



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 05:00 PM GMT

PDB ID : 1DV6
Title : PHOTOSYNTHETIC REACTION CENTER FROM RHODOBACTER SPHAEROIDES IN THE CHARGE-NEUTRAL DQAQB STATE WITH THE PROTON TRANSFER INHIBITOR ZN2+
Authors : Axelrod, H.L.; Abresch, E.C.; Paddock, M.L.; Okamura, M.Y.; Feher, G.
Deposited on : 2000-01-19
Resolution : 2.50 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>

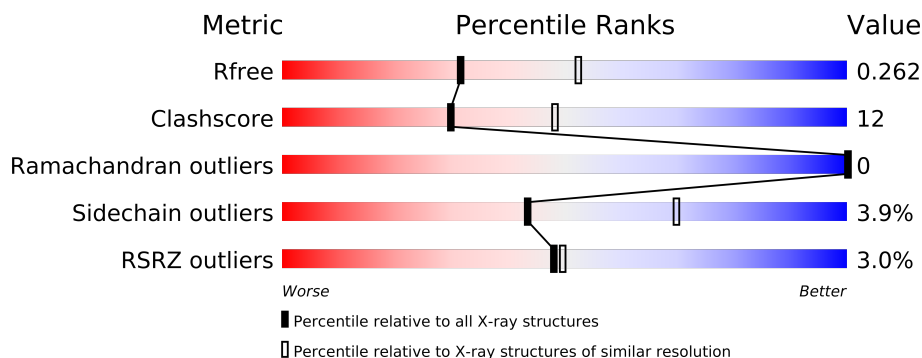
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.50 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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (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. 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
10	LDA	M	1012	-	X
10	LDA	M	1013	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Geometry	Electron density
10	LDA	M	1014	-	X
10	LDA	S	2012	-	X
9	U10	L	1009	-	X
9	U10	R	2009	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 14349 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 PHOTOSYNTHETIC REACTION CENTER.

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 PHOTOSYNTHETIC REACTION CENTER.

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 PHOTOSYNTHETIC REACTION CENTER.

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		

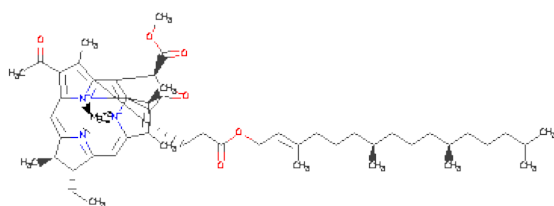
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

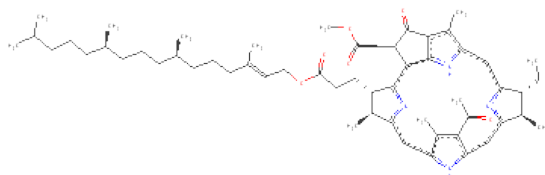
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	S	1	Total	Cl	0	0
			1	1		
6	M	1	Total	Cl	0	0
			1	1		

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



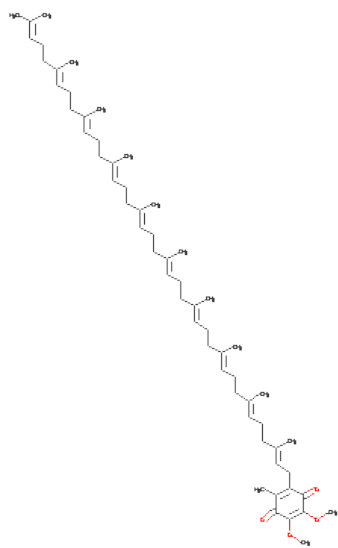
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	M	1	Total	C	Mg	N	O	
			51	40	1	4	6	
7	L	1	Total	C	Mg	N	O	
			66	55	1	4	6	
7	M	1	Total	C	Mg	N	O	
			66	55	1	4	6	
7	M	1	Total	C	Mg	N	O	
			66	55	1	4	6	
7	S	1	Total	C	Mg	N	O	
			51	40	1	4	6	
7	R	1	Total	C	Mg	N	O	
			66	55	1	4	6	
7	S	1	Total	C	Mg	N	O	
			66	55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

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



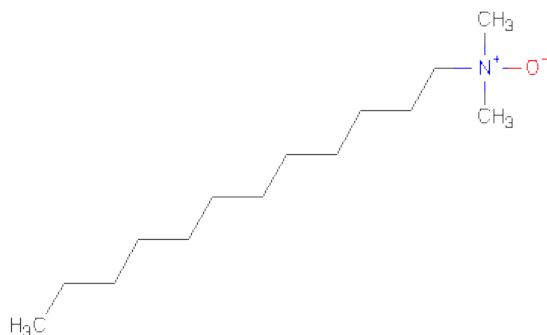
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	M	1	Total	C	N	O		
			51	41	4	6		
8	L	1	Total	C	N	O		
			65	55	4	6		
8	S	1	Total	C	N	O		
			52	42	4	6		
8	R	1	Total	C	N	O		
			65	55	4	6		

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



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

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	M	1	Total	C	N	O	0	0
			16	14	1	1		
10	M	1	Total	C	N	O	0	0
			16	14	1	1		
10	M	1	Total	C	N	O	0	0
			10	8	1	1		
10	S	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 11 is water.

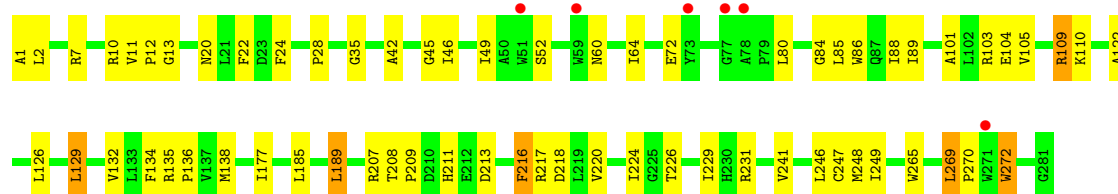
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	H	82	Total	O	0	0
			82	82		
11	L	75	Total	O	0	0
			75	75		
11	M	92	Total	O	0	0
			92	92		
11	R	55	Total	O	0	0
			55	55		
11	S	75	Total	O	0	0
			75	75		
11	T	61	Total	O	0	0
			61	61		

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.

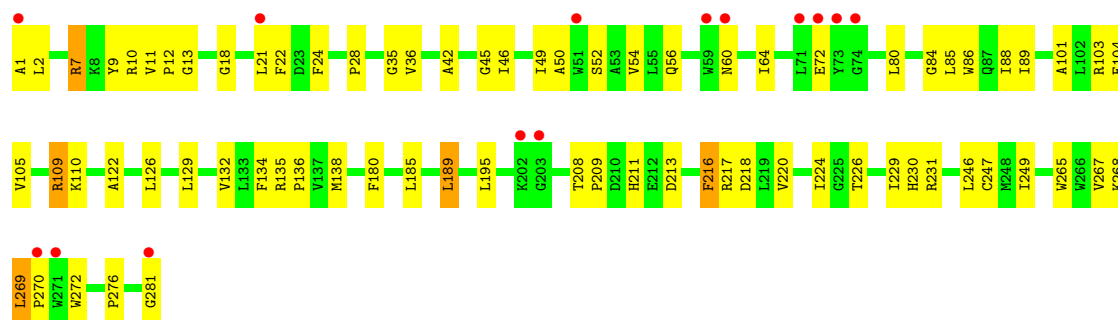
• Molecule 1: PHOTOSYNTHETIC REACTION CENTER

Chain L: 



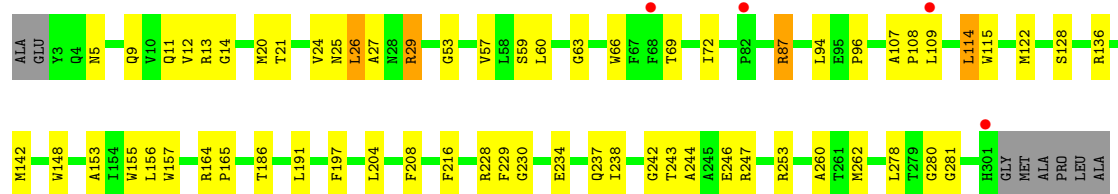
• Molecule 1: PHOTOSYNTHETIC REACTION CENTER

Chain R: 



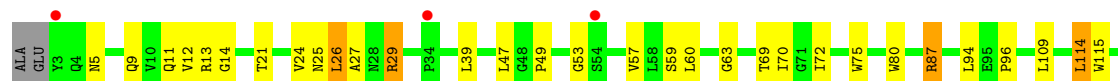
• Molecule 2: PHOTOSYNTHETIC REACTION CENTER

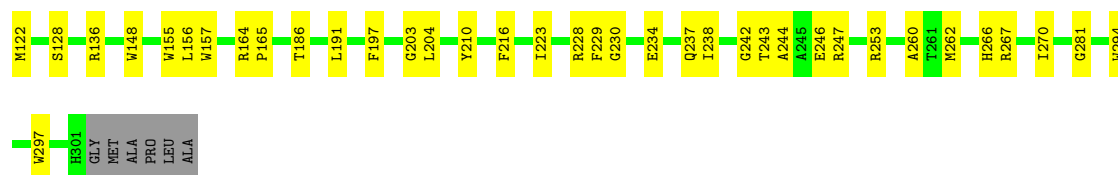
Chain M: 



• Molecule 2: PHOTOSYNTHETIC REACTION CENTER

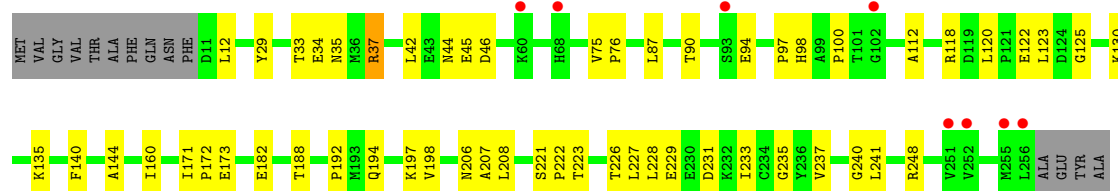
Chain S: 





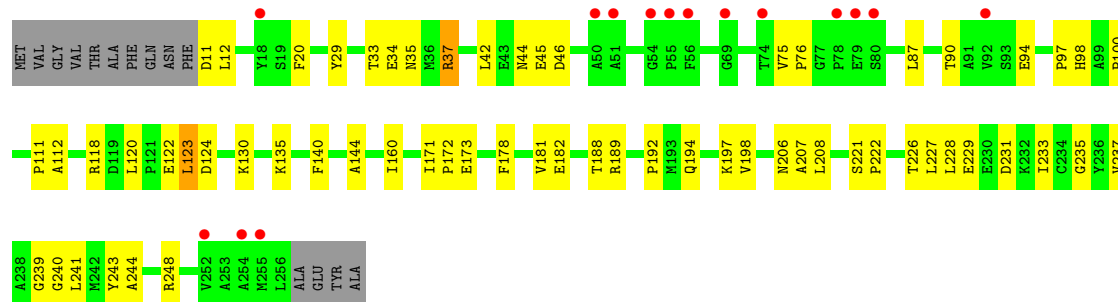
• Molecule 3: PHOTOSYNTHETIC REACTION CENTER

