



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 05:16 AM 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 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/ValidationPDFNotes.html>

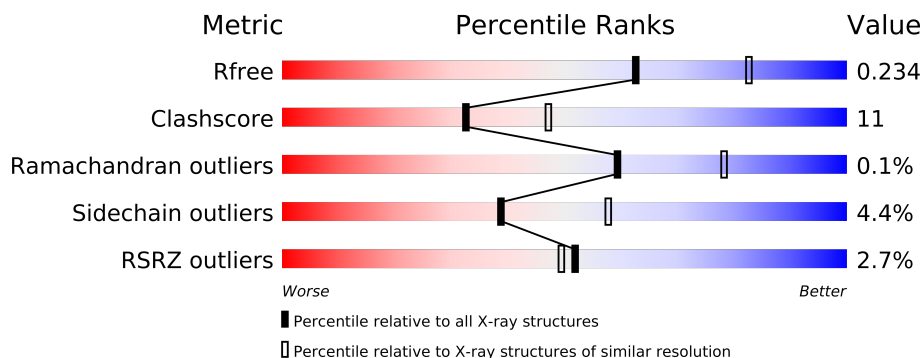
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	L	281	
1	R	281	
2	M	307	
2	S	307	
3	H	260	
3	T	260	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	BCL	R	2002	-	X
4	BCL	S	2001	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Geometry	Electron density
4	BCL	S	2003	-	X
4	BCL	S	2004	-	X
5	U10	L	1009	-	X
5	U10	R	2009	-	X
5	U10	S	2008	-	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 hydrogen and 0 are deuterium.

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			

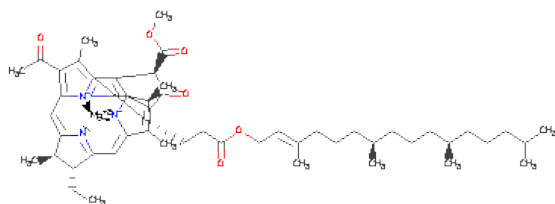
There are 2 discrepancies between the modelled and reference sequences:

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.

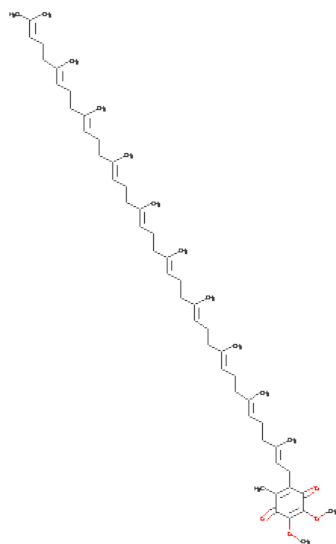
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	246	Total	C	N	O	S	0	0	0
			1869	1196	320	343	10			
3	T	246	Total	C	N	O	S	0	0	0
			1869	1196	320	343	10			

- 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: $C_{59}H_{90}O_4$).

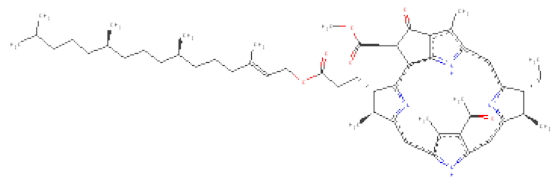


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	L	1	Total	C	O	0	0
			44	40	4		
5	M	1	Total	C	O	0	0
			38	34	4		
5	R	1	Total	C	O	0	0
			18	14	4		
5	S	1	Total	C	O	0	0
			32	28	4		

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

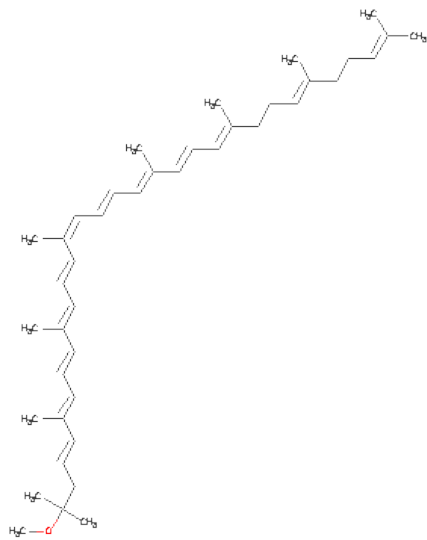
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	S	1	Total	Fe	0	0
			1	1		
6	M	1	Total	Fe	0	0
			1	1		

- Molecule 7 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: C₅₅H₇₆N₄O₆).



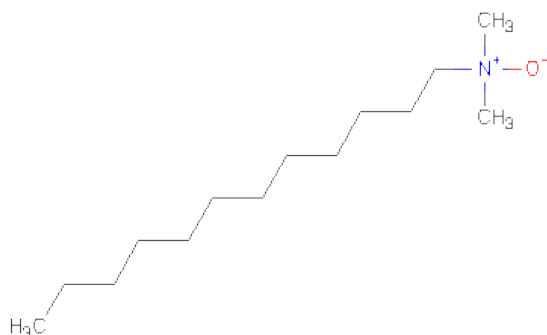
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	M	1	Total	C	N	O	0	0
			55	45	4	6		
7	M	1	Total	C	N	O	0	0
			65	55	4	6		
7	R	1	Total	C	N	O	0	0
			65	55	4	6		
7	S	1	Total	C	N	O	0	0
			55	45	4	6		

- Molecule 8 is SPHEROIDENE (three-letter code: SPO) (formula: C₄₁H₆₀O).



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

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

- Molecule 10 is water.

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

Continued on next page...

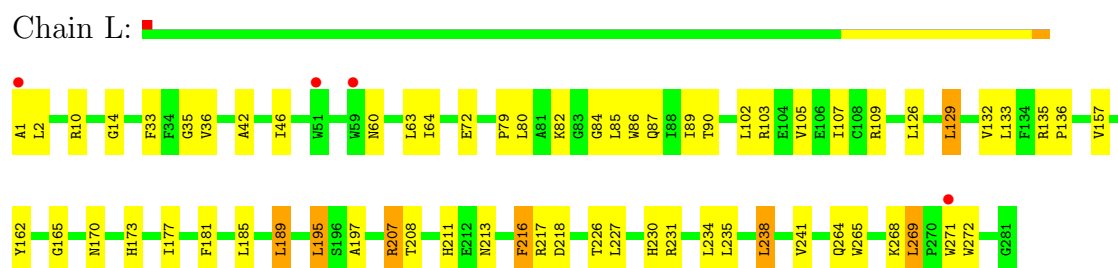
Continued from previous page...

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

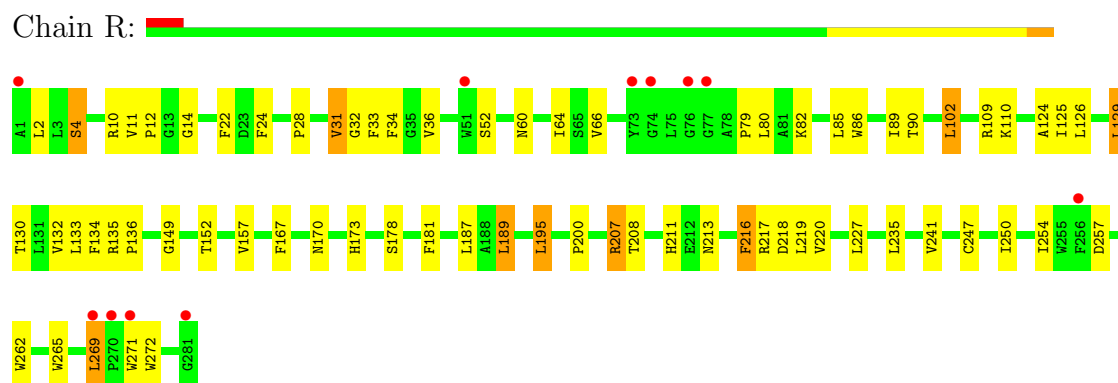
3 Residue-property plots

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.

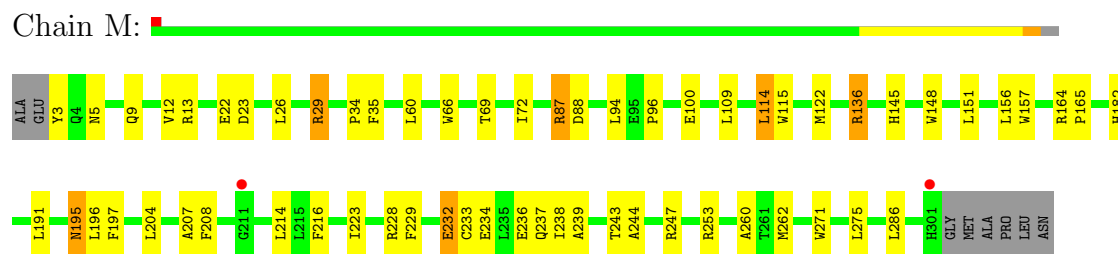
- Molecule 1: Reaction center protein L chain



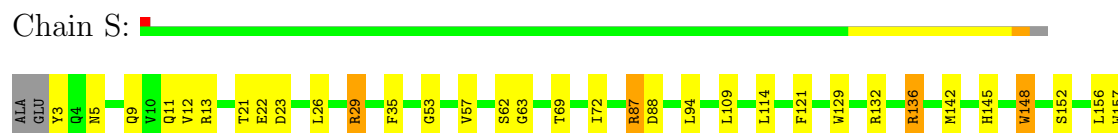
- Molecule 1: Reaction center protein L chain



