



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:39 PM GMT

PDB ID : 1L9J  
Title : X-Ray Structure of the Cytochrome-c(2)-Photosynthetic Reaction Center Electron Transfer Complex from Rhodobacter sphaeroides in Type I Crystals  
Authors : Axelrod, H.L.; Abresch, E.C.; Okamura, M.Y.; Yeh, A.P.; Rees, D.C.; Feher, G.  
Deposited on : 2002-03-24  
Resolution : 3.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

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

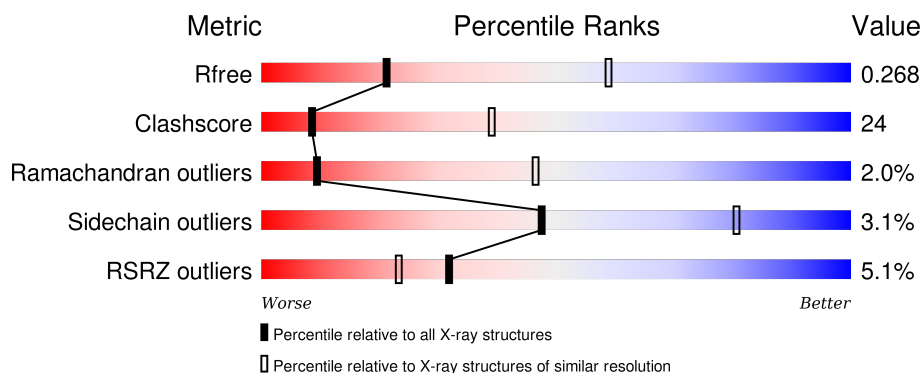
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.25 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1624 (3.32-3.20)
Clashscore	102246	1806 (3.32-3.20)
Ramachandran outliers	100387	1773 (3.32-3.20)
Sidechain outliers	100360	1771 (3.32-3.20)
RSRZ outliers	91569	1632 (3.32-3.20)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	L	281	<div> <div> <div>0%</div> <div>64%</div> <div>34%</div> <div>•</div> </div> </div>
1	R	281	<div> <div>3%</div> <div>54%</div> <div>42%</div> <div>•</div> </div>
2	M	307	<div> <div>2%</div> <div>50%</div> <div>35%</div> <div>•</div> <div>13%</div> </div>
2	S	307	<div> <div>3%</div> <div>47%</div> <div>38%</div> <div>•</div> <div>13%</div> </div>
3	H	260	<div> <div>9%</div> <div>53%</div> <div>39%</div> <div>•</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
3	T	260	
4	C	124	
4	D	124	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	LDA	M	1010	-	-	-	X
11	LDA	M	1011	-	-	-	X
11	LDA	S	2010	-	-	-	X
11	LDA	S	2011	-	-	-	X
7	BCL	L	1004	-	-	-	X
7	BCL	R	2004	-	-	-	X
8	BPH	L	1005	X	-	-	-
8	BPH	M	1006	X	-	-	-
8	BPH	R	2005	X	-	-	-
8	BPH	S	2006	X	-	-	-
9	U10	M	1008	-	-	-	X

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 15497 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	267	Total	C	N	O	S	0	0	0
			2150	1450	347	344	9			
2	S	267	Total	C	N	O	S	0	0	0
			2150	1450	347	344	9			

- 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
			1871	1197	321	344	9			
3	T	246	Total	C	N	O	S	0	0	0
			1871	1197	321	344	9			

- Molecule 4 is a protein called cytochrome c-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	124	Total	C	N	O	S	0	0	0
			949	595	166	184	4			
4	D	124	Total	C	N	O	S	0	0	0
			949	595	166	184	4			

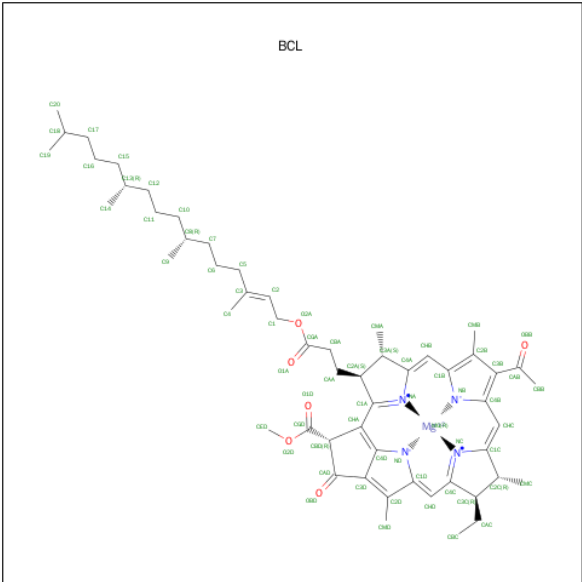
- Molecule 5 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	S	1	Total	Fe	0	0
			1	1		
5	M	1	Total	Fe	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: C<sub>55</sub>H<sub>74</sub>MgN<sub>4</sub>O<sub>6</sub>).



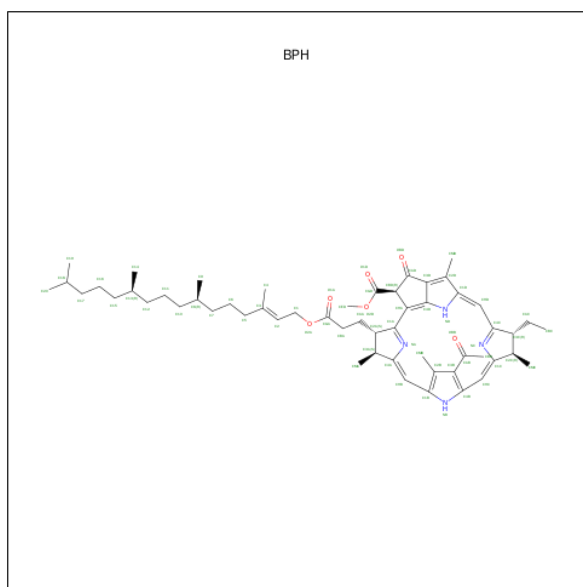
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	M	1	Total	C	Mg	N	O	0	0
			50	39	1	4	6		
7	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	S	1	Total	C	Mg	N	O	0	0
			50	39	1	4	6		
7	R	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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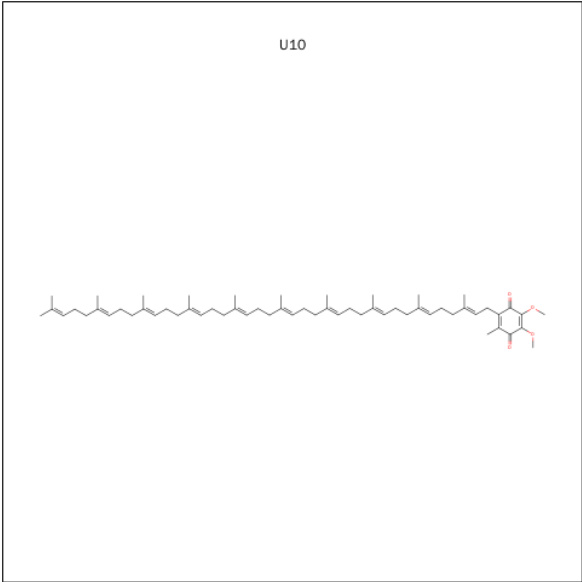
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	S	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	R	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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



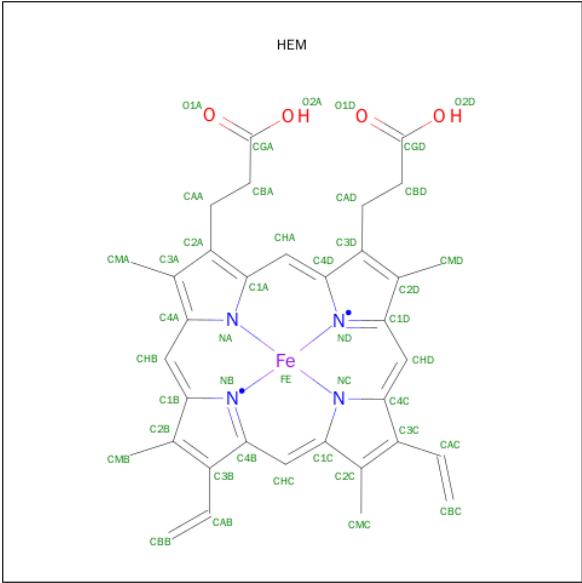
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	L	1	Total	C	N	O	0	0
			55	45	4	6		
8	M	1	Total	C	N	O	0	0
			65	55	4	6		
8	R	1	Total	C	N	O	0	0
			55	45	4	6		
8	S	1	Total	C	N	O	0	0
			65	55	4	6		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	M	1	Total	C	O	0	0
			37	33	4		
9	S	1	Total	C	O	0	0
			37	33	4		

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



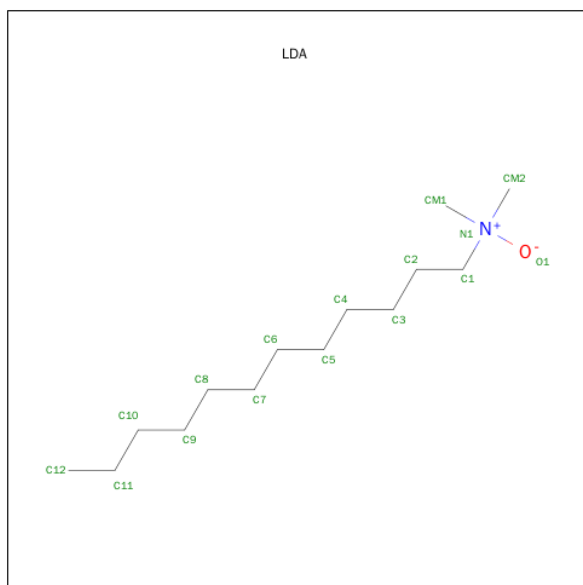
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 11 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:  $C_{14}H_{31}NO$ ).



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

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	C	10	Total	O	0	0
			10	10		
12	D	9	Total	O	0	0
			9	9		
12	H	18	Total	O	0	0
			18	18		
12	L	32	Total	O	0	0
			32	32		

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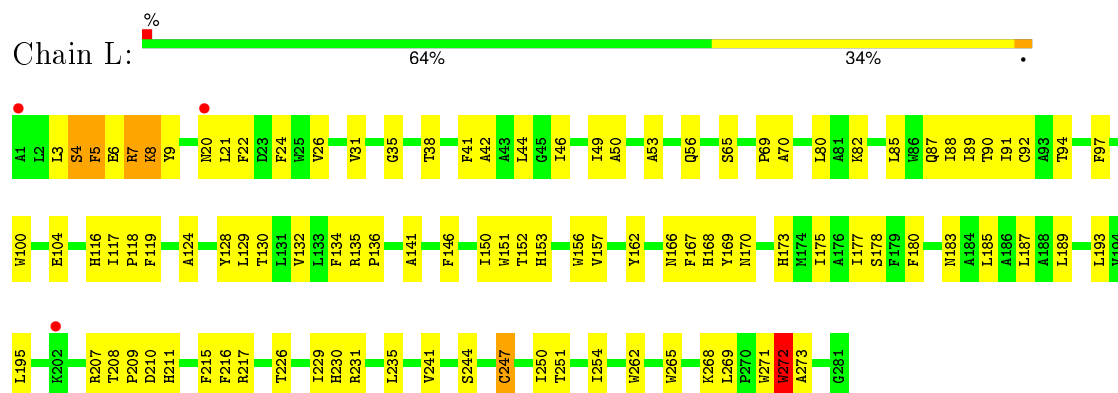
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	M	14	Total 14	O 14	0	0
12	R	18	Total 18	O 18	0	0
12	S	15	Total 15	O 15	0	0
12	T	13	Total 13	O 13	0	0

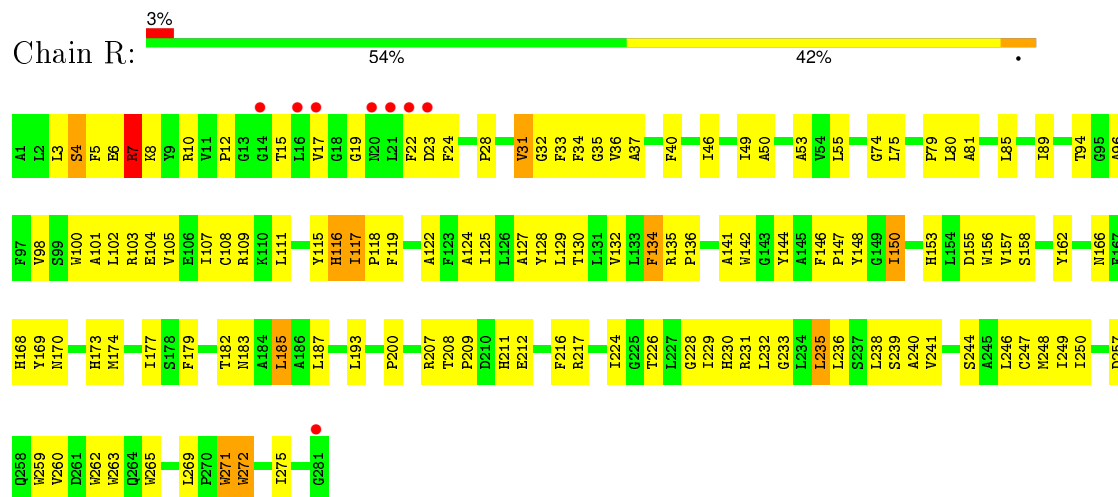
### 3 Residue-property plots

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.

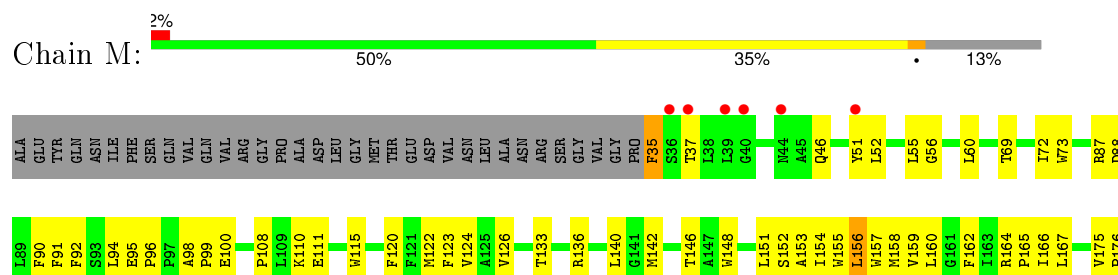
#### • Molecule 1: REACTION CENTER PROTEIN L CHAIN

