



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:58 PM GMT

PDB ID : 1Z9J
Title : Photosynthetic Reaction Center from Rhodobacter sphaeroides
Authors : Thielges, M.; Uyeda, G.; Camara-Artigas, A.; Kalman, L.; Williams, J.C.; Allen, J.P.
Deposited on : 2005-04-02
Resolution : 4.50 Å(reported)

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

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

MolProbity : 4.02b-467
Mogul : 1.7 (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

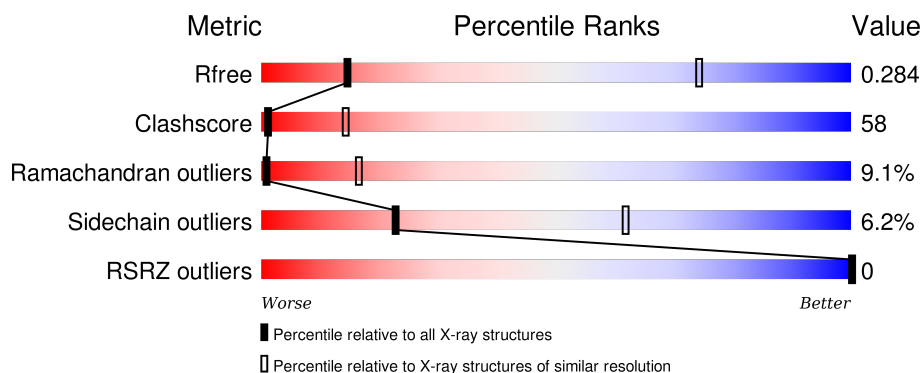
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 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}	91344	1071 (5.40-3.60)
Clashscore	102246	1003 (5.30-3.62)
Ramachandran outliers	100387	1117 (5.40-3.60)
Sidechain outliers	100360	1099 (5.40-3.60)
RSRZ outliers	91569	1075 (5.40-3.60)

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

Mol	Chain	Length	Quality of chain
1	A	281	<div> <div>25%</div> <div>62%</div> <div>12%</div> <div>.</div> </div>
2	B	307	<div> <div>26%</div> <div>62%</div> <div>10%</div> <div>..</div> </div>
3	C	260	<div> <div>36%</div> <div>49%</div> <div>7%</div> <div>8%</div> </div>

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
6	BCL	A	850	-	-	-	X
6	BCL	A	851	-	-	-	X
7	BPH	B	854	-	-	-	X
8	U10	A	857	-	-	-	X
8	U10	B	856	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6957 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	A	281	Total	C	N	O	S	0	0	0
			2234	1507	357	362	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	131	HIS	LEU	ENGINEERED	UNP P02954

- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	302	Total	C	N	O	S	0	0	0
			2415	1609	395	402	9			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	160	HIS	LEU	ENGINEERED	UNP P02953
B	164	TYR	ARG	ENGINEERED	UNP P02953
B	168	GLU	MET	ENGINEERED	UNP P02953
B	197	HIS	PHE	ENGINEERED	UNP P02953
B	288	ASP	GLY	ENGINEERED	UNP P02953

- Molecule 3 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	238	Total	C	N	O	S	0	0	0
			1814	1160	311	334	9			

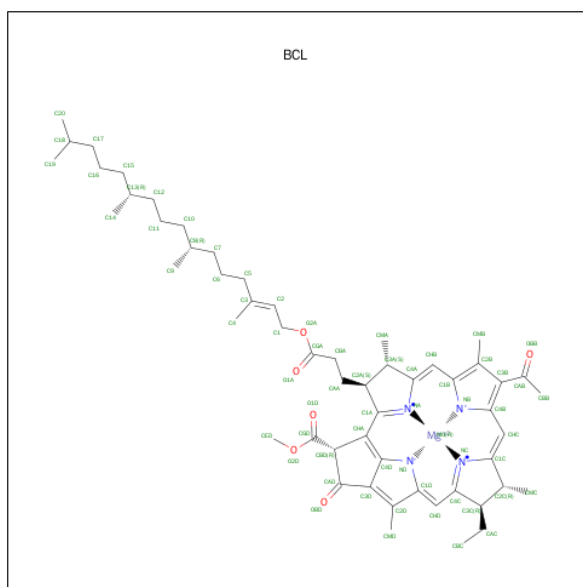
- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Fe 1 1	0	0

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

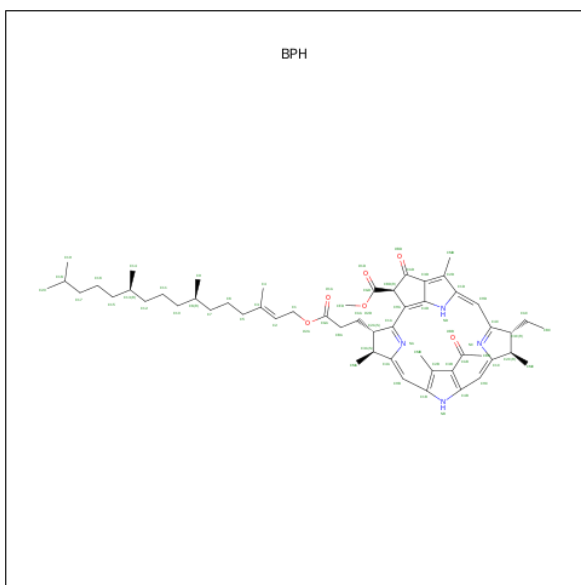
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Mn 1 1	0	0