- Molecule 2: Reaction center protein M chain



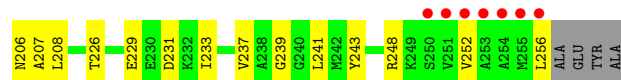
- Molecule 2: Reaction center protein M chain





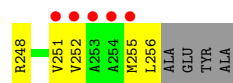
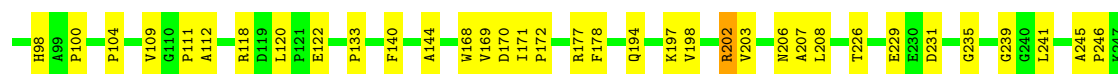
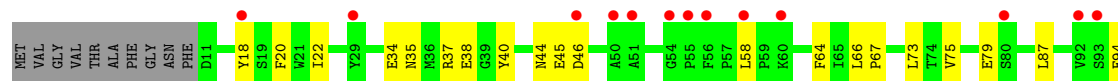
• Molecule 3: Reaction center protein H chain

Chain H:



• Molecule 3: Reaction center protein H chain

Chain T:



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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 , 38.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	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.*

¹Intensities estimated from amplitudes.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	183	0	189	22	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (317) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
1:R:208:THR:H	1:R:211:HIS:CD2	2.01	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:CB D	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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

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%)	269 (96%)	10 (4%)	0	100	100
1	R	279/281 (99%)	263 (94%)	14 (5%)	2 (1%)	30	43
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
3	T	244/260 (94%)	235 (96%)	9 (4%)	0	100	100
All	All	1640/1696 (97%)	1575 (96%)	63 (4%)	2 (0%)	59	78

All (2) Ramachandran outliers are listed below:

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

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%)	207 (94%)	13 (6%)	28	42
1	R	220/220 (100%)	208 (94%)	12 (6%)	30	46
2	M	235/240 (98%)	220 (94%)	15 (6%)	25	37
2	S	235/240 (98%)	225 (96%)	10 (4%)	40	59
3	H	199/208 (96%)	194 (98%)	5 (2%)	60	80
3	T	199/208 (96%)	196 (98%)	3 (2%)	76	90
All	All	1308/1336 (98%)	1250 (96%)	58 (4%)	39	58

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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 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	-	59,59,74	2.42	15 (25%)	77,97,115	2.05	21 (27%)
4	BCL	L	1002	-	74,74,74	2.01	13 (17%)	97,115,115	1.94	27 (27%)
4	BCL	L	1004	-	74,74,74	2.12	13 (17%)	97,115,115	2.00	27 (27%)
5	U10	L	1009	-	44,44,63	2.38	20 (45%)	55,56,79	3.15	16 (29%)
4	BCL	M	1003	-	74,74,74	2.01	12 (16%)	97,115,115	1.97	30 (30%)
7	BPH	M	1005	-	59,60,70	1.71	12 (20%)	80,89,101	2.09	26 (32%)
7	BPH	M	1006	-	70,70,70	1.71	13 (18%)	94,101,101	2.03	30 (31%)
5	U10	M	1008	-	38,38,63	2.04	13 (34%)	47,49,79	2.00	9 (19%)
8	SPO	M	1010	-	41,41,41	3.42	23 (56%)	50,50,50	3.94	17 (34%)
9	LDA	M	1011	-	15,15,15	3.64	2 (13%)	17,17,17	2.50	5 (29%)
9	LDA	M	1012	-	15,15,15	3.93	2 (13%)	17,17,17	2.45	5 (29%)
9	LDA	M	1013	-	15,15,15	3.86	2 (13%)	17,17,17	2.42	5 (29%)
9	LDA	M	1014	-	15,15,15	3.92	2 (13%)	17,17,17	2.49	5 (29%)
4	BCL	R	2002	-	74,74,74	2.10	13 (17%)	97,115,115	1.94	29 (29%)
7	BPH	R	2006	-	70,70,70	1.72	13 (18%)	94,101,101	2.04	27 (28%)
5	U10	R	2009	-	18,18,63	2.20	8 (44%)	23,25,79	2.25	6 (26%)
4	BCL	S	2001	-	59,59,74	2.33	15 (25%)	77,97,115	2.00	21 (27%)
4	BCL	S	2003	-	74,74,74	2.06	12 (16%)	97,115,115	2.04	34 (35%)
4	BCL	S	2004	-	74,74,74	2.15	15 (20%)	97,115,115	1.92	26 (26%)
7	BPH	S	2005	-	59,60,70	1.70	11 (18%)	80,89,101	2.18	28 (35%)
5	U10	S	2008	-	31,32,63	2.13	10 (32%)	39,41,79	1.99	9 (23%)
8	SPO	S	2010	-	41,41,41	3.31	24 (58%)	50,50,50	4.05	17 (34%)
9	LDA	S	2011	-	15,15,15	3.82	2 (13%)	17,17,17	2.48	5 (29%)

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	-	-	0/23/119/137	0/0/9/9
4	BCL	L	1002	-	-	0/41/137/137	0/0/9/9
4	BCL	L	1004	-	-	0/41/137/137	0/0/9/9
5	U10	L	1009	-	-	1/41/65/87	0/1/1/1
4	BCL	M	1003	-	-	0/41/137/137	0/0/9/9
7	BPH	M	1005	-	-	0/37/93/105	0/0/6/6
7	BPH	M	1006	-	-	1/49/105/105	0/0/6/6