Chain H:



• Molecule 3: PHOTOSYNTHETIC REACTION CENTER

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	141.52Å 141.52Å 278.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.52 – 2.50 27.48 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.4 (27.52-2.50) 96.8 (27.48-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.09 (at 2.51Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.238 , 0.265 0.234 , 0.262	Depositor DCC
R_{free} test set	4424 reflections (4.90%)	DCC
Wilson B-factor (Å ²)	49.8	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 94671 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14349	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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, ZN, CL, BPH, LDA, 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	0.41	0/2320	0.56	0/3175
1	R	0.41	0/2320	0.56	0/3175
2	M	0.42	0/2482	0.53	0/3389
2	S	0.43	0/2482	0.54	0/3389
3	H	0.35	0/1917	0.59	0/2608
3	T	0.36	0/1917	0.59	0/2608
All	All	0.40	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 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	2187	55	0
1	R	2232	0	2187	61	0
2	M	2390	0	2304	54	0
2	S	2390	0	2304	60	0
3	H	1869	0	1884	38	0
3	T	1869	0	1884	57	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	M	1	0	0	0	0
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	1	0
6	S	1	0	0	0	0
7	L	66	0	74	9	0
7	M	183	0	188	21	0
7	R	132	0	148	12	0
7	S	117	0	115	12	0
8	L	65	0	76	6	0
8	M	51	0	45	2	0
8	R	65	0	76	7	0
8	S	52	0	47	4	0
9	L	44	0	57	3	0
9	M	38	0	47	0	0
9	R	18	0	15	2	0
9	S	32	0	39	2	0
10	M	42	0	78	8	0
10	S	16	0	31	1	0
11	H	82	0	0	2	0
11	L	75	0	0	5	0
11	M	92	0	0	3	0
11	R	55	0	0	7	0
11	S	75	0	0	14	0
11	T	61	0	0	17	0
All	All	14349	0	13786	335	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 12.