- Molecule 6 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



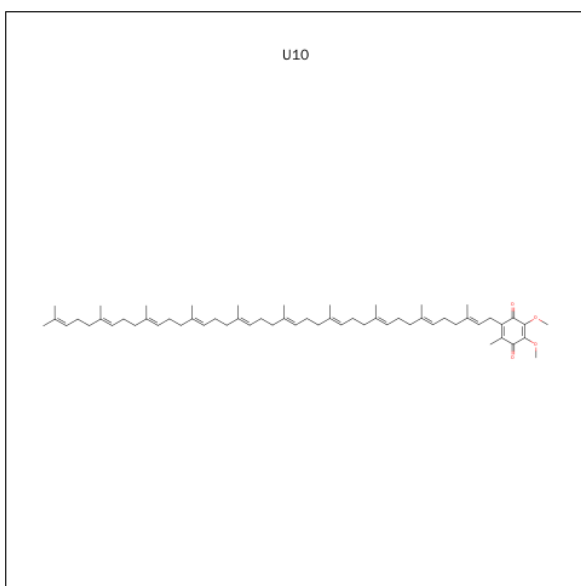
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C Mg N O 66 55 1 4 6	0	0
6	A	1	Total C Mg N O 66 55 1 4 6	0	0
6	B	1	Total C Mg N O 66 55 1 4 6	0	0
6	B	1	Total C Mg N O 66 55 1 4 6	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			65	55	4	6		
7	A	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 8 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			48	44	4		
8	A	1	Total	C	O	0	0
			48	44	4		

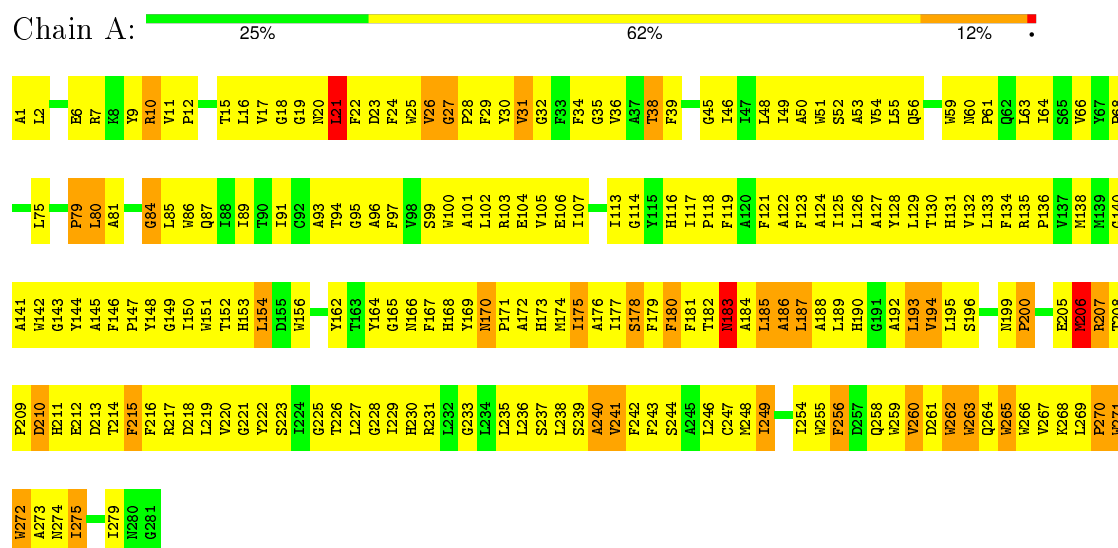
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	2	Total	O	0	0
			2	2		