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	-	0/41/137/137	0/0/9/9
7	BPH	R	2006	-	-	0/49/105/105	0/0/6/6
5	U10	R	2009	-	-	0/9/33/87	0/1/1/1
4	BCL	S	2001	-	-	0/23/119/137	0/0/9/9
4	BCL	S	2003	-	-	0/41/137/137	0/0/9/9
4	BCL	S	2004	-	-	0/41/137/137	0/0/9/9
7	BPH	S	2005	-	-	0/37/93/105	0/0/6/6
5	U10	S	2008	-	-	0/25/50/87	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 (265) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	1012	LDA	O1-N1	-14.55	1.25	1.39
9	M	1014	LDA	O1-N1	-14.46	1.25	1.39
9	M	1013	LDA	O1-N1	-14.27	1.26	1.39
9	S	2011	LDA	O1-N1	-14.11	1.26	1.39
9	M	1011	LDA	O1-N1	-13.40	1.26	1.39
4	S	2003	BCL	C3B-C4B	9.38	1.54	1.40
4	L	1002	BCL	C3B-C4B	9.36	1.54	1.40
4	S	2004	BCL	C1B-C2B	9.33	1.51	1.40
4	R	2002	BCL	C3B-C4B	9.25	1.54	1.40
4	L	1004	BCL	C1B-C2B	9.19	1.51	1.40
4	S	2001	BCL	C3B-C4B	8.70	1.53	1.40
4	L	1004	BCL	C3B-C4B	8.63	1.53	1.40
4	L	1001	BCL	C3B-C4B	8.59	1.53	1.40
4	M	1003	BCL	C3B-C4B	8.54	1.53	1.40
4	S	2004	BCL	C3B-C4B	8.37	1.53	1.40
4	L	1001	BCL	C1B-C2B	8.34	1.50	1.40
8	M	1010	SPO	C15-C16	8.20	1.56	1.34
8	M	1010	SPO	C6-C5	8.20	1.55	1.31
4	S	2001	BCL	C1B-C2B	8.05	1.50	1.40
4	R	2002	BCL	C1B-C2B	7.97	1.50	1.40
8	S	2010	SPO	C6-C5	7.81	1.54	1.31
8	M	1010	SPO	C10-C11	7.50	1.54	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	S	2010	SPO	C10-C11	7.47	1.54	1.34
4	S	2003	BCL	C1B-C2B	7.46	1.49	1.40
8	S	2010	SPO	C15-C16	7.36	1.54	1.34
4	M	1003	BCL	C1B-C2B	7.28	1.49	1.40
4	L	1002	BCL	C1B-C2B	7.19	1.49	1.40
5	L	1009	U10	C37-C36	-6.12	1.52	1.55
7	M	1006	BPH	C1D-CHD	5.89	1.42	1.35
4	R	2002	BCL	MG-ND	5.75	2.17	2.05
7	R	2006	BPH	C1D-CHD	5.48	1.41	1.35
7	S	2005	BPH	C1D-CHD	5.45	1.41	1.35
4	L	1002	BCL	MG-ND	5.42	2.17	2.05
8	M	1010	SPO	C21-C20	5.39	1.50	1.35
8	M	1010	SPO	C14-C12	5.22	1.42	1.35
4	S	2001	BCL	MG-ND	5.20	2.16	2.05
8	S	2010	SPO	C21-C20	5.19	1.49	1.35
5	L	1009	U10	C13-C14	5.19	1.43	1.32
8	S	2010	SPO	C27-C28	5.18	1.39	1.34
8	S	2010	SPO	C14-C12	5.14	1.42	1.35
4	M	1003	BCL	MG-ND	5.13	2.16	2.05
4	L	1001	BCL	MG-ND	5.13	2.16	2.05
8	M	1010	SPO	C4-C1	5.12	1.60	1.54
4	S	2003	BCL	MG-ND	4.99	2.16	2.05
7	M	1005	BPH	C1D-CHD	4.95	1.40	1.35
4	M	1003	BCL	MG-NB	-4.94	1.94	2.05
4	L	1001	BCL	C3C-C4C	-4.92	1.45	1.51
4	S	2004	BCL	MG-ND	4.91	2.15	2.05
4	R	2002	BCL	C1A-NA	4.89	1.43	1.32
4	L	1004	BCL	MG-ND	4.89	2.15	2.05
5	R	2009	U10	O4-C4	4.76	1.48	1.36
5	S	2008	U10	O4-C4	4.75	1.48	1.36
7	R	2006	BPH	C3B-C4B	4.71	1.47	1.40
5	L	1009	U10	O4-C4	4.69	1.48	1.36
7	M	1006	BPH	C11-C10	-4.65	1.29	1.52
7	R	2006	BPH	C11-C10	-4.63	1.29	1.52
4	L	1001	BCL	MG-NB	-4.62	1.94	2.05
4	S	2004	BCL	MG-NB	-4.60	1.94	2.05
4	S	2004	BCL	C1A-NA	4.58	1.42	1.32
4	S	2003	BCL	MG-NB	-4.50	1.95	2.05
4	L	1004	BCL	C1A-NA	4.50	1.42	1.32
7	M	1006	BPH	C3B-C4B	4.50	1.47	1.40
4	S	2001	BCL	C1A-NA	4.48	1.42	1.32
8	M	1010	SPO	C27-C28	4.47	1.38	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	S	2010	SPO	C26-C25	4.44	1.46	1.34
5	M	1008	U10	O4-C4	4.42	1.48	1.36
4	L	1002	BCL	C1A-NA	4.40	1.41	1.32
4	L	1001	BCL	C1A-NA	4.37	1.41	1.32
4	R	2002	BCL	MG-NB	-4.36	1.95	2.05
5	M	1008	U10	C13-C14	4.36	1.41	1.32
7	M	1005	BPH	C3B-C4B	4.35	1.47	1.40
5	L	1009	U10	C8-C9	4.35	1.41	1.32
5	S	2008	U10	C13-C14	4.34	1.41	1.32
4	S	2001	BCL	MG-NB	-4.26	1.95	2.05
8	M	1010	SPO	C26-C25	4.24	1.46	1.34
7	S	2005	BPH	C3B-C4B	4.17	1.46	1.40
5	S	2008	U10	C25-C24	4.17	1.54	1.47
8	S	2010	SPO	O1-CM1	4.17	1.56	1.43
5	M	1008	U10	C7-C8	-4.16	1.44	1.50
8	M	1010	SPO	O1-CM1	4.14	1.56	1.43
7	M	1005	BPH	O2D-CGD	4.12	1.44	1.33
4	L	1002	BCL	MG-NB	-4.05	1.96	2.05
4	S	2003	BCL	C1A-NA	4.05	1.41	1.32
4	M	1003	BCL	C1A-NA	4.04	1.41	1.32
7	S	2005	BPH	O2A-CGA	4.03	1.45	1.33
7	M	1006	BPH	C4B-NB	4.00	1.40	1.36
4	S	2001	BCL	C3C-C4C	-3.99	1.46	1.51
4	L	1004	BCL	MG-NB	-3.99	1.96	2.05
7	R	2006	BPH	O2A-CGA	3.95	1.45	1.33
7	M	1006	BPH	O2D-CGD	3.88	1.43	1.33
7	R	2006	BPH	O2D-CGD	3.86	1.43	1.33
9	M	1014	LDA	CM2-N1	-3.83	1.43	1.49
8	M	1010	SPO	C19-C17	3.81	1.40	1.35
9	S	2011	LDA	CM2-N1	-3.79	1.43	1.49
4	S	2003	BCL	C4C-NC	3.78	1.40	1.32
5	M	1008	U10	C23-C24	3.78	1.40	1.32
9	M	1012	LDA	CM2-N1	-3.76	1.43	1.49
5	L	1009	U10	C23-C24	3.75	1.40	1.32
4	M	1003	BCL	C4C-NC	3.71	1.40	1.32
8	M	1010	SPO	C9-C7	3.68	1.40	1.35
9	M	1011	LDA	CM2-N1	-3.67	1.43	1.49
9	M	1013	LDA	CM2-N1	-3.67	1.43	1.49
7	M	1005	BPH	O2A-CGA	3.66	1.44	1.33
7	S	2005	BPH	O2D-CGD	3.64	1.42	1.33
4	R	2002	BCL	C4C-NC	3.62	1.40	1.32
8	S	2010	SPO	C19-C17	3.61	1.40	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	1006	BPH	O2A-CGA	3.58	1.44	1.33
8	S	2010	SPO	C9-C7	3.53	1.40	1.35
4	L	1002	BCL	C4C-NC	3.52	1.40	1.32
4	L	1001	BCL	C3D-CAD	-3.51	1.40	1.47
4	S	2004	BCL	C3D-CAD	-3.50	1.40	1.47
4	S	2003	BCL	C4D-C3D	-3.46	1.37	1.41
5	S	2008	U10	C18-C19	3.46	1.39	1.32
7	R	2006	BPH	C2-C3	3.46	1.39	1.32
5	M	1008	U10	C18-C19	3.46	1.39	1.32
4	M	1003	BCL	C3D-CAD	-3.46	1.40	1.47
4	L	1001	BCL	C4C-NC	3.45	1.39	1.32
5	S	2008	U10	C8-C9	3.40	1.39	1.32
4	S	2004	BCL	C4C-NC	3.39	1.39	1.32
8	M	1010	SPO	C10-C9	3.34	1.53	1.43
7	R	2006	BPH	C4B-NB	3.32	1.40	1.36
8	S	2010	SPO	C4-C1	3.29	1.58	1.54
5	L	1009	U10	O3-C3	3.29	1.45	1.36
7	M	1005	BPH	CAA-C2A	3.28	1.60	1.54
5	S	2008	U10	O3-C3	3.27	1.45	1.36
8	M	1010	SPO	C32-C33	3.26	1.39	1.32
