



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 29, 2017 – 05:19 PM EDT

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

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029077
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20029077

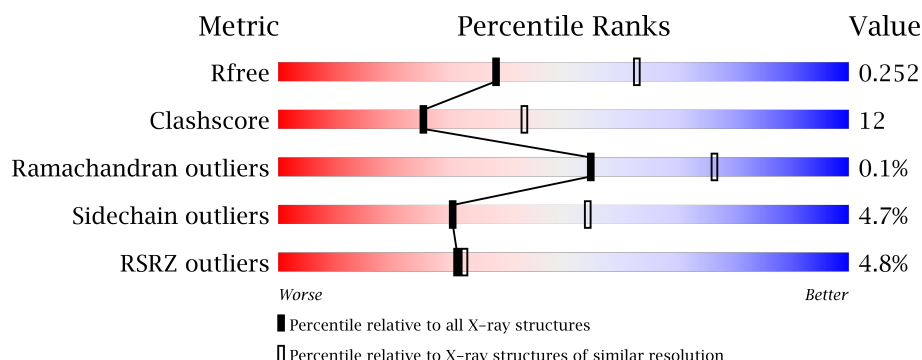
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	L	281	<div> <div>4%</div> <div>72%</div> <div>26%</div> <div>.</div> </div>
1	R	281	<div> <div>7%</div> <div>72%</div> <div>26%</div> <div>.</div> </div>
2	M	307	<div> <div>%</div> <div>79%</div> <div>17%</div> <div>..</div> </div>
2	S	307	<div> <div>2%</div> <div>79%</div> <div>17%</div> <div>..</div> </div>
3	H	260	<div> <div>3%</div> <div>73%</div> <div>20%</div> <div>5%</div> </div>

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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
10	LDA	M	1013	-	-	-	X
10	LDA	M	1014	-	-	-	X
10	LDA	S	2012	-	-	-	X
10	LDA	S	2013	-	-	-	X
10	LDA	S	2014	-	-	-	X
9	U10	L	1009	-	-	-	X
9	U10	R	2009	-	-	-	X

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 14529 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called REACTION CENTER PROTEIN L CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	281	Total	C	N	O	S	0	0	0
			2232	1507	355	362	8			
1	R	281	Total	C	N	O	S	0	0	0
			2232	1507	355	362	8			

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

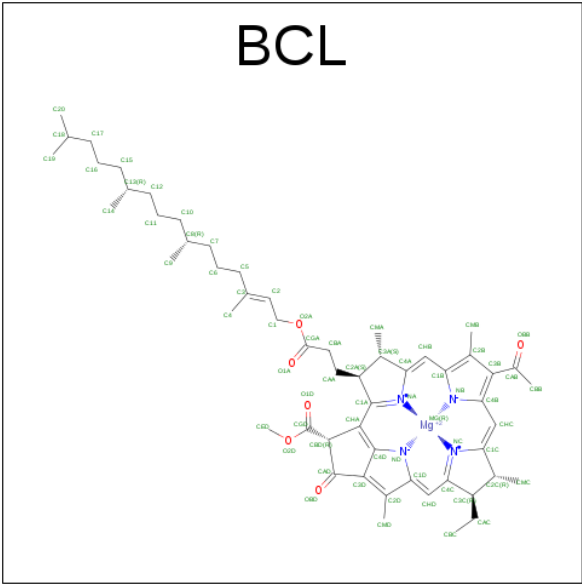
- Molecule 5 is CADMIUM ION (three-letter code: CD) (formula: Cd).

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

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

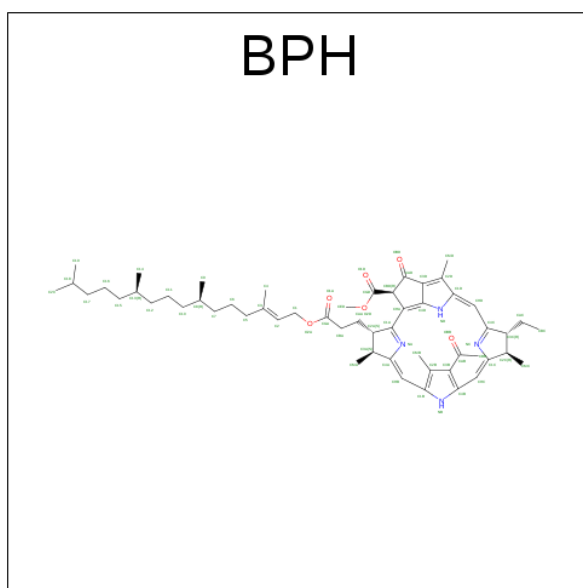
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	S	1	Total	Cl	0	0
			1	1		
6	M	1	Total	Cl	0	0
			1	1		

- Molecule 7 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



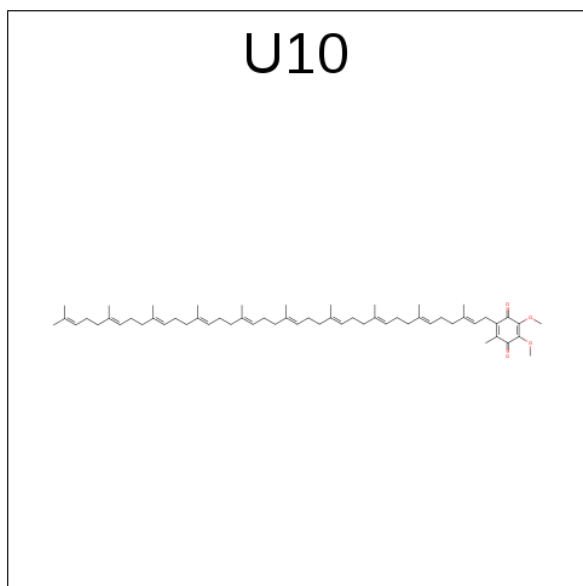
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	L	1	Total 51	C 40	Mg 1	N 4	O 6	0	0
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	R	1	Total 51	C 40	Mg 1	N 4	O 6	0	0
7	R	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	S	1	Total 66	C 55	Mg 1	N 4	O 6	0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

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



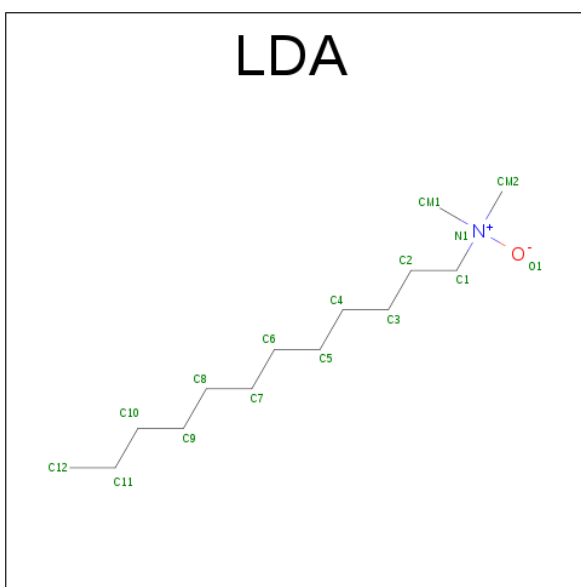
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	M	1	Total	C	N	O	0	0
			51	41	4	6		
8	L	1	Total	C	N	O	0	0
			65	55	4	6		
8	S	1	Total	C	N	O	0	0
			52	42	4	6		
8	R	1	Total	C	N	O	0	0
			65	55	4	6		

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



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

- Molecule 10 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



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

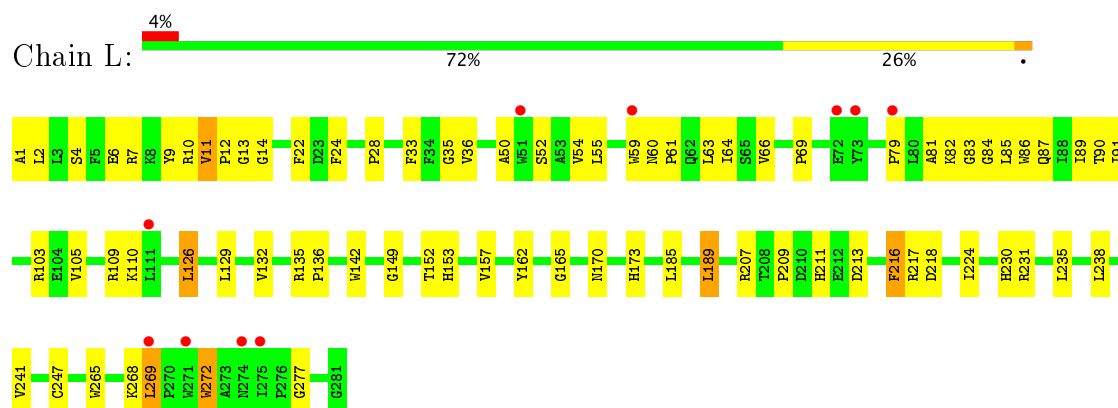
- Molecule 11 is water.