All (335) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:T:239:GLY:HA2	11:T:2042:HOH:O	1.54	1.05
2:S:267:ARG:HA	11:S:2068:HOH:O	1.66	0.94
1:R:195:LEU:HD11	11:S:2068:HOH:O	1.70	0.91
1:L:217:ARG:HD2	11:M:1077:HOH:O	1.77	0.83
3:T:178:PHE:HB3	11:T:2036:HOH:O	1.78	0.82
7:M:1001:BCL:HBB3	7:M:1003:BCL:H41	1.61	0.81
3:T:118:ARG:HD3	3:T:120:LEU:HD12	1.63	0.80
7:R:2004:BCL:HED2	2:S:203:GLY:HA3	1.64	0.80
3:H:118:ARG:HD3	3:H:120:LEU:HD12	1.64	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:S:11:GLN:HB2	3:T:144:ALA:HB3	1.67	0.76
8:L:1006:BPH:H102	7:M:1004:BCL:C19	2.15	0.76
2:S:228:ARG:HA	3:T:194:GLN:CG	2.16	0.74
2:M:122:MET:HE3	2:M:157:TRP:HE1	1.53	0.73
2:M:13:ARG:O	3:H:140:PHE:HA	1.90	0.72
2:S:21:THR:O	2:S:24:VAL:HG13	1.88	0.72
1:L:11:VAL:HG13	1:L:12:PRO:HD2	1.71	0.72
3:T:130:LYS:HB2	11:T:2044:HOH:O	1.88	0.72
2:S:53:GLY:O	2:S:57:VAL:HG23	1.89	0.72
2:S:63:GLY:HA3	8:S:2005:BPH:H5C1	1.71	0.71
1:R:11:VAL:HG13	1:R:12:PRO:HD2	1.72	0.71
2:M:21:THR:O	2:M:24:VAL:HG13	1.91	0.71
1:R:189:LEU:HG	1:R:216:PHE:HZ	1.56	0.71
7:R:2004:BCL:HED2	2:S:203:GLY:CA	2.21	0.70
2:M:53:GLY:O	2:M:57:VAL:HG23	1.92	0.70
2:M:197:PHE:HZ	7:M:1003:BCL:HBB2	1.57	0.69
2:S:294:TRP:N	11:S:2052:HOH:O	2.26	0.68
2:S:197:PHE:HZ	7:S:2003:BCL:HBB2	1.58	0.68
7:M:1001:BCL:HHC	7:M:1001:BCL:HBB2	1.76	0.68
9:S:2008:U10:H4M2	9:S:2008:U10:H3M3	1.76	0.68
7:M:1004:BCL:HMB1	7:M:1004:BCL:HBB2	1.74	0.67
1:R:7:ARG:HG3	11:R:2049:HOH:O	1.93	0.67
1:L:80:LEU:O	1:L:85:LEU:HB2	1.95	0.67
8:R:2006:BPH:HBB3	8:R:2006:BPH:HHC	1.75	0.67
1:L:52:SER:HB2	1:L:85:LEU:HD23	1.77	0.67
1:R:80:LEU:O	1:R:85:LEU:HB2	1.95	0.67
3:T:111:PRO:HG2	11:T:2042:HOH:O	1.95	0.66
2:M:9:GLN:NE2	3:H:198:VAL:H	1.93	0.66
1:L:189:LEU:HG	1:L:216:PHE:HZ	1.59	0.66
2:S:228:ARG:HA	3:T:194:GLN:HG3	1.78	0.65
1:R:276:PRO:HA	11:R:2046:HOH:O	1.97	0.65
1:R:9:TYR:HD1	11:T:2061:HOH:O	1.80	0.65
3:H:173:GLU:HG3	11:H:1081:HOH:O	1.96	0.65
3:T:173:GLU:HG3	11:T:2045:HOH:O	1.97	0.65
1:R:52:SER:HB2	1:R:85:LEU:HD23	1.79	0.64
7:L:1002:BCL:HBB3	7:L:1002:BCL:HMB1	1.79	0.64
2:M:122:MET:HE1	10:M:1014:LDA:HM22	1.80	0.64
7:R:2004:BCL:CED	2:S:203:GLY:HA3	2.28	0.63
1:R:1:ALA:HB1	3:T:42:LEU:HB3	1.80	0.63
7:R:2004:BCL:HBB2	7:R:2004:BCL:HMB1	1.79	0.63
7:S:2001:BCL:CBB	7:S:2001:BCL:HHC	2.29	0.62
1:L:208:THR:H	1:L:211:HIS:CD2	2.17	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:S:109:LEU:HD22	2:S:114:LEU:HD13	1.80	0.62
1:R:224:ILE:HG22	9:R:2009:U10:H3M3	1.81	0.62
2:M:109:LEU:HD22	2:M:114:LEU:HD13	1.81	0.62
11:L:1029:HOH:O	2:M:253:ARG:HD3	1.98	0.62
1:R:208:THR:H	1:R:211:HIS:CD2	2.16	0.61
3:T:112:ALA:N	11:T:2042:HOH:O	2.33	0.61
2:M:9:GLN:HE22	3:H:198:VAL:H	1.46	0.61
2:S:297:TRP:NE1	3:T:11:ASP:OD1	2.26	0.61
8:R:2006:BPH:HBB2	2:S:210:TYR:HB3	1.81	0.61
3:T:123:LEU:C	11:T:2044:HOH:O	2.39	0.60
1:L:49:ILE:HG12	1:L:89:ILE:HD13	1.83	0.60
3:T:37:ARG:HH11	3:T:76:PRO:HD3	1.66	0.60
2:S:197:PHE:CZ	7:S:2003:BCL:HBB2	2.37	0.60
7:M:1003:BCL:HBB2	7:M:1003:BCL:HHC	1.83	0.60
2:M:186:THR:HG23	7:M:1003:BCL:HMD2	1.83	0.60
2:M:197:PHE:CZ	7:M:1003:BCL:HBB2	2.35	0.60
11:S:2045:HOH:O	3:T:34:GLU:HG3	2.02	0.60
3:T:111:PRO:C	11:T:2042:HOH:O	2.39	0.60
1:L:1:ALA:HB1	3:H:42:LEU:HB3	1.83	0.60
3:T:189:ARG:HB2	11:T:2051:HOH:O	2.01	0.59
1:L:28:PRO:HB3	2:M:253:ARG:NH1	2.18	0.59
7:L:1002:BCL:HMB1	7:L:1002:BCL:CBB	2.32	0.59
3:T:181:VAL:HB	11:T:2051:HOH:O	2.01	0.58
1:L:60:ASN:O	1:L:64:ILE:HG13	2.04	0.58
2:S:122:MET:HE3	2:S:157:TRP:HE1	1.68	0.58
3:H:37:ARG:HH11	3:H:76:PRO:HD3	1.68	0.58
2:S:21:THR:HG23	2:S:26:LEU:HD11	1.85	0.58
3:T:87:LEU:HD23	3:T:100:PRO:HA	1.85	0.58
7:M:1001:BCL:HHC	7:M:1001:BCL:CBB	2.34	0.57
7:M:1003:BCL:CBB	7:M:1003:BCL:HHC	2.34	0.57
2:S:243:THR:O	2:S:247:ARG:HG3	2.04	0.57
1:R:60:ASN:O	1:R:64:ILE:HG13	2.03	0.57
1:R:218:ASP:OD1	2:S:29:ARG:HD2	2.04	0.57
1:L:52:SER:CB	1:L:85:LEU:HD23	2.34	0.57
3:H:87:LEU:HD23	3:H:100:PRO:HA	1.85	0.57
2:M:21:THR:HG23	2:M:26:LEU:HD11	1.86	0.57
3:T:37:ARG:NH1	3:T:76:PRO:HD3	2.20	0.57
2:S:253:ARG:HD3	11:S:2061:HOH:O	2.03	0.57
1:R:28:PRO:HB3	2:S:253:ARG:NH1	2.19	0.56
1:R:231:ARG:HD2	2:S:5:ASN:O	2.06	0.56
1:R:105:VAL:HG12	1:R:109:ARG:HD2	1.85	0.56
2:M:204:LEU:HG	10:M:1013:LDA:HM11	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:241:VAL:HG21	8:L:1006:BPH:HAC1	1.86	0.56
2:M:228:ARG:HA	3:H:194:GLN:CG	2.35	0.56
1:R:49:ILE:HG12	1:R:89:ILE:HD13	1.88	0.56
3:T:182:GLU:HA	3:T:188:THR:HG22	1.87	0.56
3:T:239:GLY:CA	11:T:2042:HOH:O	2.30	0.56
1:L:224:ILE:HG22	9:L:1009:U10:H3M3	1.87	0.56
3:H:37:ARG:NH1	3:H:76:PRO:HD3	2.21	0.55
3:T:226:THR:OG1	3:T:229:GLU:HG3	2.06	0.55
1:L:105:VAL:HG12	1:L:109:ARG:HD2	1.88	0.55
1:L:218:ASP:OD1	2:M:29:ARG:HD2	2.06	0.55
3:H:241:LEU:O	3:H:248:ARG:NH2	2.39	0.55
7:S:2001:BCL:HBB3	7:S:2003:BCL:H41	1.88	0.55
2:M:243:THR:O	2:M:247:ARG:HG3	2.07	0.55
2:S:9:GLN:HE22	3:T:198:VAL:H	1.54	0.55
2:S:228:ARG:HA	3:T:194:GLN:HG2	1.88	0.55
7:S:2003:BCL:CBB	7:S:2003:BCL:HHC	2.36	0.55
1:R:208:THR:H	1:R:211:HIS:HD2	1.53	0.55
7:R:2004:BCL:CBB	7:R:2004:BCL:HMB1	2.36	0.55
1:R:52:SER:CB	1:R:85:LEU:HD23	2.36	0.55
2:S:164:ARG:HB3	2:S:165:PRO:HD3	1.89	0.55
1:L:226:THR:HG23	11:L:1051:HOH:O	2.08	0.54
1:R:217:ARG:HD2	11:S:2017:HOH:O	2.08	0.54
7:M:1001:BCL:HBB2	10:M:1014:LDA:HM11	1.90	0.54
1:L:208:THR:H	1:L:211:HIS:HD2	1.54	0.54
3:T:90:THR:HB	3:T:97:PRO:O	2.07	0.54
7:M:1004:BCL:HMB1	7:M:1004:BCL:CBB	2.37	0.54
1:R:189:LEU:HD13	8:S:2005:BPH:HMD2	1.88	0.54
1:R:195:LEU:CD1	11:S:2068:HOH:O	2.43	0.54
3:H:226:THR:OG1	3:H:229:GLU:HG3	2.07	0.54
1:L:20:ASN:HB3	11:L:1072:HOH:O	2.06	0.54
7:R:2002:BCL:CBB	7:R:2002:BCL:HMB1	2.38	0.54
2:M:13:ARG:NH2	11:M:1100:HOH:O	2.38	0.54
2:S:13:ARG:HG2	2:S:14:GLY:N	2.23	0.53
3:T:34:GLU:O	3:T:37:ARG:HD3	2.09	0.53
1:L:2:LEU:HG	1:L:10:ARG:NH1	2.24	0.53
3:T:241:LEU:O	3:T:248:ARG:NH2	2.41	0.53
1:L:213:ASP:O	1:L:217:ARG:HB2	2.09	0.53
1:R:213:ASP:O	1:R:217:ARG:HB2	2.09	0.53
8:L:1006:BPH:H7C2	7:M:1004:BCL:H193	1.91	0.53
1:R:220:VAL:O	1:R:220:VAL:HG22	2.08	0.53
1:R:189:LEU:HG	1:R:216:PHE:CZ	2.41	0.53
1:R:2:LEU:HG	1:R:10:ARG:NH1	2.23	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:M:11:GLN:HB2	3:H:144:ALA:HB3	1.90	0.53
8:R:2006:BPH:CBB	8:R:2006:BPH:HHC	2.38	0.53
2:M:13:ARG:HG2	2:M:14:GLY:N	2.24	0.53
3:H:90:THR:HB	3:H:97:PRO:O	2.08	0.52
3:H:207:ALA:O	3:H:240:GLY:HA3	2.09	0.52
2:M:208:PHE:HE1	10:M:1013:LDA:H112	1.73	0.52
7:R:2004:BCL:H193	8:R:2006:BPH:C10	2.39	0.52
1:R:22:PHE:HA	1:R:24:PHE:HE1	1.74	0.52
3:T:207:ALA:O	3:T:240:GLY:HA3	2.10	0.52
3:H:233:ILE:O	3:H:237:VAL:HG23	2.09	0.52
3:H:34:GLU:O	3:H:37:ARG:HD3	2.10	0.52
3:H:182:GLU:HA	3:H:188:THR:HG22	1.91	0.52
1:L:189:LEU:HG	1:L:216:PHE:CZ	2.43	0.52
1:R:22:PHE:HA	1:R:24:PHE:CE1	2.45	0.52
2:M:164:ARG:HB3	2:M:165:PRO:HD3	1.90	0.52
1:L:22:PHE:HA	1:L:24:PHE:HE1	1.74	0.51
7:R:2004:BCL:H193	8:R:2006:BPH:H102	1.92	0.51
3:H:194:GLN:H	3:H:194:GLN:CD	2.14	0.51
1:L:22:PHE:HA	1:L:24:PHE:CE1	2.45	0.51
3:T:233:ILE:O	3:T:237:VAL:HG23	2.11	0.51
1:R:135:ARG:HB3	1:R:136:PRO:HD3	1.93	0.51
3:T:194:GLN:H	3:T:194:GLN:CD	2.13	0.51
1:L:265:TRP:O	1:L:269:LEU:HD13	2.11	0.51
1:R:230:HIS:CD2	2:S:223:ILE:HG13	2.47	0.50
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.94	0.50
2:M:9:GLN:HE22	3:H:197:LYS:HA	1.75	0.50
1:L:272:TRP:CD2	2:M:87:ARG:HB3	2.47	0.50
7:L:1002:BCL:HAA2	7:L:1002:BCL:HBD	1.93	0.50
2:M:230:GLY:HA2	11:M:1058:HOH:O	2.10	0.50
8:S:2005:BPH:HBB3	8:S:2005:BPH:CMB	2.42	0.49
1:L:28:PRO:HB3	2:M:253:ARG:HH11	1.76	0.49
1:R:56:GLN:HA	11:R:2059:HOH:O	2.12	0.49
11:S:2022:HOH:O	3:T:173:GLU:HG2	2.10	0.49
3:H:87:LEU:HD22	3:H:98:HIS:O	2.13	0.49
1:L:220:VAL:HG22	1:L:220:VAL:O	2.12	0.49
2:S:260:ALA:HB1	3:T:35:ASN:OD1	2.13	0.49