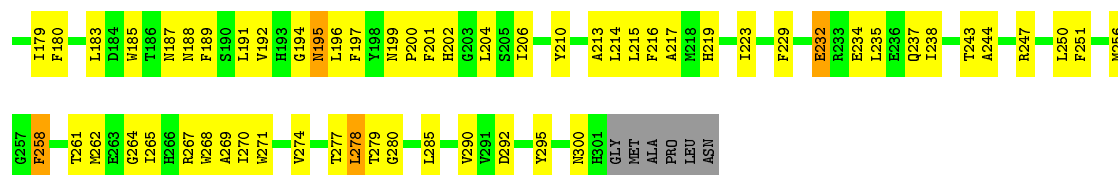


#### • Molecule 1: REACTION CENTER PROTEIN L CHAIN

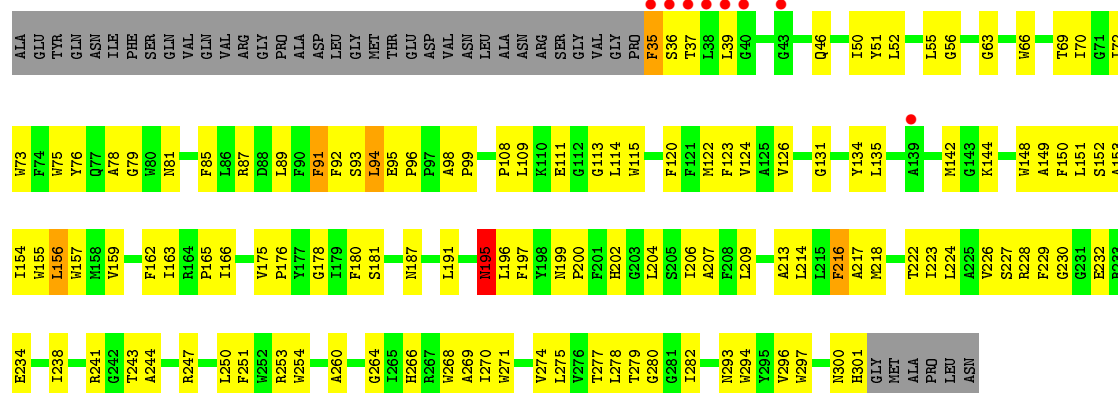


#### • Molecule 2: REACTION CENTER PROTEIN M CHAIN

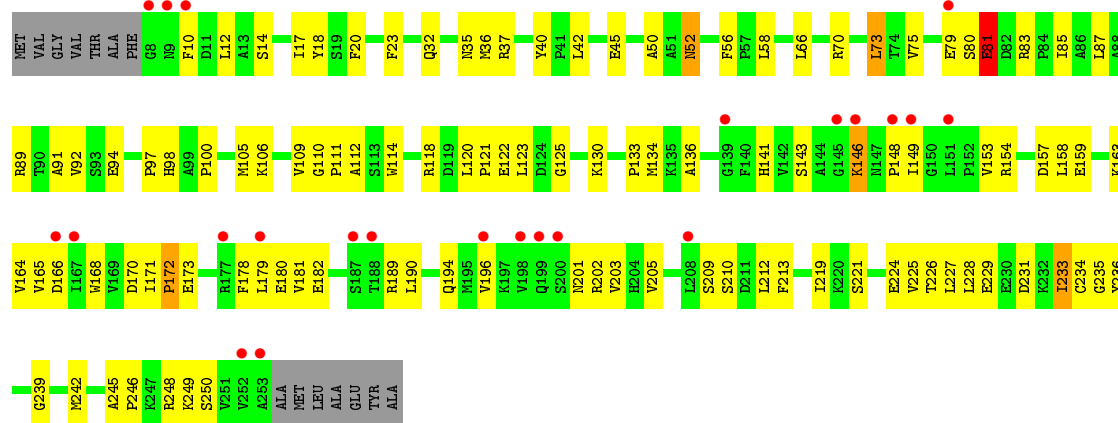




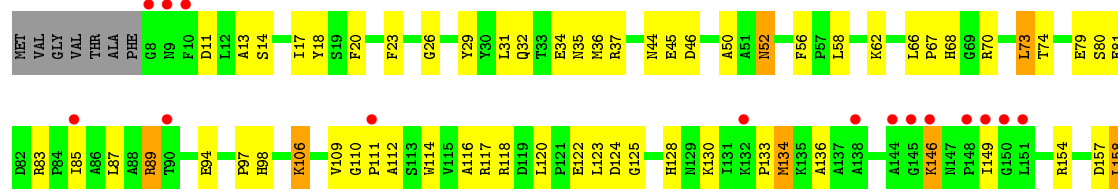
• Molecule 2: REACTION CENTER PROTEIN M CHAIN

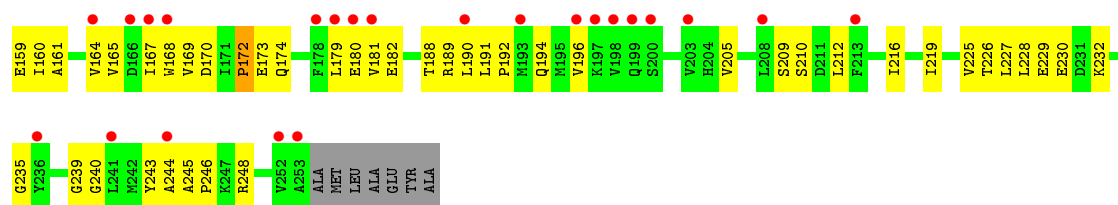


• Molecule 3: REACTION CENTER PROTEIN H CHAIN

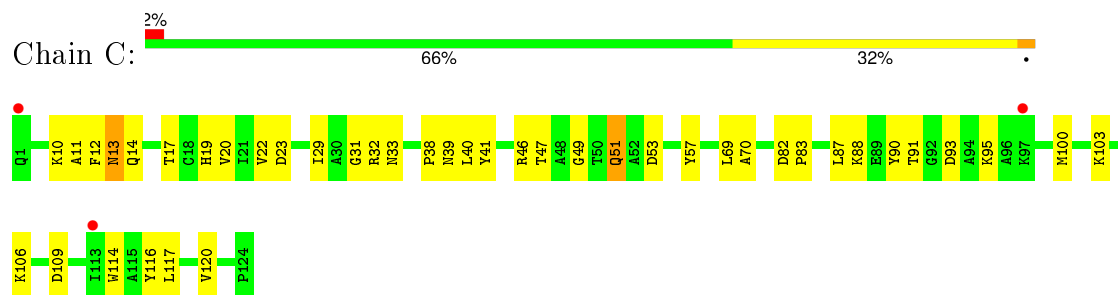


• Molecule 3: REACTION CENTER PROTEIN H CHAIN

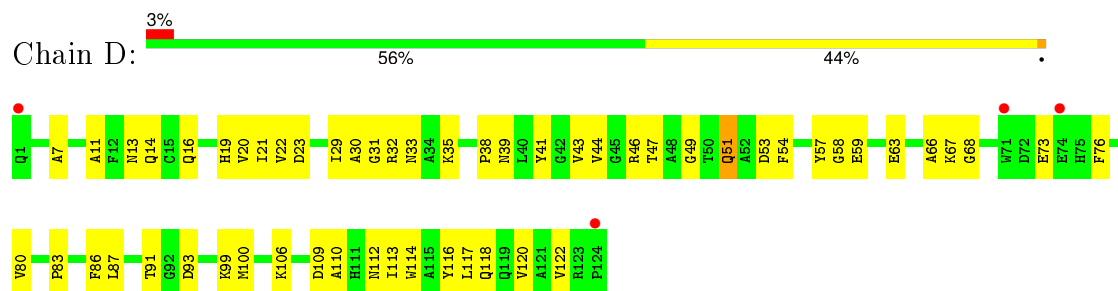




• Molecule 4: cytochrome c-2



• Molecule 4: cytochrome c-2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.93Å 80.31Å 246.57Å 90.00° 92.41° 90.00°	Depositor
Resolution (Å)	49.32 – 3.25 49.32 – 3.25	Depositor EDS
% Data completeness (in resolution range)	98.5 (49.32-3.25) 98.5 (49.32-3.25)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.31 (at 3.25Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.248 , 0.287 0.235 , 0.268	Depositor DCC
$R_{free}$ test set	2385 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	78.5	Xtriage
Anisotropy	0.711	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 53.7	EDS
Estimated twinning fraction	0.000 for -k,-h,-l 0.000 for k,h,-l 0.027 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	6 of 47695 reflections (0.013%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	15497	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.15 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.1270e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, LDA, CL, BPH, FE2, HEM, 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	0.35	0/2320	0.54	0/3175
1	R	0.35	0/2320	0.54	0/3175
2	M	0.36	0/2238	0.56	0/3057
2	S	0.36	0/2238	0.53	0/3057
3	H	0.30	0/1920	0.53	0/2612
3	T	0.30	0/1920	0.52	0/2612
4	C	0.32	0/969	0.57	0/1304
4	D	0.31	0/969	0.53	0/1304
All	All	0.34	0/14894	0.54	0/20296