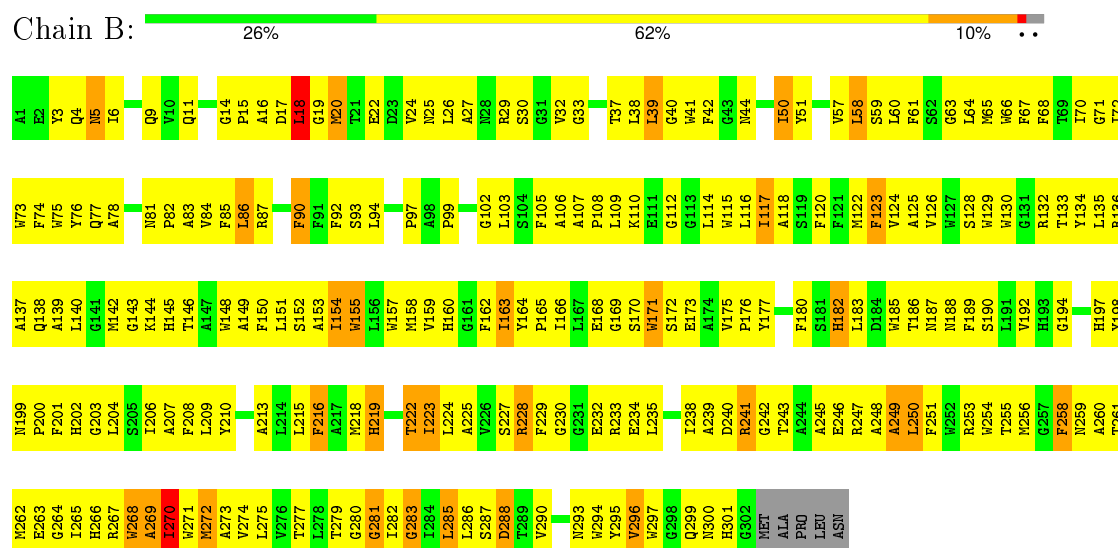
3 Residue-property plots

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

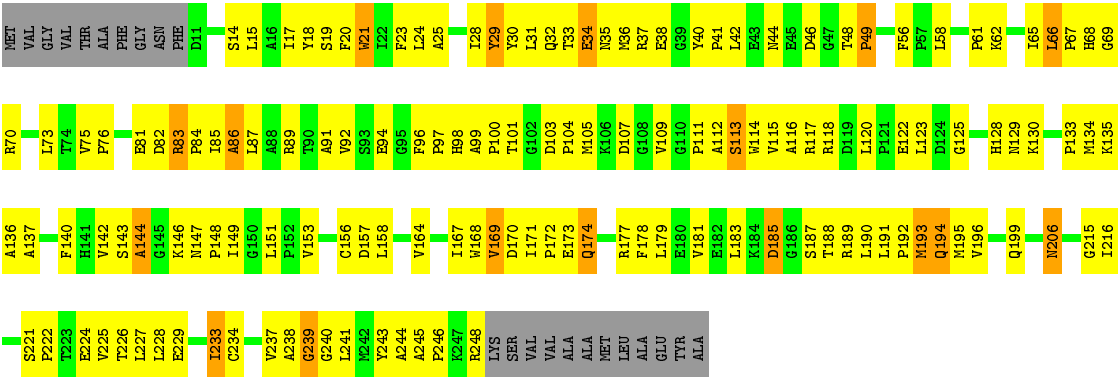


• Molecule 2: Reaction center protein M chain



• Molecule 3: Reaction center protein H chain

Chain C: 36% 49% 7% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 2 2	Depositor
Cell constants a, b, c, α , β , γ	203.84Å 203.84Å 119.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 4.50 24.90 – 4.30	Depositor EDS
% Data completeness (in resolution range)	79.9 (19.96-4.50) 80.7 (24.90-4.30)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 4.24Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.299 , 0.338 0.227 , 0.284	Depositor DCC
R_{free} test set	613 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	145.2	Xtriage
Anisotropy	0.494	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.19 , -0.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 14195 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6957	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 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, BPH, MN, FE, 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	A	0.63	0/2323	0.80	1/3179 (0.0%)
2	B	0.63	0/2509	0.79	1/3428 (0.0%)
3	C	0.62	1/1862 (0.1%)	0.80	0/2534
All	All	0.62	1/6694 (0.0%)	0.80	2/9141 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	21	TRP	CB-CG	-5.17	1.41	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	GLY	N-CA-C	-5.09	100.38	113.10
2	B	285	LEU	CA-CB-CG	-5.03	103.73	115.30

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	A	2234	0	2183	329	0
2	B	2415	0	2309	368	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1814	0	1818	187	1
4	B	1	0	0	0	0
5	B	1	0	0	0	0
6	A	132	0	148	20	0
6	B	132	0	148	18	0
7	A	65	0	76	19	0
7	B	65	0	76	14	0
8	A	48	0	63	7	0
8	B	48	0	63	15	0
9	B	2	0	0	1	0
All	All	6957	0	6884	802	1

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 58.

