79
5	R	2009	U10	O2-C2-C3	-3.21	113.83	120.79
5	R	2009	U10	C1-C6-C5	-3.20	116.47	120.12
5	S	2008	U10	O2-C2-C3	-3.18	113.89	120.79
4	S	2003	BCL	CAA-CBA-CGA	-3.17	104.04	113.32
7	M	1006	BPH	C5-C3-C2	-3.14	115.09	121.05
8	M	1010	SPO	C15-C16-C17	-3.13	117.11	126.32
4	S	2004	BCL	CBC-CAC-C3C	-3.10	105.99	113.57
4	S	2004	BCL	CAC-C3C-C4C	-3.10	105.71	112.58
4	M	1003	BCL	CAA-CBA-CGA	-3.08	104.31	113.32
4	S	2004	BCL	CAA-C2A-C3A	-3.00	104.58	113.22
4	R	2002	BCL	C11-C12-C13	-3.00	105.53	115.49
4	L	1004	BCL	CBC-CAC-C3C	-2.99	106.26	113.57
4	L	1004	BCL	C11-C12-C13	-2.98	105.61	115.49
7	S	2005	BPH	C5-C3-C2	-2.96	115.44	121.05
5	M	1008	U10	O2-C2-C3	-2.96	114.38	120.79
5	L	1009	U10	C30-C29-C31	-2.85	111.05	115.41
4	L	1002	BCL	C11-C12-C13	-2.84	106.07	115.49
4	L	1002	BCL	CAC-C3C-C4C	-2.81	106.34	112.58
8	M	1010	SPO	C6-C7-C9	-2.75	114.55	118.98
4	L	1002	BCL	CMB-C2B-C1B	-2.70	123.90	128.36
5	S	2008	U10	C1-C6-C5	-2.69	117.06	120.12
4	R	2002	BCL	CAA-C2A-C3A	-2.68	105.50	113.22
4	L	1002	BCL	CAA-C2A-C3A	-2.65	105.59	113.22
4	S	2004	BCL	CAC-C3C-C2C	-2.61	107.56	114.13
4	L	1004	BCL	CAC-C3C-C2C	-2.58	107.65	114.13
4	S	2003	BCL	CHA-C1A-NA	-2.57	119.73	126.06
4	R	2002	BCL	CMB-C2B-C1B	-2.57	124.11	128.36
4	R	2002	BCL	CAC-C3C-C4C	-2.56	106.89	112.58
9	M	1014	LDA	C6-C5-C4	-2.55	101.34	114.53
4	S	2004	BCL	CHA-C1A-NA	-2.55	119.79	126.06
4	L	1004	BCL	C16-C15-C13	-2.53	107.11	115.49
7	M	1006	BPH	O2A-CGA-O1A	-2.52	116.99	123.49
4	L	1001	BCL	CHA-C1A-NA	-2.51	119.88	126.06
4	M	1003	BCL	CHA-C1A-NA	-2.51	119.89	126.06
7	S	2005	BPH	CAA-C2A-C3A	-2.49	106.06	113.22
4	S	2001	BCL	CHA-C1A-NA	-2.46	120.01	126.06
7	M	1006	BPH	C7-C6-C5	-2.45	105.84	113.06
5	M	1008	U10	C1-C6-C5	-2.43	117.34	120.12
7	R	2006	BPH	O2A-CGA-O1A	-2.43	117.22	123.49
4	L	1002	BCL	C16-C15-C13	-2.43	107.43	115.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	S	2003	BCL	CGD-CBD-CAD	-2.42	102.42	110.62
5	L	1009	U10	C10-C9-C11	-2.41	111.73	115.41
4	L	1004	BCL	CMB-C2B-C1B	-2.40	124.39	128.36
5	M	1008	U10	C7-C6-C5	-2.40	115.74	118.56
4	L	1002	BCL	CHA-C1A-NA	-2.38	120.19	126.06
7	R	2006	BPH	CAA-C2A-C1A	-2.38	106.59	112.86
4	R	2002	BCL	CHA-C1A-NA	-2.37	120.23	126.06
8	M	1010	SPO	C10-C9-C7	-2.35	123.80	127.20
4	R	2002	BCL	C16-C15-C13	-2.33	107.76	115.49
9	M	1013	LDA	C9-C8-C7	-2.33	102.51	114.53