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2232	0	2187	93	0
1	R	2232	0	2187	123	0
2	M	2150	0	2073	118	0
2	S	2150	0	2073	145	0
3	H	1871	0	1877	105	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	T	1871	0	1877	103	0
4	C	949	0	916	36	0
4	D	949	0	916	46	0
5	M	1	0	0	0	0
5	S	1	0	0	0	0
6	M	1	0	0	0	0
6	S	1	0	0	0	0
7	L	132	0	148	15	0
7	M	116	0	115	17	0
7	R	132	0	148	16	0
7	S	116	0	115	13	0
8	L	55	0	53	2	0
8	M	65	0	74	3	0
8	R	55	0	53	2	0
8	S	65	0	74	6	0
9	M	37	0	47	1	0
9	S	37	0	47	1	0
10	C	43	0	30	2	0
10	D	43	0	30	2	0
11	M	32	0	62	5	0
11	S	32	0	62	3	0
12	C	10	0	0	3	0
12	D	9	0	0	0	0
12	H	18	0	0	2	0
12	L	32	0	0	6	0
12	M	14	0	0	1	0
12	R	18	0	0	4	0
12	S	15	0	0	2	0
12	T	13	0	0	1	0
All	All	15497	0	15164	727	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (727) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:91:THR:HG23	4:C:93:ASP:H	1.20	1.03
2:S:280:GLY:HA3	7:S:2003:BCL:CED	1.91	1.01
2:S:280:GLY:HA3	7:S:2003:BCL:HED2	1.45	0.97
2:S:122:MET:HE3	2:S:157:TRP:HE1	1.33	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:208:THR:HG22	1:L:210:ASP:H	1.37	0.90
1:L:208:THR:H	1:L:211:HIS:HD2	1.21	0.88
2:S:157:TRP:HB2	7:S:2003:BCL:H62	1.56	0.87
2:S:108:PRO:HG2	2:S:111:GLU:HB2	1.56	0.86
1:L:241:VAL:HG21	8:M:1006:BPH:HAC2	1.58	0.86
1:R:208:THR:H	1:R:211:HIS:HD2	1.23	0.84
2:M:202:HIS:CE1	2:M:206:ILE:HD11	2.12	0.84
3:H:130:LYS:HG3	3:H:172:PRO:HG3	1.59	0.84
1:R:193:LEU:HD11	1:R:216:PHE:HB2	1.60	0.83
2:S:195:ASN:ND2	2:S:197:PHE:H	1.77	0.83
1:L:42:ALA:O	1:L:46:ILE:HG12	1.80	0.82
1:R:170:ASN:HB3	1:R:173:HIS:HB3	1.60	0.82
3:T:130:LYS:HG3	3:T:172:PRO:HG3	1.64	0.80
2:M:156:LEU:HG	7:M:1003:BCL:HED1	1.62	0.80
2:S:122:MET:CE	2:S:157:TRP:HE1	1.94	0.80
3:T:245:ALA:HA	3:T:248:ARG:NH1	1.98	0.79
3:H:146:LYS:H	3:H:146:LYS:HD3	1.47	0.79
2:M:157:TRP:HB2	7:M:1003:BCL:H62	1.65	0.78
3:H:196:VAL:HG12	3:H:205:VAL:HG22	1.68	0.76
4:D:87:LEU:O	4:D:91:THR:HG22	1.86	0.76
2:S:202:HIS:CE1	2:S:206:ILE:HD11	2.22	0.75
2:M:187:ASN:O	2:M:191:LEU:HD23	1.85	0.75
1:R:241:VAL:HG21	8:S:2006:BPH:HAC2	1.68	0.75
3:T:157:ASP:OD2	3:T:159:GLU:HB2	1.87	0.74
3:T:133:PRO:HG3	3:T:168:TRP:CE2	2.22	0.74
1:R:135:ARG:HB3	1:R:136:PRO:HD3	1.69	0.74
2:S:195:ASN:HD22	2:S:195:ASN:C	1.91	0.74
2:M:234:GLU:O	2:M:238:ILE:HG13	1.87	0.74
2:M:52:LEU:HD21	2:M:60:LEU:HD12	1.67	0.74
2:M:235:LEU:HD23	2:M:238:ILE:HD12	1.69	0.73
3:T:196:VAL:HG12	3:T:205:VAL:HG22	1.69	0.73
1:R:128:TYR:HB2	7:R:2002:BCL:H62	1.68	0.73
1:R:187:LEU:HD11	2:S:269:ALA:HB1	1.70	0.73
2:M:290:VAL:HG21	3:H:12:LEU:HD23	1.70	0.73
3:H:245:ALA:HA	3:H:248:ARG:NH1	2.04	0.72
3:T:118:ARG:HD3	3:T:120:LEU:HD12	1.71	0.72
3:T:179:LEU:HD12	3:T:196:VAL:HG21	1.72	0.72
4:D:49:GLY:HA2	4:D:57:TYR:CE1	2.25	0.72
2:M:122:MET:HE3	2:M:157:TRP:HE1	1.54	0.71
1:R:166:ASN:ND2	2:S:187:ASN:HB2	2.04	0.71
3:H:36:MET:HE3	3:H:58:LEU:HD23	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:1001:BCL:HBC1	7:M:1003:BCL:CAD	2.19	0.71
2:M:195:ASN:HD22	2:M:195:ASN:C	1.93	0.71
1:L:207:ARG:HG3	2:M:142:MET:HG2	1.72	0.71
1:L:183:ASN:ND2	2:M:213:ALA:HA	2.05	0.71
4:C:51:GLN:NE2	4:C:53:ASP:H	1.88	0.71
4:D:7:ALA:HB3	4:D:112:ASN:HD22	1.56	0.71
2:M:195:ASN:ND2	2:M:197:PHE:HB2	2.05	0.71
2:S:195:ASN:HD21	2:S:197:PHE:HB2	1.54	0.71
2:M:195:ASN:HD21	2:M:197:PHE:HB2	1.55	0.70
4:C:51:GLN:HE22	4:C:53:ASP:H	1.36	0.70
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.73	0.70
8:R:2005:BPH:HAC1	2:S:153:ALA:HB2	1.72	0.70
4:C:20:VAL:HG23	4:C:31:GLY:HA3	1.72	0.70
4:D:106:LYS:HB2	4:D:109:ASP:OD2	1.92	0.69
3:H:112:ALA:HB2	3:H:239:GLY:HA3	1.73	0.69
1:R:115:TYR:O	1:R:118:PRO:HD2	1.92	0.69
2:S:260:ALA:HB2	9:S:2008:U10:H103	1.74	0.69
1:L:193:LEU:HD11	1:L:216:PHE:HB2	1.73	0.69
1:L:208:THR:HG21	3:H:125:GLY:HA2	1.73	0.69
2:M:52:LEU:O	2:M:56:GLY:HA3	1.92	0.69
2:S:123:PHE:HA	2:S:157:TRP:HH2	1.58	0.68
8:R:2005:BPH:H5C2	2:S:63:GLY:HA3	1.74	0.68
1:R:35:GLY:HA2	1:R:103:ARG:HD2	1.73	0.68
2:M:243:THR:O	2:M:247:ARG:HG3	1.93	0.68
1:R:208:THR:H	1:R:211:HIS:CD2	2.09	0.68
1:R:170:ASN:HB3	1:R:173:HIS:CB	2.23	0.68
2:M:195:ASN:ND2	2:M:197:PHE:H	1.92	0.67
7:L:1004:BCL:HAA2	11:M:1010:LDA:H31	1.76	0.67
3:T:11:ASP:HB3	3:T:14:SER:OG	1.94	0.67
2:S:35:PHE:CE1	2:S:37:THR:HB	2.30	0.67
3:H:154:ARG:NH1	3:H:158:LEU:HD22	2.10	0.67
4:C:11:ALA:O	4:C:14:GLN:HG2	1.94	0.67
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.30	0.67
1:L:208:THR:HG23	1:L:209:PRO:HD2	1.76	0.66
1:R:162:TYR:OH	2:S:191:LEU:HD21	1.94	0.66
4:D:118:GLN:HA	4:D:122:VAL:HG23	1.78	0.66
3:H:165:VAL:HG21	3:H:182:GLU:HB2	1.77	0.66
1:L:128:TYR:HB2	7:L:1002:BCL:H62	1.78	0.66
12:R:2008:HOH:O	3:T:81:GLU:HB2	1.96	0.66
2:M:136:ARG:HD3	12:M:1017:HOH:O	1.95	0.65
1:L:208:THR:H	1:L:211:HIS:CD2	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:29:ILE:HD12	4:C:29:ILE:N	2.11	0.65
1:R:111:LEU:HD21	2:S:254:TRP:CH2	2.31	0.65
2:S:280:GLY:HA3	7:S:2003:BCL:HED3	1.74	0.65
2:M:195:ASN:HD22	2:M:197:PHE:H	1.43	0.65
2:M:46:GLN:HG2	2:M:51:TYR:HA	1.78	0.65
1:R:244:SER:HB3	7:R:2002:BCL:HBA2	1.79	0.65
7:R:2004:BCL:H203	8:S:2006:BPH:H111	1.78	0.65
2:M:122:MET:O	2:M:126:VAL:HG23	1.97	0.65
4:C:49:GLY:HA2	4:C:57:TYR:CZ	2.31	0.64
3:H:89:ARG:HH21	3:H:92:VAL:HA	1.61	0.64
1:R:116:HIS:O	1:R:119:PHE:HB3	1.97	0.64
1:R:226:THR:O	1:R:229:ILE:HG22	1.96	0.64
2:M:122:MET:HE1	11:M:1011:LDA:HM22	1.80	0.64
2:M:188:ASN:O	2:M:192:VAL:HG23	1.98	0.64
1:R:37:ALA:O	1:R:40:PHE:HB3	1.97	0.64
3:T:146:LYS:HD3	3:T:146:LYS:H	1.63	0.64
2:S:78:ALA:HB2	2:S:92:PHE:CZ	2.33	0.64
2:M:90:PHE:HD1	2:M:179:ILE:HG13	1.63	0.64
1:L:175:ILE:O	1:L:178:SER:HB3	1.98	0.64
2:S:52:LEU:HG	2:S:56:GLY:HA3	1.79	0.64
2:S:155:TRP:O	2:S:159:VAL:HG23	1.97	0.63
7:L:1002:BCL:HBD	7:L:1004:BCL:CBC	2.28	0.63
4:C:106:LYS:HB2	4:C:109:ASP:OD2	1.98	0.63
2:S:187:ASN:O	2:S:191:LEU:HD23	1.98	0.63
3:H:91:ALA:HB1	12:H:262:HOH:O	1.99	0.63
3:H:225:VAL:HG23	3:H:229:GLU:HB2	1.80	0.63
1:R:246:LEU:O	1:R:249:ILE:HG22	1.98	0.63
7:R:2004:BCL:O1A	2:S:207:ALA:HA	1.99	0.62
2:M:162:PHE:O	2:M:165:PRO:HD2	1.99	0.62
2:M:194:GLY:HA2	12:C:1011:HOH:O	1.97	0.62
3:H:70:ARG:HH22	3:H:123:LEU:HD13	1.63	0.62
2:S:264:GLY:HA3	3:T:35:ASN:OD1	1.99	0.62
3:T:45:GLU:HG3	3:T:94:GLU:OE1	1.99	0.62
2:S:98:ALA:HB1	2:S:99:PRO:HD2	1.82	0.62
1:R:5:PHE:HB2	1:R:8:LYS:NZ	2.14	0.62
7:R:2004:BCL:HAA2	11:S:2010:LDA:H31	1.81	0.62
3:T:170:ASP:OD2	3:T:173:GLU:HB2	2.00	0.62
2:M:87:ARG:HG3	2:M:88:ASP:OD1	1.99	0.62
3:H:201:ASN:OD1	3:H:202:ARG:HG2	1.99	0.62
4:D:73:GLU:HB2	4:D:114:TRP:NE1	2.15	0.62
4:D:38:PRO:HB3	4:D:54:PHE:CG	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:135:ARG:HD3	12:R:2007:HOH:O	1.98	0.61
1:R:248:MET:HG2	7:R:2002:BCL:O1D	2.00	0.61
4:C:91:THR:HG23	4:C:93:ASP:N	2.03	0.61
3:H:36:MET:CE	3:H:58:LEU:HD23	2.30	0.61
4:C:49:GLY:HA2	4:C:57:TYR:CE1	2.35	0.61
3:T:122:GLU:HB2	3:T:227:LEU:HD21	1.80	0.61
2:M:72:ILE:HG23	2:M:73:TRP:N	2.16	0.61
2:M:90:PHE:CD1	2:M:179:ILE:HG13	2.36	0.61
2:M:156:LEU:HD13	7:M:1003:BCL:H43	1.82	0.61
3:T:133:PRO:HA	3:T:168:TRP:HA	1.83	0.61
2:M:122:MET:HE1	11:M:1011:LDA:CM2	2.31	0.61
1:L:183:ASN:HD21	2:M:213:ALA:HA	1.65	0.61
1:L:166:ASN:ND2	2:M:187:ASN:HB2	2.16	0.60
1:R:207:ARG:HG3	2:S:142:MET:HG2	1.83	0.60
2:S:109:LEU:HA	2:S:113:GLY:HA3	1.81	0.60
1:L:244:SER:O	1:L:247:CYS:HB3	2.01	0.60
2:S:202:HIS:HE1	2:S:206:ILE:HD11	1.66	0.60
1:R:173:HIS:CE1	1:R:177:ILE:HD11	2.37	0.60
3:H:79:GLU:HG3	3:H:81:GLU:HG2	1.84	0.60
1:L:262:TRP:O	1:L:265:TRP:HD1	1.85	0.60
2:S:123:PHE:HA	2:S:157:TRP:CH2	2.36	0.60
2:S:199:ASN:ND2	2:S:294:TRP:CE2	2.70	0.60
2:M:122:MET:CE	2:M:157:TRP:HE1	2.15	0.60
2:S:195:ASN:HD22	2:S:197:PHE:H	1.49	0.60
3:T:245:ALA:HA	3:T:248:ARG:HH12	1.65	0.60
3:H:179:LEU:HD12	3:H:196:VAL:HG21	1.82	0.60
3:H:157:ASP:OD2	3:H:159:GLU:HB2	2.02	0.60
2:M:162:PHE:C	2:M:165:PRO:HD2	2.23	0.60
1:L:94:THR:HG23	1:L:129:LEU:HD21	1.84	0.60
2:M:200:PRO:HB2	3:H:17:ILE:HD13	1.84	0.59
1:R:4:SER:HB2	3:T:79:GLU:HG2	1.84	0.59
3:T:225:VAL:HG23	3:T:229:GLU:HB2	1.84	0.59
1:R:166:ASN:HD21	2:S:187:ASN:HB2	1.68	0.59
3:H:87:LEU:HD23	3:H:100:PRO:HA	1.83	0.59
1:L:250:ILE:HB	1:L:254:ILE:HD11	1.84	0.59
3:T:149:ILE:HA	3:T:164:VAL:CG1	2.32	0.59
1:L:56:GLN:HE22	1:L:65:SER:H	1.50	0.58
2:S:297:TRP:HE1	3:T:13:ALA:HB3	1.67	0.58
3:T:120:LEU:N	3:T:226:THR:HB	2.18	0.58
2:S:96:PRO:HD3	2:S:176:PRO:HB3	1.85	0.58
1:L:269:LEU:HD13	1:L:271:TRP:CZ2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:2001:BCL:HBC1	7:S:2003:BCL:HBD	1.85	0.58
1:L:4:SER:HB2	3:H:79:GLU:HG2	1.86	0.58
1:R:6:GLU:HG2	1:R:10:ARG:HD2	1.84	0.58
2:M:235:LEU:HA	2:M:238:ILE:HD12	1.85	0.58
2:M:270:ILE:HG23	2:M:271:TRP:N	2.19	0.58
1:R:128:TYR:O	1:R:132:VAL:HG22	2.02	0.58
1:L:187:LEU:HD11	2:M:269:ALA:HB1	1.86	0.58
3:H:66:LEU:N	3:H:66:LEU:HD12	2.17	0.58
4:D:20:VAL:HG23	4:D:31:GLY:HA3	1.86	0.57
3:H:40:TYR:HB3	3:H:58:LEU:HD21	1.86	0.57
2:M:256:MET:HE2	2:M:258:PHE:HE2	1.69	0.57
2:S:301:HIS:CD2	3:T:14:SER:HB3	2.40	0.57
2:M:271:TRP:HA	2:M:274:VAL:HG22	1.86	0.57
7:R:2002:BCL:HBD	7:R:2004:BCL:CBC	2.35	0.57
7:M:1001:BCL:HBB3	7:M:1003:BCL:H61	1.86	0.57
3:H:111:PRO:HG3	3:H:242:MET:SD	2.44	0.57
2:S:206:ILE:HG23	7:S:2003:BCL:HMB3	1.86	0.57
2:S:222:THR:O	2:S:226:VAL:HG22	2.04	0.57
4:D:51:GLN:HE22	4:D:53:ASP:N	2.03	0.57
1:R:7:ARG:HG3	1:R:7:ARG:HH11	1.70	0.57
4:D:22:VAL:HB	4:D:39:ASN:ND2	2.19	0.57
7:R:2002:BCL:H2C	7:S:2003:BCL:H2C	1.87	0.56
2:S:134:TYR:HE1	2:S:144:LYS:HG3	1.70	0.56
3:H:219:ILE:O	3:H:219:ILE:HG13	2.05	0.56
2:M:295:TYR:CZ	4:C:32:ARG:HD3	2.40	0.56
3:H:105:MET:HE3	3:H:212:LEU:HD13	1.87	0.56
2:M:175:VAL:HB	11:M:1011:LDA:HM13	1.87	0.56
2:M:290:VAL:CG2	3:H:12:LEU:HD23	2.34	0.56
1:R:229:ILE:HG23	1:R:230:HIS:N	2.21	0.56
3:H:14:SER:HA	3:H:17:ILE:HG22	1.87	0.56
2:S:95:GLU:HA	2:S:176:PRO:HB3	1.88	0.56
3:T:133:PRO:HG3	3:T:168:TRP:CD2	2.41	0.56
2:M:156:LEU:CG	7:M:1003:BCL:HED1	2.33	0.56
2:S:229:PHE:CZ	2:S:247:ARG:NH1	2.73	0.56
1:L:6:GLU:HG3	2:M:250:LEU:HD22	1.86	0.56
3:T:228:LEU:O	3:T:232:LYS:HG2	2.06	0.56
1:R:115:TYR:O	1:R:117:ILE:N	2.39	0.56
3:H:225:VAL:CG2	3:H:229:GLU:HB2	2.36	0.56
3:T:161:ALA:HB2	3:T:210:SER:HB2	1.88	0.56
1:R:231:ARG:O	1:R:235:LEU:HB2	2.06	0.56
4:C:19:HIS:HA	12:C:1018:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:29:ILE:HD12	4:D:29:ILE:N	2.21	0.56
2:S:280:GLY:CA	7:S:2003:BCL:HED2	2.29	0.56
2:S:55:LEU:HD22	2:S:55:LEU:N	2.21	0.56
3:H:168:TRP:HB2	3:H:178:PHE:HB2	1.88	0.56
8:L:1005:BPH:HMB3	7:M:1001:BCL:HMB2	1.87	0.55
3:H:121:PRO:HD3	3:H:226:THR:HG22	1.88	0.55
4:C:88:LYS:O	4:C:91:THR:HG22	2.07	0.55
4:C:87:LEU:O	4:C:91:THR:HB	2.07	0.55
3:H:130:LYS:HG3	3:H:172:PRO:CG	2.36	0.55
4:D:22:VAL:HB	4:D:39:ASN:HD21	1.72	0.55
4:C:12:PHE:CE1	4:C:40:LEU:HD12	2.41	0.55
2:M:300:ASN:HD22	2:M:300:ASN:N	2.04	0.55
3:T:45:GLU:OE1	3:T:94:GLU:HA	2.07	0.55
1:L:117:ILE:HD13	2:M:251:PHE:CE2	2.41	0.55
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.88	0.55
2:M:72:ILE:HG23	2:M:73:TRP:H	1.70	0.55
2:S:96:PRO:HG3	2:S:115:TRP:NE1	2.22	0.55
1:R:85:LEU:O	1:R:89:ILE:HG13	2.07	0.54
1:L:170:ASN:HB3	1:L:173:HIS:CB	2.37	0.54
2:S:195:ASN:ND2	2:S:197:PHE:HB2	2.21	0.54