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

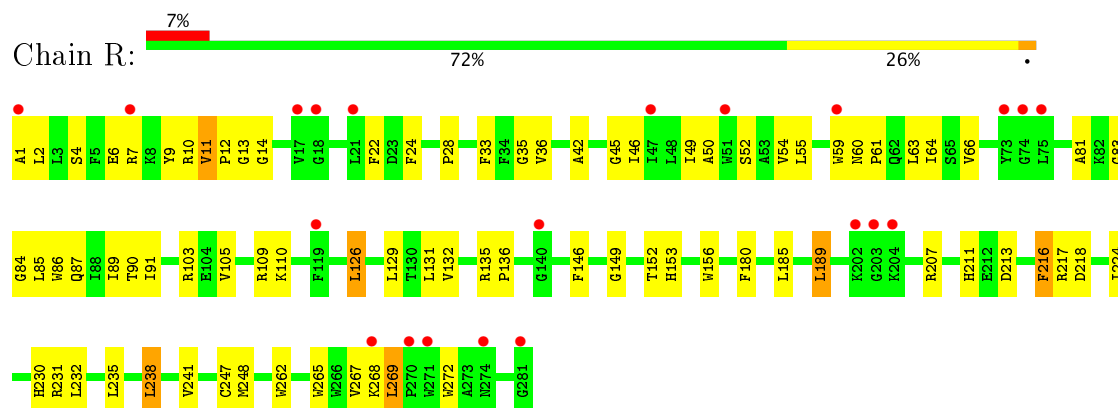
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

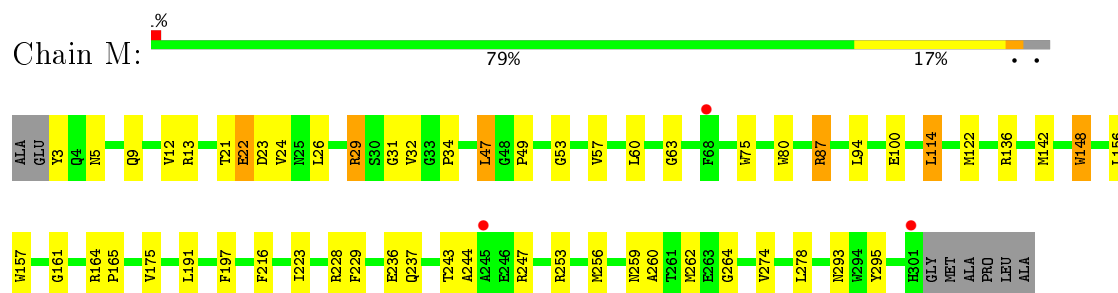
• Molecule 1: REACTION CENTER PROTEIN L CHAIN



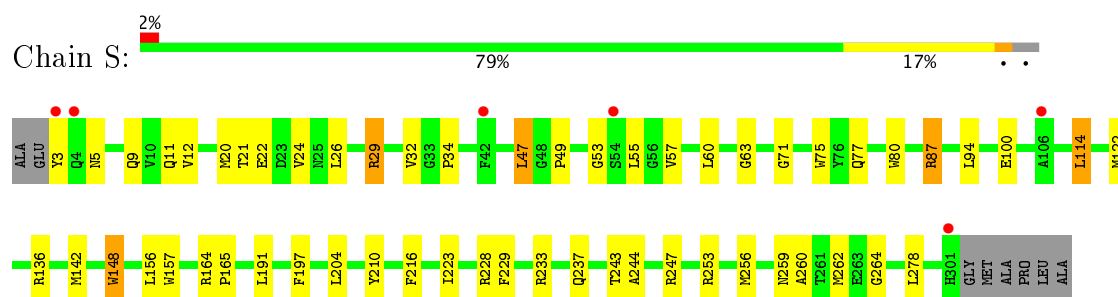
• Molecule 1: REACTION CENTER PROTEIN L CHAIN



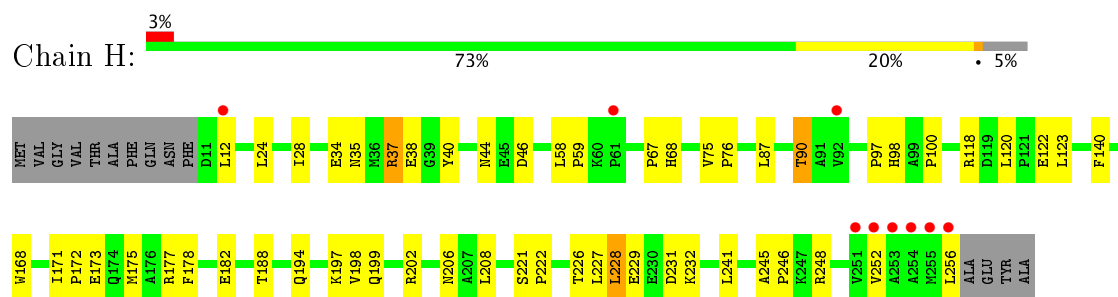
• Molecule 2: REACTION CENTER PROTEIN M CHAIN



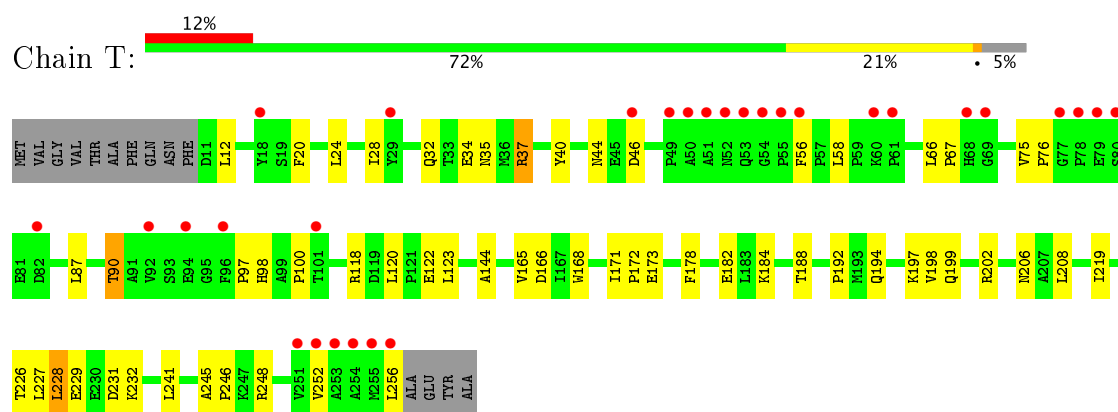
• Molecule 2: REACTION CENTER PROTEIN M CHAIN



• Molecule 3: REACTION CENTER PROTEIN H CHAIN



• Molecule 3: REACTION CENTER PROTEIN H CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	139.59Å 139.59Å 272.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 27.81 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.50) 99.6 (27.81-2.49)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.90 (at 2.51Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.227 , 0.256 0.224 , 0.252	Depositor DCC
R_{free} test set	4395 reflections (4.93%)	DCC
Wilson B-factor (Å ²)	43.2	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14529	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, LDA, CL, BPH, CD, FE2, U10

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	L	0.39	0/2320	0.55	0/3175
1	R	0.40	0/2320	0.55	0/3175
2	M	0.41	0/2482	0.54	0/3389
2	S	0.40	0/2482	0.54	0/3389
3	H	0.35	0/1917	0.60	0/2608
3	T	0.35	0/1917	0.60	0/2608
All	All	0.39	0/13438	0.56	0/18344

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2232	0	2187	59	0
1	R	2232	0	2187	63	0
2	M	2390	0	2304	53	0
2	S	2390	0	2304	49	0
3	H	1869	0	1884	49	0
3	T	1869	0	1884	45	0
4	M	1	0	0	0	0