7	M	1006	BPH	CAA-C2A	3.26	1.60	1.54
4	S	2001	BCL	C4C-NC	3.26	1.39	1.32
5	L	1009	U10	C18-C19	3.25	1.39	1.32
4	L	1001	BCL	MG-NC	-3.25	1.97	2.07
4	S	2001	BCL	C3D-CAD	-3.22	1.40	1.47
5	R	2009	U10	C8-C9	3.22	1.40	1.34
5	R	2009	U10	O3-C3	3.21	1.44	1.36
4	L	1004	BCL	C3D-CAD	-3.15	1.40	1.47
5	S	2008	U10	C7-C8	-3.15	1.45	1.50
8	S	2010	SPO	C8-C7	3.14	1.56	1.51
4	L	1004	BCL	MG-NC	-3.14	1.97	2.07
8	S	2010	SPO	C32-C33	3.13	1.39	1.32
8	S	2010	SPO	C10-C9	3.12	1.53	1.43
5	L	1009	U10	C36-C34	3.10	1.55	1.51
7	M	1005	BPH	C4B-NB	3.10	1.39	1.36
4	L	1001	BCL	C4D-C3D	-3.07	1.37	1.41
5	M	1008	U10	O3-C3M	-3.06	1.37	1.45
7	M	1005	BPH	C2-C3	3.05	1.39	1.32
4	S	2001	BCL	C4D-C3D	-3.01	1.37	1.41
4	L	1004	BCL	C3C-C4C	-2.99	1.47	1.51
7	S	2005	BPH	C2-C3	2.97	1.38	1.32
4	L	1004	BCL	C4C-NC	2.97	1.38	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	1006	BPH	C4D-ND	-2.94	1.34	1.38
5	L	1009	U10	C28-C29	2.93	1.38	1.32
8	M	1010	SPO	C15-C14	2.89	1.52	1.43
4	M	1003	BCL	C1B-NB	2.89	1.38	1.34
7	S	2005	BPH	C4D-ND	-2.89	1.34	1.38
7	S	2005	BPH	CAA-C2A	2.87	1.59	1.54
5	M	1008	U10	O3-C3	2.86	1.44	1.36
8	M	1010	SPO	C25-C23	-2.85	1.39	1.45
8	S	2010	SPO	C13-C12	2.85	1.55	1.51
7	R	2006	BPH	C4D-ND	-2.84	1.34	1.38
7	S	2005	BPH	C4B-NB	2.83	1.39	1.36
8	S	2010	SPO	C25-C23	-2.82	1.39	1.45
4	S	2004	BCL	C3C-C4C	-2.81	1.48	1.51
4	S	2004	BCL	CAA-C2A	2.80	1.59	1.54
5	R	2009	U10	O3-C3M	-2.78	1.38	1.45
7	M	1005	BPH	O2D-CED	-2.76	1.38	1.45
4	S	2003	BCL	C3D-CAD	-2.76	1.41	1.47
8	M	1010	SPO	C22-C23	2.76	1.39	1.35
8	S	2010	SPO	C24-C23	2.76	1.55	1.51
8	M	1010	SPO	C13-C12	2.75	1.55	1.51
5	S	2008	U10	O3-C3M	-2.74	1.38	1.45
4	M	1003	BCL	C4D-C3D	-2.73	1.38	1.41
8	M	1010	SPO	C37-C38	2.73	1.41	1.32
4	S	2003	BCL	MG-NA	2.73	2.15	2.07
5	R	2009	U10	C7-C8	-2.72	1.46	1.50
7	M	1006	BPH	O2D-CED	-2.72	1.38	1.45
5	M	1008	U10	C31-C29	2.69	1.55	1.40
5	L	1009	U10	C7-C8	-2.68	1.46	1.50
4	S	2003	BCL	C1B-NB	2.65	1.37	1.34
5	L	1009	U10	C32-C33	-2.65	1.42	1.50
8	M	1010	SPO	C11-C12	-2.64	1.40	1.45
8	M	1010	SPO	C8-C7	2.64	1.55	1.51
4	S	2001	BCL	MG-NC	-2.62	1.99	2.07
7	R	2006	BPH	C4C-NC	2.61	1.41	1.34
4	S	2003	BCL	C4-C3	2.61	1.57	1.50
4	R	2002	BCL	C3D-CAD	-2.61	1.42	1.47
5	L	1009	U10	O3-C3M	-2.60	1.38	1.45
7	R	2006	BPH	CAA-C2A	2.60	1.58	1.54
8	S	2010	SPO	C11-C12	-2.59	1.40	1.45
5	R	2009	U10	C6-C1	2.58	1.41	1.35
5	L	1009	U10	C6-C1	2.57	1.41	1.35
7	R	2006	BPH	C1B-NB	2.57	1.39	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	1001	BCL	C5-C3	2.56	1.54	1.40
7	M	1005	BPH	C4D-ND	-2.55	1.34	1.38
4	R	2002	BCL	C4D-C3D	-2.54	1.38	1.41
5	L	1009	U10	C7-C6	2.54	1.56	1.51
4	S	2004	BCL	MG-NC	-2.54	1.99	2.07
5	R	2009	U10	C11-C9	2.54	1.54	1.40
5	M	1008	U10	C27-C28	-2.53	1.43	1.50
8	S	2010	SPO	C37-C38	2.53	1.40	1.32
5	M	1008	U10	C6-C1	2.53	1.41	1.35
8	S	2010	SPO	C26-C27	2.53	1.51	1.43
4	L	1004	BCL	C4D-C3D	-2.52	1.38	1.41
4	S	2004	BCL	C4D-C3D	-2.50	1.38	1.41
4	S	2004	BCL	C1B-NB	2.50	1.37	1.34
5	M	1008	U10	C8-C9	2.48	1.37	1.32
5	R	2009	U10	C7-C6	2.46	1.56	1.51
4	S	2001	BCL	C5-C3	2.46	1.53	1.40
8	M	1010	SPO	O1-C1	2.46	1.57	1.41
4	R	2002	BCL	C1B-NB	2.45	1.37	1.34
7	M	1005	BPH	C1B-NB	2.45	1.39	1.36
7	M	1006	BPH	O1D-CGD	2.44	1.27	1.21
8	S	2010	SPO	O1-C1	2.43	1.57	1.41
7	R	2006	BPH	O2D-CED	-2.42	1.39	1.45
8	S	2010	SPO	C15-C14	2.41	1.50	1.43
4	L	1002	BCL	C4A-NA	-2.41	1.33	1.39
5	L	1009	U10	C31-C29	2.41	1.57	1.51
7	S	2005	BPH	C4C-NC	2.39	1.40	1.34
7	M	1005	BPH	O1D-CGD	2.39	1.27	1.21
4	L	1002	BCL	C4D-C3D	-2.37	1.38	1.41
5	L	1009	U10	C33-C34	2.37	1.37	1.32
7	M	1006	BPH	C4C-NC	2.35	1.40	1.34
7	M	1005	BPH	C4C-NC	2.35	1.40	1.34
8	S	2010	SPO	C6-C7	-2.35	1.40	1.45
7	M	1006	BPH	C2-C3	2.34	1.37	1.32
4	S	2004	BCL	C4-C3	2.33	1.56	1.50
8	M	1010	SPO	C24-C23	2.33	1.55	1.51
4	M	1003	BCL	C4-C3	2.32	1.56	1.50
5	M	1008	U10	C15-C14	2.31	1.56	1.50
5	S	2008	U10	C6-C1	2.31	1.40	1.35
4	R	2002	BCL	CBB-CAB	2.30	1.57	1.49
4	L	1001	BCL	CAA-C2A	2.29	1.58	1.54
4	S	2004	BCL	CAA-CBA	2.27	1.60	1.52
7	S	2005	BPH	O2D-CED	-2.25	1.39	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	R	2002	BCL	C4-C3	2.25	1.56	1.50
4	L	1004	BCL	C6-C5	2.24	1.60	1.52
4	L	1001	BCL	CAA-CBA	2.22	1.60	1.52
4	S	2003	BCL	MG-NC	-2.22	2.00	2.07
5	L	1009	U10	C20-C19	2.21	1.56	1.50
8	M	1010	SPO	C26-C27	2.22	1.50	1.43
7	S	2005	BPH	C2C-C3C	-2.21	1.48	1.54
5	L	1009	U10	C30-C29	2.21	1.56	1.50
4	M	1003	BCL	MG-NA	2.21	2.13	2.07
5	L	1009	U10	C15-C14	2.21	1.56	1.50
8	S	2010	SPO	C22-C23	2.19	1.38	1.35
4	L	1002	BCL	MG-NA	2.18	2.13	2.07
5	L	1009	U10	C27-C28	-2.18	1.44	1.50
4	L	1002	BCL	C3D-CAD	-2.18	1.42	1.47
7	R	2006	BPH	C2A-C1A	2.18	1.55	1.51
4	L	1001	BCL	C1B-NB	2.17	1.37	1.34
5	S	2008	U10	C15-C14	2.15	1.56	1.50
4	R	2002	BCL	MG-NA	2.14	2.13	2.07
4	L	1004	BCL	C4-C3	2.13	1.56	1.50
4	L	1004	BCL	CBB-CAB	2.13	1.56	1.49
5	M	1008	U10	C30-C29	2.12	1.55	1.48
4	S	2001	BCL	C4-C3	2.11	1.55	1.48
4	M	1003	BCL	C3C-C4C	-2.11	1.48	1.51
4	L	1002	BCL	C4-C3	2.09	1.56	1.50
4	S	2001	BCL	C4A-NA	-2.08	1.34	1.39
7	M	1006	BPH	C1B-NB	2.06	1.38	1.36
4	S	2001	BCL	C1B-NB	2.06	1.37	1.34
4	R	2002	BCL	C4A-NA	-2.06	1.34	1.39
4	S	2004	BCL	CBB-CAB	2.06	1.56	1.49
4	S	2001	BCL	CAA-CBA	2.05	1.59	1.52
4	L	1002	BCL	CHC-C1C	2.04	1.41	1.36
4	L	1002	BCL	CBB-CAB	2.03	1.56	1.49
4	L	1001	BCL	C4A-NA	-2.01	1.34	1.39