1:L:85:LEU:O	1:L:89:ILE:HG13	2.08	0.54
7:L:1002:BCL:HBD	7:L:1004:BCL:HBC3	1.88	0.54
2:S:159:VAL:HA	2:S:163:ILE:HB	1.89	0.54
1:L:230:HIS:CD2	2:M:223:ILE:HG13	2.42	0.54
2:M:108:PRO:HG2	2:M:111:GLU:HB2	1.90	0.54
4:C:12:PHE:HE1	4:C:40:LEU:HD12	1.72	0.54
4:D:38:PRO:HD3	4:D:54:PHE:CE2	2.43	0.54
3:T:112:ALA:HB2	3:T:239:GLY:HA3	1.88	0.54
2:M:264:GLY:HA3	3:H:35:ASN:OD1	2.07	0.54
2:M:96:PRO:HA	2:M:115:TRP:CG	2.43	0.54
3:T:245:ALA:HB3	3:T:246:PRO:HD3	1.88	0.54
1:R:28:PRO:HB3	2:S:253:ARG:NH1	2.23	0.54
3:T:190:LEU:C	3:T:191:LEU:HD22	2.28	0.54
1:L:88:ILE:O	1:L:91:ILE:HB	2.08	0.54
4:D:23:ASP:HA	4:D:41:TYR:CD2	2.43	0.54
2:S:271:TRP:HA	2:S:274:VAL:HG22	1.89	0.54
2:M:122:MET:HE3	2:M:157:TRP:NE1	2.21	0.53
1:R:269:LEU:HD13	1:R:271:TRP:CZ2	2.43	0.53
4:C:116:TYR:O	4:C:120:VAL:HG22	2.07	0.53
7:R:2002:BCL:HBD	7:R:2004:BCL:HBC1	1.90	0.53
4:C:22:VAL:HB	4:C:39:ASN:HD21	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:122:ALA:HA	1:R:125:ILE:HD12	1.90	0.53
4:D:49:GLY:HA2	4:D:57:TYR:CZ	2.44	0.53
3:T:165:VAL:CG2	3:T:182:GLU:H	2.22	0.53
4:D:7:ALA:CB	4:D:112:ASN:HD22	2.21	0.53
1:L:162:TYR:OH	2:M:191:LEU:HD21	2.09	0.53
1:L:22:PHE:HA	1:L:24:PHE:HE2	1.74	0.53
3:H:45:GLU:HG3	3:H:94:GLU:OE1	2.09	0.53
3:T:83:ARG:HH11	3:T:83:ARG:HG3	1.74	0.53
3:T:66:LEU:HD12	3:T:66:LEU:H	1.74	0.53
3:T:70:ARG:HH22	3:T:123:LEU:HD13	1.73	0.53
1:R:5:PHE:HB2	1:R:8:LYS:HZ1	1.72	0.53
4:D:51:GLN:NE2	4:D:54:PHE:H	2.07	0.53
2:S:162:PHE:C	2:S:165:PRO:HD2	2.29	0.53
2:S:195:ASN:HD22	2:S:196:LEU:N	2.07	0.52
1:R:6:GLU:HG3	2:S:250:LEU:CD2	2.38	0.52
1:R:6:GLU:OE2	1:R:10:ARG:NH1	2.42	0.52
3:T:114:TRP:CE3	3:T:232:LYS:HD3	2.43	0.52
2:S:148:TRP:O	2:S:151:LEU:HB3	2.10	0.52
8:L:1005:BPH:HAC1	2:M:153:ALA:HB2	1.91	0.52
1:L:135:ARG:NH1	1:L:251:THR:O	2.38	0.52
3:H:133:PRO:HB3	3:H:166:ASP:OD2	2.10	0.52
2:S:94:LEU:HA	12:S:2016:HOH:O	2.09	0.52
7:L:1002:BCL:HBD	7:L:1004:BCL:HBC1	1.90	0.52
3:T:226:THR:OG1	3:T:229:GLU:HG3	2.09	0.52
3:H:105:MET:CE	3:H:212:LEU:HD13	2.39	0.52
3:H:134:MET:C	3:H:136:ALA:H	2.13	0.52
4:C:69:LEU:HB2	4:C:90:TYR:CE2	2.45	0.52
1:L:208:THR:HG21	3:H:125:GLY:CA	2.39	0.52
3:H:80:SER:O	3:H:81:GLU:C	2.48	0.52
1:L:31:VAL:O	1:L:35:GLY:HA3	2.09	0.52
1:R:75:LEU:HA	1:R:142:TRP:NE1	2.25	0.52
4:D:46:ARG:HG2	4:D:47:THR:N	2.23	0.52
1:L:229:ILE:HG23	1:L:230:HIS:N	2.24	0.52
1:L:146:PHE:HB3	1:L:156:TRP:CD2	2.45	0.52
2:S:152:SER:O	2:S:155:TRP:HB3	2.11	0.52
3:H:118:ARG:HD3	3:H:120:LEU:HD12	1.91	0.52
2:S:268:TRP:HE1	3:T:35:ASN:ND2	2.08	0.52
3:H:97:PRO:O	3:H:98:HIS:HD2	1.93	0.52
1:R:101:ALA:O	1:R:104:GLU:HB2	2.10	0.52
4:C:100:MET:HG3	10:C:1009:HEM:C4C	2.45	0.51
1:R:150:ILE:O	7:R:2004:BCL:HED1	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:49:ILE:HG13	1:R:89:ILE:HD13	1.93	0.51
3:T:189:ARG:HH11	3:T:189:ARG:HG2	1.74	0.51
2:M:55:LEU:H	2:M:55:LEU:HD22	1.75	0.51
4:D:46:ARG:NH1	4:D:51:GLN:HB2	2.25	0.51
1:R:50:ALA:O	1:R:53:ALA:HB3	2.10	0.51
2:S:214:LEU:O	2:S:217:ALA:HB3	2.11	0.51
3:H:114:TRP:HZ3	3:H:228:LEU:HD11	1.75	0.51
1:R:262:TRP:O	1:R:265:TRP:HD1	1.92	0.51
1:R:187:LEU:CD1	2:S:269:ALA:HB1	2.40	0.51
2:S:300:ASN:HD22	2:S:300:ASN:N	2.09	0.51
1:L:226:THR:O	1:L:229:ILE:HG22	2.09	0.51
3:T:112:ALA:HA	3:T:235:GLY:O	2.11	0.51
3:T:36:MET:HE1	3:T:58:LEU:HD23	1.92	0.51
1:R:244:SER:CB	7:R:2002:BCL:HBA2	2.41	0.51
1:R:246:LEU:O	1:R:250:ILE:HG23	2.10	0.51
2:M:160:LEU:HD22	2:M:185:TRP:CH2	2.46	0.51
12:S:2027:HOH:O	3:T:34:GLU:HG3	2.10	0.51
1:R:141:ALA:HB3	1:R:144:TYR:CD2	2.46	0.51
2:S:293:ASN:HD22	4:D:13:ASN:HB3	1.76	0.51
2:M:148:TRP:O	2:M:151:LEU:HB3	2.09	0.51
1:R:193:LEU:HD22	1:R:212:GLU:HG3	1.92	0.51
1:R:183:ASN:ND2	2:S:213:ALA:HA	2.26	0.51
1:R:124:ALA:O	1:R:127:ALA:HB3	2.11	0.51
4:D:11:ALA:O	4:D:14:GLN:HG2	2.11	0.51
7:L:1004:BCL:HBB3	8:M:1006:BPH:H152	1.92	0.51
3:H:112:ALA:HA	3:H:235:GLY:O	2.11	0.51
3:H:168:TRP:CE2	3:H:190:LEU:HD21	2.46	0.50
1:L:82:LYS:HA	12:L:1027:HOH:O	2.11	0.50
3:H:50:ALA:C	3:H:52:ASN:H	2.13	0.50
1:L:128:TYR:CZ	1:L:132:VAL:HG21	2.46	0.50
3:H:226:THR:OG1	3:H:229:GLU:HG3	2.11	0.50
3:T:106:LYS:HA	3:T:106:LYS:HE2	1.92	0.50
7:S:2001:BCL:HBC1	7:S:2003:BCL:CB	2.41	0.50
1:L:177:ILE:HG12	7:L:1002:BCL:HMB3	1.93	0.50
3:H:245:ALA:N	3:H:246:PRO:CD	2.74	0.50
3:T:146:LYS:HD3	3:T:146:LYS:N	2.27	0.50
1:L:80:LEU:O	1:L:85:LEU:HG	2.11	0.50
3:H:114:TRP:CZ3	3:H:228:LEU:HD11	2.46	0.50
1:R:74:GLY:O	1:R:141:ALA:HA	2.11	0.50
3:T:225:VAL:CG2	3:T:229:GLU:HB2	2.42	0.50
2:M:88:ASP:HB2	2:M:92:PHE:CZ	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:165:VAL:HG23	3:T:182:GLU:H	1.76	0.50
3:H:163:LYS:C	3:H:181:VAL:HG23	2.31	0.50
3:T:189:ARG:HD2	3:T:216:ILE:CG2	2.41	0.50
3:H:32:GLN:HG2	3:H:56:PHE:CD2	2.47	0.50
3:T:83:ARG:O	3:T:83:ARG:HG3	2.10	0.50
2:S:79:GLY:C	2:S:81:ASN:H	2.14	0.50
2:S:72:ILE:CG2	2:S:73:TRP:N	2.75	0.50
1:L:153:HIS:O	1:L:157:VAL:HG23	2.12	0.50
3:H:73:LEU:CD2	3:H:75:VAL:HG13	2.42	0.50
2:M:265:ILE:O	2:M:268:TRP:HB2	2.12	0.50
1:R:31:VAL:HG12	1:R:32:GLY:N	2.26	0.50
4:D:66:ALA:C	4:D:68:GLY:H	2.16	0.50
1:L:170:ASN:HB3	1:L:173:HIS:HB3	1.93	0.49
2:S:55:LEU:HD22	2:S:55:LEU:H	1.75	0.49
2:S:274:VAL:HG23	2:S:275:LEU:N	2.26	0.49
3:T:180:GLU:HG3	3:T:188:THR:OG1	2.12	0.49
2:S:202:HIS:O	2:S:206:ILE:HG13	2.12	0.49
3:T:209:SER:H	3:T:212:LEU:HD12	1.76	0.49
2:S:195:ASN:ND2	2:S:195:ASN:C	2.58	0.49
2:M:35:PHE:CE1	2:M:37:THR:HB	2.47	0.49
2:S:66:TRP:NE1	2:S:70:ILE:HD11	2.28	0.49
3:H:122:GLU:HB2	3:H:227:LEU:HD21	1.94	0.49
3:T:133:PRO:O	3:T:136:ALA:N	2.46	0.49
1:L:169:TYR:HE1	2:M:180:PHE:CD2	2.30	0.49
1:R:105:VAL:O	1:R:109:ARG:HD3	2.12	0.49
4:D:21:ILE:HD12	4:D:30:ALA:HB3	1.94	0.49
2:M:280:GLY:CA	7:M:1003:BCL:HED3	2.43	0.49
2:M:206:ILE:HG23	7:M:1003:BCL:HMB3	1.94	0.49
1:R:28:PRO:O	2:S:254:TRP:HA	2.11	0.49
4:C:46:ARG:HG2	4:C:47:THR:N	2.27	0.49
1:L:241:VAL:HG21	8:M:1006:BPH:CAC	2.37	0.49
4:D:118:GLN:HA	4:D:122:VAL:CG2	2.43	0.49
2:S:275:LEU:HD23	2:S:278:LEU:HD12	1.95	0.49
3:H:73:LEU:HD22	3:H:75:VAL:HG13	1.93	0.49
2:M:155:TRP:O	2:M:159:VAL:HG23	2.11	0.49
1:R:46:ILE:HD13	7:R:2004:BCL:H201	1.95	0.49
2:S:191:LEU:HD22	2:S:191:LEU:N	2.28	0.49
3:H:120:LEU:N	3:H:226:THR:HB	2.28	0.49
1:R:117:ILE:HD13	2:S:251:PHE:CE2	2.48	0.49
2:S:46:GLN:HG2	2:S:51:TYR:HA	1.95	0.49
1:L:130:THR:HA	1:L:134:PHE:HD2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:169:TYR:CE2	1:R:260:VAL:HG23	2.48	0.49
2:S:271:TRP:O	2:S:275:LEU:HG	2.12	0.49
1:R:263:TRP:CD2	2:S:180:PHE:HZ	2.31	0.49
1:L:65:SER:HB2	1:L:152:THR:HG21	1.94	0.48
1:L:22:PHE:HA	1:L:24:PHE:CE2	2.47	0.48
1:R:179:PHE:HB3	1:R:240:ALA:HB2	1.95	0.48
3:T:124:ASP:OD1	3:T:125:GLY:N	2.46	0.48
4:D:91:THR:HG23	4:D:93:ASP:N	2.28	0.48
1:R:117:ILE:HB	1:R:118:PRO:CD	2.43	0.48
1:L:87:GLN:O	1:L:91:ILE:HG12	2.13	0.48
2:M:120:PHE:O	2:M:124:VAL:HG23	2.12	0.48
12:L:1007:HOH:O	3:H:81:GLU:HB2	2.14	0.48
3:T:181:VAL:O	3:T:181:VAL:HG13	2.14	0.48
2:M:152:SER:OG	2:M:278:LEU:HG	2.13	0.48
4:D:76:PHE:O	4:D:80:VAL:HG22	2.14	0.48
2:M:195:ASN:C	2:M:195:ASN:ND2	2.63	0.48
3:T:44:ASN:C	3:T:46:ASP:H	2.16	0.48
7:R:2002:BCL:H142	7:R:2004:BCL:HBB2	1.96	0.48
2:S:241:ARG:NH2	3:T:79:GLU:OE2	2.44	0.48
3:T:110:GLY:C	3:T:112:ALA:H	2.16	0.48
3:T:219:ILE:O	3:T:219:ILE:HG13	2.13	0.48
3:T:73:LEU:HD22	3:T:74:THR:N	2.28	0.48
1:L:124:ALA:O	7:L:1002:BCL:H51	2.13	0.48
3:H:17:ILE:HG23	3:H:18:TYR:N	2.29	0.48
1:L:6:GLU:HG3	2:M:250:LEU:CD2	2.44	0.48
3:T:70:ARG:NH2	3:T:123:LEU:HD13	2.29	0.48
3:H:32:GLN:HG2	3:H:56:PHE:CE2	2.48	0.48
4:D:83:PRO:O	4:D:86:PHE:HB3	2.13	0.48
2:S:191:LEU:CD2	2:S:191:LEU:H	2.26	0.47
3:T:161:ALA:HB2	3:T:210:SER:CB	2.43	0.47
1:R:272:TRP:HA	1:R:275:ILE:HG13	1.95	0.47
2:S:232:GLU:N	2:S:232:GLU:OE1	2.47	0.47
1:R:132:VAL:HG13	1:R:146:PHE:CE1	2.49	0.47
1:L:117:ILE:HB	1:L:118:PRO:CD	2.44	0.47
2:M:199:ASN:OD1	2:M:201:PHE:N	2.48	0.47
1:L:3:LEU:C	1:L:5:PHE:H	2.18	0.47
2:S:122:MET:O	2:S:126:VAL:HG23	2.15	0.47
1:R:166:ASN:OD1	1:R:168:HIS:HB2	2.14	0.47
2:S:50:ILE:HD12	2:S:50:ILE:C	2.34	0.47
3:T:83:ARG:O	3:T:85:ILE:HD12	2.15	0.47
2:S:209:LEU:HD22	7:S:2003:BCL:H3A	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:219:ILE:HA	3:H:229:GLU:OE2	2.15	0.47
3:T:36:MET:CE	3:T:58:LEU:HD23	2.44	0.47
1:L:38:THR:HG21	1:L:100:TRP:HE3	1.80	0.47
2:S:91:PHE:N	2:S:91:PHE:CD1	2.83	0.47
3:H:170:ASP:OD2	3:H:172:PRO:HG2	2.13	0.47
1:R:187:LEU:HD11	2:S:269:ALA:CB	2.42	0.47
4:D:100:MET:HG3	10:D:2009:HEM:C4C	2.49	0.47
2:S:156:LEU:HD13	7:S:2003:BCL:H43	1.97	0.47
1:R:182:THR:O	1:R:183:ASN:C	2.53	0.47
3:H:180:GLU:HA	3:H:189:ARG:O	2.15	0.47
3:H:87:LEU:HD21	3:H:109:VAL:HG21	1.96	0.47
2:S:134:TYR:CE1	2:S:144:LYS:HG3	2.50	0.47
3:T:165:VAL:HB	3:T:180:GLU:HG2	1.97	0.47
1:L:3:LEU:HD23	3:H:42:LEU:HD21	1.96	0.47
3:T:243:TYR:O	3:T:246:PRO:HD2	2.15	0.47
3:H:50:ALA:O	3:H:52:ASN:N	2.44	0.47
3:T:32:GLN:HG2	3:T:56:PHE:CE2	2.50	0.47
1:R:75:LEU:HA	1:R:142:TRP:CD1	2.50	0.46
4:C:46:ARG:O	4:C:70:ALA:HA	2.15	0.46
1:R:157:VAL:O	1:R:158:SER:C	2.52	0.46
4:D:51:GLN:C	4:D:51:GLN:NE2	2.68	0.46
3:T:154:ARG:HB3	3:T:160:ILE:HA	1.98	0.46
2:S:175:VAL:HB	11:S:2011:LDA:O1	2.15	0.46
1:R:135:ARG:NH1	1:R:248:MET:O	2.48	0.46
4:D:57:TYR:HA	10:D:2009:HEM:O1D	2.15	0.46
4:D:38:PRO:HB3	4:D:54:PHE:CD2	2.50	0.46
2:M:69:THR:O	2:M:72:ILE:HG22	2.16	0.46
4:C:17:THR:HA	4:C:32:ARG:HH12	1.81	0.46
2:M:278:LEU:O	2:M:279:THR:C	2.53	0.46
1:L:3:LEU:HD23	3:H:42:LEU:CD2	2.45	0.46
7:L:1004:BCL:HMD2	7:M:1003:BCL:HBB3	1.98	0.46
3:H:83:ARG:O	3:H:85:ILE:HD12	2.15	0.46
1:L:50:ALA:O	1:L:53:ALA:HB3	2.15	0.46
1:L:8:LYS:O	3:H:110:GLY:N	2.43	0.46
1:L:244:SER:HB3	7:L:1002:BCL:HED3	1.97	0.46
3:H:122:GLU:OE2	3:H:130:LYS:HD3	2.16	0.46
4:C:29:ILE:N	4:C:29:ILE:CD1	2.79	0.46
2:S:229:PHE:O	2:S:244:ALA:HB2	2.16	0.46
3:H:181:VAL:O	3:H:181:VAL:HG13	2.16	0.46
3:T:17:ILE:HG23	3:T:18:TYR:N	2.31	0.46
1:R:207:ARG:N	1:R:207:ARG:HD2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:300:ASN:ND2	2:M:300:ASN:N	2.64	0.46
3:T:32:GLN:HG2	3:T:56:PHE:CD2	2.51	0.46
3:T:154:ARG:NH1	3:T:158:LEU:HB3	2.31	0.46
7:R:2004:BCL:H3A	7:R:2004:BCL:HBA2	1.66	0.46
3:T:157:ASP:C	3:T:159:GLU:H	2.19	0.46
1:R:185:LEU:O	1:R:185:LEU:HD12	2.16	0.46
2:S:204:LEU:O	2:S:207:ALA:HB3	2.16	0.46
4:D:33:ASN:HD21	4:D:35:LYS:NZ	2.14	0.46
2:S:300:ASN:N	2:S:300:ASN:ND2	2.64	0.45
1:R:200:PRO:HB3	1:R:207:ARG:HD3	1.98	0.45
1:R:7:ARG:HG3	1:R:7:ARG:NH1	2.30	0.45
2:S:266:HIS:O	2:S:270:ILE:HG22	2.14	0.45
1:L:135:ARG:HD3	12:L:1006:HOH:O	2.16	0.45
1:R:115:TYR:O	1:R:116:HIS:C	2.54	0.45
4:C:10:LYS:O	4:C:13:ASN:HB2	2.16	0.45
1:R:135:ARG:HG3	1:R:135:ARG:HH11	1.80	0.45
1:R:162:TYR:OH	2:S:191:LEU:CD2	2.65	0.45
1:L:49:ILE:HG12	1:L:89:ILE:HD13	1.97	0.45
1:L:217:ARG:HD3	12:L:1021:HOH:O	2.16	0.45
1:R:166:ASN:ND2	2:S:187:ASN:CB	2.77	0.45
3:H:83:ARG:HH21	3:H:114:TRP:HE1	1.65	0.45
3:H:221:SER:OG	3:H:224:GLU:HG2	2.16	0.45
1:L:268:LYS:HA	1:L:273:ALA:HB2	1.97	0.45
4:C:93:ASP:OD1	4:C:95:LYS:HG2	2.16	0.45
2:M:206:ILE:HG22	2:M:210:TYR:CE2	2.52	0.45
3:T:165:VAL:HG21	3:T:182:GLU:HB2	1.98	0.45
2:M:148:TRP:CE3	2:M:148:TRP:HA	2.51	0.45
2:S:178:GLY:HA3	2:S:181:SER:OG	2.17	0.45
1:R:55:LEU:HD13	1:R:81:ALA:HB2	1.99	0.45