5	R	2009	U10	C7-C6-C5	-2.32	115.83	118.56
7	M	1006	BPH	CAA-C2A-C1A	-2.32	106.76	112.86
7	M	1005	BPH	CAA-C2A-C3A	-2.32	106.56	113.22
7	S	2005	BPH	O2A-CGA-O1A	-2.30	117.56	123.49
8	S	2010	SPO	C20-C19-C17	-2.30	123.88	127.20
5	S	2008	U10	C7-C6-C5	-2.29	115.86	118.56
4	M	1003	BCL	CBC-CAC-C3C	-2.29	107.97	113.57
7	S	2005	BPH	C2A-C1A-NA	-2.28	109.16	112.08
4	S	2003	BCL	CAA-C2A-C3A	-2.28	106.67	113.22
4	S	2003	BCL	CMB-C2B-C1B	-2.28	124.60	128.36
9	S	2011	LDA	C9-C8-C7	-2.28	102.78	114.53
7	M	1005	BPH	C2A-C1A-NA	-2.27	109.17	112.08
9	M	1012	LDA	C9-C8-C7	-2.27	102.78	114.53
4	S	2003	BCL	C11-C10-C8	-2.26	108.01	115.49
4	L	1004	BCL	CHA-C1A-NA	-2.25	120.53	126.06
4	M	1003	BCL	CAC-C3C-C4C	-2.24	107.61	112.58
8	M	1010	SPO	C4-C5-C6	-2.23	121.50	124.67
5	L	1009	U10	C7-C6-C5	-2.21	115.96	118.56
4	S	2003	BCL	C7-C6-C5	-2.21	106.53	113.06
4	R	2002	BCL	CBC-CAC-C3C	-2.20	108.18	113.57
7	M	1005	BPH	O2A-CGA-O1A	-2.19	117.84	123.49
7	M	1006	BPH	C3A-C4A-NA	-2.18	109.75	113.57
9	M	1011	LDA	C9-C8-C7	-2.18	103.25	114.53
7	R	2006	BPH	CAA-C2A-C3A	-2.18	106.95	113.22
7	R	2006	BPH	C7-C6-C5	-2.18	106.63	113.06
4	M	1003	BCL	C11-C10-C8	-2.17	108.30	115.49
4	S	2004	BCL	CMB-C2B-C1B	-2.15	124.80	128.36
9	S	2011	LDA	CM1-N1-C1	-2.15	102.84	109.77
7	M	1005	BPH	C3A-C4A-NA	-2.15	109.82	113.57
9	M	1012	LDA	CM1-N1-C1	-2.13	102.92	109.77
4	S	2004	BCL	C16-C15-C13	-2.13	108.43	115.49
4	S	2003	BCL	CBC-CAC-C3C	-2.12	108.37	113.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	1004	BCL	C12-C11-C10	-2.12	102.49	112.99
9	M	1013	LDA	CM1-N1-C1	-2.11	102.98	109.77
4	S	2003	BCL	O2A-CGA-O1A	-2.10	118.06	123.49
4	M	1003	BCL	C16-C15-C13	-2.10	108.53	115.49
4	S	2003	BCL	CAC-C3C-C2C	-2.10	108.85	114.13
8	S	2010	SPO	C10-C9-C7	-2.10	124.17	127.20
4	S	2003	BCL	C16-C15-C13	-2.10	108.54	115.49
4	M	1003	BCL	CMB-C2B-C1B	-2.09	124.90	128.36
4	M	1003	BCL	C7-C6-C5	-2.09	106.88	113.06
7	S	2005	BPH	C3A-C4A-NA	-2.08	109.92	113.57
9	M	1011	LDA	CM1-N1-C1	-2.08	103.06	109.77
9	M	1014	LDA	CM1-N1-C1	-2.08	103.08	109.77
4	S	2003	BCL	CAC-C3C-C4C	-2.07	107.98	112.58
7	M	1006	BPH	OBD-CAD-CBD	-2.07	122.81	125.94
7	S	2005	BPH	CAC-C3C-C2C	-2.06	108.94	114.13
7	S	2005	BPH	OBD-CAD-CBD	-2.06	122.83	125.94
7	M	1005	BPH	OBD-CAD-CBD	-2.06	122.83	125.94
7	R	2006	BPH	OBD-CAD-CBD	-2.03	122.88	125.94
4	L	1002	BCL	C4A-NA-C1A	-2.02	103.74	106.36