All (425) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	S	2010	SPO	C3-C1-C4	-16.32	84.02	110.97
5	L	1009	U10	C32-C33-C34	16.13	162.60	127.80
8	M	1010	SPO	C3-C1-C4	-16.00	84.55	110.97
8	S	2010	SPO	C2-C1-C4	-15.09	86.04	110.97
8	M	1010	SPO	C2-C1-C4	-14.59	86.88	110.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1009	U10	C27-C28-C29	8.47	146.07	127.80
9	M	1011	LDA	CM2-N1-CM1	-7.83	99.90	108.85
7	S	2005	BPH	O2D-CGD-CBD	7.78	127.18	111.33
8	S	2010	SPO	C26-C27-C28	-7.70	120.54	127.91
9	S	2011	LDA	CM2-N1-CM1	-7.65	100.11	108.85
9	M	1014	LDA	CM2-N1-CM1	-7.64	100.12	108.85
9	M	1012	LDA	CM2-N1-CM1	-7.42	100.37	108.85
8	M	1010	SPO	C26-C27-C28	-7.39	120.84	127.91
9	M	1013	LDA	CM2-N1-CM1	-7.37	100.42	108.85
7	R	2006	BPH	O2D-CGD-CBD	7.32	126.24	111.33
7	M	1005	BPH	O2D-CGD-CBD	7.12	125.83	111.33
7	M	1006	BPH	O2D-CGD-CBD	7.01	125.60	111.33
5	R	2009	U10	C3M-O3-C3	6.77	139.47	116.48
4	S	2003	BCL	C3A-C4A-NA	6.76	119.18	110.95
5	L	1009	U10	C3M-O3-C3	6.66	139.10	116.48
5	S	2008	U10	C3M-O3-C3	6.58	138.85	116.48
4	L	1002	BCL	C3A-C4A-NA	6.53	118.90	110.95
4	M	1003	BCL	C3A-C4A-NA	6.53	118.89	110.95
4	L	1004	BCL	O2A-C1-C2	-6.46	94.55	108.55
4	R	2002	BCL	C3A-C4A-NA	6.42	118.76	110.95
5	M	1008	U10	C3M-O3-C3	6.36	138.10	116.48
4	L	1001	BCL	C3A-C4A-NA	6.33	118.66	110.95
4	S	2001	BCL	C3A-C4A-NA	6.28	118.60	110.95
8	M	1010	SPO	O1-C1-C4	-6.26	86.08	107.08
4	S	2004	BCL	C3A-C4A-NA	6.05	118.31	110.95
8	S	2010	SPO	O1-C1-C4	-6.02	86.88	107.08
4	L	1004	BCL	C3A-C4A-NA	6.01	118.26	110.95
4	S	2001	BCL	CBC-CAC-C3C	-5.88	99.14	113.61
8	S	2010	SPO	C15-C14-C12	-5.76	118.99	127.29
7	S	2005	BPH	C1-C2-C3	5.62	136.19	126.19
7	R	2006	BPH	C1-C2-C3	5.61	136.16	126.19
7	M	1006	BPH	C1-C2-C3	5.54	136.03	126.19
8	M	1010	SPO	C20-C21-C22	-5.53	111.12	123.36
8	S	2010	SPO	C20-C21-C22	-5.44	111.31	123.36
5	M	1008	U10	C27-C28-C29	5.44	141.82	128.63
8	M	1010	SPO	C15-C14-C12	-5.31	119.64	127.29
4	L	1001	BCL	CBC-CAC-C3C	-5.23	100.75	113.61
7	M	1005	BPH	C1-C2-C3	5.21	135.44	126.19
8	S	2010	SPO	C25-C23-C22	-5.09	111.16	118.97
4	L	1001	BCL	CMD-C2D-C3D	4.97	132.80	124.97
7	M	1006	BPH	C11-C10-C8	4.95	129.39	115.14
7	R	2006	BPH	C6-C5-C3	4.86	124.33	112.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	R	2006	BPH	CBC-CAC-C3C	4.83	125.49	113.61
8	M	1010	SPO	C25-C23-C22	-4.75	111.67	118.97
7	S	2005	BPH	C6-C5-C3	4.73	124.02	112.78
4	S	2003	BCL	OBD-CAD-CBD	-4.72	118.81	125.94
7	R	2006	BPH	C11-C10-C8	4.72	128.72	115.14
7	M	1005	BPH	C6-C5-C3	4.71	123.98	112.78
4	R	2002	BCL	CMD-C2D-C3D	4.70	132.37	124.97
4	S	2003	BCL	C11-C12-C13	-4.64	101.77	115.14
4	S	2004	BCL	C2C-C1C-NC	4.63	116.58	110.95
4	L	1004	BCL	CMD-C2D-C3D	4.62	132.25	124.97
4	M	1003	BCL	CMD-C2D-C3D	4.62	132.25	124.97
4	M	1003	BCL	C1D-C2D-C3D	-4.51	103.09	106.78
4	L	1001	BCL	C1D-C2D-C3D	-4.49	103.11	106.78
4	S	2003	BCL	CMD-C2D-C3D	4.48	132.02	124.97
4	S	2003	BCL	C2C-C1C-NC	4.46	116.38	110.95
4	S	2004	BCL	CMD-C2D-C3D	4.45	131.97	124.97
4	S	2001	BCL	CMD-C2D-C3D	4.43	131.95	124.97
7	M	1006	BPH	C6-C5-C3	4.42	123.28	112.78
4	L	1001	BCL	C2C-C1C-NC	4.41	116.31	110.95
4	M	1003	BCL	C2C-C1C-NC	4.41	116.31	110.95
4	L	1002	BCL	CMD-C2D-C3D	4.39	131.88	124.97
4	L	1004	BCL	C1D-C2D-C3D	-4.39	103.19	106.78
4	M	1003	BCL	C11-C12-C13	-4.38	102.52	115.14
8	M	1010	SPO	C18-C17-C19	-4.32	116.78	122.92
4	S	2003	BCL	C1D-C2D-C3D	-4.32	103.25	106.78
5	M	1008	U10	C20-C19-C21	-4.32	108.82	115.39
4	L	1004	BCL	C2C-C1C-NC	4.31	116.19	110.95
9	M	1013	LDA	O1-N1-C1	4.25	116.12	110.19
9	M	1014	LDA	O1-N1-C1	4.24	116.10	110.19
4	S	2004	BCL	C11-C12-C13	-4.24	102.93	115.14
9	M	1012	LDA	O1-N1-C1	4.23	116.09	110.19
9	S	2011	LDA	O1-N1-C1	4.21	116.06	110.19
4	R	2002	BCL	C1D-C2D-C3D	-4.21	103.34	106.78
4	S	2001	BCL	C2C-C1C-NC	4.21	116.07	110.95
9	M	1011	LDA	O1-N1-C1	4.16	115.99	110.19
4	S	2001	BCL	C1D-C2D-C3D	-4.14	103.39	106.78
4	R	2002	BCL	C2C-C1C-NC	4.14	115.99	110.95
4	L	1002	BCL	C2C-C1C-NC	4.12	115.96	110.95
4	L	1002	BCL	C1D-C2D-C3D	-4.10	103.43	106.78
7	M	1006	BPH	CED-O2D-CGD	4.08	125.73	116.02
8	S	2010	SPO	C18-C17-C19	-4.07	117.14	122.92
4	M	1003	BCL	OBD-CAD-CBD	-4.05	119.82	125.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	S	2004	BCL	C1D-C2D-C3D	-4.03	103.49	106.78
4	L	1001	BCL	C2C-C3C-C4C	3.97	106.56	101.05
4	L	1004	BCL	C1-O2A-CGA	3.97	128.11	116.98
8	S	2010	SPO	C24-C23-C25	3.94	124.47	118.09
7	R	2006	BPH	CED-O2D-CGD	3.93	125.37	116.02
4	S	2001	BCL	CAA-C2A-C3A	-3.87	103.89	113.04
4	L	1001	BCL	CAA-C2A-C3A	-3.86	103.90	113.04
5	R	2009	U10	O5-C5-C6	-3.86	114.58	121.67
7	M	1005	BPH	CED-O2D-CGD	3.85	125.17	116.02
7	S	2005	BPH	CED-O2D-CGD	3.85	125.17	116.02
7	S	2005	BPH	O2D-CGD-O1D	-3.84	115.99	123.79
4	S	2003	BCL	C4-C3-C5	3.83	121.22	115.39
4	R	2002	BCL	OBD-CAD-CBD	-3.83	120.16	125.94
5	L	1009	U10	C20-C19-C21	-3.82	109.58	115.39
5	L	1009	U10	O5-C5-C6	-3.80	114.68	121.67
4	S	2001	BCL	C2C-C3C-C4C	3.77	106.28	101.05
4	L	1002	BCL	CMB-C2B-C3B	3.74	130.87	124.97
4	L	1002	BCL	C1-C2-C3	-3.74	119.54	126.19
4	L	1004	BCL	OBD-CAD-CBD	-3.74	120.30	125.94
7	S	2005	BPH	O1D-CGD-CBD	-3.71	116.81	124.42
4	R	2002	BCL	CMB-C2B-C3B	3.71	130.81	124.97
4	L	1002	BCL	OBD-CAD-CBD	-3.69	120.38	125.94
4	M	1003	BCL	C4-C3-C5	3.69	121.00	115.39
5	S	2008	U10	O5-C5-C6	-3.69	114.90	121.67
4	L	1004	BCL	C2C-C3C-C4C	3.67	106.13	101.05
5	M	1008	U10	O5-C5-C6	-3.66	114.94	121.67
4	L	1001	BCL	CAC-C3C-C4C	-3.65	104.49	112.58
7	R	2006	BPH	O2D-CGD-O1D	-3.64	116.40	123.79
4	L	1004	BCL	CAC-C3C-C4C	-3.63	104.52	112.58
8	M	1010	SPO	C24-C23-C25	3.62	123.95	118.09
4	S	2004	BCL	C2C-C3C-C4C	3.60	106.05	101.05
7	M	1005	BPH	O1D-CGD-CBD	-3.60	117.04	124.42
4	S	2004	BCL	CAA-C2A-C3A	-3.58	104.58	113.04
7	R	2006	BPH	CMB-C2B-C1B	-3.54	123.26	128.65
5	S	2008	U10	C20-C19-C21	-3.48	110.09	115.39
7	R	2006	BPH	C3C-C4C-CHD	3.47	129.03	121.83
4	L	1001	BCL	OBD-CAD-CBD	-3.46	120.71	125.94
7	S	2005	BPH	CBC-CAC-C3C	3.46	122.11	113.61
7	R	2006	BPH	O1D-CGD-CBD	-3.45	117.34	124.42
4	S	2001	BCL	OBD-CAD-CBD	-3.44	120.74	125.94
7	M	1005	BPH	C3C-C4C-CHD	3.44	128.97	121.83
7	M	1006	BPH	C2C-C1C-NC	-3.43	108.28	112.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	R	2006	BPH	C2C-C1C-NC	-3.43	108.28	112.90
7	M	1006	BPH	CMB-C2B-C1B	-3.42	123.44	128.65
8	S	2010	SPO	C15-C16-C17	-3.42	116.63	126.38
4	R	2002	BCL	C7-C6-C5	-3.40	102.98	113.01
7	S	2005	BPH	C3C-C4C-CHD	3.40	128.90	121.83
7	M	1006	BPH	O2D-CGD-O1D	-3.40	116.89	123.79
7	M	1006	BPH	O1D-CGD-CBD	-3.40	117.46	124.42
4	L	1004	BCL	CMB-C2B-C3B	3.39	130.31	124.97
8	S	2010	SPO	C6-C7-C9	-3.38	113.77	118.97