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:252:VAL:O	3:H:256:LEU:HD13	2.02	0.60
1:L:60:ASN:HB3	1:L:63:LEU:HD23	1.84	0.60
2:M:9:GLN:HE22	3:H:198:VAL:H	1.49	0.60
2:M:161:GLY:HA3	10:M:1014:LDA:HM23	1.83	0.60
1:L:265:TRP:O	1:L:269:LEU:HD13	2.00	0.60
1:L:60:ASN:O	1:L:64:ILE:HG13	2.02	0.60
11:S:2020:HOH:O	3:T:173:GLU:HG2	2.01	0.59
1:L:218:ASP:OD1	2:M:29:ARG:HD2	2.02	0.59
1:R:238:LEU:HD12	8:R:2006:BPH:CBC	2.33	0.59
1:R:28:PRO:HB3	2:S:253:ARG:NH1	2.18	0.59
3:T:226:THR:OG1	3:T:229:GLU:HG3	2.03	0.59
7:L:1001:BCL:CBB	7:L:1001:BCL:HHC	2.33	0.58
1:R:60:ASN:HB3	1:R:63:LEU:HD23	1.84	0.58
2:M:63:GLY:HA3	8:M:1005:BPH:H5C2	1.84	0.58
3:T:252:VAL:O	3:T:256:LEU:HD13	2.03	0.58
9:M:1008:U10:H4M2	9:M:1008:U10:H3M3	1.83	0.58
1:R:60:ASN:O	1:R:64:ILE:HG13	2.02	0.58
1:R:86:TRP:CH2	1:R:132:VAL:HG13	2.39	0.58
1:L:272:TRP:CD2	2:M:87:ARG:HB3	2.38	0.58
1:L:86:TRP:CH2	1:L:132:VAL:HG13	2.38	0.58
3:T:118:ARG:HD3	3:T:120:LEU:HD12	1.86	0.58
7:S:2003:BCL:CBB	7:S:2003:BCL:HHC	2.34	0.58
1:R:13:GLY:O	1:R:110:LYS:HE2	2.04	0.57
1:L:13:GLY:O	1:L:110:LYS:HE2	2.04	0.57
1:R:189:LEU:HD13	8:S:2005:BPH:HMD2	1.86	0.57
2:S:256:MET:CE	9:S:2008:U10:H102	2.35	0.57
7:R:2004:BCL:CBB	7:R:2004:BCL:HMB1	2.35	0.57
1:R:248:MET:HG3	7:R:2002:BCL:HED2	1.85	0.57
3:H:118:ARG:HD3	3:H:120:LEU:HD12	1.86	0.57
7:R:2002:BCL:CBB	7:R:2002:BCL:HMB1	2.35	0.57
2:S:148:TRP:HD1	10:S:2013:LDA:H12	1.70	0.56
9:L:1009:U10:H311	2:M:31:GLY:O	2.06	0.56
2:S:122:MET:HE3	2:S:157:TRP:HE1	1.68	0.56
2:S:20:MET:HA	11:T:2085:HOH:O	2.04	0.56
2:M:122:MET:HE1	2:M:157:TRP:HE1	1.69	0.55
1:L:189:LEU:HG	1:L:216:PHE:HZ	1.72	0.55
1:R:135:ARG:HB3	1:R:136:PRO:HD3	1.89	0.55
1:L:28:PRO:HB3	2:M:253:ARG:NH1	2.22	0.55
7:R:2002:BCL:H192	8:R:2006:BPH:HMA1	1.88	0.54
1:R:267:VAL:HG13	2:S:87:ARG:HD2	1.90	0.54
2:M:228:ARG:HA	3:H:194:GLN:HG2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:9:GLN:HE22	3:T:198:VAL:H	1.55	0.54
7:L:1004:BCL:HMB1	7:L:1004:BCL:CBB	2.38	0.54
7:L:1004:BCL:O1D	10:M:1013:LDA:H21	2.08	0.54
7:L:1002:BCL:HBB3	7:L:1002:BCL:HMB1	1.89	0.54
7:L:1001:BCL:HBB3	7:M:1003:BCL:H41	1.90	0.54
1:L:231:ARG:HD2	2:M:5:ASN:O	2.08	0.54
1:R:189:LEU:HG	1:R:216:PHE:HZ	1.72	0.54
2:S:164:ARG:HB3	2:S:165:PRO:HD3	1.90	0.53
1:R:230:HIS:CD2	2:S:223:ILE:HG13	2.44	0.53
2:M:13:ARG:O	3:H:140:PHE:HA	2.07	0.53
1:R:54:VAL:HA	11:R:2068:HOH:O	2.09	0.53
1:L:14:GLY:O	1:L:109:ARG:HD3	2.08	0.53
1:R:14:GLY:O	1:R:109:ARG:HD3	2.08	0.53
1:R:87:GLN:O	1:R:91:ILE:HG12	2.08	0.53
3:T:199:GLN:HE22	3:T:202:ARG:NH1	2.07	0.53
11:L:1054:HOH:O	3:H:67:PRO:HG2	2.08	0.53
3:H:199:GLN:HE22	3:H:202:ARG:NH1	2.08	0.52
1:L:241:VAL:HG21	8:L:1006:BPH:HAC1	1.91	0.52
3:T:34:GLU:O	3:T:37:ARG:HD3	2.09	0.52
2:M:164:ARG:HB3	2:M:165:PRO:HD3	1.90	0.52
7:S:2003:BCL:HBB2	7:S:2003:BCL:HHC	1.91	0.52
11:R:2018:HOH:O	2:S:233:ARG:HA	2.10	0.52
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.91	0.52
3:H:37:ARG:HH11	3:H:76:PRO:HD3	1.75	0.51
3:H:34:GLU:O	3:H:37:ARG:HD3	2.09	0.51
2:M:122:MET:HE3	2:M:157:TRP:HE1	1.76	0.51
7:R:2002:BCL:H122	8:R:2006:BPH:H3A	1.93	0.51
1:L:52:SER:HB2	1:L:85:LEU:HD23	1.91	0.51
1:L:83:GLY:O	1:L:87:GLN:HG3	2.10	0.51
1:R:6:GLU:OE2	1:R:10:ARG:HD3	2.10	0.51
1:L:272:TRP:CE2	2:M:87:ARG:HB3	2.45	0.51
1:L:28:PRO:HB3	2:M:253:ARG:HH11	1.75	0.51
3:H:226:THR:OG1	3:H:229:GLU:HG3	2.11	0.51
1:R:42:ALA:HA	8:R:2006:BPH:H9C2	1.93	0.51
2:S:9:GLN:NE2	3:T:198:VAL:H	2.07	0.51
2:M:228:ARG:HA	3:H:194:GLN:CG	2.41	0.51
2:M:32:VAL:HG22	2:M:49:PRO:HD3	1.92	0.51
3:T:87:LEU:HD22	3:T:98:HIS:O	2.11	0.51
1:R:45:GLY:HA3	8:R:2006:BPH:H9C1	1.93	0.50
3:T:37:ARG:HH11	3:T:76:PRO:HD3	1.75	0.50
2:M:148:TRP:HA	2:M:148:TRP:CE3	2.47	0.50