9	M	1014	LDA	C9-C8-C7	-2.01	104.15	114.53
4	L	1002	BCL	C12-C11-C10	-2.01	103.03	112.99
7	R	2006	BPH	C3A-C4A-NA	-2.00	110.07	113.57
4	R	2002	BCL	C3D-CAD-CBD	2.04	110.49	107.60
4	S	2001	BCL	CBB-CAB-C3B	2.12	126.62	120.33
4	S	2003	BCL	O2A-CGA-CBA	2.14	118.43	111.90
4	S	2001	BCL	O1D-CGD-CBD	2.16	127.72	124.62
4	L	1004	BCL	C3D-CAD-CBD	2.16	110.66	107.60
4	L	1001	BCL	CBB-CAB-C3B	2.17	126.75	120.33
7	M	1006	BPH	CMD-C2D-C3D	2.17	129.34	125.09
4	S	2004	BCL	O1D-CGD-CBD	2.17	127.74	124.62
8	M	1010	SPO	C16-C17-C19	2.18	122.49	118.98
4	L	1001	BCL	CHD-C4C-NC	2.25	127.66	125.06
4	L	1001	BCL	C3D-CAD-CBD	2.25	110.77	107.60
4	R	2002	BCL	C4-C3-C5	2.25	118.85	115.41
7	R	2006	BPH	CAC-C3C-C4C	2.26	118.47	112.67
4	S	2004	BCL	C3D-CAD-CBD	2.27	110.80	107.60
4	S	2001	BCL	C3D-CAD-CBD	2.29	110.83	107.60
7	S	2005	BPH	CMD-C2D-C3D	2.29	129.57	125.09
5	L	1009	U10	C8-C7-C6	2.30	118.54	111.64
4	L	1001	BCL	CMB-C2B-C3B	2.32	129.63	125.09
5	R	2009	U10	C8-C7-C6	2.37	118.75	111.64
4	R	2002	BCL	CBB-CAB-C3B	2.38	127.39	120.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	1002	BCL	CBB-CAB-C3B	2.38	127.40	120.33
5	S	2008	U10	C17-C18-C19	2.40	132.97	127.76
4	S	2001	BCL	CMB-C2B-C3B	2.41	129.81	125.09
7	S	2005	BPH	C2C-C3C-C4C	2.43	105.62	101.50
5	L	1009	U10	C31-C32-C33	2.44	118.07	111.69
7	M	1005	BPH	C2C-C3C-C4C	2.46	105.67	101.50
4	S	2003	BCL	CBB-CAB-C3B	2.47	127.66	120.33
4	M	1003	BCL	CBB-CAB-C3B	2.48	127.69	120.33
7	M	1006	BPH	C2C-C3C-C4C	2.49	105.72	101.50
4	M	1003	BCL	CMB-C2B-C3B	2.50	129.99	125.09
4	M	1003	BCL	C3D-CAD-CBD	2.53	111.17	107.60
5	L	1009	U10	C22-C21-C19	2.54	121.00	112.71
5	S	2008	U10	C21-C19-C18	2.55	125.88	121.05
4	S	2003	BCL	CMB-C2B-C3B	2.58	130.13	125.09
4	S	2004	BCL	CMB-C2B-C3B	2.58	130.14	125.09
7	R	2006	BPH	C2C-C3C-C4C	2.61	105.92	101.50
4	L	1004	BCL	CBB-CAB-C3B	2.63	128.14	120.33
4	S	2003	BCL	CBA-CAA-C2A	2.65	121.21	113.73
4	L	1004	BCL	CMB-C2B-C3B	2.67	130.31	125.09
4	S	2004	BCL	C2C-C3C-C4C	2.68	106.05	101.50
4	S	2004	BCL	CBB-CAB-C3B	2.70	128.35	120.33
4	L	1004	BCL	CBA-CAA-C2A	2.72	121.41	113.73
4	L	1004	BCL	C2C-C3C-C4C	2.73	106.13	101.50
4	S	2001	BCL	C2C-C3C-C4C	2.82	106.28	101.50
4	M	1003	BCL	CBA-CAA-C2A	2.83	121.73	113.73
5	L	1009	U10	C31-C29-C28	2.85	126.47	121.05
5	S	2008	U10	C16-C14-C13	2.86	126.47	121.05
5	M	1008	U10	C16-C14-C13	2.87	126.49	121.05