4	L	1004	BCL	OBB-CAB-CBB	-3.37	111.76	120.13
7	M	1005	BPH	CMB-C2B-C1B	-3.36	123.54	128.65
5	L	1009	U10	O2-C2-C3	-3.35	113.54	120.96
4	R	2002	BCL	C11-C12-C13	-3.34	105.53	115.14
7	R	2006	BPH	CMB-C2B-C3B	3.33	130.21	124.97
4	L	1002	BCL	C7-C6-C5	-3.32	103.22	113.01
4	L	1004	BCL	C11-C12-C13	-3.31	105.61	115.14
4	S	2004	BCL	OBD-CAD-CBD	-3.30	120.96	125.94
4	S	2003	BCL	OBB-CAB-CBB	-3.29	111.96	120.13
4	S	2004	BCL	OBB-CAB-CBB	-3.29	111.96	120.13
4	S	2004	BCL	CMB-C2B-C3B	3.28	130.14	124.97
7	M	1005	BPH	O2D-CGD-O1D	-3.28	117.13	123.79
4	S	2003	BCL	CMB-C2B-C3B	3.28	130.13	124.97
8	S	2010	SPO	C8-C7-C6	3.27	123.38	118.09
7	M	1006	BPH	CBC-CAC-C3C	3.26	121.62	113.61
8	S	2010	SPO	C3-C1-C2	3.26	117.04	110.24
7	S	2005	BPH	C2C-C1C-NC	-3.26	108.51	112.90
7	M	1005	BPH	CMB-C2B-C3B	3.25	130.09	124.97
8	M	1010	SPO	C15-C16-C17	-3.25	117.11	126.38
7	M	1006	BPH	C3C-C4C-CHD	3.22	128.52	121.83
4	M	1003	BCL	OBB-CAB-CBB	-3.22	112.13	120.13
5	R	2009	U10	O2-C2-C3	-3.21	113.83	120.96
7	M	1006	BPH	CMB-C2B-C3B	3.20	130.00	124.97
4	L	1001	BCL	OBB-CAB-CBB	-3.20	112.19	120.13
4	S	2001	BCL	OBB-CAB-CBB	-3.19	112.20	120.13
4	R	2002	BCL	CAA-C2A-C3A	-3.19	105.50	113.04
5	S	2008	U10	O2-C2-C3	-3.19	113.89	120.96
4	M	1003	BCL	CMB-C2B-C3B	3.18	129.99	124.97
4	R	2002	BCL	OBB-CAB-CBB	-3.17	112.25	120.13
4	L	1002	BCL	OBB-CAB-CBB	-3.17	112.25	120.13
4	S	2003	BCL	CHA-C1A-NA	-3.16	119.73	126.22
7	M	1005	BPH	C2C-C1C-NC	-3.16	108.65	112.90
8	M	1010	SPO	C8-C7-C6	3.15	123.19	118.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	1002	BCL	CAA-C2A-C3A	-3.15	105.59	113.04
4	L	1002	BCL	C11-C12-C13	-3.15	106.07	115.14
5	M	1008	U10	C21-C19-C18	3.15	127.14	121.08
5	L	1009	U10	C1-C6-C5	-3.14	116.31	120.26
4	S	2004	BCL	CHA-C1A-NA	-3.13	119.79	126.22
5	L	1009	U10	C16-C14-C13	3.13	127.11	121.08
7	S	2005	BPH	CMB-C2B-C1B	-3.13	123.89	128.65
4	S	2001	BCL	C1-C2-C3	-3.12	120.64	126.19
8	S	2010	SPO	C4-C5-C6	-3.12	119.80	124.95
7	M	1006	BPH	C5-C3-C2	-3.11	115.09	121.08
8	M	1010	SPO	C3-C1-C2	3.10	116.72	110.24
4	S	2004	BCL	CAC-C3C-C4C	-3.10	105.71	112.58
4	S	2004	BCL	CBC-CAC-C3C	-3.10	105.99	113.61
4	L	1001	BCL	CHA-C1A-NA	-3.09	119.88	126.22
4	R	2002	BCL	O1D-CGD-CBD	3.09	130.75	124.42
4	M	1003	BCL	CHA-C1A-NA	-3.08	119.89	126.22
5	L	1009	U10	C21-C19-C18	3.08	127.00	121.08
4	L	1002	BCL	CMB-C2B-C1B	-3.07	123.90	128.62
4	S	2001	BCL	CMB-C2B-C3B	3.07	129.81	124.97
4	S	2004	BCL	O2A-C1-C2	-3.05	101.95	108.55
4	S	2003	BCL	C3D-CAD-CBD	3.03	111.88	107.60
4	S	2001	BCL	CHA-C1A-NA	-3.03	120.01	126.22
5	R	2009	U10	C1-C6-C5	-3.01	116.47	120.26
7	S	2005	BPH	C4-C3-C5	3.00	119.95	115.39
7	M	1005	BPH	CBC-CAC-C3C	2.99	120.96	113.61
4	L	1004	BCL	CBC-CAC-C3C	-2.98	106.26	113.61
4	L	1004	BCL	C2A-C1A-NA	2.97	114.53	111.24
7	M	1006	BPH	C4-C3-C5	2.97	119.91	115.39
5	M	1008	U10	O2-C2-C3	-2.97	114.38	120.96
4	L	1001	BCL	CMB-C2B-C3B	2.96	129.63	124.97
7	S	2005	BPH	CMB-C2B-C3B	2.95	129.62	124.97
7	S	2005	BPH	CAA-C2A-C3A	-2.95	106.06	113.04
7	S	2005	BPH	C5-C3-C2	-2.93	115.44	121.08
4	L	1002	BCL	CHA-C1A-NA	-2.94	120.19	126.22
4	R	2002	BCL	CMB-C2B-C1B	-2.93	124.11	128.62
7	S	2005	BPH	CMD-C2D-C3D	2.92	129.57	124.97
4	R	2002	BCL	CHA-C1A-NA	-2.92	120.23	126.22
8	M	1010	SPO	C6-C7-C9	-2.88	114.55	118.97
4	S	2003	BCL	CAA-CBA-CGA	-2.86	104.04	113.27
5	L	1009	U10	C30-C29-C31	-2.85	111.05	115.39
7	R	2006	BPH	C2C-C3C-C4C	2.83	105.92	102.06
4	L	1002	BCL	CAC-C3C-C4C	-2.81	106.34	112.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	1001	BCL	C3A-C4A-CHB	-2.81	118.49	124.33
5	M	1008	U10	C16-C14-C13	2.81	126.49	121.08
4	L	1002	BCL	C3A-C4A-CHB	-2.80	118.50	124.33
5	S	2008	U10	C16-C14-C13	2.80	126.47	121.08
5	L	1009	U10	C31-C29-C28	2.80	126.47	121.08
4	L	1004	BCL	C16-C15-C13	-2.79	107.11	115.14
5	M	1008	U10	C7-C6-C5	-2.78	115.74	118.75
4	M	1003	BCL	CAA-CBA-CGA	-2.78	104.31	113.27
7	M	1006	BPH	CMD-C2D-C3D	2.77	129.34	124.97
4	S	2003	BCL	C2A-C1A-NA	2.77	114.31	111.24
4	L	1004	BCL	CHA-C1A-NA	-2.77	120.53	126.22
7	R	2006	BPH	C1D-C2D-C3D	-2.77	104.52	106.89
4	S	2004	BCL	CAC-C3C-C2C	-2.76	107.56	113.89
4	S	2004	BCL	CBB-CAB-C3B	2.76	128.35	120.30
4	L	1004	BCL	CMB-C2B-C1B	-2.75	124.39	128.62
4	S	2003	BCL	C4D-C3D-C2D	2.74	110.78	107.42
7	M	1005	BPH	CAA-C2A-C3A	-2.74	106.56	113.04
4	L	1002	BCL	C2C-C3C-C4C	2.74	104.85	101.05
7	S	2005	BPH	C1D-C2D-C3D	-2.74	104.54	106.89
4	S	2001	BCL	C3A-C4A-CHB	-2.74	118.64	124.33
7	R	2006	BPH	C3C-C4C-NC	-2.72	108.75	113.49
4	L	1004	BCL	CAC-C3C-C2C	-2.72	107.65	113.89
4	R	2002	BCL	CGD-CBD-CHA	2.71	120.18	110.96
4	S	2003	BCL	CAA-C2A-C3A	-2.69	106.67	113.04
5	R	2009	U10	C7-C6-C5	-2.69	115.83	118.75
4	L	1004	BCL	CBB-CAB-C3B	2.69	128.14	120.30
4	S	2004	BCL	C1-C2-C3	-2.69	121.41	126.19
7	M	1006	BPH	C2C-C3C-C4C	2.68	105.72	102.06
4	L	1002	BCL	C16-C15-C13	-2.68	107.43	115.14
4	R	2002	BCL	C3A-C4A-CHB	-2.67	118.77	124.33
4	S	2003	BCL	C2C-C3C-C4C	2.67	104.75	101.05
4	R	2002	BCL	O2D-CGD-CBD	-2.67	105.90	111.33
7	M	1006	BPH	C1D-C2D-C3D	-2.67	104.60	106.89
5	S	2008	U10	C7-C6-C5	-2.67	115.86	118.75
7	M	1005	BPH	C1D-C2D-C3D	-2.65	104.62	106.89
4	M	1003	BCL	C2A-C1A-NA	2.64	114.17	111.24
7	M	1005	BPH	C2C-C3C-C4C	2.64	105.67	102.06
4	L	1002	BCL	C2A-C1A-NA	2.64	114.16	111.24
7	S	2005	BPH	CBD-CHA-C1A	2.62	130.44	123.62
4	S	2003	BCL	C4D-ND-C1D	2.62	109.73	106.57
4	R	2002	BCL	C2C-C3C-C4C	2.62	104.68	101.05
4	S	2003	BCL	CMB-C2B-C1B	-2.62	124.60	128.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	S	2005	BPH	C2C-C3C-C4C	2.61	105.62	102.06
7	M	1005	BPH	C3B-C4B-NB	2.60	110.04	107.10
4	M	1003	BCL	CBA-CAA-C2A	2.60	121.73	114.01
4	S	2003	BCL	C3A-C4A-CHB	-2.60	118.93	124.33
4	M	1003	BCL	C4D-C3D-C2D	2.59	110.59	107.42
4	L	1002	BCL	CGD-CBD-CHA	2.59	119.75	110.96
5	L	1009	U10	C7-C6-C5	-2.58	115.96	118.75
7	R	2006	BPH	CAA-C2A-C3A	-2.58	106.95	113.04
4	L	1002	BCL	O1D-CGD-CBD	2.58	129.71	124.42
7	S	2005	BPH	C3C-C4C-NC	-2.57	109.01	113.49
4	R	2002	BCL	CAC-C3C-C4C	-2.56	106.89	112.58
4	R	2002	BCL	C16-C15-C13	-2.56	107.76	115.14
5	S	2008	U10	C1-C6-C5	-2.55	117.06	120.26
7	M	1005	BPH	O2A-C1-C2	-2.53	103.06	108.55
7	M	1005	BPH	C3C-C4C-NC	-2.53	109.08	113.49
7	S	2005	BPH	C3B-C4B-NB	2.53	109.96	107.10
4	M	1003	BCL	CBB-CAB-C3B	2.53	127.69	120.30
4	M	1003	BCL	C3D-CAD-CBD	2.53	111.17	107.60
4	R	2002	BCL	C2A-C1A-NA	2.53	114.04	111.24
7	M	1005	BPH	CBD-CHA-C1A	2.52	130.18	123.62
4	S	2003	BCL	CBB-CAB-C3B	2.52	127.66	120.30
4	S	2003	BCL	CGD-CBD-CAD	-2.51	102.42	110.96
4	L	1002	BCL	C2B-C1B-NB	2.49	111.29	109.41
5	L	1009	U10	C22-C21-C19	2.50	121.00	112.74