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:90:THR:HG23	1:R:132:VAL:HG11	1.99	0.44
3:T:24:LEU:O	3:T:28:ILE:HG13	2.17	0.44
1:R:153:HIS:CE1	8:R:2006:BPH:H201	2.53	0.44
1:R:238:LEU:HD12	8:R:2006:BPH:HBC3	1.99	0.44
2:M:278:LEU:HD12	2:M:278:LEU:HA	1.88	0.44
2:S:34:PRO:O	2:S:47:LEU:HB2	2.18	0.44
3:H:87:LEU:HD23	3:H:100:PRO:CA	2.44	0.44
2:M:260:ALA:HB1	3:H:35:ASN:OD1	2.18	0.44
2:M:264:GLY:HA3	3:H:35:ASN:OD1	2.16	0.44
3:H:44:ASN:HB2	3:H:46:ASP:OD1	2.18	0.44
7:R:2004:BCL:HED1	10:S:2014:LDA:O1	2.18	0.44
3:T:194:GLN:H	3:T:194:GLN:NE2	2.15	0.44
3:H:40:TYR:HB3	3:H:58:LEU:HD21	2.00	0.44
1:L:90:THR:HG23	1:L:132:VAL:HG11	2.00	0.44
2:S:264:GLY:HA3	3:T:35:ASN:OD1	2.18	0.44
3:T:75:VAL:HA	3:T:76:PRO:C	2.37	0.44
3:T:182:GLU:HA	3:T:188:THR:HG22	2.00	0.43
1:L:9:TYR:O	1:L:11:VAL:N	2.50	0.43
3:T:44:ASN:HB2	3:T:46:ASP:OD1	2.19	0.43
3:H:194:GLN:H	3:H:194:GLN:NE2	2.16	0.43
3:H:206:ASN:HD21	3:H:248:ARG:HD2	1.83	0.43
3:T:219:ILE:HG12	11:T:2062:HOH:O	2.19	0.43
1:L:66:VAL:HG12	1:L:86:TRP:HB2	2.00	0.43
1:R:213:ASP:O	1:R:217:ARG:HB2	2.18	0.43
1:R:268:LYS:HA	1:R:268:LYS:HD3	1.83	0.43
7:L:1002:BCL:HBD	7:L:1004:BCL:HAC1	2.00	0.43
1:R:2:LEU:HB3	1:R:6:GLU:HB3	1.99	0.43
3:H:177:ARG:NH1	3:H:177:ARG:HG2	2.33	0.43
1:L:213:ASP:O	1:L:217:ARG:HB2	2.19	0.43
1:L:84:GLY:HA2	1:L:87:GLN:HE21	1.83	0.43
1:L:185:LEU:HD13	8:M:1005:BPH:ND	2.32	0.43
7:R:2002:BCL:HBB3	7:R:2002:BCL:HMB1	2.01	0.43
7:S:2003:BCL:H2C	7:S:2003:BCL:HBC2	1.88	0.43
2:S:55:LEU:HD12	2:S:55:LEU:HA	1.89	0.43
1:L:33:PHE:O	1:L:36:VAL:HG22	2.19	0.43
1:R:22:PHE:HA	1:R:24:PHE:CE2	2.54	0.43
2:S:11:GLN:HB2	3:T:144:ALA:HB3	2.01	0.43
8:S:2005:BPH:HBB3	8:S:2005:BPH:CMB	2.49	0.43
2:S:253:ARG:HB2	2:S:259:ASN:OD1	2.19	0.43
1:R:60:ASN:HA	1:R:61:PRO:HD3	1.85	0.43
1:R:207:ARG:HG3	1:R:211:HIS:CG	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:84:GLY:HA2	1:R:87:GLN:HE21	1.83	0.43
1:R:9:TYR:O	1:R:11:VAL:N	2.49	0.43
1:L:162:TYR:HA	1:L:165:GLY:O	2.19	0.42
1:L:185:LEU:HD12	1:L:189:LEU:HD22	2.01	0.42
1:R:238:LEU:HD12	8:R:2006:BPH:HBC1	2.00	0.42
1:R:33:PHE:O	1:R:36:VAL:HG22	2.18	0.42
1:R:45:GLY:O	1:R:49:ILE:HG13	2.20	0.42
2:S:237:GLN:HB2	2:S:262:MET:HG2	2.02	0.42
3:T:245:ALA:N	3:T:246:PRO:CD	2.82	0.42
2:S:260:ALA:HB1	3:T:35:ASN:OD1	2.19	0.42
2:M:253:ARG:HB2	2:M:259:ASN:OD1	2.20	0.42
3:H:228:LEU:HD22	3:H:232:LYS:HE3	2.00	0.42
7:L:1001:BCL:HBC1	7:M:1003:BCL:HAA2	2.02	0.42
7:L:1002:BCL:CBA	7:L:1004:BCL:HBC1	2.50	0.42
2:M:237:GLN:HB2	2:M:262:MET:HG2	2.02	0.42
3:T:37:ARG:NH1	3:T:76:PRO:HD3	2.35	0.42
3:H:245:ALA:N	3:H:246:PRO:CD	2.82	0.42
3:H:34:GLU:HG3	11:H:1021:HOH:O	2.20	0.42
7:L:1002:BCL:H192	8:L:1006:BPH:HMA1	2.02	0.42
1:L:85:LEU:O	1:L:89:ILE:HG13	2.19	0.42
7:M:1003:BCL:HBB2	7:M:1003:BCL:HHC	2.00	0.42
2:M:53:GLY:O	2:M:57:VAL:HG23	2.19	0.42
3:H:221:SER:HA	3:H:222:PRO:HD3	1.84	0.42
1:L:11:VAL:HG13	11:L:1086:HOH:O	2.19	0.42
1:L:149:GLY:HA3	1:L:152:THR:OG1	2.19	0.42
1:L:1:ALA:C	1:L:2:LEU:HD12	2.40	0.42
7:M:1003:BCL:HMB1	7:M:1003:BCL:OBB	2.20	0.42
2:M:293:ASN:OD1	2:M:295:TYR:HB3	2.20	0.42
1:R:241:VAL:HG21	8:R:2006:BPH:HAC2	2.01	0.42
3:H:182:GLU:HA	3:H:188:THR:HG22	2.01	0.42
1:L:241:VAL:HG21	8:L:1006:BPH:CAC	2.50	0.42
7:M:1003:BCL:HBB3	7:M:1003:BCL:HHC	2.02	0.42
1:R:185:LEU:HD12	1:R:189:LEU:HD22	2.01	0.42
1:R:1:ALA:C	1:R:2:LEU:HD12	2.40	0.42
1:R:66:VAL:HG12	1:R:86:TRP:HB2	2.01	0.42
10:M:1014:LDA:HM11	10:M:1014:LDA:H22	1.68	0.42
1:R:185:LEU:HD13	8:S:2005:BPH:ND	2.35	0.42
1:L:60:ASN:HA	1:L:61:PRO:HD3	1.84	0.41
3:H:175:MET:CE	11:H:1028:HOH:O	2.61	0.41
1:L:152:THR:HG23	11:L:1081:HOH:O	2.20	0.41
1:L:268:LYS:HA	1:L:268:LYS:HD3	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:114:LEU:HD12	2:M:114:LEU:HA	1.92	0.41
11:L:1069:HOH:O	2:M:29:ARG:HD2	2.20	0.41
7:L:1002:BCL:OBB	7:L:1002:BCL:HHC	2.20	0.41
3:H:68:HIS:HD2	11:H:1030:HOH:O	2.04	0.41
1:L:126:LEU:HD12	1:L:126:LEU:HA	1.87	0.41
1:R:262:TRP:O	1:R:265:TRP:HD1	2.03	0.41
2:S:278:LEU:HD12	2:S:278:LEU:HA	1.86	0.41
3:T:206:ASN:HD21	3:T:248:ARG:HD2	1.85	0.41
2:S:114:LEU:HA	2:S:114:LEU:HD12	1.91	0.41
7:R:2001:BCL:HBB2	10:S:2012:LDA:H123	2.03	0.41
2:S:229:PHE:HB2	2:S:244:ALA:HB2	2.02	0.41
3:T:66:LEU:HA	3:T:67:PRO:HD3	1.77	0.41
1:R:180:PHE:HE2	7:R:2002:BCL:HMA2	1.85	0.41
1:L:69:PRO:HD2	1:L:142:TRP:HB2	2.03	0.41
1:L:60:ASN:CB	1:L:63:LEU:HD23	2.49	0.41
3:H:177:ARG:HG2	3:H:177:ARG:HH11	1.86	0.41
3:H:37:ARG:C	3:H:38:GLU:HG2	2.41	0.41
7:R:2002:BCL:H203	9:S:2008:U10:H252	2.03	0.41
1:R:207:ARG:HG2	2:S:142:MET:HG2	2.03	0.41
2:S:75:TRP:HB3	2:S:80:TRP:CE3	2.56	0.41
3:H:37:ARG:NH1	3:H:76:PRO:HD3	2.36	0.40
1:L:153:HIS:O	1:L:157:VAL:HG23	2.21	0.40
1:L:170:ASN:HB3	1:L:173:HIS:CB	2.51	0.40
1:L:79:PRO:HB2	1:L:82:LYS:HB2	2.02	0.40
1:R:126:LEU:HA	1:R:126:LEU:HD12	1.87	0.40
7:L:1004:BCL:H193	8:L:1006:BPH:H102	2.02	0.40
1:L:22:PHE:HA	1:L:24:PHE:CE2	2.55	0.40
2:S:9:GLN:HE22	3:T:197:LYS:HA	1.87	0.40
1:L:207:ARG:HG3	1:L:211:HIS:CG	2.56	0.40
2:M:75:TRP:HB3	2:M:80:TRP:CE3	2.56	0.40
3:T:192:PRO:HB3	3:T:194:GLN:HE21	1.87	0.40
3:T:32:GLN:HG2	3:T:56:PHE:CD2	2.57	0.40
3:H:37:ARG:HD2	3:H:59:PRO:HG3	2.03	0.40
3:T:165:VAL:O	3:T:166:ASP:HB2	2.20	0.40
1:L:230:HIS:CD2	2:M:223:ILE:HG13	2.56	0.40
2:M:22:GLU:HB3	2:M:23:ASP:H	1.69	0.40
1:R:146:PHE:HB3	1:R:156:TRP:CD2	2.56	0.40
7:S:2003:BCL:OBB	7:S:2003:BCL:HMB1	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	279/281 (99%)	266 (95%)	12 (4%)	1 (0%)	38	59
1	R	279/281 (99%)	266 (95%)	12 (4%)	1 (0%)	38	59
2	M	297/307 (97%)	288 (97%)	9 (3%)	0	100	100
2	S	297/307 (97%)	289 (97%)	8 (3%)	0	100	100
3	H	244/260 (94%)	236 (97%)	8 (3%)	0	100	100
3	T	244/260 (94%)	234 (96%)	10 (4%)	0	100	100
All	All	1640/1696 (97%)	1579 (96%)	59 (4%)	2 (0%)	55	76