2:S:59:SER:HB2	2:S:128:SER:OG	2.13	0.49
2:M:59:SER:HB2	2:M:128:SER:OG	2.12	0.49
2:S:270:ILE:CG2	11:S:2068:HOH:O	2.61	0.48
7:S:2003:BCL:HBB2	7:S:2003:BCL:HHC	1.94	0.48
3:T:29:TYR:O	3:T:33:THR:HG23	2.13	0.48
7:R:2002:BCL:HBB3	7:R:2002:BCL:HMB1	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:S:2001:BCL:HMB1	7:S:2001:BCL:OBB	2.13	0.48
1:R:281:GLY:C	11:R:2046:HOH:O	2.50	0.48
2:S:49:PRO:HG2	11:S:2025:HOH:O	2.13	0.48
11:R:2017:HOH:O	3:T:130:LYS:HE2	2.14	0.48
1:L:185:LEU:HD12	1:L:189:LEU:HD22	1.96	0.48
1:R:267:VAL:HG13	2:S:87:ARG:HD2	1.95	0.48
2:M:260:ALA:HB1	3:H:35:ASN:OD1	2.13	0.48
2:S:21:THR:HG22	11:S:2049:HOH:O	2.13	0.48
9:S:2008:U10:C3M	9:S:2008:U10:H4M2	2.42	0.48
1:R:265:TRP:O	1:R:269:LEU:HD13	2.13	0.48
2:S:204:LEU:HD13	3:T:20:PHE:CE2	2.48	0.48
1:R:28:PRO:HB3	2:S:253:ARG:HH11	1.77	0.47
1:L:86:TRP:CH2	1:L:132:VAL:HG13	2.49	0.47
2:M:242:GLY:O	2:M:246:GLU:HG3	2.14	0.47
1:R:86:TRP:CH2	1:R:132:VAL:HG13	2.50	0.47
1:R:72:GLU:CD	1:R:72:GLU:H	2.17	0.47
1:L:72:GLU:H	1:L:72:GLU:CD	2.17	0.47
8:R:2006:BPH:H192	8:R:2006:BPH:H151	1.95	0.47
11:L:1018:HOH:O	3:H:130:LYS:HE2	2.13	0.47
3:T:87:LEU:HD22	3:T:98:HIS:O	2.14	0.47
1:L:231:ARG:HD2	2:M:5:ASN:O	2.14	0.47
2:S:242:GLY:O	2:S:246:GLU:HG3	2.14	0.47
8:S:2005:BPH:HMB3	8:S:2005:BPH:HBB3	1.96	0.47
6:M:1011:CL:CL	10:M:1012:LDA:CM2	3.00	0.47
1:L:11:VAL:CG1	11:L:1055:HOH:O	2.63	0.47
3:H:29:TYR:O	3:H:33:THR:HG23	2.15	0.47
2:M:155:TRP:NE1	2:M:281:GLY:HA3	2.29	0.47
3:T:130:LYS:CB	11:T:2044:HOH:O	2.54	0.47
2:S:9:GLN:NE2	3:T:198:VAL:H	2.12	0.47
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.96	0.47
1:L:208:THR:HB	1:L:209:PRO:HD2	1.97	0.47
3:T:45:GLU:HG3	3:T:94:GLU:OE1	2.15	0.47
2:M:114:LEU:HD12	2:M:114:LEU:HA	1.76	0.47
1:L:35:GLY:HA2	1:L:103:ARG:HD2	1.97	0.47
1:R:45:GLY:O	1:R:49:ILE:HG13	2.14	0.46
2:S:234:GLU:O	2:S:238:ILE:HG13	2.15	0.46
1:L:208:THR:HB	1:L:209:PRO:CD	2.46	0.46
3:H:75:VAL:HA	3:H:76:PRO:C	2.36	0.46
3:T:192:PRO:HB3	3:T:194:GLN:HE21	1.80	0.46
1:R:85:LEU:O	1:R:89:ILE:HG13	2.15	0.46
1:R:42:ALA:O	1:R:46:ILE:HG13	2.16	0.46
1:R:35:GLY:HA2	1:R:103:ARG:HD2	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:M:1001:BCL:OBB	10:M:1014:LDA:H12	2.16	0.46
2:S:155:TRP:NE1	2:S:281:GLY:HA3	2.31	0.46
1:R:189:LEU:HB3	9:R:2009:U10:H4M3	1.97	0.46
1:L:45:GLY:O	1:L:49:ILE:HG13	2.15	0.46
1:L:42:ALA:O	1:L:46:ILE:HG13	2.16	0.46
1:L:101:ALA:O	1:L:104:GLU:HB2	2.16	0.46
1:L:49:ILE:CG1	1:L:89:ILE:HD13	2.45	0.45
2:M:153:ALA:HB2	8:M:1005:BPH:HAC1	1.99	0.45
2:S:25:ASN:OD1	2:S:27:ALA:HB3	2.17	0.45
2:M:25:ASN:OD1	2:M:27:ALA:HB3	2.16	0.45
1:L:248:MET:CG	7:L:1002:BCL:HED2	2.47	0.45
2:M:148:TRP:HA	2:M:148:TRP:CE3	2.52	0.45
3:T:122:GLU:HB2	3:T:227:LEU:HD21	1.99	0.45
3:T:112:ALA:HB2	11:T:2042:HOH:O	2.15	0.45
7:R:2002:BCL:H192	8:R:2006:BPH:HMA1	1.98	0.45
2:S:229:PHE:HB2	2:S:244:ALA:HB2	1.97	0.45
3:T:75:VAL:HA	3:T:76:PRO:C	2.36	0.45
2:S:69:THR:O	2:S:72:ILE:HG22	2.16	0.45
1:R:185:LEU:HD12	1:R:189:LEU:HD22	1.98	0.45
7:S:2003:BCL:HBC2	7:S:2003:BCL:H2C	1.82	0.45
2:M:280:GLY:HA2	7:M:1003:BCL:HED2	1.97	0.45
3:H:192:PRO:HB3	3:H:194:GLN:HE21	1.82	0.45
1:L:84:GLY:O	1:L:88:ILE:HG12	2.17	0.45
2:S:148:TRP:CE3	2:S:148:TRP:HA	2.52	0.45
1:R:122:ALA:O	1:R:126:LEU:HD13	2.17	0.45
2:M:69:THR:O	2:M:72:ILE:HG22	2.17	0.45
2:S:148:TRP:HA	2:S:148:TRP:HE3	1.82	0.45
3:H:223:THR:HB	11:H:1067:HOH:O	2.16	0.44
1:R:208:THR:HB	1:R:209:PRO:CD	2.47	0.44
1:R:208:THR:HB	1:R:209:PRO:HD2	1.98	0.44
2:M:148:TRP:HA	2:M:148:TRP:HE3	1.82	0.44
3:H:44:ASN:HB2	3:H:46:ASP:OD1	2.17	0.44
1:L:220:VAL:HG21	9:L:1009:U10:C15	2.47	0.44
2:S:21:THR:HG23	2:S:26:LEU:CD1	2.48	0.44
3:T:124:ASP:N	11:T:2044:HOH:O	2.51	0.44
1:L:246:LEU:HA	1:L:249:ILE:HG22	2.00	0.44
7:M:1001:BCL:CBB	10:M:1014:LDA:HM11	2.47	0.44
7:L:1002:BCL:CGA	7:M:1004:BCL:HBC1	2.48	0.44
1:R:84:GLY:O	1:R:88:ILE:HG12	2.18	0.44
3:H:122:GLU:HB2	3:H:227:LEU:HD21	2.00	0.44
1:R:11:VAL:HG11	3:T:243:TYR:OH	2.17	0.44
3:H:45:GLU:HG3	3:H:94:GLU:OE1	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:S:2001:BCL:HHC	7:S:2001:BCL:HBB2	1.98	0.44
9:L:1009:U10:H1M1	9:L:1009:U10:C8	2.48	0.43
1:R:269:LEU:HA	1:R:270:PRO:HD3	1.88	0.43
3:T:44:ASN:HB2	3:T:46:ASP:OD1	2.18	0.43
1:L:122:ALA:O	1:L:126:LEU:HD13	2.18	0.43
1:L:134:PHE:O	1:L:138:MET:HG3	2.18	0.43
1:R:246:LEU:HA	1:R:249:ILE:HG22	1.99	0.43
3:T:112:ALA:HA	3:T:235:GLY:O	2.17	0.43
1:R:110:LYS:NZ	11:R:2051:HOH:O	2.52	0.43
1:L:177:ILE:HG12	7:L:1002:BCL:HMB3	1.99	0.43
1:L:85:LEU:O	1:L:89:ILE:HG13	2.18	0.43
2:M:228:ARG:HA	3:H:194:GLN:HG2	2.01	0.43
1:L:248:MET:HG3	7:L:1002:BCL:HED2	2.01	0.43
2:S:13:ARG:HG2	2:S:14:GLY:H	1.83	0.43
1:R:18:GLY:O	1:R:21:LEU:HG	2.18	0.43
2:S:186:THR:OG1	7:S:2001:BCL:H3C	2.18	0.43
1:L:207:ARG:HG2	2:M:142:MET:HG2	2.01	0.43
1:R:101:ALA:O	1:R:104:GLU:HB2	2.19	0.43
2:M:122:MET:CE	10:M:1014:LDA:HM22	2.47	0.42
1:R:49:ILE:CG1	1:R:89:ILE:HD13	2.49	0.42
3:T:240:GLY:O	3:T:244:ALA:HB3	2.19	0.42
2:S:26:LEU:HB2	11:S:2077:HOH:O	2.19	0.42
7:S:2003:BCL:OBB	7:S:2003:BCL:HMB1	2.19	0.42
2:S:70:ILE:HG21	10:S:2012:LDA:H22	2.01	0.42
3:H:221:SER:HA	3:H:222:PRO:HD3	1.80	0.42
2:M:66:TRP:CD1	2:M:122:MET:HB2	2.55	0.42
7:L:1002:BCL:CBA	7:M:1004:BCL:HBC1	2.49	0.42
2:M:63:GLY:HA3	8:M:1005:BPH:H5C2	2.00	0.42
2:M:237:GLN:HB2	2:M:262:MET:HG2	2.01	0.42
2:M:234:GLU:O	2:M:238:ILE:HG13	2.19	0.42
2:S:237:GLN:HB2	2:S:262:MET:HG2	2.02	0.42
1:L:13:GLY:O	1:L:110:LYS:HE2	2.20	0.42
7:R:2002:BCL:CGA	7:R:2004:BCL:HBC1	2.49	0.42
3:H:206:ASN:HD21	3:H:248:ARG:HD2	1.84	0.42
3:T:206:ASN:HD21	3:T:248:ARG:HD2	1.85	0.42
1:R:134:PHE:O	1:R:138:MET:HG3	2.20	0.42
3:T:171:ILE:HB	3:T:172:PRO:HD3	2.01	0.42
3:H:171:ILE:HB	3:H:172:PRO:HD3	2.02	0.42
7:M:1003:BCL:HMB1	7:M:1003:BCL:OBB	2.19	0.41
2:M:21:THR:HG23	2:M:26:LEU:CD1	2.49	0.41
2:S:230:GLY:HA2	11:S:2019:HOH:O	2.20	0.41
3:T:160:ILE:N	3:T:160:ILE:HD12	2.34	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:S:266:HIS:O	11:S:2068:HOH:O	2.21	0.41
1:L:226:THR:O	1:L:229:ILE:HG22	2.19	0.41
2:S:96:PRO:HB3	2:S:115:TRP:CE2	2.55	0.41
2:S:39:LEU:HD12	2:S:47:LEU:HD11	2.02	0.41
8:L:1006:BPH:H102	7:M:1004:BCL:H192	1.96	0.41
3:T:241:LEU:HB2	11:T:2035:HOH:O	2.19	0.41
3:T:197:LYS:NZ	11:T:2059:HOH:O	2.53	0.41
1:L:129:LEU:HD12	1:L:129:LEU:HA	1.90	0.41
3:H:112:ALA:HA	3:H:235:GLY:O	2.20	0.41
7:L:1002:BCL:H122	8:L:1006:BPH:H3A	2.03	0.41
2:M:136:ARG:NE	2:M:136:ARG:HA	2.35	0.41
1:R:50:ALA:O	1:R:54:VAL:HG23	2.21	0.41
3:T:221:SER:HA	3:T:222:PRO:HD3	1.80	0.41
2:S:13:ARG:O	3:T:140:PHE:HA	2.21	0.41
1:R:185:LEU:HD23	7:S:2001:BCL:H43	2.02	0.41
1:L:269:LEU:HA	1:L:270:PRO:HD3	1.89	0.41
2:S:136:ARG:NE	2:S:136:ARG:HA	2.35	0.41
2:M:278:LEU:HD12	2:M:278:LEU:HA	1.92	0.41
8:L:1006:BPH:H102	7:M:1004:BCL:H191	1.98	0.41
2:M:107:ALA:HA	2:M:108:PRO:HD3	1.94	0.41
3:H:160:ILE:HD12	3:H:160:ILE:N	2.36	0.41
2:M:228:ARG:HA	3:H:194:GLN:HG3	2.03	0.40
2:S:228:ARG:CA	3:T:194:GLN:HG3	2.50	0.40
2:M:96:PRO:HB3	2:M:115:TRP:CE2	2.56	0.40
1:R:268:LYS:HG3	11:R:2048:HOH:O	2.20	0.40
1:R:180:PHE:CE2	7:R:2002:BCL:HMA2	2.56	0.40
2:S:24:VAL:O	2:S:26:LEU:HD13	2.21	0.40
2:S:75:TRP:HB3	2:S:80:TRP:CZ3	2.56	0.40
2:M:20:MET:SD	3:H:125:GLY:HA3	2.62	0.40
1:R:226:THR:O	1:R:229:ILE:HG22	2.20	0.40
1:L:85:LEU:HD12	1:L:85:LEU:HA	1.88	0.40
1:R:13:GLY:O	1:R:110:LYS:HE2	2.21	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%)	262 (94%)	17 (6%)	0	100	100
1	R	279/281 (99%)	262 (94%)	17 (6%)	0	100	100
2	M	297/307 (97%)	288 (97%)	9 (3%)	0	100	100
2	S	297/307 (97%)	288 (97%)	9 (3%)	0	100	100
3	H	244/260 (94%)	234 (96%)	10 (4%)	0	100	100
3	T	244/260 (94%)	234 (96%)	10 (4%)	0	100	100
All	All	1640/1696 (97%)	1568 (96%)	72 (4%)	0	100	100