5	S	2008	U10	C21-C19-C18	2.49	125.88	121.08
4	L	1004	BCL	CBA-CAA-C2A	2.49	121.41	114.01
7	M	1006	BPH	C3C-C4C-NC	-2.49	109.15	113.49
4	S	2004	BCL	CMB-C2B-C1B	-2.48	124.80	128.62
7	M	1005	BPH	CMD-C2D-C3D	2.48	128.88	124.97
4	S	2003	BCL	C11-C10-C8	-2.48	108.01	115.14
4	S	2004	BCL	C3A-C4A-CHB	-2.47	119.20	124.33
7	R	2006	BPH	CMD-C2D-C3D	2.46	128.85	124.97
9	M	1014	LDA	C6-C5-C4	-2.45	101.34	114.61
4	R	2002	BCL	C1-C2-C3	-2.44	121.85	126.19
7	M	1006	BPH	C7-C6-C5	-2.43	105.84	113.01
4	L	1002	BCL	CBB-CAB-C3B	2.43	127.40	120.30
4	R	2002	BCL	CBB-CAB-C3B	2.43	127.39	120.30
4	S	2004	BCL	C4D-C3D-C2D	2.43	110.39	107.42
8	M	1010	SPO	C10-C9-C7	-2.43	123.80	127.29
4	S	2003	BCL	CBA-CAA-C2A	2.42	121.21	114.01
4	L	1002	BCL	O2D-CGD-CBD	-2.42	106.40	111.33
4	M	1003	BCL	CMB-C2B-C1B	-2.42	124.90	128.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	1001	BCL	C4D-C3D-C2D	2.42	110.38	107.42
4	M	1003	BCL	C2C-C3C-C4C	2.42	104.40	101.05
4	M	1003	BCL	C3A-C4A-CHB	-2.42	119.31	124.33
5	L	1009	U10	C10-C9-C11	-2.40	111.73	115.39
4	S	2003	BCL	C4D-C3D-CAD	-2.40	105.10	108.05
4	M	1003	BCL	C4D-ND-C1D	2.40	109.47	106.57
5	S	2008	U10	C17-C18-C19	2.40	132.97	127.80
7	M	1006	BPH	C3B-C4B-NB	2.39	109.80	107.10
9	M	1011	LDA	C2-C1-N1	2.39	117.92	113.80
9	M	1012	LDA	C2-C1-N1	2.39	117.92	113.80
4	M	1003	BCL	C1-C2-C3	-2.38	121.95	126.19
4	S	2001	BCL	C4D-C3D-C2D	2.38	110.33	107.42
4	L	1001	BCL	C4D-ND-C1D	2.38	109.44	106.57
4	M	1003	BCL	C11-C10-C8	-2.38	108.30	115.14
8	S	2010	SPO	C20-C19-C17	-2.37	123.88	127.29
7	R	2006	BPH	C4A-NA-C1A	2.36	112.28	107.76
4	L	1004	BCL	C3A-C4A-CHB	-2.36	119.41	124.33
7	M	1006	BPH	O2A-CGA-O1A	-2.36	116.99	123.43
9	S	2011	LDA	C2-C1-N1	2.36	117.86	113.80
4	L	1004	BCL	C2C-C1C-CHC	-2.34	119.46	124.33
4	M	1003	BCL	CHB-C4A-NA	-2.34	121.80	124.58
7	M	1006	BPH	C3A-C4A-NA	-2.34	109.75	112.90
4	L	1001	BCL	C4D-C3D-CAD	-2.34	105.18	108.05
7	R	2006	BPH	CAA-C2A-C1A	-2.33	106.59	112.72
4	S	2004	BCL	C16-C15-C13	-2.33	108.43	115.14
4	L	1002	BCL	C4D-ND-C1D	2.32	109.37	106.57
5	M	1008	U10	C1-C6-C5	-2.32	117.34	120.26
7	S	2005	BPH	C2A-C1A-NA	-2.32	109.16	112.61
7	R	2006	BPH	CBD-CHA-C1A	2.31	129.64	123.62
7	M	1005	BPH	C2A-C1A-NA	-2.31	109.17	112.61
4	S	2004	BCL	C2C-C1C-CHC	-2.31	119.54	124.33
7	M	1006	BPH	CBD-CHA-C1A	2.30	129.61	123.62
4	S	2001	BCL	C4D-ND-C1D	2.30	109.34	106.57
4	M	1003	BCL	C16-C15-C13	-2.30	108.53	115.14
7	M	1006	BPH	C4A-NA-C1A	2.29	112.15	107.76
4	S	2003	BCL	C16-C15-C13	-2.29	108.54	115.14
8	M	1010	SPO	C16-C17-C19	2.29	122.49	118.97
4	M	1003	BCL	CBC-CAC-C3C	-2.29	107.97	113.61
7	M	1005	BPH	C3A-C4A-NA	-2.29	109.82	112.90
4	S	2001	BCL	C3D-CAD-CBD	2.29	110.83	107.60
4	S	2004	BCL	C4D-ND-C1D	2.28	109.32	106.57
7	M	1006	BPH	CAA-C2A-C3A	-2.28	107.66	113.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	R	2006	BPH	O2A-CGA-O1A	-2.27	117.22	123.43
4	R	2002	BCL	C4-C3-C5	2.27	118.85	115.39
9	M	1014	LDA	C2-C1-N1	2.27	117.71	113.80
4	M	1003	BCL	C4D-C3D-CAD	-2.27	105.26	108.05
7	M	1006	BPH	CAA-C2A-C1A	-2.27	106.76	112.72
4	S	2003	BCL	CHB-C4A-NA	-2.27	121.89	124.58
4	S	2004	BCL	C3D-CAD-CBD	2.27	110.80	107.60
5	L	1009	U10	C31-C32-C33	2.26	118.07	111.62
4	L	1004	BCL	C4D-ND-C1D	2.25	109.29	106.57
4	S	2001	BCL	CMB-C2B-C1B	-2.25	125.16	128.62
4	L	1001	BCL	C3D-CAD-CBD	2.25	110.77	107.60
7	R	2006	BPH	C3C-C2C-C1C	2.24	106.16	101.11
4	S	2003	BCL	C1-C2-C3	-2.24	122.20	126.19
5	R	2009	U10	C8-C7-C6	2.24	118.75	111.61
4	M	1003	BCL	CAC-C3C-C4C	-2.24	107.61	112.58
9	M	1013	LDA	C9-C8-C7	-2.24	102.51	114.61
7	M	1005	BPH	C4A-NA-C1A	2.24	112.04	107.76
4	R	2002	BCL	C4D-ND-C1D	2.23	109.26	106.57
4	S	2003	BCL	O1D-CGD-CBD	2.22	128.98	124.42
7	S	2005	BPH	C3C-C2C-C1C	2.22	106.11	101.11
4	L	1001	BCL	C2C-C1C-CHC	-2.22	119.71	124.33
4	L	1001	BCL	CBB-CAB-C3B	2.21	126.75	120.30
7	S	2005	BPH	C3A-C4A-NA	-2.21	109.92	112.90
4	R	2002	BCL	CBC-CAC-C3C	-2.21	108.18	113.61
4	S	2003	BCL	C7-C6-C5	-2.20	106.53	113.01
4	S	2003	BCL	CAC-C3C-C2C	-2.19	108.85	113.89
9	M	1012	LDA	C9-C8-C7	-2.19	102.78	114.61
9	S	2011	LDA	C9-C8-C7	-2.19	102.78	114.61
9	M	1013	LDA	C2-C1-N1	2.18	117.55	113.80
4	S	2001	BCL	C2A-C1A-NA	2.17	113.65	111.24
7	M	1006	BPH	C3C-C2C-C1C	2.17	106.00	101.11
8	S	2010	SPO	C10-C9-C7	-2.17	124.17	127.29
5	L	1009	U10	C8-C7-C6	2.17	118.54	111.61
7	R	2006	BPH	C7-C6-C5	-2.16	106.63	113.01
4	S	2001	BCL	CBB-CAB-C3B	2.16	126.62	120.30
4	L	1004	BCL	C3D-CAD-CBD	2.16	110.66	107.60
4	R	2002	BCL	C4D-C3D-CAD	-2.16	105.40	108.05
7	S	2005	BPH	CAC-C3C-C2C	-2.15	108.94	113.89
7	S	2005	BPH	O2A-CGA-O1A	-2.15	117.56	123.43
9	S	2011	LDA	CM1-N1-C1	-2.14	102.84	109.86
4	R	2002	BCL	C4D-C3D-C2D	2.14	110.04	107.42
7	S	2005	BPH	C4A-NA-C1A	2.14	111.85	107.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	1002	BCL	C4D-C3D-CAD	-2.14	105.43	108.05
4	S	2003	BCL	CBC-CAC-C3C	-2.13	108.37	113.61
9	M	1012	LDA	CM1-N1-C1	-2.12	102.92	109.86
4	M	1003	BCL	CAA-C2A-C3A	-2.12	108.03	113.04
7	M	1005	BPH	OBB-CAB-C3B	2.12	123.25	120.07
4	S	2004	BCL	C11-C10-C8	-2.11	109.05	115.14
4	S	2004	BCL	C2A-C1A-NA	2.11	113.58	111.24
4	M	1003	BCL	O1D-CGD-CBD	2.11	128.74	124.42
7	R	2006	BPH	C3A-C4A-NA	-2.10	110.07	112.90
9	M	1013	LDA	CM1-N1-C1	-2.10	102.98	109.86
4	L	1001	BCL	CMB-C2B-C1B	-2.10	125.39	128.62
7	R	2006	BPH	CAC-C3C-C4C	2.10	118.47	112.68
4	S	2001	BCL	C2C-C1C-CHC	-2.10	119.96	124.33
9	M	1011	LDA	C9-C8-C7	-2.10	103.25	114.61
4	L	1002	BCL	C4D-C3D-C2D	2.10	109.99	107.42
8	M	1010	SPO	C4-C5-C6	-2.09	121.50	124.95
8	S	2010	SPO	C1-C4-C5	2.08	119.11	113.57
4	L	1001	BCL	C2A-C1A-NA	2.08	113.55	111.24
4	M	1003	BCL	C7-C6-C5	-2.08	106.88	113.01
9	M	1011	LDA	CM1-N1-C1	-2.08	103.06	109.86
4	S	2003	BCL	C2C-C1C-CHC	-2.08	120.01	124.33
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
9	M	1014	LDA	CM1-N1-C1	-2.07	103.08	109.86
4	S	2001	BCL	C4D-C3D-CAD	-2.06	105.51	108.05
4	R	2002	BCL	C2B-C1B-NB	2.06	110.97	109.41
7	M	1005	BPH	C3C-C2C-C1C	2.06	105.76	101.11
4	S	2003	BCL	O2A-CGA-CBA	2.06	118.43	111.94
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	M	1006	BPH	C2A-C1A-NA	-2.06	109.54	112.61
4	L	1004	BCL	C4D-C3D-C2D	2.06	109.94	107.42
4	L	1004	BCL	C12-C11-C10	-2.05	102.49	113.02
7	M	1005	BPH	O2A-CGA-O1A	-2.05	117.84	123.43
8	M	1010	SPO	C1-C4-C5	2.05	119.01	113.57
4	R	2002	BCL	C3D-CAD-CBD	2.04	110.49	107.60
7	R	2006	BPH	OBD-CAD-CBD	-2.03	122.88	125.94
7	R	2006	BPH	C3B-C4B-NB	2.02	109.38	107.10
7	S	2005	BPH	C6-C7-C8	-2.02	109.73	114.92
4	L	1002	BCL	C4A-NA-C1A	-2.02	103.74	106.52
7	M	1006	BPH	CAC-C3C-C2C	-2.01	109.27	113.89
4	L	1004	BCL	C4D-C3D-CAD	-2.01	105.58	108.05