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	220/220 (100%)	209 (95%)	11 (5%)	28	51
1	R	220/220 (100%)	209 (95%)	11 (5%)	28	51
2	M	235/239 (98%)	222 (94%)	13 (6%)	25	46
2	S	235/239 (98%)	222 (94%)	13 (6%)	25	46
3	H	199/209 (95%)	192 (96%)	7 (4%)	41	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	T	199/209 (95%)	192 (96%)	7 (4%)	41 68
All	All	1308/1336 (98%)	1246 (95%)	62 (5%)	30 54

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

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

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

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

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

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 6 are monoatomic - leaving 22 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	BCL	L	1001	2	40,59,74	1.43	6 (15%)	47,97,115	1.80	14 (29%)
7	BCL	L	1002	1	55,74,74	1.32	6 (10%)	65,115,115	1.38	13 (20%)
7	BCL	L	1004	1	55,74,74	1.19	6 (10%)	65,115,115	1.55	14 (21%)
8	BPH	L	1006	-	65,70,70	1.19	7 (10%)	75,101,101	1.75	14 (18%)
9	U10	L	1009	-	44,44,63	1.58	8 (18%)	53,56,79	1.38	6 (11%)
7	BCL	M	1003	2	55,74,74	1.20	6 (10%)	65,115,115	1.43	15 (23%)
8	BPH	M	1005	-	51,56,70	1.17	8 (15%)	58,84,101	2.16	11 (18%)
9	U10	M	1008	-	38,38,63	1.74	9 (23%)	46,49,79	1.21	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	LDA	M	1012	-	13,15,15	2.52	1 (7%)	14,17,17	2.45	3 (21%)
10	LDA	M	1013	-	13,15,15	2.70	1 (7%)	14,17,17	2.37	3 (21%)
10	LDA	M	1014	-	13,15,15	2.74	1 (7%)	14,17,17	2.29	4 (28%)
7	BCL	R	2001	2	40,59,74	1.33	7 (17%)	47,97,115	1.74	11 (23%)
7	BCL	R	2002	1	55,74,74	1.41	5 (9%)	65,115,115	1.35	10 (15%)
7	BCL	R	2004	1	55,74,74	1.24	7 (12%)	65,115,115	1.55	8 (12%)
8	BPH	R	2006	-	65,70,70	1.05	6 (9%)	75,101,101	1.64	10 (13%)
9	U10	R	2009	-	18,18,63	1.90	3 (16%)	22,25,79	1.24	3 (13%)
7	BCL	S	2003	2	55,74,74	1.25	7 (12%)	65,115,115	1.49	11 (16%)
8	BPH	S	2005	-	52,57,70	1.20	5 (9%)	59,85,101	1.90	12 (20%)
9	U10	S	2008	-	32,32,63	1.58	7 (21%)	38,41,79	1.10	3 (7%)
10	LDA	S	2012	-	13,15,15	2.78	1 (7%)	14,17,17	2.45	2 (14%)
10	LDA	S	2013	-	13,15,15	2.66	1 (7%)	14,17,17	2.45	2 (14%)
10	LDA	S	2014	-	13,15,15	2.88	1 (7%)	14,17,17	2.32	2 (14%)

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

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

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

All (109) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	S	2014	LDA	O1-N1	-10.09	1.22	1.42
10	S	2012	LDA	O1-N1	-9.72	1.23	1.42
10	M	1014	LDA	O1-N1	-9.68	1.23	1.42
10	M	1013	LDA	O1-N1	-9.45	1.23	1.42
10	S	2013	LDA	O1-N1	-9.36	1.23	1.42
10	M	1012	LDA	O1-N1	-8.87	1.24	1.42
8	L	1006	BPH	C1B-C2B	-3.40	1.38	1.45
8	R	2006	BPH	C1B-C2B	-3.37	1.38	1.45
8	L	1006	BPH	C3D-CAD	-3.34	1.39	1.47
7	R	2004	BCL	C3D-CAD	-3.26	1.36	1.46
7	R	2004	BCL	O2D-CGD	-3.18	1.25	1.33
8	S	2005	BPH	C3D-CAD	-3.17	1.39	1.47
7	L	1001	BCL	O2D-CGD	-3.14	1.25	1.33
8	R	2006	BPH	C3D-CAD	-3.11	1.40	1.47
7	R	2002	BCL	O2D-CGD	-3.02	1.25	1.33
7	M	1003	BCL	C3B-CAB	-3.00	1.41	1.49
8	R	2006	BPH	O2D-CGD	-2.95	1.25	1.33
8	S	2005	BPH	O2D-CGD	-2.93	1.25	1.33
9	L	1009	U10	C7-C8	-2.92	1.46	1.50
7	M	1003	BCL	C3D-CAD	-2.91	1.37	1.46
7	S	2003	BCL	O2D-CGD	-2.90	1.25	1.33
7	L	1004	BCL	O2D-CGD	-2.88	1.25	1.33
7	R	2001	BCL	O2D-CGD	-2.83	1.26	1.33
8	S	2005	BPH	C1B-C2B	-2.83	1.39	1.45
8	L	1006	BPH	O2A-CGA	-2.83	1.24	1.33
9	S	2008	U10	C7-C8	-2.83	1.46	1.50
7	L	1001	BCL	O2A-CGA	-2.81	1.25	1.33
8	M	1005	BPH	O2A-CGA	-2.77	1.25	1.33
7	L	1004	BCL	C3D-CAD	-2.76	1.38	1.46
8	M	1005	BPH	C3D-CAD	-2.75	1.40	1.47
7	M	1003	BCL	O2D-CGD	-2.74	1.26	1.33
7	L	1002	BCL	O2D-CGD	-2.73	1.26	1.33
7	M	1003	BCL	O2A-CGA	-2.68	1.25	1.33
9	M	1008	U10	C7-C8	-2.67	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	R	2002	BCL	O2A-CGA	-2.64	1.25	1.33
8	S	2005	BPH	O2A-CGA	-2.61	1.25	1.33
7	S	2003	BCL	O2A-CGA	-2.57	1.25	1.33
8	L	1006	BPH	O2D-CGD	-2.56	1.26	1.33
7	L	1002	BCL	C3B-CAB	-2.55	1.42	1.49
8	M	1005	BPH	O2D-CGD	-2.55	1.26	1.33
7	R	2001	BCL	O2A-CGA	-2.54	1.25	1.33
7	S	2003	BCL	C3B-CAB	-2.51	1.42	1.49
7	L	1002	BCL	O2A-CGA	-2.51	1.25	1.33
7	L	1004	BCL	O2A-CGA	-2.48	1.26	1.33
8	R	2006	BPH	O2A-CGA	-2.47	1.26	1.33
7	R	2001	BCL	C3B-CAB	-2.45	1.42	1.49
7	S	2003	BCL	C3D-CAD	-2.43	1.39	1.46
9	S	2008	U10	C4-C5	-2.42	1.42	1.48
7	L	1001	BCL	C3B-CAB	-2.37	1.42	1.49
7	R	2001	BCL	C3D-CAD	-2.32	1.39	1.46
7	L	1001	BCL	C3D-CAD	-2.31	1.39	1.46
8	M	1005	BPH	C1B-C2B	-2.23	1.41	1.45
7	R	2004	BCL	O2A-CGA	-2.23	1.26	1.33
7	R	2004	BCL	C3B-CAB	-2.17	1.43	1.49
9	M	1008	U10	C3-C2	-2.13	1.42	1.48
7	M	1003	BCL	C2-C3	2.07	1.38	1.33
8	M	1005	BPH	CHC-C1C	2.07	1.40	1.36
9	S	2008	U10	C13-C14	2.07	1.38	1.33
8	M	1005	BPH	CMB-C2B	2.08	1.55	1.50
8	M	1005	BPH	C2-C3	2.10	1.38	1.33
7	L	1004	BCL	C2-C3	2.10	1.38	1.33
9	L	1009	U10	C23-C24	2.12	1.38	1.33
9	M	1008	U10	C28-C29	2.13	1.38	1.32
9	S	2008	U10	C4-C3	2.23	1.45	1.35
9	M	1008	U10	O3-C3	2.28	1.42	1.36
7	L	1002	BCL	C2-C3	2.28	1.38	1.33
9	M	1008	U10	C8-C9	2.32	1.38	1.33
8	M	1005	BPH	C3C-C4C	2.38	1.54	1.50
8	R	2006	BPH	C3C-C4C	2.39	1.54	1.50
7	R	2001	BCL	C2-C3	2.40	1.39	1.32
9	L	1009	U10	C18-C19	2.41	1.39	1.33
9	L	1009	U10	C13-C14	2.47	1.39	1.33
9	S	2008	U10	C8-C9	2.68	1.39	1.33
7	R	2004	BCL	C2-C3	2.71	1.39	1.33
9	M	1008	U10	C7-C6	2.73	1.56	1.51
8	R	2006	BPH	C2-C3	2.78	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	1008	U10	C18-C19	2.82	1.40	1.33
8	L	1006	BPH	CBB-CAB	2.86	1.56	1.50
8	S	2005	BPH	C2-C3	2.96	1.40	1.33
9	L	1009	U10	C8-C9	2.99	1.40	1.33
9	L	1009	U10	C33-C34	3.00	1.40	1.33
9	L	1009	U10	C28-C29	3.11	1.40	1.33
8	L	1006	BPH	C2-C3	3.17	1.40	1.33
7	R	2002	BCL	C2-C3	3.20	1.41	1.33
9	S	2008	U10	C18-C19	3.20	1.41	1.33
9	R	2009	U10	C8-C9	3.24	1.41	1.32
7	S	2003	BCL	C2-C3	3.29	1.41	1.33
7	R	2001	BCL	CHC-C1C	3.30	1.37	1.33
8	L	1006	BPH	CHC-C1C	3.36	1.43	1.36
7	L	1001	BCL	CHC-C1C	3.40	1.37	1.33
9	M	1008	U10	C13-C14	3.44	1.41	1.33
9	R	2009	U10	C7-C6	3.52	1.57	1.51
7	R	2004	BCL	CHC-C1C	3.54	1.38	1.33
7	L	1004	BCL	CHB-C4A	3.61	1.38	1.33
7	L	1004	BCL	CHC-C1C	3.89	1.38	1.33
7	R	2001	BCL	CHB-C4A	4.07	1.38	1.33
7	S	2003	BCL	CHB-C4A	4.17	1.38	1.33
9	L	1009	U10	C6-C1	4.28	1.44	1.35
9	S	2008	U10	C6-C1	4.35	1.44	1.35
7	R	2004	BCL	CHB-C4A	4.55	1.39	1.33
9	R	2009	U10	C6-C1	4.69	1.45	1.35
7	S	2003	BCL	CHC-C1C	4.70	1.39	1.33
7	L	1002	BCL	CHC-C1C	4.95	1.39	1.33
7	L	1001	BCL	CHB-C4A	5.01	1.39	1.33
7	M	1003	BCL	CHB-C4A	5.16	1.40	1.33
7	L	1002	BCL	CHB-C4A	5.20	1.40	1.33
7	R	2002	BCL	CHC-C1C	5.25	1.40	1.33
9	M	1008	U10	C6-C1	5.50	1.47	1.35
7	R	2002	BCL	CHB-C4A	5.80	1.40	1.33