There are no Ramachandran outliers to report.

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%)	212 (96%)	8 (4%)	47	73
1	R	220/220 (100%)	211 (96%)	9 (4%)	41	67
2	M	235/239 (98%)	225 (96%)	10 (4%)	40	65
2	S	235/239 (98%)	225 (96%)	10 (4%)	40	65
3	H	199/209 (95%)	192 (96%)	7 (4%)	48	74
3	T	199/209 (95%)	192 (96%)	7 (4%)	48	74
All	All	1308/1336 (98%)	1257 (96%)	51 (4%)	43	70

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	7	ARG
1	L	109	ARG
1	L	129	LEU
1	L	189	LEU
1	L	216	PHE
1	L	247	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	269	LEU
1	L	272	TRP
2	M	12	VAL
2	M	26	LEU
2	M	29	ARG
2	M	60	LEU
2	M	87	ARG
2	M	94	LEU
2	M	114	LEU
2	M	156	LEU
2	M	191	LEU
2	M	216	PHE
3	H	12	LEU
3	H	37	ARG
3	H	123	LEU
3	H	135	LYS
3	H	208	LEU
3	H	228	LEU
3	H	231	ASP
1	R	7	ARG
1	R	36	VAL
1	R	109	ARG
1	R	129	LEU
1	R	189	LEU
1	R	216	PHE
1	R	247	CYS
1	R	269	LEU
1	R	272	TRP
2	S	12	VAL
2	S	26	LEU
2	S	29	ARG
2	S	60	LEU
2	S	87	ARG
2	S	94	LEU
2	S	114	LEU
2	S	156	LEU
2	S	191	LEU
2	S	216	PHE
3	T	12	LEU
3	T	37	ARG
3	T	123	LEU
3	T	135	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	87	GLN
1	L	211	HIS
1	L	274	ASN
2	M	4	GLN
2	M	9	GLN
2	M	300	ASN
3	H	194	GLN
3	H	199	GLN
3	H	206	ASN
1	R	87	GLN
1	R	211	HIS
1	R	274	ASN
2	S	4	GLN
2	S	9	GLN
2	S	300	ASN
3	T	194	GLN
3	T	199	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 26 ligands modelled in this entry, 6 are monoatomic - leaving 20 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	1002	1	74,74,74	1.26	7 (9%)	97,115,115	1.61	20 (20%)
8	BPH	L	1006	-	70,70,70	1.32	8 (11%)	94,101,101	1.60	19 (20%)
9	U10	L	1009	-	44,44,63	1.99	10 (22%)	55,56,79	1.38	4 (7%)
7	BCL	M	1001	2	59,59,74	1.34	10 (16%)	77,97,115	1.82	22 (28%)
7	BCL	M	1003	2	74,74,74	1.18	8 (10%)	97,115,115	1.59	20 (20%)
7	BCL	M	1004	1	74,74,74	1.19	6 (8%)	97,115,115	1.76	25 (25%)
8	BPH	M	1005	-	56,56,70	1.81	8 (14%)	76,84,101	2.03	23 (30%)
9	U10	M	1008	-	38,38,63	1.92	9 (23%)	47,49,79	1.18	5 (10%)
10	LDA	M	1012	-	15,15,15	4.39	3 (20%)	17,17,17	3.16	3 (17%)
10	LDA	M	1013	-	15,15,15	4.74	3 (20%)	17,17,17	2.77	3 (17%)
10	LDA	M	1014	-	9,9,15	6.20	3 (33%)	11,11,17	3.90	3 (27%)
7	BCL	R	2002	1	74,74,74	1.27	7 (9%)	97,115,115	1.69	22 (22%)
7	BCL	R	2004	1	74,74,74	1.13	7 (9%)	97,115,115	1.68	23 (23%)
8	BPH	R	2006	-	70,70,70	1.11	6 (8%)	94,101,101	1.60	21 (22%)
9	U10	R	2009	-	18,18,63	1.85	4 (22%)	23,25,79	1.34	2 (8%)
7	BCL	S	2001	2	59,59,74	1.29	10 (16%)	77,97,115	1.90	23 (29%)
7	BCL	S	2003	2	74,74,74	1.19	8 (10%)	97,115,115	1.68	22 (22%)
8	BPH	S	2005	-	57,57,70	1.52	7 (12%)	78,85,101	1.79	18 (23%)
9	U10	S	2008	-	31,32,63	1.77	6 (19%)	39,41,79	1.09	3 (7%)
10	LDA	S	2012	-	15,15,15	4.66	3 (20%)	17,17,17	3.02	2 (11%)

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	1002	1	-	0/41/137/137	0/0/9/9
8	BPH	L	1006	-	2/2/18/22	0/49/105/105	0/0/6/6
9	U10	L	1009	-	-	0/41/65/87	0/1/1/1
7	BCL	M	1001	2	-	0/23/119/137	0/0/9/9
7	BCL	M	1003	2	-	0/41/137/137	0/0/9/9
7	BCL	M	1004	1	-	0/41/137/137	0/0/9/9
8	BPH	M	1005	-	-	0/33/89/105	0/0/6/6
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	-	-	0/7/7/13	0/0/0/0
7	BCL	R	2002	1	-	0/41/137/137	0/0/9/9
7	BCL	R	2004	1	-	0/41/137/137	0/0/9/9
8	BPH	R	2006	-	2/2/18/22	0/49/105/105	0/0/6/6
9	U10	R	2009	-	-	0/9/33/87	0/1/1/1
7	BCL	S	2001	2	-	0/23/119/137	0/0/9/9
7	BCL	S	2003	2	-	0/41/137/137	0/0/9/9
8	BPH	S	2005	-	-	0/34/90/105	0/0/6/6
9	U10	S	2008	-	-	0/25/50/87	0/1/1/1
10	LDA	S	2012	-	-	0/13/13/13	0/0/0/0

All (133) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	1014	LDA	O1-N1	-18.20	1.22	1.39
10	M	1013	LDA	O1-N1	-17.93	1.22	1.39
10	S	2012	LDA	O1-N1	-17.55	1.22	1.39
10	M	1012	LDA	O1-N1	-16.34	1.24	1.39
8	M	1005	BPH	C1D-CHD	7.70	1.44	1.35
8	M	1005	BPH	C6-C5	-7.04	1.52	1.55
8	S	2005	BPH	C7-C6	-5.73	1.52	1.55
9	L	1009	U10	C37-C36	-5.62	1.52	1.55
8	L	1006	BPH	C1D-CHD	5.21	1.41	1.35
8	S	2005	BPH	C1D-CHD	4.97	1.40	1.35
9	M	1008	U10	C6-C1	4.94	1.47	1.35
7	R	2002	BCL	C2-C3	4.79	1.42	1.32
7	R	2002	BCL	C1A-NA	4.78	1.42	1.32
7	M	1004	BCL	C3D-CAD	-4.63	1.37	1.47
9	S	2008	U10	C6-C1	4.56	1.46	1.35
7	R	2004	BCL	C3D-CAD	-4.54	1.38	1.47
7	L	1002	BCL	C1A-NA	4.50	1.42	1.32
9	M	1008	U10	C8-C9	4.39	1.41	1.32
7	M	1003	BCL	C3D-CAD	-4.38	1.38	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	R	2009	U10	C6-C1	4.35	1.45	1.35
8	L	1006	BPH	C2-C3	4.29	1.41	1.32
7	L	1002	BCL	C4B-NB	4.28	1.39	1.34
9	L	1009	U10	C28-C29	4.19	1.41	1.32
8	R	2006	BPH	C1D-CHD	4.19	1.40	1.35
9	L	1009	U10	C6-C1	4.12	1.45	1.35
9	S	2008	U10	C13-C14	3.97	1.40	1.32
7	S	2001	BCL	C1A-NA	3.86	1.40	1.32
9	L	1009	U10	C7-C8	-3.81	1.44	1.50
7	M	1001	BCL	C3D-CAD	-3.77	1.39	1.47
7	M	1003	BCL	C1A-NA	3.75	1.40	1.32
9	S	2008	U10	C18-C19	3.74	1.40	1.32
7	L	1002	BCL	C4C-NC	3.74	1.40	1.32
9	M	1008	U10	C23-C24	3.72	1.40	1.32
7	M	1001	BCL	C1A-NA	3.67	1.40	1.32
9	M	1008	U10	C18-C19	3.66	1.40	1.32
7	L	1002	BCL	C2-C3	3.65	1.40	1.32
10	M	1012	LDA	CM2-N1	-3.63	1.43	1.49
9	L	1009	U10	C8-C9	3.60	1.40	1.32
7	S	2001	BCL	C3D-CAD	-3.46	1.40	1.47
7	M	1004	BCL	C1A-NA	3.44	1.39	1.32
7	R	2002	BCL	C4C-NC	3.41	1.39	1.32
7	S	2003	BCL	C1A-NA	3.39	1.39	1.32
7	S	2003	BCL	C2-C3	3.39	1.39	1.32
8	L	1006	BPH	C3D-CAD	-3.38	1.40	1.47
9	L	1009	U10	C18-C19	3.37	1.39	1.32
7	S	2003	BCL	C4B-NB	3.35	1.38	1.34
9	L	1009	U10	C33-C34	3.35	1.39	1.32
7	R	2004	BCL	C1A-NA	3.32	1.39	1.32
7	R	2004	BCL	C2-C3	3.31	1.39	1.32
9	M	1008	U10	C13-C14	3.29	1.39	1.32
7	R	2002	BCL	C3D-CAD	-3.27	1.40	1.47
8	S	2005	BPH	C3D-CAD	-3.27	1.40	1.47
9	R	2009	U10	C8-C9	3.26	1.41	1.34
7	S	2003	BCL	C3D-CAD	-3.26	1.40	1.47
9	S	2008	U10	C8-C9	3.25	1.39	1.32
8	R	2006	BPH	C3D-CAD	-3.24	1.40	1.47
8	M	1005	BPH	C2-C3	3.21	1.39	1.32
7	M	1004	BCL	C4B-NB	3.18	1.38	1.34
8	S	2005	BPH	C3B-CAB	-3.17	1.40	1.49
9	M	1008	U10	C28-C29	3.16	1.40	1.34
7	M	1001	BCL	C4B-NB	3.14	1.38	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	S	2001	BCL	C4C-NC	3.13	1.39	1.32
9	M	1008	U10	C7-C8	-3.12	1.45	1.50
8	M	1005	BPH	C3D-CAD	-3.09	1.41	1.47
9	L	1009	U10	C13-C14	3.07	1.39	1.32
7	S	2003	BCL	C4C-NC	3.07	1.39	1.32
7	M	1003	BCL	C4C-NC	3.02	1.38	1.32
9	L	1009	U10	C23-C24	2.97	1.38	1.32
7	M	1004	BCL	O2D-CGD	-2.96	1.25	1.33
7	R	2004	BCL	O2D-CGD	-2.95	1.25	1.33
7	S	2001	BCL	O2D-CGD	-2.94	1.25	1.33
9	S	2008	U10	C25-C24	2.94	1.52	1.47
7	M	1003	BCL	C4B-NB	2.93	1.38	1.34
7	M	1004	BCL	C2-C3	2.91	1.38	1.32
8	S	2005	BPH	O2D-CGD	-2.90	1.25	1.33
7	R	2002	BCL	O2D-CGD	-2.82	1.25	1.33
7	L	1002	BCL	O2D-CGD	-2.82	1.25	1.33
8	M	1005	BPH	O2D-CGD	-2.81	1.25	1.33
7	M	1003	BCL	C2-C3	2.81	1.38	1.32
7	M	1001	BCL	O2D-CGD	-2.81	1.25	1.33
7	M	1001	BCL	C4C-NC	2.78	1.38	1.32
10	M	1014	LDA	CM2-N1	-2.74	1.45	1.49
8	R	2006	BPH	C2-C3	2.73	1.38	1.32
8	R	2006	BPH	O2D-CGD	-2.73	1.25	1.33
8	S	2005	BPH	C2-C3	2.70	1.38	1.32
7	S	2003	BCL	O2D-CGD	-2.69	1.26	1.33
7	R	2002	BCL	C4B-NB	2.68	1.38	1.34
7	M	1001	BCL	C3B-CAB	-2.67	1.41	1.49
9	R	2009	U10	C7-C6	2.64	1.56	1.51
8	R	2006	BPH	O2A-CGA	-2.62	1.24	1.33
7	M	1003	BCL	O2D-CGD	-2.61	1.26	1.33
8	L	1006	BPH	O2A-CGA	-2.59	1.25	1.33
10	S	2012	LDA	CM1-N1	-2.57	1.45	1.49
7	S	2001	BCL	C3B-CAB	-2.56	1.42	1.49
8	L	1006	BPH	O2D-CGD	-2.55	1.26	1.33
7	R	2004	BCL	C4C-NC	2.54	1.37	1.32
10	M	1013	LDA	CM1-N1	-2.50	1.45	1.49
7	R	2004	BCL	C3B-CAB	-2.48	1.42	1.49
8	M	1005	BPH	O2A-CGA	-2.45	1.25	1.33
7	S	2001	BCL	C1B-NB	2.43	1.37	1.34
7	M	1003	BCL	O2A-CGA	-2.41	1.25	1.33
7	M	1003	BCL	C3B-CAB	-2.39	1.42	1.49
10	S	2012	LDA	CM2-N1	-2.39	1.45	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	1008	U10	C30-C29	2.38	1.56	1.48
8	R	2006	BPH	C3B-CAB	-2.36	1.42	1.49
7	M	1004	BCL	O2A-CGA	-2.35	1.25	1.33
9	M	1008	U10	C31-C29	2.34	1.53	1.40
8	S	2005	BPH	O2A-CGA	-2.34	1.25	1.33
7	M	1001	BCL	O2A-CGA	-2.34	1.25	1.33
7	S	2001	BCL	C2A-C1A	2.33	1.56	1.52
8	L	1006	BPH	C4C-NC	2.29	1.40	1.34
7	M	1001	BCL	C5-C3	2.27	1.52	1.40
7	S	2003	BCL	O2A-CGA	-2.25	1.26	1.33
9	R	2009	U10	C11-C9	2.21	1.52	1.40
7	L	1002	BCL	O2A-CGA	-2.21	1.26	1.33
7	R	2002	BCL	O2A-CGA	-2.20	1.26	1.33
7	S	2001	BCL	O2A-CGA	-2.20	1.26	1.33
10	M	1012	LDA	CM1-N1	-2.20	1.46	1.49
7	S	2001	BCL	C3C-C4C	2.17	1.54	1.51
7	R	2004	BCL	O2A-CGA	-2.17	1.26	1.33
7	M	1001	BCL	C2-C3	2.16	1.38	1.34
7	S	2001	BCL	C2-C3	2.15	1.38	1.34
10	M	1014	LDA	CM1-N1	-2.13	1.46	1.49
8	M	1005	BPH	C3B-CAB	-2.13	1.43	1.49
8	L	1006	BPH	C3B-CAB	-2.10	1.43	1.49
8	M	1005	BPH	CHA-C1A	-2.10	1.38	1.45
7	L	1002	BCL	C3D-CAD	-2.09	1.43	1.47
8	L	1006	BPH	C1B-CHB	-2.07	1.38	1.46
9	L	1009	U10	C4-C3	2.06	1.44	1.35
7	M	1001	BCL	OBD-CAD	2.06	1.25	1.22
10	M	1013	LDA	CM2-N1	-2.04	1.46	1.49
7	S	2003	BCL	OBD-CAD	2.03	1.25	1.22
9	S	2008	U10	C7-C6	2.01	1.55	1.51