4	M	1003	BCL	O1D-CGD-CBD	2.87	128.74	124.62
4	R	2002	BCL	CMB-C2B-C3B	2.93	130.81	125.09
7	M	1006	BPH	C4-C3-C5	2.95	119.91	115.41
4	L	1002	BCL	CMB-C2B-C3B	2.95	130.87	125.09
7	S	2005	BPH	C4-C3-C5	2.98	119.95	115.41
4	L	1001	BCL	C2C-C3C-C4C	2.98	106.56	101.50
7	M	1005	BPH	CBC-CAC-C3C	3.02	120.96	113.57
4	S	2003	BCL	C3D-CAD-CBD	3.03	111.88	107.60
4	S	2003	BCL	O1D-CGD-CBD	3.04	128.98	124.62
8	M	1010	SPO	C8-C7-C6	3.06	123.19	118.10
5	L	1009	U10	C21-C19-C18	3.14	127.00	121.05
8	S	2010	SPO	C8-C7-C6	3.18	123.38	118.10
5	L	1009	U10	C16-C14-C13	3.19	127.11	121.05
5	M	1008	U10	C21-C19-C18	3.21	127.14	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	M	1010	SPO	C3-C1-C2	3.22	116.72	110.22
7	M	1006	BPH	CBC-CAC-C3C	3.30	121.62	113.57
8	S	2010	SPO	C3-C1-C2	3.38	117.04	110.22
4	L	1002	BCL	CMD-C2D-C3D	3.48	131.88	125.09
7	S	2005	BPH	CBC-CAC-C3C	3.49	122.11	113.57
4	S	2001	BCL	CMD-C2D-C3D	3.51	131.95	125.09
8	M	1010	SPO	C24-C23-C25	3.52	123.95	118.10
4	S	2004	BCL	CMD-C2D-C3D	3.52	131.97	125.09
4	S	2003	BCL	CMD-C2D-C3D	3.54	132.02	125.09
4	L	1002	BCL	O1D-CGD-CBD	3.55	129.71	124.62
5	M	1008	U10	C27-C28-C29	3.66	141.82	127.73
4	M	1003	BCL	C4-C3-C5	3.66	121.00	115.41
4	M	1003	BCL	CMD-C2D-C3D	3.66	132.25	125.09
4	L	1004	BCL	CMD-C2D-C3D	3.66	132.25	125.09
4	R	2002	BCL	CMD-C2D-C3D	3.72	132.37	125.09
4	S	2003	BCL	C4-C3-C5	3.80	121.22	115.41
8	S	2010	SPO	C24-C23-C25	3.83	124.47	118.10
7	M	1005	BPH	CED-O2D-CGD	3.92	125.17	115.99
7	S	2005	BPH	CED-O2D-CGD	3.92	125.17	115.99
4	L	1001	BCL	CMD-C2D-C3D	3.94	132.80	125.09
7	R	2006	BPH	C11-C10-C8	3.99	128.72	115.49
7	R	2006	BPH	CED-O2D-CGD	4.00	125.37	115.99
7	S	2005	BPH	C4A-NA-C1A	4.08	111.85	108.21
7	M	1006	BPH	CED-O2D-CGD	4.15	125.73	115.99
7	M	1006	BPH	C11-C10-C8	4.19	129.39	115.49
4	R	2002	BCL	O1D-CGD-CBD	4.27	130.75	124.62
7	M	1005	BPH	C4A-NA-C1A	4.29	112.04	108.21
7	M	1006	BPH	C4A-NA-C1A	4.41	112.15	108.21
7	R	2006	BPH	C4A-NA-C1A	4.56	112.28	108.21
7	R	2006	BPH	CBC-CAC-C3C	4.88	125.49	113.57
7	M	1006	BPH	C6-C5-C3	4.92	123.28	112.48
9	M	1011	LDA	O1-N1-C1	5.08	115.99	110.27
9	S	2011	LDA	O1-N1-C1	5.15	116.06	110.27
9	M	1012	LDA	O1-N1-C1	5.17	116.09	110.27
9	M	1014	LDA	O1-N1-C1	5.18	116.10	110.27
9	M	1013	LDA	O1-N1-C1	5.19	116.12	110.27
7	M	1005	BPH	C6-C5-C3	5.24	123.98	112.48