All (176) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	1005	BPH	C4D-C3D-CAD	-8.48	102.93	107.78
8	L	1006	BPH	C4D-C3D-CAD	-8.01	103.20	107.78
10	S	2012	LDA	CM2-N1-CM1	-7.90	95.87	110.99
10	S	2013	LDA	CM2-N1-CM1	-7.79	96.08	110.99
10	M	1012	LDA	CM2-N1-CM1	-7.77	96.11	110.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	R	2006	BPH	C4D-C3D-CAD	-7.69	103.38	107.78
10	M	1013	LDA	CM2-N1-CM1	-7.52	96.59	110.99
8	S	2005	BPH	C4D-C3D-CAD	-7.37	103.56	107.78
10	S	2014	LDA	CM2-N1-CM1	-7.28	97.06	110.99
10	M	1014	LDA	CM2-N1-CM1	-6.99	97.62	110.99
7	R	2004	BCL	OBD-CAD-C3D	-5.72	117.48	128.03
8	L	1006	BPH	OBD-CAD-C3D	-3.78	121.06	128.03
7	S	2003	BCL	OBD-CAD-CBD	-3.43	120.76	125.94
7	M	1003	BCL	C7-C6-C5	-3.36	103.77	113.11
7	L	1001	BCL	OBD-CAD-C3D	-3.31	121.93	128.03
7	R	2001	BCL	OBD-CAD-C3D	-3.14	122.23	128.03
7	S	2003	BCL	CMB-C2B-C1B	-3.04	123.80	128.46
7	R	2002	BCL	CMB-C2B-C1B	-3.03	123.81	128.46
7	L	1004	BCL	OBD-CAD-CBD	-2.96	121.47	125.94
7	M	1003	BCL	CMB-C2B-C1B	-2.89	124.02	128.46
9	M	1008	U10	O5-C5-C6	-2.89	116.50	121.82
7	R	2004	BCL	C7-C6-C5	-2.87	105.14	113.11
7	M	1003	BCL	OBD-CAD-C3D	-2.82	122.83	128.03
7	R	2004	BCL	CED-O2D-CGD	-2.81	109.38	115.97
7	L	1001	BCL	CMA-C3A-C4A	-2.80	104.25	111.77
7	L	1002	BCL	CMA-C3A-C4A	-2.79	104.27	111.77
7	L	1001	BCL	OBB-CAB-CBB	-2.79	113.80	120.16
7	L	1004	BCL	C1-C2-C3	-2.73	120.93	125.96
8	R	2006	BPH	C1C-NC-C4C	-2.73	108.09	110.54
8	M	1005	BPH	O1D-CGD-CBD	-2.72	119.72	124.60
7	L	1004	BCL	OBD-CAD-C3D	-2.65	123.14	128.03
8	M	1005	BPH	OBD-CAD-CBD	-2.63	121.96	125.94
7	L	1004	BCL	CAC-C3C-C4C	-2.63	106.75	112.58
8	L	1006	BPH	C7-C6-C5	-2.62	105.84	113.11
7	L	1002	BCL	CMB-C2B-C1B	-2.58	124.50	128.46
8	L	1006	BPH	O1D-CGD-CBD	-2.58	119.97	124.60
7	L	1001	BCL	CMB-C2B-C1B	-2.56	124.52	128.46
7	R	2002	BCL	CMA-C3A-C4A	-2.56	104.90	111.77
7	S	2003	BCL	CAC-C3C-C4C	-2.55	106.93	112.58
7	R	2004	BCL	CAC-C3C-C4C	-2.54	106.95	112.58
7	L	1002	BCL	CHA-C1A-NA	-2.49	120.41	126.18
7	R	2001	BCL	CMA-C3A-C4A	-2.46	105.15	111.77
7	L	1001	BCL	CHA-C1A-NA	-2.46	120.46	126.18
8	S	2005	BPH	C1C-NC-C4C	-2.45	108.34	110.54
7	L	1004	BCL	CMB-C2B-C1B	-2.44	124.71	128.46
9	M	1008	U10	C17-C18-C19	-2.44	121.55	127.68
8	R	2006	BPH	C7-C6-C5	-2.43	106.35	113.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	S	2003	BCL	CHA-C1A-NA	-2.40	120.61	126.18
8	R	2006	BPH	OBD-CAD-C3D	-2.39	123.63	128.03
8	S	2005	BPH	OBD-CAD-CBD	-2.37	122.36	125.94
7	L	1004	BCL	O1D-CGD-CBD	-2.36	120.36	124.60
8	S	2005	BPH	O1D-CGD-CBD	-2.35	120.39	124.60
7	R	2001	BCL	CMB-C2B-C1B	-2.33	124.88	128.46
7	M	1003	BCL	CAC-C3C-C4C	-2.33	107.41	112.58
10	M	1014	LDA	C6-C5-C4	-2.32	102.48	114.45
9	L	1009	U10	C16-C17-C18	-2.32	104.00	111.97
9	M	1008	U10	C12-C13-C14	-2.32	121.85	127.68
8	R	2006	BPH	O1D-CGD-CBD	-2.30	120.47	124.60
7	L	1002	BCL	CAC-C3C-C4C	-2.28	107.52	112.58
7	L	1004	BCL	C15-C13-C12	-2.27	101.18	112.10
7	R	2001	BCL	O1D-CGD-CBD	-2.27	120.52	124.60
7	R	2002	BCL	CAC-C3C-C4C	-2.25	107.58	112.58
7	L	1004	BCL	CHA-C1A-NA	-2.23	121.00	126.18
10	M	1013	LDA	C6-C5-C4	-2.20	103.09	114.45
7	R	2002	BCL	CHA-C1A-NA	-2.18	121.11	126.18
10	M	1012	LDA	C6-C5-C4	-2.18	103.24	114.45
7	S	2003	BCL	O1D-CGD-CBD	-2.17	120.70	124.60
7	M	1003	BCL	O1D-CGD-CBD	-2.17	120.71	124.60
8	L	1006	BPH	C1C-NC-C4C	-2.12	108.63	110.54
8	R	2006	BPH	OBD-CAD-CBD	-2.11	122.75	125.94
7	M	1003	BCL	CHA-C1A-NA	-2.09	121.33	126.18
9	R	2009	U10	O5-C5-C6	-2.08	117.98	121.82
7	L	1002	BCL	O1D-CGD-CBD	-2.08	120.87	124.60
8	L	1006	BPH	CMA-C3A-C4A	-2.06	106.17	112.37
7	L	1002	BCL	CAA-C2A-C1A	-2.04	105.29	111.97
10	M	1014	LDA	C4-C3-C2	-2.03	103.97	114.45
7	R	2004	BCL	C6-C5-C3	-2.03	108.05	112.66
9	M	1008	U10	C1M-C1-C6	-2.02	120.10	124.20
7	R	2002	BCL	CMC-C2C-C3C	-2.02	105.57	113.77
10	S	2014	LDA	C4-C3-C2	-2.02	104.04	114.45
8	L	1006	BPH	O2A-CGA-CBA	2.00	117.73	111.90
7	M	1003	BCL	C2A-C1A-CHA	2.02	127.50	123.92
7	M	1003	BCL	C4A-NA-C1A	2.03	108.97	106.45
9	L	1009	U10	C7-C6-C5	2.04	121.08	118.47
7	L	1004	BCL	CHB-C4A-NA	2.04	127.33	124.51
7	L	1002	BCL	C2A-C3A-C4A	2.04	105.16	101.87
8	S	2005	BPH	CED-O2D-CGD	2.04	120.75	115.97