All (283) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	M	1012	LDA	CM2-N1-CM1	-11.57	95.62	108.85
10	S	2012	LDA	CM2-N1-CM1	-11.25	96.00	108.85
10	M	1014	LDA	CM2-N1-CM1	-11.12	96.14	108.85
10	M	1013	LDA	CM2-N1-CM1	-10.01	97.40	108.85
7	S	2001	BCL	C4D-C3D-C2D	-6.95	98.93	107.42
7	S	2003	BCL	C4D-C3D-C2D	-6.74	99.18	107.42
7	L	1002	BCL	C4D-C3D-C2D	-6.18	99.87	107.42
7	M	1003	BCL	C4D-C3D-C2D	-5.89	100.22	107.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	S	2005	BPH	C4D-C3D-C2D	-5.88	100.26	107.37
7	M	1004	BCL	C4D-C3D-C2D	-5.74	100.41	107.42
7	R	2004	BCL	C4D-C3D-C2D	-5.70	100.45	107.42
7	M	1001	BCL	C4D-C3D-C2D	-5.62	100.55	107.42
8	M	1005	BPH	C1D-C2D-C3D	5.62	111.71	106.89
8	R	2006	BPH	C4D-C3D-C2D	-5.57	100.63	107.37
7	R	2002	BCL	C4D-C3D-C2D	-5.54	100.66	107.42
8	L	1006	BPH	C4D-C3D-C2D	-5.51	100.71	107.37
7	S	2001	BCL	C1D-C2D-C3D	5.29	111.11	106.78
10	M	1014	LDA	C6-C5-C4	-5.21	102.75	114.46
8	M	1005	BPH	C4D-C3D-C2D	-5.19	101.09	107.37
8	M	1005	BPH	O2A-C1-C2	-5.09	97.52	108.55
9	L	1009	U10	C25-C24-C26	4.84	122.75	115.39
7	M	1004	BCL	C3B-C4B-NB	4.70	113.21	108.64
8	S	2005	BPH	O2A-C1-C2	-4.58	98.64	108.55
10	M	1012	LDA	O1-N1-C1	4.47	116.42	110.19
7	R	2002	BCL	C2B-C1B-NB	4.29	112.65	109.41
7	R	2004	BCL	C2B-C1B-NB	4.28	112.64	109.41
8	S	2005	BPH	C3B-C4B-NB	4.27	111.92	107.10
7	M	1003	BCL	C2B-C1B-NB	4.22	112.60	109.41
8	R	2006	BPH	C3D-CAD-CBD	4.16	113.48	107.60
7	M	1004	BCL	C4-C3-C5	3.97	121.43	115.39
8	M	1005	BPH	C3D-CAD-CBD	3.95	113.18	107.60
8	R	2006	BPH	C7-C6-C5	-3.89	101.56	113.01
7	M	1001	BCL	C3D-CAD-CBD	3.87	113.07	107.60
7	S	2003	BCL	C1D-C2D-C3D	3.86	109.94	106.78
7	M	1004	BCL	C2B-C1B-NB	3.83	112.30	109.41
8	L	1006	BPH	C3D-CAD-CBD	3.80	112.97	107.60
8	L	1006	BPH	C1D-C2D-C3D	3.79	110.14	106.89
7	S	2003	BCL	C2B-C1B-NB	3.78	112.26	109.41
8	S	2005	BPH	C3D-CAD-CBD	3.76	112.91	107.60
7	R	2002	BCL	OBD-CAD-C3D	-3.75	120.92	127.91
7	S	2001	BCL	C3B-C4B-NB	3.73	112.27	108.64
7	M	1001	BCL	C2A-C3A-C4A	3.71	107.10	101.40
7	R	2004	BCL	CMB-C2B-C3B	3.71	130.81	124.97
7	R	2004	BCL	C3B-C4B-NB	3.69	112.23	108.64
8	L	1006	BPH	C3B-C2B-C1B	-3.67	104.82	107.01
7	L	1002	BCL	C3B-C4B-NB	3.65	112.19	108.64
7	R	2004	BCL	C1-C2-C3	-3.64	119.72	126.19
7	R	2002	BCL	CED-O2D-CGD	3.63	124.66	116.02
10	S	2012	LDA	O1-N1-C1	3.58	115.18	110.19
7	M	1001	BCL	C4D-C3D-CAD	-3.57	103.66	108.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	1005	BPH	C1-O2A-CGA	3.57	126.97	116.98
7	L	1002	BCL	C4-C3-C5	3.56	120.81	115.39
8	M	1005	BPH	CMD-C2D-C3D	-3.56	119.36	124.97
7	S	2003	BCL	C3A-C2A-C1A	3.55	106.09	101.08
8	M	1005	BPH	C3B-C4B-NB	3.53	111.09	107.10
8	R	2006	BPH	C3B-C4B-NB	3.53	111.08	107.10
8	M	1005	BPH	C3A-C4A-NA	-3.48	108.22	112.90
8	L	1006	BPH	O2D-CGD-CBD	3.44	118.33	111.33
7	M	1003	BCL	C1D-C2D-C3D	3.43	109.59	106.78
7	M	1001	BCL	C1D-C2D-C3D	3.41	109.58	106.78
7	M	1001	BCL	OBD-CAD-C3D	-3.42	121.55	127.91
7	R	2002	BCL	C1D-C2D-C3D	3.41	109.58	106.78
8	M	1005	BPH	O2D-CGD-CBD	3.36	118.18	111.33
7	S	2003	BCL	C4D-ND-C1D	-3.35	102.52	106.57
7	S	2001	BCL	C4D-C3D-CAD	-3.35	103.94	108.05
8	M	1005	BPH	OBD-CAD-C3D	-3.34	121.69	127.91
7	R	2004	BCL	C3D-CAD-CBD	3.34	112.32	107.60
10	M	1013	LDA	O1-N1-C1	3.32	114.81	110.19
7	M	1004	BCL	C2A-C3A-C4A	3.32	106.50	101.40
7	S	2001	BCL	C3D-CAD-CBD	3.31	112.28	107.60
7	R	2004	BCL	OBD-CAD-C3D	-3.30	121.76	127.91
7	L	1002	BCL	C2B-C1B-NB	3.29	111.89	109.41
7	M	1003	BCL	C3D-CAD-CBD	3.27	112.22	107.60
7	M	1004	BCL	C4D-ND-C1D	-3.25	102.64	106.57
7	R	2004	BCL	CMB-C2B-C1B	-3.24	123.64	128.62
7	M	1004	BCL	C1D-C2D-C3D	3.23	109.42	106.78
8	S	2005	BPH	O2D-CGD-CBD	3.23	117.90	111.33
7	R	2002	BCL	CMB-C2B-C3B	3.22	130.04	124.97
7	R	2002	BCL	CHA-C1A-NA	-3.20	119.64	126.22
7	R	2002	BCL	C2A-C3A-C4A	3.20	106.33	101.40
7	R	2004	BCL	C4D-C3D-CAD	-3.20	104.12	108.05
10	M	1014	LDA	O1-N1-C1	3.19	114.64	110.19
8	L	1006	BPH	CMB-C2B-C3B	3.18	129.98	124.97
7	S	2001	BCL	C2A-C3A-C4A	3.18	106.29	101.40
7	M	1003	BCL	C4D-C3D-CAD	-3.18	104.15	108.05
8	R	2006	BPH	CMB-C2B-C3B	3.14	129.92	124.97
8	S	2005	BPH	C1-O2A-CGA	3.14	125.79	116.98
7	S	2003	BCL	C4D-C3D-CAD	-3.10	104.25	108.05
7	R	2002	BCL	C4D-C3D-CAD	-3.08	104.27	108.05
8	M	1005	BPH	C4-C3-C5	3.05	121.73	114.77
7	M	1001	BCL	CMB-C2B-C1B	-3.05	123.94	128.62
8	S	2005	BPH	C4D-ND-C1D	-3.05	101.73	108.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	1005	BPH	CMB-C2B-C3B	3.04	129.76	124.97
8	L	1006	BPH	C3B-C4B-NB	3.00	110.48	107.10
7	S	2003	BCL	C3D-CAD-CBD	2.99	111.83	107.60
8	L	1006	BPH	C2B-C1B-NB	2.98	113.96	108.16
7	M	1004	BCL	C3D-CAD-CBD	2.97	111.79	107.60
9	S	2008	U10	C10-C9-C11	2.97	119.90	115.39
7	R	2002	BCL	C3D-CAD-CBD	2.96	111.79	107.60
8	S	2005	BPH	C1D-C2D-C3D	2.96	109.43	106.89
7	M	1003	BCL	C15-C13-C12	2.96	127.17	111.92
7	R	2004	BCL	C4D-ND-C1D	-2.95	103.00	106.57
7	M	1003	BCL	OBD-CAD-C3D	-2.92	122.48	127.91
7	L	1002	BCL	C1D-C2D-C3D	2.91	109.17	106.78
7	L	1002	BCL	C4D-ND-C1D	-2.91	103.06	106.57
7	M	1003	BCL	CMB-C2B-C3B	2.90	129.54	124.97
7	M	1004	BCL	CAC-C3C-C4C	-2.90	106.15	112.58
7	M	1001	BCL	C3B-C4B-NB	2.90	111.46	108.64
8	M	1005	BPH	C2A-C3A-C4A	2.89	107.61	101.11
7	M	1001	BCL	C1-O2A-CGA	2.87	125.03	116.98
8	S	2005	BPH	C3B-C2B-C1B	-2.85	105.31	107.01
7	M	1004	BCL	C4D-C3D-CAD	-2.84	104.56	108.05
7	R	2002	BCL	CMB-C2B-C1B	-2.84	124.26	128.62
8	R	2006	BPH	CMB-C2B-C1B	-2.83	124.33	128.65
8	S	2005	BPH	OBD-CAD-C3D	-2.83	122.63	127.91
8	R	2006	BPH	O2D-CGD-CBD	2.83	117.09	111.33
7	L	1002	BCL	C4D-C3D-CAD	-2.82	104.58	108.05
8	R	2006	BPH	C1D-C2D-C3D	2.82	109.31	106.89
8	R	2006	BPH	C1-O2A-CGA	2.81	124.86	116.98
8	R	2006	BPH	C4D-ND-C1D	-2.80	102.29	108.72
8	L	1006	BPH	OBD-CAD-C3D	-2.79	122.73	127.91
7	L	1002	BCL	C2A-C3A-C4A	2.78	105.68	101.40
7	S	2001	BCL	C2D-C3D-CAD	2.78	157.12	138.46
7	R	2004	BCL	C2A-C3A-C4A	2.77	105.66	101.40
8	M	1005	BPH	C3C-C4C-CHD	2.77	127.58	121.83
9	M	1008	U10	C4M-O4-C4	2.76	125.86	116.48
7	R	2002	BCL	C3B-C4B-NB	2.76	111.32	108.64
7	M	1004	BCL	C2C-C3C-C4C	2.75	104.87	101.05
7	M	1004	BCL	CHA-C1A-NA	-2.74	120.60	126.22
8	R	2006	BPH	O2A-C1-C2	-2.73	102.64	108.55
7	M	1003	BCL	O2D-CGD-CBD	2.72	116.88	111.33
7	S	2003	BCL	OBD-CAD-CBD	-2.71	121.84	125.94
8	M	1005	BPH	CMB-C2B-C1B	-2.70	124.55	128.65
7	S	2003	BCL	C2D-C3D-CAD	2.70	156.57	138.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	S	2005	BPH	C2D-C3D-CAD	2.70	156.57	138.46
7	L	1002	BCL	CMB-C2B-C1B	-2.68	124.50	128.62
8	R	2006	BPH	C2D-C3D-CAD	2.67	156.43	138.46
7	M	1001	BCL	CHA-C1A-NA	-2.67	120.74	126.22
7	M	1001	BCL	CMB-C2B-C3B	2.67	129.18	124.97
7	S	2001	BCL	C1-O2A-CGA	2.65	124.41	116.98