3:T:50:ALA:C	3:T:52:ASN:H	2.19	0.45
3:T:149:ILE:HA	3:T:164:VAL:HG12	1.99	0.45
4:D:116:TYR:O	4:D:120:VAL:HG22	2.16	0.45
4:C:87:LEU:O	4:C:91:THR:CG2	2.65	0.45
3:H:229:GLU:O	3:H:233:ILE:HG13	2.17	0.45
2:M:153:ALA:HA	2:M:277:THR:HG21	1.99	0.45
2:S:149:ALA:O	2:S:152:SER:HB3	2.17	0.45
3:H:201:ASN:OD1	3:H:202:ARG:NH1	2.49	0.45
1:R:6:GLU:HG3	2:S:250:LEU:HD21	1.97	0.45
4:C:19:HIS:HE1	4:C:38:PRO:HD2	1.82	0.45
1:L:49:ILE:CG1	1:L:89:ILE:HD13	2.47	0.45
3:T:181:VAL:HG12	3:T:191:LEU:HD23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:7:ARG:O	1:L:9:TYR:N	2.50	0.45
1:L:208:THR:C	1:L:210:ASP:N	2.71	0.45
3:H:173:GLU:HG2	12:H:276:HOH:O	2.17	0.45
1:R:233:GLY:HA3	2:S:216:PHE:CZ	2.52	0.45
2:M:55:LEU:N	2:M:55:LEU:HD22	2.32	0.44
3:H:20:PHE:O	3:H:23:PHE:HB3	2.16	0.44
1:R:216:PHE:HE2	1:R:224:ILE:HG22	1.82	0.44
1:L:193:LEU:CD1	1:L:216:PHE:HB2	2.45	0.44
3:H:163:LYS:O	3:H:181:VAL:HG23	2.17	0.44
2:S:204:LEU:HD13	3:T:20:PHE:CE2	2.53	0.44
2:M:154:ILE:HG23	2:M:157:TRP:HE3	1.83	0.44
3:H:79:GLU:CG	3:H:81:GLU:HG2	2.47	0.44
3:H:81:GLU:HG3	3:H:81:GLU:O	2.16	0.44
3:T:106:LYS:HA	3:T:106:LYS:CE	2.46	0.44
3:T:44:ASN:C	3:T:46:ASP:N	2.71	0.44
3:H:148:PRO:O	3:H:164:VAL:HB	2.17	0.44
3:T:240:GLY:O	3:T:244:ALA:N	2.44	0.44
1:L:195:LEU:HD21	2:M:267:ARG:HG3	1.99	0.44
1:L:44:LEU:HD23	1:L:92:CYS:SG	2.58	0.44
2:S:36:SER:O	2:S:39:LEU:HB3	2.18	0.44
4:D:58:GLY:HA2	4:D:99:LYS:HE2	1.99	0.44
1:R:94:THR:HG23	1:R:129:LEU:HD21	1.98	0.44
4:C:114:TRP:HA	4:C:117:LEU:HD12	1.98	0.44
2:S:300:ASN:C	2:S:301:HIS:ND1	2.71	0.44
3:H:225:VAL:HG23	3:H:229:GLU:CB	2.46	0.44
3:T:169:VAL:HG12	3:T:170:ASP:N	2.32	0.44
2:S:228:ARG:C	2:S:230:GLY:H	2.21	0.44
7:L:1004:BCL:HBA2	7:L:1004:BCL:H3A	1.67	0.44
2:M:162:PHE:O	2:M:166:ILE:HG13	2.18	0.44
4:D:38:PRO:HD3	4:D:54:PHE:CZ	2.53	0.44
2:M:219:HIS:HA	9:M:1008:U10:O2	2.17	0.44
2:S:243:THR:HG23	2:S:244:ALA:N	2.33	0.44
2:S:73:TRP:HE3	2:S:114:LEU:HD12	1.83	0.44
1:R:130:THR:HA	1:R:134:PHE:HD2	1.82	0.44
2:S:131:GLY:O	2:S:135:LEU:HG	2.17	0.44
3:H:170:ASP:OD2	3:H:173:GLU:HB2	2.18	0.44
3:H:146:LYS:H	3:H:146:LYS:CD	2.23	0.44
2:S:73:TRP:CE3	2:S:114:LEU:HD12	2.53	0.44
3:T:154:ARG:HD2	3:T:158:LEU:O	2.18	0.44
2:M:237:GLN:HB2	2:M:262:MET:HG2	1.99	0.44
2:S:204:LEU:HG	11:S:2010:LDA:HM11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:224:ILE:HG12	1:R:228:GLY:HA3	2.00	0.44
2:S:89:LEU:HA	2:S:92:PHE:CD2	2.53	0.44
4:C:23:ASP:HA	4:C:41:TYR:CD2	2.53	0.44
1:L:150:ILE:HG22	1:L:151:TRP:N	2.32	0.44
7:R:2002:BCL:HBA1	7:R:2004:BCL:HBC1	2.00	0.44
1:L:170:ASN:HB3	1:L:173:HIS:HB2	2.00	0.44
3:H:165:VAL:HG23	3:H:182:GLU:H	1.83	0.44
1:R:111:LEU:HD21	2:S:254:TRP:CZ3	2.52	0.44
3:H:14:SER:O	3:H:17:ILE:HG22	2.18	0.44
1:R:49:ILE:CG1	1:R:89:ILE:HD13	2.48	0.43
2:M:280:GLY:C	7:M:1003:BCL:CED	2.86	0.43
2:M:290:VAL:HG11	3:H:12:LEU:HB3	1.99	0.43
1:R:230:HIS:CD2	2:S:223:ILE:HG13	2.53	0.43
1:R:94:THR:CG2	1:R:129:LEU:HD21	2.48	0.43
2:M:164:ARG:HH11	2:M:164:ARG:HG2	1.83	0.43
1:R:148:TYR:HB3	8:S:2006:BPH:H161	2.00	0.43
3:H:66:LEU:HD12	3:H:66:LEU:H	1.83	0.43
3:H:133:PRO:HG3	3:H:168:TRP:CE2	2.54	0.43
2:S:293:ASN:ND2	4:D:13:ASN:HB3	2.32	0.43
1:L:100:TRP:O	1:L:104:GLU:HG3	2.19	0.43
3:T:20:PHE:O	3:T:23:PHE:HB3	2.18	0.43
1:R:209:PRO:O	1:R:212:GLU:HB3	2.17	0.43
2:S:52:LEU:O	2:S:56:GLY:HA3	2.18	0.43
2:M:200:PRO:HB2	3:H:17:ILE:CD1	2.49	0.43
2:S:96:PRO:HG3	2:S:115:TRP:CE2	2.53	0.43
2:S:162:PHE:O	2:S:165:PRO:HD2	2.18	0.43
4:C:33:ASN:HA	12:C:1010:HOH:O	2.17	0.43
1:L:128:TYR:CE2	1:L:132:VAL:HG21	2.54	0.43
3:T:85:ILE:HD12	3:T:85:ILE:N	2.33	0.43
1:R:153:HIS:O	1:R:156:TRP:HB3	2.18	0.43
1:L:97:PHE:CE1	7:L:1002:BCL:H121	2.53	0.43
1:L:7:ARG:HH11	1:L:7:ARG:HG3	1.84	0.43
2:S:120:PHE:O	2:S:124:VAL:HG23	2.18	0.43
1:R:49:ILE:HD11	8:S:2006:BPH:H122	2.01	0.43
2:S:93:SER:HB2	2:S:181:SER:HB3	2.00	0.43
1:R:130:THR:HA	1:R:134:PHE:CD2	2.53	0.43
2:M:268:TRP:HE1	3:H:35:ASN:ND2	2.17	0.43
1:R:170:ASN:O	1:R:174:MET:HG3	2.18	0.43
2:S:150:PHE:CE2	2:S:154:ILE:HD11	2.54	0.43
2:S:199:ASN:ND2	2:S:294:TRP:CZ2	2.87	0.43
3:T:227:LEU:O	3:T:230:GLU:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:67:PRO:O	3:T:68:HIS:HB2	2.18	0.43
2:S:195:ASN:ND2	2:S:197:PHE:N	2.55	0.43
1:R:217:ARG:HD3	12:R:2011:HOH:O	2.19	0.43
1:R:107:ILE:HG23	2:S:254:TRP:HE3	1.84	0.42
2:S:268:TRP:CE3	3:T:31:LEU:HD13	2.54	0.42
2:S:297:TRP:NE1	3:T:13:ALA:HB3	2.33	0.42
2:M:258:PHE:H	2:M:258:PHE:HD2	1.67	0.42
3:H:37:ARG:HB3	3:H:75:VAL:HB	2.01	0.42
2:S:200:PRO:HB2	3:T:17:ILE:HD13	2.01	0.42
2:M:157:TRP:HD1	7:M:1001:BCL:HBB1	1.84	0.42
3:T:79:GLU:HG3	3:T:81:GLU:HG2	2.01	0.42
3:T:188:THR:O	3:T:189:ARG:HG2	2.18	0.42
4:D:59:GLU:O	4:D:63:GLU:HG3	2.19	0.42
7:M:1003:BCL:HAA2	7:M:1003:BCL:HBD	2.01	0.42
4:D:109:ASP:O	4:D:110:ALA:C	2.58	0.42
1:R:111:LEU:HD21	2:S:254:TRP:HH2	1.83	0.42
3:T:173:GLU:O	3:T:174:GLN:HB3	2.19	0.42
1:L:117:ILE:HB	12:L:1016:HOH:O	2.18	0.42
1:R:33:PHE:O	1:R:36:VAL:HG22	2.19	0.42
1:L:185:LEU:CD2	1:L:189:LEU:HD12	2.49	0.42
3:T:134:MET:HB2	3:T:167:ILE:O	2.19	0.42
2:M:214:LEU:HG	2:M:215:LEU:N	2.34	0.42
1:R:238:LEU:O	1:R:239:SER:C	2.58	0.42
3:T:130:LYS:HG3	3:T:172:PRO:CG	2.41	0.42
2:M:195:ASN:HD21	2:M:197:PHE:CB	2.27	0.42
2:M:271:TRP:HA	2:M:274:VAL:CG2	2.49	0.42
2:M:270:ILE:HG23	2:M:271:TRP:H	1.83	0.42
2:S:162:PHE:O	2:S:166:ILE:HG13	2.19	0.42
3:H:83:ARG:HG3	3:H:83:ARG:HH11	1.84	0.42
1:L:90:THR:HG22	1:L:90:THR:O	2.18	0.42
1:R:173:HIS:HE1	1:R:177:ILE:HD11	1.80	0.42
1:R:169:TYR:HE1	2:S:180:PHE:CD2	2.38	0.42
3:T:26:GLY:O	3:T:29:TYR:HB3	2.20	0.42
2:M:148:TRP:HA	2:M:148:TRP:HE3	1.84	0.42
4:C:41:TYR:O	4:C:46:ARG:NH2	2.53	0.42
3:T:154:ARG:HD2	3:T:158:LEU:HA	2.00	0.42
2:M:133:THR:HG21	2:M:146:THR:HG22	2.01	0.42
2:S:150:PHE:O	2:S:154:ILE:HG13	2.19	0.42
3:H:157:ASP:HA	3:H:249:LYS:HG2	2.01	0.42
3:H:159:GLU:HB2	3:H:210:SER:HG	1.84	0.42
3:T:66:LEU:HD12	3:T:66:LEU:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:125:ILE:O	1:R:128:TYR:HB3	2.20	0.42
2:S:195:ASN:HD21	2:S:197:PHE:CB	2.28	0.42
4:D:91:THR:HG23	4:D:93:ASP:H	1.84	0.42
4:C:57:TYR:HA	10:C:1009:HEM:O1D	2.20	0.42
3:H:233:ILE:O	3:H:236:TYR:N	2.53	0.42
1:L:269:LEU:HD12	1:L:272:TRP:CZ2	2.55	0.42
3:T:191:LEU:HA	3:T:192:PRO:HD3	1.83	0.42
2:M:55:LEU:CD2	2:M:55:LEU:H	2.33	0.42
1:R:34:PHE:CZ	1:R:102:LEU:HD13	2.55	0.42
2:S:75:TRP:O	2:S:76:TYR:C	2.58	0.42
1:L:41:PHE:O	1:L:42:ALA:C	2.58	0.42
2:S:279:THR:O	2:S:282:ILE:HB	2.20	0.42
3:H:209:SER:O	3:H:213:PHE:HD1	2.02	0.42
1:R:79:PRO:O	1:R:80:LEU:C	2.57	0.42
4:C:51:GLN:NE2	4:C:53:ASP:N	2.64	0.42
1:L:229:ILE:CG2	1:L:230:HIS:N	2.82	0.42
3:H:149:ILE:HA	3:H:164:VAL:HG12	2.01	0.42
1:R:177:ILE:HD13	7:S:2001:BCL:HMD1	2.02	0.41
2:S:199:ASN:HB3	2:S:202:HIS:HB3	2.02	0.41
1:R:6:GLU:HG3	2:S:250:LEU:HD22	2.01	0.41
3:H:149:ILE:HA	3:H:164:VAL:CG1	2.50	0.41
2:M:95:GLU:OE1	2:M:176:PRO:HB3	2.19	0.41
1:L:141:ALA:HB1	12:L:1018:HOH:O	2.20	0.41
1:L:116:HIS:O	1:L:119:PHE:HB3	2.19	0.41
2:M:91:PHE:N	2:M:91:PHE:CD1	2.88	0.41
1:L:215:PHE:HD1	2:M:140:LEU:HD12	1.85	0.41
1:R:80:LEU:O	1:R:85:LEU:HG	2.21	0.41
2:S:191:LEU:CD2	2:S:191:LEU:N	2.83	0.41
3:H:66:LEU:N	3:H:66:LEU:CD1	2.83	0.41
4:D:32:ARG:O	4:D:33:ASN:HB3	2.19	0.41
2:M:204:LEU:HG	11:M:1010:LDA:HM11	2.03	0.41
1:R:185:LEU:C	1:R:185:LEU:HD12	2.41	0.41
2:M:156:LEU:HD12	2:M:277:THR:HG22	2.02	0.41
3:H:225:VAL:HA	3:H:229:GLU:OE1	2.20	0.41
3:T:117:ARG:O	3:T:228:LEU:HB2	2.20	0.41
2:S:50:ILE:O	2:S:50:ILE:HD12	2.21	0.41
1:R:147:PRO:HD2	1:R:156:TRP:HB2	2.02	0.41
3:H:141:HIS:CD2	3:H:143:SER:HB3	2.56	0.41
1:L:69:PRO:O	1:L:70:ALA:C	2.59	0.41
1:R:238:LEU:HD23	8:S:2006:BPH:CBC	2.51	0.41
2:M:235:LEU:O	2:M:238:ILE:HB	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:49:GLY:HA2	4:D:57:TYR:CD1	2.56	0.41
2:S:69:THR:O	2:S:72:ILE:HG22	2.19	0.41
1:R:94:THR:O	1:R:98:VAL:HG23	2.21	0.41
2:M:232:GLU:OE1	2:M:232:GLU:N	2.54	0.41
7:R:2002:BCL:HBD	7:R:2004:BCL:HBC3	2.01	0.41
2:M:123:PHE:HA	2:M:157:TRP:HH2	1.85	0.41
4:D:16:GLN:HE21	4:D:32:ARG:HG3	1.86	0.41
2:M:167:LEU:HD12	2:M:285:LEU:HD11	2.01	0.41
3:H:153:VAL:HG22	3:H:203:VAL:HB	2.03	0.41
4:D:43:VAL:HG13	4:D:44:VAL:N	2.36	0.41
7:L:1002:BCL:H2C	7:M:1003:BCL:H2C	2.02	0.41
3:H:171:ILE:N	3:H:172:PRO:HD2	2.36	0.41
3:H:146:LYS:N	3:H:146:LYS:HD3	2.25	0.41
2:S:191:LEU:HD22	2:S:191:LEU:H	1.86	0.41
2:M:110:LYS:O	2:M:111:GLU:HG3	2.20	0.41
4:D:116:TYR:CZ	4:D:120:VAL:HG21	2.55	0.41
3:T:87:LEU:HD21	3:T:109:VAL:HG21	2.03	0.41
1:R:96:ALA:HB1	8:S:2006:BPH:H2	2.02	0.41
2:M:280:GLY:C	7:M:1003:BCL:HED3	2.41	0.41
1:R:229:ILE:CG2	1:R:230:HIS:N	2.83	0.41
2:S:234:GLU:O	2:S:238:ILE:HG13	2.21	0.41
3:T:37:ARG:NE	3:T:62:LYS:HD2	2.36	0.41
7:S:2001:BCL:HHC	7:S:2001:BCL:HBB2	2.03	0.41
1:L:166:ASN:HD21	2:M:187:ASN:HB2	1.83	0.41
3:T:159:GLU:HG3	12:T:268:HOH:O	2.21	0.41
3:T:70:ARG:HH22	3:T:123:LEU:CD1	2.34	0.41
2:S:79:GLY:C	2:S:81:ASN:N	2.74	0.41
2:M:278:LEU:HD23	2:M:278:LEU:HA	1.94	0.41
2:S:224:LEU:HA	2:S:227:SER:HB3	2.02	0.41
2:M:98:ALA:HB1	2:M:99:PRO:HD2	2.03	0.41
2:S:296:VAL:O	2:S:297:TRP:C	2.57	0.41
3:T:110:GLY:O	3:T:112:ALA:N	2.53	0.41
1:L:26:VAL:HG23	1:L:31:VAL:CG2	2.50	0.41
2:M:261:THR:O	2:M:262:MET:C	2.59	0.41
4:C:82:ASP:OD2	4:C:103:LYS:HE2	2.21	0.41
2:S:156:LEU:HD12	2:S:277:THR:HG22	2.03	0.40
7:L:1002:BCL:HBC2	7:M:1003:BCL:HBC2	2.02	0.40
2:M:154:ILE:HG22	2:M:158:MET:HG2	2.03	0.40
2:S:148:TRP:CE3	2:S:148:TRP:HA	2.56	0.40
1:R:17:VAL:HB	1:R:33:PHE:CD2	2.56	0.40
3:T:89:ARG:HA	3:T:98:HIS:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:154:ILE:HG23	2:S:157:TRP:HE3	1.85	0.40
1:L:208:THR:C	1:L:210:ASP:H	2.24	0.40
1:R:117:ILE:HG21	2:S:251:PHE:CZ	2.56	0.40
4:C:17:THR:HG22	4:C:17:THR:O	2.21	0.40
2:M:214:LEU:O	2:M:217:ALA:HB3	2.21	0.40
1:L:231:ARG:O	1:L:235:LEU:HB2	2.21	0.40
1:R:155:ASP:HA	12:R:2018:HOH:O	2.21	0.40
1:R:12:PRO:HD3	3:T:97:PRO:HB3	2.02	0.40
1:R:128:TYR:CE2	1:R:132:VAL:HG21	2.56	0.40
2:S:196:LEU:HD23	2:S:196:LEU:HA	1.94	0.40
1:R:3:LEU:O	1:R:5:PHE:N	2.55	0.40
3:H:81:GLU:O	3:H:81:GLU:CG	2.69	0.40
2:S:95:GLU:HA	2:S:96:PRO:HD3	1.91	0.40
1:R:232:LEU:O	1:R:236:LEU:HG	2.21	0.40
1:R:22:PHE:O	1:R:24:PHE:N	2.55	0.40
2:S:55:LEU:CD2	2:S:55:LEU:H	2.34	0.40
3:T:70:ARG:NH2	3:T:123:LEU:CD1	2.85	0.40
1:R:100:TRP:O	1:R:104:GLU:HG3	2.22	0.40
1:L:268:LYS:HA	1:L:273:ALA:CB	2.51	0.40
4:D:113:ILE:O	4:D:117:LEU:HG	2.21	0.40
2:M:189:PHE:CD1	2:M:189:PHE:C	2.95	0.40
1:L:180:PHE:HE2	7:L:1002:BCL:HMA2	1.87	0.40
2:M:206:ILE:HG12	7:M:1003:BCL:CHB	2.52	0.40
3:H:233:ILE:O	3:H:234:CYS:C	2.60	0.40
4:D:19:HIS:HE1	4:D:38:PRO:HD2	1.86	0.40
1:L:168:HIS:HB3	2:M:183:LEU:HD13	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	279/281 (99%)	227 (81%)	46 (16%)	6 (2%)	8	43
1	R	279/281 (99%)	231 (83%)	36 (13%)	12 (4%)	3	25
2	M	265/307 (86%)	228 (86%)	36 (14%)	1 (0%)	39	78
2	S	265/307 (86%)	220 (83%)	42 (16%)	3 (1%)	17	60
3	H	244/260 (94%)	198 (81%)	42 (17%)	4 (2%)	12	52
3	T	244/260 (94%)	199 (82%)	37 (15%)	8 (3%)	5	32
4	C	122/124 (98%)	109 (89%)	12 (10%)	1 (1%)	24	66
4	D	122/124 (98%)	105 (86%)	16 (13%)	1 (1%)	24	66
All	All	1820/1944 (94%)	1517 (83%)	267 (15%)	36 (2%)	9	46