All (802) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:64:LEU:HD21	7:B:854:BPH:H112	1.32	1.10
2:B:267:ARG:O	2:B:270:ILE:HG22	1.65	0.96
1:A:171:PRO:HA	1:A:174:MET:HG3	1.48	0.95
2:B:242:GLY:HA2	3:C:117:ARG:HD2	1.49	0.94
1:A:114:GLY:H	2:B:225:ALA:HB1	1.32	0.93
2:B:287:SER:CB	2:B:294:TRP:HE1	1.82	0.92
7:A:855:BPH:HBB2	6:B:853:BCL:H11	1.49	0.91
3:C:87:LEU:HD22	3:C:98:HIS:O	1.72	0.90
1:A:22:PHE:HA	1:A:24:PHE:CE2	2.06	0.90
3:C:61:PRO:HA	3:C:76:PRO:HD2	1.54	0.89
3:C:86:ALA:HB1	3:C:101:THR:OG1	1.75	0.87
1:A:146:PHE:HA	1:A:156:TRP:CD1	2.08	0.87
2:B:299:GLN:HA	2:B:299:GLN:HE21	1.38	0.87
1:A:9:TYR:O	1:A:11:VAL:HG13	1.74	0.87
1:A:229:ILE:HD12	8:A:857:U10:H3M2	1.55	0.86
1:A:34:PHE:O	1:A:38:THR:HG23	1.76	0.86
3:C:233:ILE:O	3:C:237:VAL:HG23	1.75	0.86
2:B:202:HIS:CE1	2:B:206:ILE:HD11	2.10	0.86
1:A:227:LEU:HD21	2:B:5:ASN:ND2	1.90	0.85
1:A:116:HIS:CD2	2:B:224:LEU:HB3	2.12	0.85
3:C:117:ARG:O	3:C:228:LEU:HB2	1.75	0.85
1:A:38:THR:HG22	1:A:99:SER:CB	2.08	0.83
1:A:227:LEU:HD21	2:B:5:ASN:HD21	1.44	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ASN:O	1:A:64:ILE:HG12	1.79	0.82
1:A:229:ILE:CG2	1:A:230:HIS:N	2.42	0.82
2:B:299:GLN:HA	2:B:299:GLN:NE2	1.94	0.82
1:A:114:GLY:N	2:B:225:ALA:HB1	1.94	0.81
2:B:97:PRO:HB3	2:B:112:GLY:HA3	1.60	0.81
2:B:271:TRP:O	2:B:273:ALA:N	2.13	0.81
2:B:64:LEU:CD2	7:B:854:BPH:H112	2.09	0.81
1:A:185:LEU:O	1:A:188:ALA:HB3	1.80	0.81
1:A:38:THR:HG22	1:A:99:SER:HB3	1.62	0.79
2:B:180:PHE:O	2:B:183:LEU:HB2	1.82	0.79
3:C:83:ARG:HB2	3:C:84:PRO:HD2	1.64	0.79
3:C:189:ARG:HD2	3:C:216:ILE:HB	1.62	0.79
3:C:87:LEU:HD23	3:C:100:PRO:HA	1.65	0.79
1:A:173:HIS:CE1	1:A:177:ILE:HD11	2.17	0.79
2:B:247:ARG:NH2	3:C:111:PRO:O	2.15	0.78
2:B:241:ARG:HD3	3:C:38:GLU:OE1	1.84	0.78
2:B:26:LEU:HD22	2:B:29:ARG:HD2	1.65	0.78
2:B:227:SER:C	2:B:229:PHE:H	1.85	0.77
1:A:177:ILE:HD12	6:A:850:BCL:OBD	1.84	0.77
1:A:193:LEU:O	1:A:196:SER:N	2.16	0.77
1:A:219:LEU:HD12	2:B:132:ARG:NH1	1.99	0.77
1:A:124:ALA:HB1	6:A:851:BCL:H62	1.67	0.76
1:A:12:PRO:HG3	3:C:97:PRO:HB2	1.65	0.76
1:A:150:ILE:HG22	1:A:151:TRP:CD1	2.21	0.76
3:C:89:ARG:HD3	3:C:91:ALA:O	1.85	0.76
2:B:74:PHE:CE2	2:B:92:PHE:HB2	2.20	0.76
1:A:241:VAL:HG21	7:A:855:BPH:HAC2	1.68	0.76
1:A:12:PRO:HG3	3:C:97:PRO:CB	2.16	0.76
2:B:14:GLY:HA3	3:C:140:PHE:CE1	2.20	0.76
1:A:239:SER:O	1:A:242:PHE:N	2.19	0.76
2:B:281:GLY:O	2:B:285:LEU:HB2	1.86	0.76
2:B:102:GLY:HA2	2:B:170:SER:CB	2.16	0.75
1:A:173:HIS:HE1	1:A:177:ILE:HD11	1.51	0.75
2:B:153:ALA:HB1	6:B:852:BCL:H62	1.67	0.75
2:B:207:ALA:HA	6:B:853:BCL:O1A	1.86	0.75
2:B:103:LEU:HG	2:B:169:GLY:O	1.87	0.75
1:A:183:ASN:O	1:A:186:ALA:HB3	1.86	0.74
3:C:29:TYR:HD1	3:C:56:PHE:HE1	1.32	0.74
1:A:22:PHE:HA	1:A:24:PHE:HE2	1.50	0.74