7	S	2001	BCL	C2B-C1B-NB	2.64	111.40	109.41
7	M	1004	BCL	OBD-CAD-C3D	-2.62	123.03	127.91
9	L	1009	U10	C30-C29-C31	2.62	119.36	115.39
7	R	2002	BCL	CMA-C3A-C4A	-2.59	104.24	111.76
9	M	1008	U10	C3M-O3-C3	2.59	125.26	116.48
7	S	2003	BCL	CMB-C2B-C3B	2.58	129.04	124.97
7	M	1001	BCL	C2D-C3D-CAD	2.58	155.79	138.46
7	L	1002	BCL	CAA-C2A-C1A	-2.57	105.20	111.62
7	S	2003	BCL	CMB-C2B-C1B	-2.57	124.66	128.62
8	S	2005	BPH	C3D-C4D-ND	2.57	116.54	108.80
8	L	1006	BPH	C2D-C3D-CAD	2.56	155.66	138.46
7	M	1001	BCL	CHB-C4A-NA	2.56	127.61	124.58
7	M	1003	BCL	C2D-C3D-CAD	2.56	155.63	138.46
7	S	2001	BCL	CHA-C1A-NA	-2.55	120.98	126.22
7	M	1004	BCL	CMD-C2D-C3D	-2.54	120.97	124.97
7	R	2002	BCL	CAC-C3C-C4C	-2.54	106.96	112.58
7	R	2004	BCL	CAC-C3C-C4C	-2.54	106.96	112.58
7	M	1004	BCL	C4B-C3B-C2B	-2.53	103.91	106.97
7	L	1002	BCL	C2D-C3D-CAD	2.53	155.44	138.46
7	M	1003	BCL	C4D-ND-C1D	-2.53	103.52	106.57
7	R	2004	BCL	C2D-C3D-CAD	2.52	155.43	138.46
7	S	2001	BCL	OBD-CAD-C3D	-2.52	123.22	127.91
7	L	1002	BCL	CHA-C1A-NA	-2.51	121.07	126.22
8	M	1005	BPH	C2C-C3C-C4C	2.51	105.48	102.06
8	S	2005	BPH	C7-C6-C5	-2.50	108.84	114.46
7	M	1003	BCL	C3A-C2A-C1A	2.50	104.61	101.08
8	M	1005	BPH	C2D-C3D-CAD	2.49	155.21	138.46
8	L	1006	BPH	C7-C6-C5	-2.49	105.68	113.01
7	S	2001	BCL	C4D-ND-C1D	-2.48	103.58	106.57
7	R	2004	BCL	CHB-C4A-NA	2.47	127.50	124.58
7	M	1004	BCL	C2D-C3D-CAD	2.47	155.04	138.46
7	R	2002	BCL	C2D-C3D-CAD	2.46	155.00	138.46
8	M	1005	BPH	C4D-ND-C1D	-2.46	103.08	108.72
8	S	2005	BPH	CMB-C2B-C3B	2.44	128.82	124.97
7	M	1004	BCL	C4D-CHA-C1A	2.44	127.38	120.32
7	R	2004	BCL	C1D-C2D-C3D	2.44	108.78	106.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	1001	BCL	C2C-C3C-C4C	2.43	104.42	101.05
7	R	2002	BCL	C6-C5-C3	2.43	118.56	112.78
8	S	2005	BPH	C2C-C3C-C4C	2.42	105.37	102.06
7	M	1004	BCL	C4D-CHA-CBD	-2.42	103.68	109.37
7	L	1002	BCL	C2D-C1D-ND	2.42	111.24	109.41
7	S	2001	BCL	C2C-C3C-C4C	2.41	104.39	101.05
7	S	2003	BCL	CAC-C3C-C4C	-2.40	107.25	112.58
9	R	2009	U10	C1-C6-C5	-2.40	117.24	120.26
7	R	2004	BCL	O2D-CGD-CBD	2.40	116.22	111.33
9	L	1009	U10	C4M-O4-C4	2.38	124.57	116.48
9	M	1008	U10	C25-C24-C26	2.38	119.01	115.39
7	S	2003	BCL	OBB-CAB-C3B	2.37	123.63	120.07
8	R	2006	BPH	CED-O2D-CGD	2.37	121.66	116.02
7	L	1002	BCL	C6-C5-C3	2.37	118.42	112.78
7	S	2001	BCL	O2D-CGD-CBD	2.37	116.15	111.33
7	M	1004	BCL	C15-C13-C12	-2.36	99.74	111.92
8	R	2006	BPH	C3D-C4D-ND	2.36	115.90	108.80
7	M	1003	BCL	C4D-CHA-C1A	2.35	127.14	120.32
9	R	2009	U10	C3M-O3-C3	2.35	124.48	116.48
8	M	1005	BPH	CED-O2D-CGD	2.35	121.61	116.02
8	L	1006	BPH	CMA-C3A-C4A	-2.34	105.48	112.94
9	L	1009	U10	C16-C17-C18	-2.33	104.96	111.62
7	S	2001	BCL	C1-C2-C3	2.32	130.30	126.19
7	S	2001	BCL	CHC-C4B-NB	-2.30	120.73	124.58
8	M	1005	BPH	C3C-C4C-NC	-2.29	109.50	113.49
7	R	2004	BCL	C4D-CHA-C1A	2.28	126.92	120.32
7	S	2003	BCL	C4D-CHA-C1A	2.27	126.91	120.32
7	M	1004	BCL	C1-C2-C3	-2.27	122.14	126.19
8	L	1006	BPH	CMB-C2B-C1B	-2.27	125.19	128.65
7	S	2001	BCL	CMA-C3A-C4A	-2.27	105.18	111.76
8	L	1006	BPH	C3C-C4C-CHD	2.26	126.53	121.83
7	M	1001	BCL	O2D-CGD-CBD	2.26	115.93	111.33
7	L	1002	BCL	C4B-C3B-C2B	-2.25	104.25	106.97
7	L	1002	BCL	C4D-CHA-C1A	2.25	126.82	120.32
7	M	1003	BCL	CMB-C2B-C1B	-2.24	125.17	128.62
7	M	1003	BCL	CGD-CBD-CHA	-2.24	103.34	110.96
7	L	1002	BCL	C2C-C3C-C4C	2.23	104.15	101.05
7	R	2004	BCL	CHA-C1A-NA	-2.23	121.63	126.22
8	R	2006	BPH	OBD-CAD-C3D	-2.23	123.76	127.91
7	S	2001	BCL	CMB-C2B-C3B	2.23	128.48	124.97
7	M	1004	BCL	C4B-NB-C1B	-2.22	103.84	106.76
7	M	1004	BCL	O1D-CGD-CBD	-2.21	119.90	124.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	1005	BPH	C3B-C2B-C1B	-2.21	105.69	107.01
8	L	1006	BPH	C4D-CHA-CBD	-2.21	104.69	110.15
7	S	2003	BCL	C3B-C4B-NB	2.21	110.79	108.64
7	R	2004	BCL	CAA-C2A-C3A	-2.20	107.83	113.04
7	M	1001	BCL	C2B-C1B-NB	2.19	111.07	109.41
7	S	2003	BCL	CHC-C4B-NB	-2.19	120.92	124.58
8	R	2006	BPH	O1D-CGD-CBD	-2.19	119.94	124.42
7	R	2002	BCL	C1D-CHD-C4C	2.18	129.31	125.55
7	M	1003	BCL	C1-O2A-CGA	2.18	123.09	116.98
7	R	2002	BCL	C4D-ND-C1D	-2.18	103.93	106.57
7	M	1001	BCL	CMC-C2C-C1C	-2.18	105.43	111.76
8	L	1006	BPH	C4D-ND-C1D	-2.18	103.72	108.72
7	S	2003	BCL	C2C-C3C-C4C	2.18	104.07	101.05
7	S	2001	BCL	C4D-CHA-C1A	2.17	126.59	120.32
7	M	1001	BCL	OB B-CAB-CBB	-2.16	114.77	120.13
7	S	2003	BCL	C4-C3-C5	2.16	118.67	115.39
7	S	2001	BCL	C2C-C1C-NC	2.16	113.58	110.95
7	M	1003	BCL	C4D-CHA-CBD	-2.15	104.30	109.37
7	R	2004	BCL	C6-C5-C3	-2.15	107.67	112.78
9	S	2008	U10	C17-C18-C19	-2.15	123.16	127.80
7	M	1001	BCL	C4D-CHA-C1A	2.15	126.54	120.32
7	R	2002	BCL	O2D-CGD-CBD	2.14	115.69	111.33
7	S	2001	BCL	C4D-CHA-CBD	-2.14	104.33	109.37
7	R	2002	BCL	C3C-C2C-C1C	2.13	104.68	101.40
7	S	2001	BCL	C1D-CHD-C4C	2.13	129.22	125.55
7	L	1002	BCL	C3D-CAD-CBD	2.13	110.61	107.60
7	L	1002	BCL	CMA-C3A-C4A	-2.11	105.62	111.76
8	R	2006	BPH	C3B-C2B-C1B	-2.11	105.75	107.01
8	L	1006	BPH	C3D-C4D-ND	2.11	115.15	108.80
7	R	2004	BCL	C3A-C4A-CHB	-2.11	119.94	124.33
8	R	2006	BPH	OBD-CAD-CBD	-2.10	122.76	125.94
8	R	2006	BPH	CMA-C3A-C4A	-2.10	106.24	112.94
7	S	2003	BCL	C4D-CHA-CBD	-2.10	104.42	109.37
7	M	1001	BCL	C4D-ND-C1D	-2.10	104.03	106.57
9	M	1008	U10	C27-C28-C29	-2.10	123.53	128.63
7	R	2004	BCL	CHC-C4B-NB	-2.10	121.07	124.58
7	M	1001	BCL	CMA-C3A-C4A	-2.09	105.68	111.76
9	S	2008	U10	C3M-O3-C3	2.09	123.59	116.48
8	R	2006	BPH	C4D-CHA-CBD	-2.09	104.97	110.15
10	M	1012	LDA	C6-C5-C4	-2.09	103.32	114.61
8	M	1005	BPH	C3D-C4D-ND	2.08	115.07	108.80
7	S	2003	BCL	O2D-CGD-CBD	2.08	115.57	111.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	R	2002	BCL	C4D-CHA-CBD	-2.06	104.52	109.37
8	R	2006	BPH	C2A-C3A-C4A	2.06	105.75	101.11
7	M	1003	BCL	O2A-CGA-CBA	2.05	118.40	111.94
8	S	2005	BPH	C4D-CHA-CBD	-2.05	105.07	110.15
7	M	1003	BCL	CAC-C3C-C2C	-2.05	109.18	113.89
7	S	2001	BCL	C2A-C1A-CHA	2.05	127.39	123.83
7	M	1004	BCL	CAC-C3C-C2C	-2.05	109.19	113.89
10	M	1013	LDA	C6-C5-C4	-2.05	103.54	114.61
8	L	1006	BPH	CAC-C3C-C4C	2.04	118.31	112.68
7	R	2004	BCL	C4D-CHA-CBD	-2.04	104.56	109.37
7	M	1004	BCL	CAA-C2A-C3A	-2.04	108.22	113.04
8	S	2005	BPH	O1D-CGD-CBD	-2.04	120.25	124.42
7	L	1002	BCL	OB B-CAB-CBB	-2.03	115.08	120.13
7	M	1001	BCL	CAA-C2A-C3A	-2.03	108.24	113.04
7	S	2003	BCL	C1-O2A-CGA	2.03	122.66	116.98
7	M	1003	BCL	CHA-C1A-NA	-2.02	122.08	126.22
8	M	1005	BPH	CMA-C3A-C4A	-2.01	106.53	112.94
9	M	1008	U10	C22-C23-C24	-2.01	123.46	127.80
8	L	1006	BPH	C1B-NB-C4B	-2.01	104.12	108.72
8	S	2005	BPH	C2B-C1B-NB	2.01	112.06	108.16
7	M	1004	BCL	C5-C3-C2	-2.00	117.23	121.08
7	S	2003	BCL	O2A-CGA-CBA	2.00	118.24	111.94
7	R	2002	BCL	C2A-C1A-CHA	2.00	127.30	123.83