7	R	2004	BCL	CMB-C2B-C3B	2.04	128.68	124.89
8	L	1006	BPH	C4A-NA-C1A	2.06	109.83	108.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	1005	BPH	C3C-C2C-C1C	2.06	105.20	101.87
7	L	1002	BCL	C2C-C3C-C4C	2.08	104.45	101.34
7	L	1001	BCL	C4A-NA-C1A	2.10	109.06	106.45
8	M	1005	BPH	C2A-C3A-C4A	2.12	105.56	101.33
8	L	1006	BPH	CED-O2D-CGD	2.12	120.95	115.97
7	R	2002	BCL	C2C-C3C-C4C	2.12	104.52	101.34
7	L	1001	BCL	C1-C2-C3	2.13	130.04	126.68
7	M	1003	BCL	C1-O2A-CGA	2.14	121.91	116.77
7	L	1001	BCL	C2C-C3C-C4C	2.15	104.55	101.34
7	S	2003	BCL	C1-O2A-CGA	2.16	121.96	116.77
9	L	1009	U10	C35-C34-C36	2.17	118.41	115.85
7	R	2001	BCL	C2C-C3C-C4C	2.17	104.58	101.34
9	L	1009	U10	C15-C14-C16	2.17	119.05	115.29
7	M	1003	BCL	O2D-CGD-CBD	2.17	115.18	111.30
7	L	1001	BCL	CMB-C2B-C3B	2.24	129.04	124.89
8	S	2005	BPH	C2B-C1B-NB	2.25	113.15	109.82
8	L	1006	BPH	C1-O2A-CGA	2.30	122.29	116.77
7	L	1001	BCL	CHB-C4A-NA	2.30	127.69	124.51
7	R	2002	BCL	C1D-CHD-C4C	2.35	129.43	125.92
8	S	2005	BPH	C3C-C4C-NC	2.39	110.22	107.97
7	M	1003	BCL	C2C-C3C-C4C	2.41	104.94	101.34
10	M	1014	LDA	O1-N1-C1	2.41	115.19	109.27
7	L	1001	BCL	O2D-CGD-CBD	2.42	115.62	111.30
9	S	2008	U10	C4M-O4-C4	2.42	125.11	116.44
7	L	1004	BCL	CMB-C2B-C3B	2.46	129.45	124.89
8	L	1006	BPH	CAC-C3C-C4C	2.46	118.98	112.67
9	S	2008	U10	C10-C9-C11	2.46	119.55	115.29
7	L	1002	BCL	CMB-C2B-C3B	2.50	129.52	124.89
7	S	2003	BCL	O2A-CGA-CBA	2.50	119.17	111.90
7	R	2001	BCL	C2A-C3A-C4A	2.50	105.92	101.87
9	S	2008	U10	C15-C14-C16	2.52	119.66	115.29
7	M	1003	BCL	CED-O2D-CGD	2.54	121.91	115.97
9	R	2009	U10	C8-C7-C6	2.56	119.06	111.85
7	L	1004	BCL	C4-C3-C5	2.59	119.79	115.29
10	M	1013	LDA	O1-N1-C1	2.65	115.78	109.27
7	L	1002	BCL	C6-C5-C3	2.68	118.73	112.66
9	M	1008	U10	C31-C29-C30	2.71	120.92	114.60
7	R	2001	BCL	C1-C2-C3	2.71	130.97	126.68
7	R	2004	BCL	O2D-CGD-CBD	2.72	116.15	111.30
7	S	2003	BCL	O2D-CGD-CBD	2.72	116.16	111.30
7	R	2002	BCL	CMB-C2B-C3B	2.73	129.95	124.89
7	R	2002	BCL	CED-O2D-CGD	2.73	122.37	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	1002	BCL	C3D-CAD-CBD	2.74	111.46	107.60
10	S	2012	LDA	O1-N1-C1	2.74	115.99	109.27
7	M	1003	BCL	C3D-CAD-CBD	2.74	111.47	107.60
8	M	1005	BPH	O2D-CGD-CBD	2.80	116.30	111.30
9	R	2009	U10	C3M-O3-C3	2.81	126.49	116.44
10	M	1012	LDA	O1-N1-C1	2.83	116.22	109.27
7	R	2002	BCL	C6-C5-C3	2.93	119.29	112.66
9	L	1009	U10	C30-C29-C31	2.94	120.39	115.29
7	M	1003	BCL	CMB-C2B-C3B	2.98	130.41	124.89
7	L	1002	BCL	C4-C3-C5	3.02	120.53	115.29
7	R	2001	BCL	CMB-C2B-C3B	3.04	130.54	124.89
7	M	1003	BCL	C15-C13-C12	3.05	126.77	112.10
10	S	2013	LDA	O1-N1-C1	3.10	116.89	109.27
8	R	2006	BPH	C1-O2A-CGA	3.11	124.23	116.77
7	L	1004	BCL	O2D-CGD-CBD	3.17	116.96	111.30
7	S	2003	BCL	CMB-C2B-C3B	3.18	130.78	124.89
7	L	1002	BCL	CED-O2D-CGD	3.18	123.41	115.97
7	S	2003	BCL	CED-O2D-CGD	3.19	123.44	115.97
7	L	1004	BCL	C2A-C3A-C4A	3.26	107.13	101.87
8	L	1006	BPH	O2D-CGD-CBD	3.28	117.16	111.30
8	M	1005	BPH	CED-O2D-CGD	3.36	123.85	115.97
8	S	2005	BPH	O2D-CGD-CBD	3.37	117.33	111.30
7	R	2001	BCL	O2D-CGD-CBD	3.38	117.34	111.30
8	R	2006	BPH	O2D-CGD-CBD	3.63	117.78	111.30
8	S	2005	BPH	C2C-C3C-C4C	3.63	106.78	101.34
7	L	1001	BCL	C2A-C3A-C4A	3.70	107.84	101.87
7	L	1001	BCL	C3D-CAD-CBD	3.87	113.07	107.60
8	S	2005	BPH	C3D-CAD-CBD	3.90	113.11	107.60
7	R	2001	BCL	C1-O2A-CGA	4.05	126.49	116.77
9	L	1009	U10	C25-C24-C26	4.07	122.36	115.29
8	S	2005	BPH	C4-C3-C5	4.08	122.37	115.29
7	L	1001	BCL	C1-O2A-CGA	4.09	126.58	116.77
8	M	1005	BPH	C3D-CAD-CBD	4.17	113.49	107.60
7	R	2001	BCL	C3D-CAD-CBD	4.23	113.57	107.60
8	R	2006	BPH	C3D-CAD-CBD	4.26	113.62	107.60
8	M	1005	BPH	C1-O2A-CGA	4.30	127.09	116.77
7	R	2004	BCL	C3D-CAD-CBD	4.37	113.78	107.60
8	L	1006	BPH	C3D-CAD-CBD	4.53	114.00	107.60
7	S	2003	BCL	C3D-CAD-CBD	4.64	114.15	107.60
8	R	2006	BPH	C3C-C4C-NC	4.64	112.34	107.97
8	S	2005	BPH	C1-O2A-CGA	4.85	128.40	116.77
7	L	1004	BCL	C3D-CAD-CBD	4.90	114.52	107.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	1005	BPH	C3C-C4C-NC	5.05	112.72	107.97
8	L	1006	BPH	C3C-C4C-NC	5.64	113.28	107.97
8	M	1005	BPH	C4-C3-C5	6.69	123.77	115.85