7	S	2005	BPH	C6-C5-C3	5.26	124.02	112.48
7	R	2006	BPH	C6-C5-C3	5.40	124.33	112.48
5	M	1008	U10	C3M-O3-C3	6.05	138.10	116.61
5	S	2008	U10	C3M-O3-C3	6.25	138.85	116.61
5	L	1009	U10	C3M-O3-C3	6.33	139.10	116.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	R	2009	U10	C3M-O3-C3	6.43	139.47	116.61
5	L	1009	U10	C27-C28-C29	8.42	146.07	127.76
7	M	1006	BPH	O2D-CGD-CBD	10.43	125.60	111.30
7	M	1005	BPH	O2D-CGD-CBD	10.59	125.83	111.30
7	R	2006	BPH	O2D-CGD-CBD	10.89	126.24	111.30
7	S	2005	BPH	O2D-CGD-CBD	11.58	127.18	111.30
5	L	1009	U10	C32-C33-C34	16.02	162.60	127.76

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	M	1005	BPH	C8
7	S	2005	BPH	C8
7	M	1006	BPH	C8
7	M	1006	BPH	C13
7	R	2006	BPH	C8
7	R	2006	BPH	C13

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	M	1006	BPH	C1-C2-C3-C4
5	L	1009	U10	C34-C33-C32-C31

There are no ring outliers.

19 monomers are involved in 71 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	1001	BCL	11	0
4	L	1002	BCL	6	0
4	L	1004	BCL	9	0
5	L	1009	U10	3	0
4	M	1003	BCL	13	0
7	M	1005	BPH	2	0
7	M	1006	BPH	4	0
5	M	1008	U10	4	0
8	M	1010	SPO	4	0
9	M	1012	LDA	1	0
9	M	1014	LDA	2	0
4	R	2002	BCL	5	0
7	R	2006	BPH	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	S	2001	BCL	8	0
4	S	2003	BCL	11	0
4	S	2004	BCL	5	0
7	S	2005	BPH	2	0
5	S	2008	U10	1	0
8	S	2010	SPO	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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%)	0.16	7 (2%) 61 60	17, 32, 49, 58	0
1	R	281/281 (100%)	0.35	16 (5%) 27 27	23, 41, 58, 69	0
2	M	299/307 (97%)	0.01	14 (4%) 35 36	17, 27, 41, 67	0
2	S	299/307 (97%)	0.10	10 (3%) 50 50	24, 35, 48, 69	0
3	H	246/260 (94%)	0.14	10 (4%) 41 42	22, 34, 54, 88	0
3	T	246/260 (94%)	0.55	25 (10%) 9 8	31, 45, 70, 80	0
All	All	1652/1696 (97%)	0.21	82 (4%) 32 33	17, 36, 57, 88	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	252	VAL	6.4
3	H	254	ALA	5.8
3	H	255	MET	5.3
3	T	254	ALA	5.3
3	T	252	VAL	5.0
3	H	251	VAL	4.8
3	T	80	SER	4.8
3	T	51	ALA	4.7
3	T	92	VAL	4.7
1	R	1	ALA	4.5
3	T	54	GLY	4.3
2	S	301	HIS	4.2
3	H	256	LEU	4.1
3	H	253	ALA	4.0
1	R	140	GLY	4.0
3	T	255	MET	3.8
3	T	46	ASP	3.8
3	T	55	PRO	3.8
3	T	251	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
3	H	51	ALA	3.7
3	T	60	LYS	3.7
1	R	74	GLY	3.5
3	T	93	SER	3.5
1	R	73	TYR	3.5
3	T	79	GLU	3.5
3	T	18	TYR	3.4
2	S	223	ILE	3.4