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.12	4 (1%) 72 71	17, 32, 49, 58	0
1	R	281/281 (100%)	0.04	11 (3%) 37 35	23, 41, 58, 69	0
2	M	299/307 (97%)	-0.27	2 (0%) 84 84	17, 27, 41, 67	0
2	S	299/307 (97%)	-0.14	2 (0%) 84 84	24, 35, 48, 69	0
3	H	246/260 (94%)	-0.14	8 (3%) 44 42	22, 34, 54, 88	0
3	T	246/260 (94%)	0.16	18 (7%) 15 13	31, 45, 70, 80	0
All	All	1652/1696 (97%)	-0.08	45 (2%) 52 49	17, 36, 57, 88	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	252	VAL	5.4
3	H	255	MET	4.8
3	H	254	ALA	4.7
3	H	256	LEU	4.6
1	R	1	ALA	4.4
3	T	54	GLY	3.7
3	T	255	MET	3.7
3	T	254	ALA	3.6
3	T	92	VAL	3.6
3	H	251	VAL	3.4
3	T	252	VAL	3.3
3	T	55	PRO	3.2
3	H	253	ALA	3.2
3	T	51	ALA	3.2
1	R	73	TYR	3.2
2	S	301	HIS	3.1
3	T	251	VAL	3.0
1	R	269	LEU	2.9
1	R	271	TRP	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	T	93	SER	2.8
3	T	253	ALA	2.7
1	R	270	PRO	2.7
1	R	76	GLY	2.7
3	T	80	SER	2.6
1	L	271	TRP	2.6
3	H	250	SER	2.6
3	T	60	LYS	2.5
3	T	58	LEU	2.5
1	L	1	ALA	2.5
3	H	51	ALA	2.5
3	T	56	PHE	2.4
1	L	51	TRP	2.4
3	T	29	TYR	2.4
2	M	301	HIS	2.4
3	T	50	ALA	2.4
1	R	77	GLY	2.3
3	T	46	ASP	2.3
1	R	281	GLY	2.3
1	R	51	TRP	2.3
1	R	74	GLY	2.3
2	S	223	ILE	2.2
1	R	256	PHE	2.1
1	L	59	TRP	2.1
3	T	18	TYR	2.1
2	M	211	GLY	2.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	U10	R	2009	18/63	0.37	8.08	81,85,86,87	0
9	LDA	M	1011	16/16	0.25	5.08	49,57,74,74	0
5	U10	L	1009	44/63	0.32	4.31	66,72,79,79	0
9	LDA	M	1013	16/16	0.28	4.13	69,71,80,80	0
9	LDA	S	2011	16/16	0.34	3.82	74,79,85,85	0
8	SPO	M	1010	42/42	0.22	3.32	16,28,47,51	0
9	LDA	M	1014	16/16	0.31	3.29	50,55,59,60	0
8	SPO	S	2010	42/42	0.21	3.16	24,35,51,54	0
5	U10	S	2008	32/63	0.29	2.96	36,42,51,54	0
4	BCL	S	2001	51/66	0.18	2.91	28,31,41,43	0
4	BCL	S	2003	66/66	0.19	2.63	27,33,48,55	0
9	LDA	M	1012	16/16	0.26	2.42	60,62,65,65	0
4	BCL	R	2002	66/66	0.17	2.31	29,35,44,48	0
4	BCL	S	2004	66/66	0.20	2.09	26,34,58,60	0
7	BPH	S	2005	55/65	0.17	1.85	25,30,55,58	0
4	BCL	L	1001	51/66	0.21	1.83	17,24,51,55	0
7	BPH	M	1006	65/65	0.22	1.75	23,28,37,40	0
4	BCL	L	1002	66/66	0.18	1.65	20,26,29,33	0
5	U10	M	1008	38/63	0.25	1.60	23,30,53,53	0
4	BCL	L	1004	66/66	0.25	1.57	16,25,45,52	0
7	BPH	R	2006	65/65	0.17	1.48	31,38,45,46	0
4	BCL	M	1003	66/66	0.17	1.42	20,25,39,44	0
7	BPH	M	1005	55/65	0.16	0.78	17,23,43,46	0
6	FE2	S	2007	1/1	0.13	-1.29	30,30,30,30	0
6	FE2	M	1007	1/1	0.12	-2.95	20,20,20,20	0

6.5 Other polymers ⓘ

There are no such residues in this entry.