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

22 monomers are involved in 84 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	L	1001	BCL	4	0
7	L	1002	BCL	9	0
7	L	1004	BCL	7	0
8	L	1006	BPH	5	0
9	L	1009	U10	2	0
7	M	1003	BCL	8	0
8	M	1005	BPH	5	0
9	M	1008	U10	2	0
10	M	1012	LDA	1	0
10	M	1013	LDA	1	0
10	M	1014	LDA	5	0
7	R	2001	BCL	3	0
7	R	2002	BCL	9	0
7	R	2004	BCL	6	0
8	R	2006	BPH	14	0
9	R	2009	U10	3	0
7	S	2003	BCL	6	0
8	S	2005	BPH	4	0
9	S	2008	U10	2	0
10	S	2012	LDA	2	0
10	S	2013	LDA	1	0
10	S	2014	LDA	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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, 95th 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%)	0.29	10 (3%) 43 45	26, 43, 67, 75	0
1	R	281/281 (100%)	0.15	21 (7%) 15 15	26, 44, 67, 75	0
2	M	299/307 (97%)	0.08	3 (1%) 82 83	28, 36, 48, 67	0
2	S	299/307 (97%)	-0.12	6 (2%) 65 67	29, 37, 49, 67	0
3	H	246/260 (94%)	0.09	9 (3%) 42 44	33, 43, 66, 82	0
3	T	246/260 (94%)	0.40	30 (12%) 5 4	34, 44, 66, 82	0
All	All	1652/1696 (97%)	0.14	79 (4%) 31 32	26, 40, 65, 82	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	S	301	HIS	6.5
2	M	301	HIS	6.3
3	H	255	MET	5.4
3	T	69	GLY	5.2
3	H	252	VAL	5.2
3	T	92	VAL	5.1
1	R	1	ALA	4.9
3	T	80	SER	4.7
1	L	51	TRP	4.4
1	L	79	PRO	4.3
3	T	79	GLU	4.2
1	R	203	GLY	4.1
3	T	252	VAL	4.1
3	T	51	ALA	4.0
1	L	59	TRP	4.0
1	L	271	TRP	3.9
1	R	51	TRP	3.9
3	T	255	MET	3.9
3	H	256	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	R	202	LYS	3.8
3	T	46	ASP	3.8
3	T	78	PRO	3.8
1	R	270	PRO	3.6
1	R	59	TRP	3.5
3	H	254	ALA	3.4
3	T	29	TYR	3.4
2	S	3	TYR	3.3
3	T	55	PRO	3.2
1	R	140	GLY	3.2
1	R	281	GLY	3.1
1	R	17	VAL	3.1
3	T	68	HIS	3.1
1	R	21	LEU	3.0
3	T	56	PHE	2.9
1	L	269	LEU	2.9
3	T	50	ALA	2.8
1	L	274	ASN	2.8
3	H	251	VAL	2.7
1	R	75	LEU	2.7
3	T	18	TYR	2.7
3	T	52	ASN	2.7
1	R	204	LYS	2.6
1	R	271	TRP	2.6
3	T	61	PRO	2.6
3	T	60	LYS	2.6
3	T	96	PHE	2.6
2	S	4	GLN	2.6
1	R	73	TYR	2.6
3	T	254	ALA	2.5
1	L	111	LEU	2.5
3	H	61	PRO	2.5
3	T	256	LEU	2.5
2	S	42	PHE	2.5
1	L	275	ILE	2.4
3	T	251	VAL	2.4
3	T	82	ASP	2.4
1	R	74	GLY	2.4
3	T	54	GLY	2.4
3	T	101	THR	2.4
3	H	253	ALA	2.3
3	T	253	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	R	7	ARG	2.3
2	M	68	PHE	2.3
3	T	49	PRO	2.2
2	M	245	ALA	2.2
2	S	54	SER	2.2
3	T	94	GLU	2.2
1	R	119	PHE	2.2
1	R	274	ASN	2.2
1	L	73	TYR	2.2
2	S	106	ALA	2.2
3	T	77	GLY	2.1
1	L	72	GLU	2.1
1	R	18	GLY	2.1
3	H	12	LEU	2.1
3	H	92	VAL	2.0
1	R	47	ILE	2.0
1	R	268	LYS	2.0
3	T	53	GLN	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, 95th 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
10	LDA	M	1014	16/16	0.70	0.39	13.65	51,52,55,55	0
10	LDA	S	2012	16/16	0.61	0.42	7.07	50,54,58,58	0
9	U10	L	1009	44/63	0.68	0.36	4.86	67,78,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
10	LDA	S	2014	16/16	0.69	0.28	4.68	54,57,60,60	0
9	U10	R	2009	18/63	0.79	0.28	4.34	61,62,63,63	0
10	LDA	S	2013	16/16	0.66	0.28	3.59	58,59,63,63	0
10	LDA	M	1013	16/16	0.77	0.24	3.42	47,51,55,55	0
7	BCL	R	2002	66/66	0.93	0.19	1.98	36,38,43,44	0
10	LDA	M	1012	16/16	0.76	0.25	1.74	54,56,59,59	0
8	BPH	R	2006	65/65	0.92	0.17	1.63	42,45,51,51	0
7	BCL	S	2003	66/66	0.94	0.17	1.62	33,34,48,49	0
7	BCL	M	1003	66/66	0.95	0.19	1.50	27,29,39,43	0
7	BCL	L	1002	66/66	0.94	0.18	0.96	27,32,33,36	0
9	U10	S	2008	32/63	0.94	0.17	0.86	41,43,46,47	0
7	BCL	R	2001	51/66	0.94	0.13	0.50	30,32,41,43	0
7	BCL	R	2004	66/66	0.94	0.15	0.36	30,33,53,54	0
8	BPH	L	1006	65/65	0.92	0.16	0.21	26,30,39,39	0
7	BCL	L	1001	51/66	0.97	0.15	0.21	26,28,33,34	0
9	U10	M	1008	38/63	0.92	0.18	-0.29	27,30,45,45	0
8	BPH	S	2005	52/65	0.96	0.12	-0.48	30,32,41,41	0
7	BCL	L	1004	66/66	0.95	0.15	-0.49	25,27,43,44	0
8	BPH	M	1005	51/65	0.96	0.14	-0.64	23,25,33,34	0
4	FE2	M	1007	1/1	0.99	0.12	-2.22	28,28,28,28	0
4	FE2	S	2007	1/1	0.99	0.05	-2.22	32,32,32,32	0
6	CL	M	1011	1/1	0.97	0.18	-	48,48,48,48	0
6	CL	S	2011	1/1	0.96	0.20	-	59,59,59,59	0
5	CD	H	1010	1/1	0.99	0.05	-	41,41,41,41	0
5	CD	T	2010	1/1	0.99	0.04	-	53,53,53,53	0

6.5 Other polymers ⓘ

There are no such residues in this entry.