1	R	270	PRO	3.4
3	H	250	SER	3.4
1	L	51	TRP	3.2
2	S	226	VAL	3.1
2	S	54	SER	3.1
3	T	29	TYR	3.0
3	T	253	ALA	3.0
3	T	58	LEU	3.0
1	R	75	LEU	2.9
1	R	76	GLY	2.9
3	T	157	ASP	2.9
2	M	226	VAL	2.9
2	M	231	GLY	2.9
2	M	225	ALA	2.8
1	R	51	TRP	2.8
2	S	3	TYR	2.8
1	R	271	TRP	2.8
1	R	281	GLY	2.7
2	M	222	THR	2.7
1	L	271	TRP	2.6
1	R	202	LYS	2.5
1	R	59	TRP	2.5
2	M	214	LEU	2.5
2	M	215	LEU	2.5
3	T	69	GLY	2.5
1	R	142	TRP	2.4
3	T	256	LEU	2.4
1	L	113	ILE	2.4
3	T	48	THR	2.4
3	T	50	ALA	2.4
1	R	269	LEU	2.4
2	M	224	LEU	2.4
2	M	221	ALA	2.3
2	M	301	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	L	88	ILE	2.3
1	R	267	VAL	2.3
2	M	211	GLY	2.3
3	T	56	PHE	2.3
3	T	49	PRO	2.3
1	R	256	PHE	2.2
3	H	52	ASN	2.2
3	H	18	TYR	2.2
2	M	223	ILE	2.2
1	L	185	LEU	2.2
2	M	227	SER	2.1
2	S	102	GLY	2.1
2	S	265	ILE	2.1
2	S	224	LEU	2.1
2	S	242	GLY	2.1
2	S	231	GLY	2.1
1	L	269	LEU	2.1
2	M	218	MET	2.1
3	T	61	PRO	2.1
2	M	105	PHE	2.0
1	L	138	MET	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
5	U10	R	2009	18/63	0.65	0.41	6.72	81,85,86,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
9	LDA	S	2011	16/16	0.60	0.42	5.44	74,79,85,85	0
9	LDA	M	1011	16/16	0.64	0.27	4.47	49,57,74,74	0
9	LDA	M	1013	16/16	0.62	0.31	4.34	69,71,80,80	0
9	LDA	M	1014	16/16	0.78	0.34	3.71	50,55,59,60	0
5	U10	L	1009	44/63	0.66	0.34	3.40	66,72,79,79	0
4	BCL	S	2003	66/66	0.90	0.21	3.03	27,33,48,55	0
8	SPO	S	2010	42/42	0.87	0.22	2.84	24,35,51,54	0
4	BCL	S	2001	51/66	0.90	0.20	2.72	28,31,41,43	0
4	BCL	R	2002	66/66	0.88	0.19	2.57	29,35,44,48	0
5	U10	S	2008	32/63	0.94	0.34	2.38	36,42,51,54	0
8	SPO	M	1010	42/42	0.87	0.21	2.26	16,28,47,51	0
9	LDA	M	1012	16/16	0.75	0.26	2.11	60,62,65,65	0
4	BCL	L	1002	66/66	0.90	0.22	2.03	20,26,29,33	0
4	BCL	M	1003	66/66	0.92	0.20	1.85	20,25,39,44	0
7	BPH	M	1006	65/65	0.92	0.25	1.65	23,28,37,40	0
4	BCL	S	2004	66/66	0.91	0.21	1.65	26,34,58,60	0
5	U10	M	1008	38/63	0.92	0.30	1.54	23,30,53,53	0
4	BCL	L	1001	51/66	0.89	0.22	1.52	17,24,51,55	0
4	BCL	L	1004	66/66	0.91	0.27	1.49	16,25,45,52	0
7	BPH	R	2006	65/65	0.92	0.19	1.30	31,38,45,46	0
7	BPH	S	2005	55/65	0.94	0.17	1.11	25,30,55,58	0
7	BPH	M	1005	55/65	0.94	0.19	0.80	17,23,43,46	0
6	FE2	S	2007	1/1	0.99	0.13	-1.52	30,30,30,30	0
6	FE2	M	1007	1/1	0.99	0.14	-2.15	20,20,20,20	0

6.5 Other polymers (i)

There are no such residues in this entry.