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	R	7	ARG
1	R	23	ASP
1	R	116	HIS
3	T	80	SER
3	T	89	ARG
1	L	5	PHE
1	L	7	ARG
1	L	8	LYS
3	H	81	GLU
3	H	233	ILE
3	H	250	SER
1	R	4	SER
1	R	259	TRP
3	T	116	ALA
3	T	128	HIS
3	T	172	PRO
1	L	4	SER
1	L	20	ASN
1	L	272	TRP
2	M	278	LEU
3	H	172	PRO
1	R	15	THR
1	R	271	TRP
2	S	195	ASN
2	S	218	MET
1	R	31	VAL
1	R	117	ILE

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Mol	Chain	Res	Type
1	R	134	PHE
2	S	85	PHE
3	T	134	MET
3	T	158	LEU
4	D	67	LYS
4	C	83	PRO
3	T	111	PRO
1	R	150	ILE
1	R	19	GLY

### 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%)	216 (98%)	4 (2%)	66	88
1	R	220/220 (100%)	213 (97%)	7 (3%)	46	80
2	M	209/240 (87%)	199 (95%)	10 (5%)	31	71
2	S	209/240 (87%)	202 (97%)	7 (3%)	45	79
3	H	199/208 (96%)	191 (96%)	8 (4%)	38	76
3	T	199/208 (96%)	194 (98%)	5 (2%)	55	84
4	C	93/93 (100%)	91 (98%)	2 (2%)	60	86
4	D	93/93 (100%)	92 (99%)	1 (1%)	80	92
All	All	1442/1522 (95%)	1398 (97%)	44 (3%)	47	80

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	21	LEU
1	L	167	PHE
1	L	247	CYS
1	L	272	TRP
2	M	35	PHE
2	M	94	LEU

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Mol	Chain	Res	Type
2	M	100	GLU
2	M	156	LEU
2	M	195	ASN
2	M	196	LEU
2	M	216	PHE
2	M	232	GLU
2	M	258	PHE
2	M	292	ASP
3	H	10	PHE
3	H	52	ASN
3	H	73	LEU
3	H	81	GLU
3	H	106	LYS
3	H	146	LYS
3	H	194	GLN
3	H	231	ASP
4	C	13	ASN
4	C	51	GLN
1	R	7	ARG
1	R	108	CYS
1	R	185	LEU
1	R	235	LEU
1	R	247	CYS
1	R	257	ASP
1	R	272	TRP
2	S	35	PHE
2	S	87	ARG
2	S	91	PHE
2	S	94	LEU
2	S	156	LEU
2	S	195	ASN
2	S	216	PHE
3	T	52	ASN
3	T	73	LEU
3	T	106	LYS
3	T	146	LYS
3	T	194	GLN
4	D	51	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	56	GLN
1	L	87	GLN
1	L	173	HIS
1	L	183	ASN
1	L	211	HIS
2	M	44	ASN
2	M	46	GLN
2	M	195	ASN
2	M	300	ASN
3	H	52	ASN
3	H	98	HIS
3	H	194	GLN
4	C	13	ASN
4	C	16	GLN
4	C	33	ASN
4	C	51	GLN
4	C	81	GLN
1	R	56	GLN
1	R	87	GLN
1	R	173	HIS
1	R	211	HIS
2	S	44	ASN
2	S	46	GLN
2	S	195	ASN
2	S	202	HIS
2	S	300	ASN
3	T	52	ASN
3	T	68	HIS
3	T	194	GLN
4	D	16	GLN
4	D	33	ASN
4	D	51	GLN
4	D	112	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 4 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$
10	HEM	C	1009	4	30,50,50	2.49	10 (33%)	24,82,82	3.11	12 (50%)
10	HEM	D	2009	4	30,50,50	2.51	7 (23%)	24,82,82	3.09	11 (45%)
7	BCL	L	1002	1	53,74,74	1.02	3 (5%)	57,115,115	1.82	17 (29%)
7	BCL	L	1004	1	53,74,74	1.18	5 (9%)	57,115,115	1.72	16 (28%)
8	BPH	L	1005	-	54,60,70	1.45	9 (16%)	61,89,101	2.29	16 (26%)
7	BCL	M	1001	2	37,58,74	1.30	4 (10%)	39,95,115	1.97	12 (30%)
7	BCL	M	1003	2	53,74,74	1.18	3 (5%)	57,115,115	2.05	20 (35%)
8	BPH	M	1006	-	64,70,70	1.50	10 (15%)	73,101,101	2.19	21 (28%)
9	U10	M	1008	-	37,37,63	1.99	10 (27%)	44,47,79	1.84	10 (22%)
11	LDA	M	1010	-	15,15,15	3.83	3 (20%)	16,17,17	2.72	3 (18%)
11	LDA	M	1011	-	15,15,15	4.00	2 (13%)	16,17,17	2.75	4 (25%)
7	BCL	R	2002	1	53,74,74	1.05	2 (3%)	57,115,115	1.89	18 (31%)
7	BCL	R	2004	1	53,74,74	1.17	4 (7%)	57,115,115	1.72	17 (29%)
8	BPH	R	2005	-	54,60,70	1.52	10 (18%)	61,89,101	2.31	18 (29%)
7	BCL	S	2001	2	37,58,74	1.25	3 (8%)	39,95,115	1.99	13 (33%)
7	BCL	S	2003	2	53,74,74	1.12	4 (7%)	57,115,115	2.02	18 (31%)
8	BPH	S	2006	-	64,70,70	1.49	11 (17%)	73,101,101	2.27	20 (27%)
9	U10	S	2008	-	37,37,63	2.05	12 (32%)	44,47,79	1.87	10 (22%)
11	LDA	S	2010	-	15,15,15	3.53	3 (20%)	16,17,17	2.85	3 (18%)
11	LDA	S	2011	-	15,15,15	4.05	3 (20%)	16,17,17	2.41	3 (18%)

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
10	HEM	C	1009	4	-	0/10/54/54	0/0/8/8
10	HEM	D	2009	4	-	0/10/54/54	0/0/8/8
7	BCL	L	1002	1	-	0/37/137/137	0/0/9/9
7	BCL	L	1004	1	-	0/37/137/137	0/0/9/9
8	BPH	L	1005	-	1/1/16/22	0/42/93/105	0/1/6/6
7	BCL	M	1001	2	-	0/18/118/137	0/0/9/9
7	BCL	M	1003	2	-	0/37/137/137	0/0/9/9
8	BPH	M	1006	-	2/2/18/22	1/54/105/105	0/1/6/6
9	U10	M	1008	-	-	0/32/56/87	0/1/1/1
11	LDA	M	1010	-	-	0/13/13/13	0/0/0/0
11	LDA	M	1011	-	-	0/13/13/13	0/0/0/0
7	BCL	R	2002	1	-	0/37/137/137	0/0/9/9
7	BCL	R	2004	1	-	0/37/137/137	0/0/9/9
8	BPH	R	2005	-	1/1/16/22	0/42/93/105	0/1/6/6
7	BCL	S	2001	2	-	0/18/118/137	0/0/9/9
7	BCL	S	2003	2	-	0/37/137/137	0/0/9/9
8	BPH	S	2006	-	2/2/18/22	0/54/105/105	0/1/6/6
9	U10	S	2008	-	-	0/32/56/87	0/1/1/1
11	LDA	S	2010	-	-	0/13/13/13	0/0/0/0
11	LDA	S	2011	-	-	0/13/13/13	0/0/0/0

All (118) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	S	2011	LDA	O1-N1	-14.85	1.25	1.39
11	M	1011	LDA	O1-N1	-14.51	1.25	1.39
11	M	1010	LDA	O1-N1	-14.03	1.26	1.39
11	S	2010	LDA	O1-N1	-12.81	1.27	1.39
10	C	1009	HEM	C2D-C3D	-7.05	1.33	1.54
10	D	2009	HEM	C2D-C3D	-6.98	1.33	1.54
10	D	2009	HEM	C3B-C4B	-5.71	1.46	1.51
8	M	1006	BPH	C11-C10	-5.03	1.29	1.52
8	S	2006	BPH	C11-C10	-4.98	1.29	1.52
10	C	1009	HEM	C3B-C4B	-4.88	1.47	1.51
11	M	1011	LDA	CM2-N1	-4.76	1.42	1.49
10	C	1009	HEM	C2C-C1C	-4.50	1.44	1.52
10	D	2009	HEM	C2C-C1C	-4.35	1.44	1.52
7	M	1001	BCL	C3C-C4C	-3.92	1.46	1.51
11	S	2011	LDA	CM2-N1	-3.83	1.43	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	1010	LDA	CM2-N1	-3.79	1.43	1.49
11	S	2010	LDA	CM2-N1	-3.61	1.43	1.49
9	M	1008	U10	C7-C8	-3.15	1.45	1.50
7	S	2001	BCL	C3C-C4C	-3.03	1.47	1.51
9	S	2008	U10	C7-C8	-3.02	1.46	1.50
9	M	1008	U10	O3-C3M	-3.01	1.38	1.45
9	S	2008	U10	O3-C3M	-3.01	1.38	1.45
10	D	2009	HEM	C2B-C1B	-2.88	1.42	1.51
10	C	1009	HEM	CAD-C3D	-2.83	1.48	1.54
7	L	1004	BCL	C3C-C4C	-2.77	1.48	1.51
7	R	2004	BCL	C3C-C4C	-2.73	1.48	1.51
8	M	1006	BPH	O2D-CED	-2.71	1.38	1.45
8	R	2005	BPH	O2D-CED	-2.66	1.38	1.45
8	S	2006	BPH	O2D-CED	-2.65	1.38	1.45
10	C	1009	HEM	C2B-C1B	-2.64	1.43	1.51
11	S	2011	LDA	CM1-N1	-2.62	1.45	1.49
8	L	1005	BPH	O2D-CED	-2.47	1.39	1.45
8	M	1006	BPH	C2C-C3C	-2.41	1.47	1.54
7	M	1003	BCL	C3D-CAD	-2.39	1.39	1.45
8	L	1005	BPH	C2C-C3C	-2.34	1.47	1.54
7	S	2003	BCL	C3D-CAD	-2.21	1.39	1.45
10	D	2009	HEM	CAD-C3D	-2.21	1.49	1.54
7	S	2003	BCL	OBD-CAD	-2.19	1.19	1.22
8	R	2005	BPH	C2C-C3C	-2.18	1.48	1.54
11	S	2010	LDA	CM1-N1	-2.17	1.46	1.49
7	L	1002	BCL	C3C-C4C	-2.16	1.48	1.51
11	M	1010	LDA	CM1-N1	-2.15	1.46	1.49
8	S	2006	BPH	C2C-C3C	-2.15	1.48	1.54
7	L	1004	BCL	C1A-CHA	-2.06	1.34	1.43
8	S	2006	BPH	C3D-C2D	-2.03	1.35	1.40
7	R	2004	BCL	OBD-CAD	-2.01	1.19	1.22
10	C	1009	HEM	C3D-C4D	-2.00	1.49	1.51
7	R	2004	BCL	C6-C5	2.01	1.59	1.52
10	C	1009	HEM	C3B-CAB	2.05	1.55	1.51
7	L	1002	BCL	CBB-CAB	2.05	1.55	1.49
7	M	1001	BCL	CAA-C2A	2.07	1.58	1.54
8	L	1005	BPH	C2A-C1A	2.07	1.55	1.51
7	M	1001	BCL	CAA-CBA	2.08	1.59	1.52
9	S	2008	U10	C20-C19	2.10	1.55	1.50
8	M	1006	BPH	O1D-CGD	2.12	1.26	1.21
7	S	2003	BCL	CBB-CAB	2.13	1.56	1.49
8	R	2005	BPH	CHA-C1A	2.13	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	S	2001	BCL	CAA-C2A	2.14	1.58	1.54
7	M	1001	BCL	CBB-CAB	2.14	1.56	1.49
8	L	1005	BPH	O1D-CGD	2.14	1.26	1.21
9	S	2008	U10	C7-C6	2.14	1.55	1.51
8	M	1006	BPH	CHC-C1C	2.14	1.40	1.36
8	L	1005	BPH	CHA-C1A	2.15	1.42	1.37
7	S	2003	BCL	C4-C3	2.16	1.55	1.50
7	L	1004	BCL	CBB-CAB	2.17	1.56	1.49
7	L	1002	BCL	C4-C3	2.18	1.56	1.50
8	S	2006	BPH	CHC-C1C	2.18	1.40	1.36
10	C	1009	HEM	CAA-C2A	2.18	1.55	1.52
8	S	2006	BPH	CHA-C1A	2.19	1.42	1.37
7	L	1004	BCL	C6-C5	2.19	1.60	1.52
7	R	2002	BCL	CBB-CAB	2.19	1.56	1.49
9	M	1008	U10	C6-C1	2.20	1.40	1.35
7	R	2002	BCL	C4-C3	2.23	1.56	1.50
8	R	2005	BPH	O1D-CGD	2.23	1.26	1.21
8	M	1006	BPH	C2A-C1A	2.28	1.55	1.51
9	M	1008	U10	C15-C14	2.28	1.56	1.50
7	M	1003	BCL	CBB-CAB	2.29	1.56	1.49
7	L	1004	BCL	C4-C3	2.30	1.56	1.50
8	S	2006	BPH	C2A-C1A	2.33	1.55	1.51
7	M	1003	BCL	C4-C3	2.34	1.56	1.50
7	S	2001	BCL	CBB-CAB	2.34	1.56	1.49
9	S	2008	U10	C15-C14	2.48	1.56	1.50
7	R	2004	BCL	C4-C3	2.49	1.56	1.50
8	R	2005	BPH	C2A-C1A	2.51	1.55	1.51
8	S	2006	BPH	CAA-C2A	2.60	1.59	1.54
8	R	2005	BPH	CAA-C2A	2.74	1.59	1.54
8	M	1006	BPH	CAA-C2A	2.77	1.59	1.54
9	M	1008	U10	O3-C3	2.80	1.44	1.37
9	S	2008	U10	C6-C1	2.83	1.41	1.35
8	L	1005	BPH	CAA-C2A	2.83	1.59	1.54
8	R	2005	BPH	CHC-C1C	2.85	1.42	1.36
9	S	2008	U10	O3-C3	2.92	1.44	1.37
8	S	2006	BPH	C2-C3	3.06	1.39	1.33
8	R	2005	BPH	C2-C3	3.11	1.39	1.33
9	S	2008	U10	C18-C19	3.34	1.39	1.33
8	M	1006	BPH	C2-C3	3.38	1.39	1.33
9	M	1008	U10	C18-C19	3.50	1.39	1.33
8	L	1005	BPH	C2-C3	3.52	1.39	1.33
8	S	2006	BPH	O2D-CGD	3.73	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	S	2008	U10	C8-C9	3.76	1.40	1.33
9	M	1008	U10	O4-C4	3.83	1.47	1.37
8	M	1006	BPH	O2D-CGD	3.83	1.43	1.33
9	M	1008	U10	C8-C9	3.83	1.40	1.33
8	L	1005	BPH	O2D-CGD	3.95	1.43	1.33
8	L	1005	BPH	O2A-CGA	4.01	1.45	1.33
8	R	2005	BPH	O2D-CGD	4.01	1.43	1.33
9	S	2008	U10	C23-C24	4.08	1.41	1.33
8	S	2006	BPH	O2A-CGA	4.24	1.46	1.33
8	R	2005	BPH	O2A-CGA	4.24	1.46	1.33
9	M	1008	U10	C23-C24	4.25	1.41	1.33
8	M	1006	BPH	O2A-CGA	4.26	1.46	1.33
9	S	2008	U10	O4-C4	4.42	1.48	1.37
10	D	2009	HEM	CBC-CAC	4.46	1.55	1.29
10	C	1009	HEM	CBC-CAC	4.49	1.55	1.29
9	S	2008	U10	C13-C14	4.57	1.41	1.33
9	M	1008	U10	C13-C14	4.63	1.42	1.33
10	C	1009	HEM	CBB-CAB	4.97	1.58	1.29
10	D	2009	HEM	CBB-CAB	5.07	1.58	1.29