3:C:193:MET:HE3	3:C:196:VAL:HG21	1.70	0.74
1:A:190:HIS:HA	8:A:857:U10:H4M1	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:LEU:HD12	1:A:106:GLU:HG2	1.69	0.74
1:A:229:ILE:HG22	1:A:230:HIS:H	1.53	0.74
2:B:3:TYR:CD2	3:C:194:GLN:HA	2.22	0.73
1:A:173:HIS:O	1:A:173:HIS:ND1	2.21	0.73
1:A:39:PHE:HB2	8:B:856:U10:H352	1.70	0.73
2:B:164:TYR:HB3	2:B:165:PRO:HD3	1.71	0.73
2:B:280:GLY:O	2:B:282:ILE:N	2.21	0.73
1:A:182:THR:O	1:A:185:LEU:N	2.21	0.73
3:C:140:PHE:CD2	3:C:169:VAL:HG21	2.24	0.73
2:B:253:ARG:HH11	2:B:259:ASN:ND2	1.87	0.72
2:B:103:LEU:HD22	2:B:166:ILE:HD13	1.70	0.72
3:C:14:SER:O	3:C:17:ILE:HG22	1.89	0.72
1:A:35:GLY:HA2	1:A:103:ARG:HD2	1.71	0.72
6:B:852:BCL:H201	7:B:854:BPH:H9C2	1.71	0.72
2:B:19:GLY:O	2:B:20:MET:O	2.08	0.72
3:C:115:VAL:HG12	3:C:116:ALA:N	2.04	0.72
1:A:9:TYR:O	1:A:11:VAL:N	2.22	0.72
1:A:145:ALA:O	1:A:156:TRP:NE1	2.23	0.72
2:B:63:GLY:HA3	7:B:854:BPH:H5C1	1.72	0.72
2:B:3:TYR:CE2	3:C:194:GLN:HA	2.25	0.71
2:B:242:GLY:CA	3:C:117:ARG:HD2	2.19	0.71
1:A:229:ILE:HG23	1:A:230:HIS:N	2.06	0.71
1:A:46:ILE:HG12	6:B:853:BCL:H191	1.72	0.71
2:B:18:LEU:HD22	2:B:18:LEU:H	1.55	0.71
6:B:852:BCL:HBB3	6:B:853:BCL:HMD2	1.73	0.71
1:A:100:TRP:HZ3	8:B:856:U10:H321	1.54	0.70
1:A:28:PRO:HB3	2:B:253:ARG:HE	1.56	0.70
1:A:135:ARG:HB3	1:A:136:PRO:HD3	1.72	0.70
1:A:51:TRP:O	1:A:54:VAL:HG22	1.92	0.70
2:B:38:LEU:O	2:B:40:GLY:N	2.24	0.70
3:C:193:MET:O	3:C:196:VAL:HG22	1.91	0.70
1:A:271:TRP:CD1	1:A:271:TRP:N	2.59	0.70
3:C:192:PRO:O	3:C:195:MET:N	2.24	0.70
1:A:187:LEU:HB2	2:B:216:PHE:CD2	2.27	0.69
1:A:183:ASN:HA	1:A:236:LEU:HD12	1.73	0.69
2:B:182:HIS:ND1	2:B:183:LEU:N	2.40	0.69
3:C:61:PRO:CA	3:C:76:PRO:HD2	2.21	0.69
1:A:217:ARG:HH21	2:B:44:ASN:HD22	1.39	0.69
1:A:20:ASN:HA	1:A:23:ASP:HB2	1.74	0.69
1:A:180:PHE:O	2:B:209:LEU:HD11	1.93	0.69
2:B:168:GLU:HG2	2:B:173:GLU:HG3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ALA:HB1	7:A:855:BPH:H4C2	1.74	0.69
3:C:133:PRO:HB3	3:C:168:TRP:CE2	2.28	0.69
3:C:18:TYR:O	3:C:21:TRP:N	2.26	0.68
6:A:850:BCL:H11	7:B:854:BPH:HBB3	1.74	0.68
2:B:287:SER:OG	2:B:294:TRP:NE1	2.26	0.68
2:B:26:LEU:CD2	2:B:29:ARG:HD2	2.23	0.68
2:B:90:PHE:N	2:B:90:PHE:HD1	1.91	0.68
1:A:183:ASN:HD22	1:A:184:ALA:N	1.92	0.68
3:C:148:PRO:HA	3:C:151:LEU:HD12	1.74	0.68
3:C:170:ASP:OD1	3:C:172:PRO:HG2	1.94	0.68
1:A:267:VAL:HG23	2:B:87:ARG:HD2	1.76	0.68
2:B:153:ALA:O	2:B:155:TRP:N	2.27	0.67
6:A:850:BCL:HBC1	6:B:852:BCL:HBD	1.74	0.67
6:B:852:BCL:CBB	6:B:853:BCL:HMD2	2.25	0.67
1:A:189:LEU:O	1:A:192:ALA:N	2.27	0.67
1:A:186:ALA:O	1:A:189:LEU:N	2.27	0.67
3:C:37:ARG:CZ	3:C:62:LYS:HD2	2.25	0.67
2:B:270:ILE:HD13	2:B:270:ILE:O	1.94	0.67
1:A:16:LEU:HD12	1:A:106:GLU:CG	2.25	0.66