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	L	1006	BPH	C8
8	L	1006	BPH	C13
8	R	2006	BPH	C8
8	R	2006	BPH	C13

There are no torsion outliers.

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%)	0.08	6 (2%) 60 63	30, 49, 74, 85	0
1	R	281/281 (100%)	-0.04	14 (4%) 28 28	33, 50, 73, 85	0
2	M	299/307 (97%)	-0.00	4 (1%) 74 76	34, 44, 59, 76	0
2	S	299/307 (97%)	-0.16	3 (1%) 79 81	36, 46, 59, 75	0
3	H	246/260 (94%)	0.01	8 (3%) 44 45	40, 52, 73, 90	0
3	T	246/260 (94%)	0.25	15 (6%) 21 20	42, 53, 74, 90	0
All	All	1652/1696 (97%)	0.02	50 (3%) 48 50	30, 49, 71, 90	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	255	MET	4.5
1	L	59	TRP	4.3
3	T	55	PRO	4.3
3	H	252	VAL	4.1
3	T	79	GLU	4.0
3	T	92	VAL	3.8
3	T	255	MET	3.7
3	T	80	SER	3.4
1	R	51	TRP	3.0
1	R	1	ALA	3.0
3	T	54	GLY	2.9
1	R	73	TYR	2.9
1	R	59	TRP	2.8
3	H	256	LEU	2.8
3	H	251	VAL	2.8
2	M	301	HIS	2.8
3	H	93	SER	2.7
1	L	73	TYR	2.7
1	L	51	TRP	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	T	51	ALA	2.7
3	T	74	THR	2.7
2	S	3	TYR	2.7
1	R	270	PRO	2.6
1	L	77	GLY	2.6
3	T	252	VAL	2.6
1	R	74	GLY	2.5
3	H	68	HIS	2.5
1	L	78	ALA	2.5
1	R	203	GLY	2.5
1	L	271	TRP	2.5
1	R	202	LYS	2.4
1	R	21	LEU	2.4
3	T	18	TYR	2.4
2	M	109	LEU	2.4
3	T	254	ALA	2.3
1	R	271	TRP	2.3
3	H	60	LYS	2.3
3	H	102	GLY	2.3
2	S	34	PRO	2.3
3	T	56	PHE	2.3
2	M	68	PHE	2.2
3	T	69	GLY	2.2
2	S	54	SER	2.1
1	R	60	ASN	2.1
2	M	82	PRO	2.1
1	R	71	LEU	2.1
1	R	281	GLY	2.1
3	T	50	ALA	2.1
1	R	72	GLU	2.0
3	T	78	PRO	2.0

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(Å ²)	Q<0.9
10	LDA	M	1014	10/16	0.36	7.46	51,53,57,58	0
10	LDA	S	2012	16/16	0.40	6.53	51,61,69,70	0
9	U10	L	1009	44/63	0.31	4.96	70,83,97,97	0
10	LDA	M	1013	16/16	0.24	3.81	53,56,58,58	0
9	U10	R	2009	18/63	0.22	3.41	73,75,76,76	0
10	LDA	M	1012	16/16	0.24	3.29	57,61,69,69	0
8	BPH	R	2006	65/65	0.16	1.77	50,56,60,62	0
9	U10	S	2008	32/63	0.16	1.70	52,54,56,56	0
7	BCL	S	2003	66/66	0.17	1.62	41,42,55,56	0
6	CL	S	2011	1/1	0.14	1.03	66,66,66,66	0
7	BCL	R	2002	66/66	0.15	0.96	40,44,51,54	0
7	BCL	L	1002	66/66	0.16	0.79	34,38,41,43	0
7	BCL	S	2001	51/66	0.12	0.26	38,42,49,51	0
8	BPH	S	2005	52/65	0.13	0.23	41,44,59,62	0
8	BPH	L	1006	65/65	0.14	0.23	31,40,43,44	0
7	BCL	R	2004	66/66	0.13	0.13	35,42,66,68	0
9	U10	M	1008	38/63	0.16	0.10	31,37,54,54	0
7	BCL	M	1003	66/66	0.14	-0.19	29,35,44,49	0
7	BCL	M	1004	66/66	0.16	-0.22	29,33,53,57	0
6	CL	M	1011	1/1	0.11	-0.69	45,45,45,45	0
7	BCL	M	1001	51/66	0.11	-0.73	33,35,45,47	0
8	BPH	M	1005	51/65	0.12	-0.79	31,33,40,42	0
4	FE2	M	1007	1/1	0.12	-1.39	35,35,35,35	0
4	FE2	S	2007	1/1	0.07	-2.59	42,42,42,42	0
5	ZN	T	2010	1/1	0.04	-3.55	60,60,60,60	0
5	ZN	H	1010	1/1	0.03	-4.11	57,57,57,57	0

6.5 Other polymers ⓘ

There are no such residues in this entry.