All (262) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	1011	LDA	CM2-N1-CM1	-8.20	99.58	108.83
11	S	2010	LDA	CM2-N1-CM1	-8.20	99.59	108.83
11	M	1010	LDA	CM2-N1-CM1	-7.66	100.19	108.83
11	S	2011	LDA	CM2-N1-CM1	-7.47	100.40	108.83
10	D	2009	HEM	C3B-CAB-CBB	-6.98	113.75	124.46
10	C	1009	HEM	C3B-CAB-CBB	-6.89	113.88	124.46
10	D	2009	HEM	C3C-CAC-CBC	-6.41	114.62	124.46
10	C	1009	HEM	C3C-CAC-CBC	-5.93	115.35	124.46
8	S	2006	BPH	O1D-CGD-CBD	-5.33	116.99	124.62
7	M	1001	BCL	CBC-CAC-C3C	-5.17	100.92	113.57
8	R	2005	BPH	O1D-CGD-CBD	-5.09	117.33	124.62
7	S	2003	BCL	O2D-CGD-CBD	-5.06	104.35	111.30
7	M	1003	BCL	O2D-CGD-CBD	-4.96	104.49	111.30
8	L	1005	BPH	O1D-CGD-CBD	-4.81	117.73	124.62
8	M	1006	BPH	O1D-CGD-CBD	-4.67	117.94	124.62
7	M	1001	BCL	OBD-CAD-CBD	-4.24	119.55	125.94
7	M	1003	BCL	OBD-CAD-CBD	-4.20	119.61	125.94
7	S	2001	BCL	OBD-CAD-CBD	-4.02	119.87	125.94
7	S	2001	BCL	CBC-CAC-C3C	-4.00	103.79	113.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	1004	BCL	OBD-CAD-CBD	-4.00	119.91	125.94
7	R	2002	BCL	O2D-CGD-CBD	-3.98	105.84	111.30
7	S	2003	BCL	OBD-CAD-CBD	-3.92	120.02	125.94
8	M	1006	BPH	O2D-CGD-O1D	-3.89	115.76	123.79
7	S	2003	BCL	C11-C12-C13	-3.78	102.94	115.49
8	S	2006	BPH	O2D-CGD-O1D	-3.78	115.99	123.79
7	R	2004	BCL	OBD-CAD-CBD	-3.76	120.26	125.94
7	L	1002	BCL	O2D-CGD-CBD	-3.70	106.23	111.30
8	L	1005	BPH	O2D-CGD-O1D	-3.69	116.16	123.79
7	R	2002	BCL	OBD-CAD-CBD	-3.67	120.41	125.94
9	S	2008	U10	O5-C5-C6	-3.65	114.81	121.68
9	M	1008	U10	O5-C5-C6	-3.61	114.89	121.68
7	R	2002	BCL	C11-C12-C13	-3.56	103.68	115.49
7	S	2003	BCL	OBB-CAB-CBB	-3.53	111.67	120.13
7	L	1002	BCL	OBD-CAD-CBD	-3.52	120.63	125.94
8	R	2005	BPH	O2D-CGD-O1D	-3.51	116.54	123.79
7	S	2001	BCL	OBB-CAB-CBB	-3.50	111.75	120.13
7	L	1004	BCL	OBB-CAB-CBB	-3.48	111.79	120.13
7	S	2001	BCL	CAC-C3C-C4C	-3.45	104.93	112.58
7	R	2004	BCL	C11-C12-C13	-3.44	104.08	115.49
7	R	2002	BCL	OBB-CAB-CBB	-3.43	111.90	120.13
9	S	2008	U10	C20-C19-C21	-3.42	110.18	115.41
7	R	2004	BCL	OBB-CAB-CBB	-3.39	112.00	120.13
7	M	1003	BCL	C11-C12-C13	-3.37	104.32	115.49
9	M	1008	U10	C20-C19-C21	-3.35	110.28	115.41
7	M	1003	BCL	OBB-CAB-CBB	-3.33	112.14	120.13
7	L	1004	BCL	CBC-CAC-C3C	-3.31	105.48	113.57
10	C	1009	HEM	CBD-CAD-C3D	-3.27	104.03	113.55
7	L	1004	BCL	C11-C12-C13	-3.21	104.84	115.49
7	R	2004	BCL	CBC-CAC-C3C	-3.17	105.82	113.57
7	M	1001	BCL	OBB-CAB-CBB	-3.11	112.68	120.13
7	R	2004	BCL	C16-C15-C13	-3.07	105.29	115.49
7	L	1004	BCL	C16-C15-C13	-3.07	105.32	115.49
9	S	2008	U10	O2-C2-C3	-3.06	114.17	120.79
7	L	1002	BCL	C11-C12-C13	-3.05	105.39	115.49
9	S	2008	U10	C1-C6-C5	-3.04	116.65	120.12
9	M	1008	U10	C1-C6-C5	-3.00	116.69	120.12
7	L	1002	BCL	OBB-CAB-CBB	-2.97	113.02	120.13
7	M	1001	BCL	CAA-C2A-C3A	-2.94	104.75	113.22
9	M	1008	U10	O2-C2-C3	-2.92	114.46	120.79
7	S	2003	BCL	C16-C15-C13	-2.92	105.80	115.49
7	R	2002	BCL	C16-C15-C13	-2.90	105.86	115.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	S	2001	BCL	CAA-C2A-C3A	-2.85	105.02	113.22
8	S	2006	BPH	O2A-CGA-O1A	-2.81	116.23	123.49
7	R	2004	BCL	CAC-C3C-C4C	-2.78	106.41	112.58
7	M	1003	BCL	CHA-C1A-NA	-2.76	119.28	126.06
10	D	2009	HEM	CBD-CAD-C3D	-2.75	105.55	113.55
7	S	2003	BCL	CHA-C1A-NA	-2.74	119.32	126.06
8	M	1006	BPH	CAA-C2A-C1A	-2.73	105.68	112.86
8	R	2005	BPH	C5-C3-C2	-2.71	115.92	121.05
7	M	1003	BCL	CMB-C2B-C1B	-2.69	123.91	128.36
7	L	1002	BCL	CAC-C3C-C4C	-2.69	106.62	112.58
8	S	2006	BPH	CBB-CAB-C3B	-2.68	114.56	120.52
8	L	1005	BPH	C5-C3-C2	-2.66	116.00	121.05
7	M	1003	BCL	C16-C15-C13	-2.66	106.66	115.49
7	R	2002	BCL	CMB-C2B-C1B	-2.63	124.02	128.36
7	M	1003	BCL	CAA-CBA-CGA	-2.62	105.65	113.32
8	M	1006	BPH	O2A-CGA-O1A	-2.62	116.74	123.49
8	S	2006	BPH	CAA-C2A-C1A	-2.57	106.10	112.86
7	R	2004	BCL	CMB-C2B-C1B	-2.55	124.14	128.36
7	R	2002	BCL	CHA-C1A-NA	-2.55	119.79	126.06
8	M	1006	BPH	CBB-CAB-C3B	-2.54	114.87	120.52
7	L	1002	BCL	CHA-C1A-NA	-2.52	119.85	126.06
7	S	2003	BCL	CMB-C2B-C1B	-2.50	124.22	128.36
7	L	1002	BCL	C16-C15-C13	-2.50	107.20	115.49
7	L	1004	BCL	CAC-C3C-C2C	-2.49	107.87	114.13
7	S	2001	BCL	CGD-CBD-CAD	-2.49	102.20	110.62
10	C	1009	HEM	CMA-C3A-C4A	-2.48	124.27	128.36
8	S	2006	BPH	C7-C6-C5	-2.47	105.75	113.06
8	R	2005	BPH	CBB-CAB-C3B	-2.47	115.04	120.52
7	L	1004	BCL	CMB-C2B-C1B	-2.46	124.29	128.36
7	R	2002	BCL	CAC-C3C-C4C	-2.46	107.12	112.58
8	R	2005	BPH	OBD-CAD-CBD	-2.43	122.26	125.94
7	M	1001	BCL	CHA-C1A-NA	-2.42	120.11	126.06
7	S	2003	BCL	CBC-CAC-C3C	-2.42	107.66	113.57
7	L	1002	BCL	CAA-CBA-CGA	-2.40	106.28	113.32
9	S	2008	U10	C7-C6-C5	-2.39	115.74	118.56
7	M	1003	BCL	CGD-CBD-CAD	-2.39	102.53	110.62
7	L	1002	BCL	CMB-C2B-C1B	-2.37	124.44	128.36
8	L	1005	BPH	CAC-C3C-C2C	-2.37	108.17	114.13
8	M	1006	BPH	C5-C3-C2	-2.36	116.57	121.05
11	M	1010	LDA	CM1-N1-C1	-2.35	102.20	109.77
11	S	2010	LDA	CM1-N1-C1	-2.33	102.25	109.77
8	S	2006	BPH	CAC-C3C-C2C	-2.32	108.29	114.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	1009	HEM	CBA-CAA-C2A	-2.32	108.37	112.53
7	L	1004	BCL	CHA-C1A-NA	-2.32	120.36	126.06
7	S	2001	BCL	CHA-C1A-NA	-2.31	120.37	126.06
7	L	1004	BCL	CAC-C3C-C4C	-2.31	107.47	112.58
9	M	1008	U10	C7-C6-C5	-2.30	115.85	118.56
7	R	2004	BCL	CHA-C1A-NA	-2.30	120.41	126.06
11	S	2011	LDA	C6-C5-C4	-2.30	102.67	114.53
7	R	2002	BCL	CBC-CAC-C3C	-2.29	107.96	113.57
10	D	2009	HEM	CMA-C3A-C4A	-2.29	124.58	128.36
7	M	1003	BCL	CAC-C3C-C4C	-2.28	107.53	112.58
8	L	1005	BPH	O2A-CGA-O1A	-2.27	117.64	123.49
8	L	1005	BPH	CBB-CAB-C3B	-2.26	115.49	120.52
8	R	2005	BPH	O2A-CGA-O1A	-2.24	117.70	123.49
8	L	1005	BPH	CAA-C2A-C3A	-2.24	106.76	113.22
8	M	1006	BPH	C7-C6-C5	-2.24	106.44	113.06
10	D	2009	HEM	CBA-CAA-C2A	-2.24	108.52	112.53
7	S	2003	BCL	C7-C6-C5	-2.23	106.46	113.06
8	S	2006	BPH	C5-C3-C2	-2.22	116.84	121.05
7	L	1002	BCL	CAA-C2A-C3A	-2.21	106.86	113.22
11	M	1011	LDA	CM1-N1-C1	-2.21	102.65	109.77
7	R	2002	BCL	CAA-C2A-C3A	-2.21	106.87	113.22
8	L	1005	BPH	C2A-C1A-NA	-2.18	109.29	112.08
7	R	2004	BCL	C7-C6-C5	-2.17	106.66	113.06
8	R	2005	BPH	CAA-C2A-C3A	-2.16	107.00	113.22
7	M	1003	BCL	CBC-CAC-C3C	-2.16	108.28	113.57
11	M	1011	LDA	C9-C8-C7	-2.16	103.38	114.53
7	M	1003	BCL	CHB-C4A-NA	-2.15	121.54	124.51
8	R	2005	BPH	CAC-C3C-C2C	-2.15	108.72	114.13
8	M	1006	BPH	CAC-C3C-C2C	-2.15	108.72	114.13
8	S	2006	BPH	CAA-C2A-C3A	-2.13	107.10	113.22
7	S	2003	BCL	CHB-C4A-NA	-2.11	121.59	124.51
8	M	1006	BPH	C2A-C1A-NA	-2.11	109.38	112.08
7	R	2004	BCL	CAC-C3C-C2C	-2.10	108.84	114.13
8	S	2006	BPH	C3A-C4A-NA	-2.10	109.89	113.57
8	M	1006	BPH	CAA-C2A-C3A	-2.10	107.17	113.22
7	L	1002	BCL	CBC-CAC-C3C	-2.07	108.50	113.57
7	R	2002	BCL	CAA-CBA-CGA	-2.07	107.27	113.32
8	M	1006	BPH	OBD-CAD-CBD	-2.05	122.85	125.94
8	M	1006	BPH	C3A-C4A-NA	-2.04	110.00	113.57
8	S	2006	BPH	OBD-CAD-CBD	-2.04	122.86	125.94
8	R	2005	BPH	C2A-C1A-NA	-2.03	109.48	112.08
8	L	1005	BPH	OBD-CAD-CBD	-2.02	122.89	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	R	2005	BPH	C3A-C4A-NA	-2.02	110.03	113.57
7	M	1001	BCL	CGD-CBD-CAD	-2.02	103.77	110.62
8	S	2006	BPH	C2A-C1A-NA	-2.02	109.50	112.08
7	M	1003	BCL	CAA-C2A-C3A	-2.01	107.43	113.22
7	S	2003	BCL	CAA-C2A-C3A	-2.00	107.46	113.22
7	S	2001	BCL	CMB-C2B-C3B	2.00	129.00	125.09
7	R	2002	BCL	C3D-CAD-CBD	2.00	110.43	107.60
8	R	2005	BPH	CMD-C2D-C3D	2.01	129.01	125.09
8	M	1006	BPH	O2A-CGA-CBA	2.01	118.01	111.90
10	C	1009	HEM	C2D-C3D-C4D	2.02	104.92	101.50
8	M	1006	BPH	CMD-C2D-C3D	2.02	129.04	125.09
7	S	2003	BCL	CBA-CAA-C2A	2.04	119.48	113.73
10	D	2009	HEM	CAA-CBA-CGA	2.05	116.50	112.75
7	R	2002	BCL	C2C-C3C-C4C	2.05	104.98	101.50
7	R	2002	BCL	C4-C3-C5	2.06	118.55	115.41
7	R	2004	BCL	O1D-CGD-CBD	2.06	127.58	124.62
7	L	1002	BCL	C2C-C3C-C4C	2.08	105.02	101.50
7	M	1001	BCL	CMB-C2B-C3B	2.13	129.25	125.09
8	L	1005	BPH	C4-C3-C5	2.13	118.66	115.41
7	L	1004	BCL	O1D-CGD-CBD	2.14	127.68	124.62
9	M	1008	U10	C21-C19-C18	2.17	125.17	121.05
8	S	2006	BPH	O2A-CGA-CBA	2.18	118.55	111.90
7	L	1002	BCL	C4-C3-C5	2.19	118.75	115.41
7	S	2001	BCL	C2C-C3C-C4C	2.19	105.22	101.50
7	L	1002	BCL	CBB-CAB-C3B	2.20	126.87	120.33
7	L	1004	BCL	CBA-CAA-C2A	2.22	120.00	113.73
7	R	2004	BCL	CBA-CAA-C2A	2.22	120.01	113.73
8	R	2005	BPH	C4-C3-C5	2.29	118.91	115.41
7	R	2004	BCL	C3D-CAD-CBD	2.34	110.91	107.60
7	L	1004	BCL	C3D-CAD-CBD	2.35	110.92	107.60
7	M	1001	BCL	CBB-CAB-C3B	2.36	127.32	120.33
7	M	1003	BCL	CBA-CAA-C2A	2.38	120.46	113.73
9	S	2008	U10	C21-C19-C18	2.41	125.62	121.05
7	S	2003	BCL	C3D-CAD-CBD	2.43	111.03	107.60
7	R	2004	BCL	C2C-C3C-C4C	2.44	105.64	101.50
9	S	2008	U10	C17-C18-C19	2.48	133.15	127.76
7	L	1004	BCL	CBB-CAB-C3B	2.49	127.73	120.33
9	M	1008	U10	C7-C8-C9	2.51	130.94	126.70
7	R	2002	BCL	CBB-CAB-C3B	2.51	127.77	120.33
7	R	2004	BCL	CBB-CAB-C3B	2.52	127.81	120.33
7	S	2001	BCL	C3D-CAD-CBD	2.53	111.18	107.60
7	L	1004	BCL	C2C-C3C-C4C	2.55	105.81	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	S	2003	BCL	CBB-CAB-C3B	2.63	128.13	120.33
7	M	1001	BCL	O1D-CGD-CBD	2.63	128.40	124.62
7	M	1003	BCL	CBB-CAB-C3B	2.65	128.20	120.33
8	L	1005	BPH	C2C-C3C-C4C	2.67	106.03	101.50
7	M	1001	BCL	C3D-CAD-CBD	2.68	111.38	107.60
9	M	1008	U10	C17-C18-C19	2.69	133.62	127.76
7	M	1003	BCL	C3D-CAD-CBD	2.70	111.41	107.60
8	S	2006	BPH	C2C-C3C-C4C	2.72	106.10	101.50
9	M	1008	U10	C16-C14-C13	2.75	126.26	121.05
8	R	2005	BPH	C2C-C3C-C4C	2.75	106.16	101.50
7	L	1002	BCL	CMB-C2B-C3B	2.76	130.48	125.09
7	S	2003	BCL	CMB-C2B-C3B	2.76	130.48	125.09
8	M	1006	BPH	C2C-C3C-C4C	2.76	106.18	101.50
7	M	1001	BCL	C2C-C3C-C4C	2.77	106.20	101.50
10	C	1009	HEM	CAA-CBA-CGA	2.78	117.83	112.75
9	S	2008	U10	C7-C8-C9	2.80	131.43	126.70
7	L	1004	BCL	CMB-C2B-C3B	2.80	130.56	125.09
9	S	2008	U10	C16-C14-C13	2.82	126.40	121.05
7	R	2002	BCL	CMB-C2B-C3B	2.84	130.64	125.09
7	R	2004	BCL	CMB-C2B-C3B	2.84	130.65	125.09
7	S	2001	BCL	CBB-CAB-C3B	2.87	128.84	120.33
7	M	1003	BCL	CMB-C2B-C3B	2.96	130.88	125.09
7	S	2003	BCL	C4-C3-C5	2.98	119.96	115.41
7	S	2001	BCL	O1D-CGD-CBD	3.05	128.99	124.62
8	M	1006	BPH	CBC-CAC-C3C	3.06	121.05	113.57
8	L	1005	BPH	CBC-CAC-C3C	3.17	121.32	113.57
7	S	2001	BCL	CMD-C2D-C3D	3.20	131.35	125.09
10	D	2009	HEM	CMD-C2D-C3D	3.23	128.64	114.35
10	C	1009	HEM	CMD-C2D-C3D	3.23	128.66	114.35
8	R	2005	BPH	CBC-CAC-C3C	3.24	121.49	113.57
8	S	2006	BPH	CBC-CAC-C3C	3.26	121.55	113.57
7	M	1003	BCL	C4-C3-C5	3.30	120.44	115.41
7	L	1004	BCL	CMD-C2D-C3D	3.54	132.01	125.09
7	R	2004	BCL	CMD-C2D-C3D	3.55	132.03	125.09
7	L	1002	BCL	CMD-C2D-C3D	3.57	132.06	125.09
7	M	1001	BCL	CMD-C2D-C3D	3.72	132.36	125.09
7	S	2003	BCL	CMD-C2D-C3D	3.73	132.39	125.09
7	L	1002	BCL	O1D-CGD-CBD	3.74	129.98	124.62
7	M	1003	BCL	CMD-C2D-C3D	3.74	132.41	125.09
8	S	2006	BPH	CED-O2D-CGD	3.74	124.77	115.99
8	M	1006	BPH	C11-C10-C8	3.77	128.01	115.49
7	R	2002	BCL	CMD-C2D-C3D	3.77	132.47	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	S	2006	BPH	C11-C10-C8	3.84	128.23	115.49
11	S	2011	LDA	O1-N1-C1	3.91	114.68	110.27
8	M	1006	BPH	CED-O2D-CGD	3.94	125.23	115.99
8	L	1005	BPH	CED-O2D-CGD	4.06	125.52	115.99
8	R	2005	BPH	CED-O2D-CGD	4.08	125.55	115.99
7	R	2002	BCL	O1D-CGD-CBD	4.18	130.61	124.62
7	M	1003	BCL	O1D-CGD-CBD	4.34	130.85	124.62
8	R	2005	BPH	C4A-NA-C1A	4.40	112.14	108.21
8	L	1005	BPH	C4A-NA-C1A	4.45	112.18	108.21
10	D	2009	HEM	CAD-C3D-C4D	4.47	128.22	112.47
10	C	1009	HEM	CAD-C3D-C4D	4.49	128.30	112.47
8	L	1005	BPH	C6-C5-C3	4.49	122.34	112.48
8	M	1006	BPH	C4A-NA-C1A	4.61	112.32	108.21
8	R	2005	BPH	C6-C5-C3	4.63	122.64	112.48
7	S	2003	BCL	O1D-CGD-CBD	4.64	131.27	124.62
10	C	1009	HEM	CAD-C3D-C2D	4.72	126.78	113.22
10	C	1009	HEM	CMB-C2B-C3B	4.77	128.45	116.53
8	S	2006	BPH	C4A-NA-C1A	4.84	112.53	108.21
10	D	2009	HEM	CAD-C3D-C2D	4.85	127.17	113.22
10	D	2009	HEM	CMB-C2B-C3B	4.88	128.71	116.53
8	M	1006	BPH	C6-C5-C3	4.92	123.28	112.48
10	D	2009	HEM	CMC-C2C-C3C	4.93	128.84	116.53
10	C	1009	HEM	CMC-C2C-C3C	5.12	129.31	116.53
8	S	2006	BPH	C6-C5-C3	5.27	124.04	112.48
11	M	1011	LDA	O1-N1-C1	5.52	116.48	110.27
11	M	1010	LDA	O1-N1-C1	6.12	117.16	110.27
11	S	2010	LDA	O1-N1-C1	6.33	117.40	110.27
9	M	1008	U10	C3M-O3-C3	6.38	139.30	116.61
9	S	2008	U10	C3M-O3-C3	6.39	139.33	116.61
8	L	1005	BPH	O2D-CGD-CBD	10.78	126.09	111.30
8	R	2005	BPH	O2D-CGD-CBD	10.81	126.13	111.30
8	M	1006	BPH	O2D-CGD-CBD	10.93	126.30	111.30
8	S	2006	BPH	O2D-CGD-CBD	11.46	127.02	111.30