2:B:123:PHE:HA	2:B:157:TRP:HH2	1.60	0.66
1:A:261:ASP:O	1:A:263:TRP:N	2.28	0.66
3:C:173:GLU:O	3:C:174:GLN:C	2.33	0.66
1:A:97:PHE:HB3	1:A:125:ILE:CD1	2.26	0.66
2:B:102:GLY:HA2	2:B:170:SER:HB3	1.77	0.66
1:A:229:ILE:CG2	1:A:230:HIS:H	2.07	0.66
3:C:37:ARG:NH1	3:C:62:LYS:HG2	2.11	0.66
3:C:29:TYR:CD1	3:C:56:PHE:HE1	2.13	0.66
2:B:202:HIS:CE1	2:B:206:ILE:CD1	2.78	0.66
1:A:114:GLY:CA	2:B:225:ALA:HB1	2.25	0.66
2:B:227:SER:O	2:B:229:PHE:N	2.27	0.66
3:C:75:VAL:HA	3:C:76:PRO:C	2.16	0.66
3:C:142:VAL:HG21	3:C:147:ASN:ND2	2.11	0.66
1:A:173:HIS:O	1:A:177:ILE:HG13	1.95	0.66
2:B:32:VAL:HG12	2:B:33:GLY:O	1.96	0.65
3:C:36:MET:HG2	3:C:40:TYR:CE1	2.31	0.65
2:B:287:SER:HG	2:B:294:TRP:HE1	1.42	0.65
3:C:68:HIS:CD2	3:C:123:LEU:HD12	2.30	0.65
2:B:149:ALA:O	2:B:152:SER:HB3	1.96	0.65
2:B:275:LEU:O	2:B:279:THR:HG23	1.95	0.65
1:A:222:TYR:CZ	2:B:39:LEU:HD13	2.32	0.65
2:B:243:THR:O	2:B:247:ARG:HG3	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:GLY:CA	2:B:50:ILE:HG12	2.27	0.65
3:C:221:SER:HB3	3:C:224:GLU:HG3	1.79	0.65
3:C:179:LEU:O	3:C:181:VAL:HG23	1.97	0.64
2:B:287:SER:HB3	2:B:294:TRP:HE1	1.60	0.64
3:C:226:THR:OG1	3:C:229:GLU:HG3	1.97	0.64
1:A:233:GLY:HA3	2:B:216:PHE:CE1	2.33	0.64
2:B:287:SER:O	2:B:288:ASP:HB3	1.98	0.64
2:B:140:LEU:O	2:B:142:MET:HG3	1.98	0.64
2:B:18:LEU:HD22	2:B:18:LEU:N	2.13	0.64
1:A:193:LEU:O	1:A:194:VAL:C	2.35	0.63
2:B:222:THR:HG22	2:B:223:ILE:N	2.11	0.63
1:A:194:VAL:HG11	2:B:266:HIS:CD2	2.33	0.63
3:C:70:ARG:NH2	3:C:120:LEU:HD22	2.13	0.63
2:B:90:PHE:N	2:B:90:PHE:CD1	2.62	0.63
2:B:270:ILE:HG23	2:B:271:TRP:N	2.13	0.63
1:A:174:MET:HB3	6:A:850:BCL:O1D	1.97	0.63
3:C:61:PRO:HG3	3:C:76:PRO:HG2	1.81	0.63
1:A:146:PHE:HB2	1:A:147:PRO:HD2	1.81	0.63
1:A:53:ALA:HB1	1:A:64:ILE:HD12	1.80	0.63
3:C:41:PRO:HG3	3:C:58:LEU:HD11	1.79	0.63
2:B:187:ASN:O	2:B:190:SER:HB3	1.98	0.63
3:C:65:ILE:H	3:C:65:ILE:HD12	1.64	0.63
1:A:219:LEU:HD12	2:B:132:ARG:HH12	1.63	0.63
1:A:269:LEU:HB2	1:A:272:TRP:NE1	2.13	0.63
1:A:216:PHE:O	1:A:219:LEU:N	2.31	0.63
1:A:194:VAL:HG21	2:B:266:HIS:CD2	2.33	0.63
1:A:168:HIS:HB3	2:B:183:LEU:HD13	1.81	0.63
3:C:115:VAL:CG1	3:C:116:ALA:N	2.62	0.63
1:A:171:PRO:HD2	1:A:259:TRP:CZ3	2.34	0.62
3:C:153:VAL:HG21	3:C:181:VAL:HG13	1.81	0.62
2:B:233:ARG:NE	3:C:122:GLU:OE1	2.30	0.62
2:B:175:VAL:HG22	2:B:185:TRP:CE2	2.34	0.62
2:B:66:TRP:CD1	2:B:122:MET:HB2	2.33	0.62
1:A:38:THR:HG22	1:A:99:SER:HB2	1.79	0.62
3:C:96:PHE:HB3	3:C:97:PRO:CD	2.30	0.62
1:A:45:GLY:HA3	7:A:855:BPH:H9C1	1.79	0.62
3:C:83:ARG:HD2	3:C:114:TRP:CH2	2.35	0.62
1:A:269:LEU:HB2	1:A:272:TRP:HE1	1.64	0.62
3:C:134:MET:O	3:C:136:ALA:N	2.33	0.62
2:B:199:ASN:HA	2:B:294:TRP:CE3	2.35	0.61
2:B:76:TYR:OH	2:B:110:LYS:NZ	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:223:ILE:HD11	2:B:234:GLU:OE2	2.00	0.61