All (6) chirality outliers are listed below:

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

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Mol	Chain	Res	Type	Atom
8	M	1006	BPH	C13

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	M	1006	BPH	C4B-C3B-CAB-CBB

There are no ring outliers.

20 monomers are involved in 79 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	1009	HEM	2	0
10	D	2009	HEM	2	0
7	L	1002	BCL	11	0
7	L	1004	BCL	7	0
8	L	1005	BPH	2	0
7	M	1001	BCL	4	0
7	M	1003	BCL	15	0
8	M	1006	BPH	3	0
9	M	1008	U10	1	0
11	M	1010	LDA	2	0
11	M	1011	LDA	3	0
7	R	2002	BCL	10	0
7	R	2004	BCL	11	0
8	R	2005	BPH	2	0
7	S	2001	BCL	4	0
7	S	2003	BCL	11	0
8	S	2006	BPH	6	0
9	S	2008	U10	1	0
11	S	2010	LDA	2	0
11	S	2011	LDA	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	L	281/281 (100%)	-0.26	3 (1%) 82 75	34, 59, 84, 103	0
1	R	281/281 (100%)	-0.23	8 (2%) 56 47	38, 72, 106, 122	0
2	M	267/307 (86%)	-0.28	6 (2%) 65 55	25, 52, 109, 134	0
2	S	267/307 (86%)	-0.13	8 (2%) 54 44	33, 61, 110, 139	0
3	H	246/260 (94%)	0.29	23 (9%) 11 8	44, 98, 148, 167	0
3	T	246/260 (94%)	0.74	38 (15%) 3 2	42, 121, 157, 172	0
4	C	124/124 (100%)	0.17	3 (2%) 62 52	40, 70, 95, 140	0
4	D	124/124 (100%)	0.19	4 (3%) 51 42	50, 82, 105, 146	0
All	All	1836/1944 (94%)	0.03	93 (5%) 32 23	25, 71, 131, 172	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	T	8	GLY	8.6
3	T	9	ASN	7.3
2	S	37	THR	7.3
3	T	179	LEU	6.9
3	T	167	ILE	6.1
2	S	36	SER	5.6
3	T	144	ALA	5.4
3	T	168	TRP	5.4
3	T	196	VAL	5.3
3	H	253	ALA	5.2
3	H	252	VAL	4.9
3	T	148	PRO	4.9
3	H	9	ASN	4.7
2	S	38	LEU	4.6
3	H	8	GLY	4.6
3	T	178	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
2	M	37	THR	4.5
4	D	1	GLN	4.4
3	T	198	VAL	4.4
3	H	10	PHE	4.2
3	T	208	LEU	4.2
4	C	1	GLN	4.1
2	S	39	LEU	4.0
3	H	167	ILE	4.0
3	H	179	LEU	3.8
3	T	149	ILE	3.8
3	T	241	LEU	3.8
3	T	138	ALA	3.8
3	T	151	LEU	3.7
3	T	197	LYS	3.6
2	S	35	PHE	3.6
2	M	36	SER	3.6
3	H	196	VAL	3.6
1	R	22	PHE	3.5
3	T	213	PHE	3.5
3	T	200	SER	3.5
3	T	10	PHE	3.5
3	T	244	ALA	3.4
3	T	164	VAL	3.4
1	R	21	LEU	3.4
1	R	281	GLY	3.3
4	D	71	TRP	3.2
3	T	193	MET	3.2
3	T	166	ASP	3.2
3	H	148	PRO	3.2
3	T	203	VAL	3.0
3	T	252	VAL	3.0
4	D	124	PRO	2.9
3	H	166	ASP	2.9
4	D	74	GLU	2.9
2	M	44	ASN	2.8
3	T	181	VAL	2.8
3	H	208	LEU	2.7
3	H	199	GLN	2.7
3	T	145	GLY	2.7
3	T	199	GLN	2.7
1	L	1	ALA	2.7
3	T	190	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	R	14	GLY	2.6
3	T	85	ILE	2.6
3	T	253	ALA	2.6
3	T	150	GLY	2.6
3	T	111	PRO	2.6
3	T	132	LYS	2.6
3	H	200	SER	2.5
2	S	43	GLY	2.5
3	T	90	THR	2.5
3	T	180	GLU	2.5
3	T	236	TYR	2.4
3	H	146	LYS	2.4
3	H	198	VAL	2.4
2	M	39	LEU	2.3
1	R	17	VAL	2.3
2	S	40	GLY	2.3
3	H	139	GLY	2.3
3	H	177	ARG	2.3
3	H	145	GLY	2.2
1	R	23	ASP	2.2
2	M	51	TYR	2.2
3	H	79	GLU	2.2
1	L	202	LYS	2.2
1	R	16	LEU	2.2
3	H	151	LEU	2.2
3	H	149	ILE	2.1
4	C	113	ILE	2.1
2	M	40	GLY	2.1
2	S	139	ALA	2.1
1	R	20	ASN	2.1
3	T	146	LYS	2.1
1	L	20	ASN	2.1
3	H	188	THR	2.0
4	C	97	LYS	2.0
3	H	187	SER	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
11	LDA	S	2011	16/16	0.78	0.56	6.78	91,98,110,111	0
11	LDA	S	2010	16/16	0.86	0.35	5.79	59,82,94,94	0
11	LDA	M	1011	16/16	0.79	0.53	4.86	86,89,95,95	0
7	BCL	L	1004	66/66	0.93	0.28	2.95	42,48,67,71	0
7	BCL	R	2004	66/66	0.94	0.29	2.30	46,52,69,74	0
11	LDA	M	1010	16/16	0.90	0.27	2.26	50,54,57,59	0
9	U10	M	1008	37/63	0.93	0.26	2.19	44,54,68,69	0
8	BPH	S	2006	65/65	0.92	0.29	1.97	50,57,67,70	0
8	BPH	R	2005	55/65	0.92	0.29	1.93	63,70,94,96	0
7	BCL	R	2002	66/66	0.94	0.27	1.75	38,43,56,58	0
7	BCL	M	1003	66/66	0.93	0.26	1.59	33,40,55,59	0
7	BCL	L	1002	66/66	0.95	0.25	1.55	29,40,50,55	0
7	BCL	S	2003	66/66	0.95	0.25	1.53	36,42,73,75	0
8	BPH	L	1005	55/65	0.94	0.28	1.40	43,52,91,93	0
9	U10	S	2008	37/63	0.94	0.27	1.30	52,62,87,87	0
8	BPH	M	1006	65/65	0.95	0.23	1.19	48,56,67,69	0
7	BCL	S	2001	50/66	0.94	0.23	0.93	51,60,71,76	0
10	HEM	D	2009	43/43	0.96	0.26	0.28	49,52,64,70	0
7	BCL	M	1001	50/66	0.95	0.22	-0.03	37,46,58,61	0
10	HEM	C	1009	43/43	0.97	0.23	-0.19	35,42,52,55	0
5	FE2	M	1007	1/1	0.99	0.15	-1.42	45,45,45,45	0
5	FE2	S	2007	1/1	0.99	0.14	-2.66	54,54,54,54	0
6	CL	M	1012	1/1	0.96	0.35	-	66,66,66,66	0
6	CL	S	2012	1/1	0.94	0.39	-	71,71,71,71	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.