1:A:1:ALA:O	1:A:2:LEU:HD23	1.99	0.61
1:A:172:ALA:HB3	1:A:247:CYS:CB	2.31	0.61
2:B:82:PRO:O	2:B:86:LEU:HD23	2.00	0.61
1:A:180:PHE:CD2	1:A:240:ALA:HB1	2.35	0.61
2:B:102:GLY:HA2	2:B:170:SER:HB2	1.83	0.61
2:B:150:PHE:CA	7:B:854:BPH:HMD3	2.31	0.61
2:B:153:ALA:C	2:B:155:TRP:N	2.54	0.61
1:A:138:MET:SD	1:A:249:ILE:HD11	2.41	0.61
2:B:97:PRO:CB	2:B:112:GLY:HA3	2.31	0.60
1:A:52:SER:O	1:A:56:GLN:HB2	2.02	0.60
2:B:11:GLN:HB2	3:C:144:ALA:HB3	1.83	0.60
3:C:143:SER:O	3:C:144:ALA:HB2	2.01	0.60
1:A:192:ALA:HB1	2:B:146:THR:HA	1.82	0.60
2:B:64:LEU:HD21	7:B:854:BPH:C11	2.21	0.60
3:C:238:ALA:O	3:C:240:GLY:N	2.34	0.60
3:C:111:PRO:HD2	3:C:243:TYR:OH	2.02	0.60
6:A:851:BCL:CAA	6:B:853:BCL:HBC1	2.31	0.60
2:B:268:TRP:O	2:B:269:ALA:C	2.40	0.60
2:B:125:ALA:O	7:B:854:BPH:H1C2	2.02	0.60
1:A:183:ASN:ND2	1:A:184:ALA:N	2.48	0.60
1:A:147:PRO:HD3	1:A:156:TRP:CD1	2.36	0.60
1:A:265:TRP:CH2	1:A:266:TRP:HE3	2.19	0.60
2:B:287:SER:O	2:B:288:ASP:CB	2.48	0.60
1:A:186:ALA:O	1:A:188:ALA:N	2.35	0.60
1:A:239:SER:O	1:A:241:VAL:N	2.35	0.60
2:B:288:ASP:OD2	9:B:911:HOH:O	2.17	0.60
2:B:150:PHE:HA	7:B:854:BPH:HMD3	1.83	0.59
2:B:159:VAL:HA	2:B:163:ILE:HB	1.83	0.59
3:C:94:GLU:O	3:C:96:PHE:HD1	1.85	0.59
2:B:18:LEU:H	2:B:18:LEU:CD2	2.14	0.59
2:B:238:ILE:HG22	2:B:239:ALA:N	2.16	0.59
2:B:82:PRO:O	2:B:85:PHE:HB3	2.01	0.59
2:B:260:ALA:C	8:B:856:U10:H4M3	2.21	0.59
2:B:229:PHE:CZ	2:B:247:ARG:NH1	2.71	0.59
2:B:175:VAL:HG13	2:B:176:PRO:HD2	1.83	0.59
2:B:267:ARG:O	2:B:268:TRP:O	2.21	0.59
3:C:193:MET:HE3	3:C:196:VAL:CG2	2.32	0.59
3:C:151:LEU:O	3:C:164:VAL:HG23	2.03	0.59
1:A:46:ILE:HG12	6:B:853:BCL:C19	2.33	0.59
3:C:68:HIS:HD2	3:C:123:LEU:HD12	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:THR:OG1	1:A:210:ASP:HB2	2.03	0.58
3:C:156:CYS:SG	3:C:248:ARG:HB2	2.42	0.58
1:A:182:THR:O	1:A:183:ASN:C	2.39	0.58
2:B:227:SER:O	2:B:230:GLY:N	2.35	0.58
2:B:271:TRP:C	2:B:273:ALA:N	2.56	0.58
1:A:164:TYR:CE1	1:A:256:PHE:O	2.57	0.58
1:A:175:ILE:HG21	1:A:243:PHE:CD2	2.39	0.58
2:B:267:ARG:O	2:B:268:TRP:C	2.41	0.58
2:B:279:THR:O	2:B:282:ILE:HB	2.04	0.58
3:C:192:PRO:O	3:C:193:MET:C	2.43	0.57
1:A:39:PHE:HB2	8:B:856:U10:C35	2.34	0.57
1:A:164:TYR:HE1	1:A:256:PHE:O	1.87	0.57
1:A:193:LEU:HD21	1:A:212:GLU:HB3	1.85	0.57
1:A:101:ALA:O	1:A:104:GLU:HB2	2.04	0.57
1:A:185:LEU:HD23	1:A:185:LEU:O	2.04	0.57
1:A:187:LEU:H	2:B:216:PHE:HE2	1.52	0.57
3:C:193:MET:CE	3:C:196:VAL:CG2	2.83	0.57
2:B:153:ALA:O	2:B:154:ILE:C	2.43	0.57
2:B:204:LEU:O	2:B:207:ALA:HB3	2.04	0.57
2:B:97:PRO:HG2	2:B:171:TRP:HB2	1.86	0.57
1:A:187:LEU:HD13	2:B:216:PHE:CG	2.39	0.57
1:A:179:PHE:HB3	1:A:240:ALA:HB2	1.86	0.57
2:B:270:ILE:CG2	2:B:271:TRP:N	2.68	0.57
3:C:29:TYR:CD1	3:C:56:PHE:CE1	2.93	0.57
1:A:179:PHE:O	1:A:181:PHE:N	2.37	0.57
1:A:193:LEU:HD22	8:A:857:U10:H4M2	1.86	0.57
3:C:112:ALA:O	3:C:113:SER:O	2.23	0.57
3:C:133:PRO:HB3	3:C:168:TRP:CD2	2.40	0.57
1:A:272:TRP:CZ3	2:B:86:LEU:CB	2.88	0.57
1:A:87:GLN:O	1:A:91:ILE:HG12	2.05	0.57
2:B:242:GLY:O	2:B:246:GLU:HG3	2.05	0.57
2:B:246:GLU:O	2:B:249:ALA:HB3	2.05	0.56
1:A:170:ASN:HA	1:A:259:TRP:CD2	2.40	0.56
1:A:272:TRP:HB3	2:B:83:ALA:HB1	1.86	0.56
3:C:89:ARG:NH1	3:C:92:VAL:O	2.38	0.56
1:A:255:TRP:HZ2	1:A:258:GLN:O	1.88	0.56
2:B:64:LEU:O	2:B:65:MET:C	2.44	0.56
1:A:35:GLY:O	8:B:856:U10:C35	2.54	0.56
2:B:3:TYR:CE2	2:B:5:ASN:OD1	2.58	0.56
1:A:54:VAL:HG12	1:A:59:TRP:HZ2	1.70	0.56
1:A:130:THR:HA	1:A:134:PHE:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:TYR:CG	1:A:31:VAL:N	2.74	0.56
1:A:97:PHE:HB3	1:A:125:ILE:HD11	1.86	0.56
1:A:97:PHE:CE1	6:A:851:BCL:H101	2.40	0.55
1:A:153:HIS:O	1:A:156:TRP:HB3	2.06	0.55
2:B:280:GLY:C	2:B:282:ILE:N	2.59	0.55
2:B:198:TYR:O	2:B:199:ASN:C	2.44	0.55
3:C:226:THR:O	3:C:229:GLU:N	2.39	0.55
2:B:228:ARG:HH12	3:C:241:LEU:HD11	1.72	0.55
3:C:193:MET:O	3:C:195:MET:N	2.40	0.55
3:C:46:ASP:OD1	3:C:48:THR:HG23	2.06	0.55
1:A:93:ALA:O	1:A:97:PHE:CD2	2.60	0.55
2:B:280:GLY:HA2	6:B:852:BCL:HED2	1.88	0.55
3:C:227:LEU:O	3:C:228:LEU:C	2.45	0.55
1:A:261:ASP:O	1:A:262:TRP:C	2.45	0.55
2:B:129:TRP:O	2:B:130:TRP:C	2.44	0.55
2:B:143:GLY:C	2:B:145:HIS:H	2.09	0.55
2:B:168:GLU:O	2:B:168:GLU:HG3	2.06	0.55
1:A:194:VAL:HG11	2:B:266:HIS:CG	2.42	0.55
3:C:33:THR:O	3:C:35:ASN:N	2.40	0.55
1:A:223:SER:HA	8:A:857:U10:O2	2.06	0.55
7:A:855:BPH:CBB	2:B:210:TYR:HB3	2.37	0.55
2:B:68:PHE:O	2:B:71:GLY:N	2.40	0.55
3:C:229:GLU:O	3:C:233:ILE:HG13	2.07	0.55
6:A:850:BCL:HBD	6:A:850:BCL:HAA2	1.88	0.54
1:A:6:GLU:OE2	1:A:10:ARG:NH2	2.40	0.54
2:B:251:PHE:CD1	2:B:251:PHE:C	2.80	0.54
3:C:37:ARG:NH2	3:C:62:LYS:HD2	2.22	0.54
2:B:269:ALA:O	2:B:271:TRP:N	2.40	0.54
2:B:282:ILE:O	2:B:285:LEU:N	2.41	0.54
1:A:149:GLY:HA3	1:A:152:THR:OG1	2.08	0.54
3:C:86:ALA:HB1	3:C:101:THR:HG1	1.70	0.54
1:A:12:PRO:HG3	3:C:97:PRO:HB3	1.88	0.54
1:A:230:HIS:CD2	2:B:223:ILE:HG13	2.42	0.54
2:B:299:GLN:CA	2:B:299:GLN:NE2	2.61	0.54
1:A:168:HIS:CD2	6:A:851:BCL:HMC2	2.43	0.54
1:A:192:ALA:HB1	2:B:146:THR:CA	2.37	0.54
3:C:111:PRO:HG2	3:C:243:TYR:HE2	1.73	0.54
2:B:171:TRP:HE3	2:B:171:TRP:HA	1.73	0.54
1:A:20:ASN:HA	1:A:23:ASP:CB	2.38	0.54
2:B:37:THR:HG22	2:B:37:THR:O	2.07	0.54
1:A:175:ILE:O	1:A:176:ALA:C	2.46	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:LEU:O	1:A:190:HIS:C	2.46	0.54
1:A:272:TRP:CZ3	2:B:86:LEU:HB3	2.43	0.54
7:A:855:BPH:HBB1	2:B:210:TYR:CG	2.43	0.53
2:B:130:TRP:HD1	2:B:150:PHE:CD2	2.26	0.53
3:C:146:LYS:HE3	3:C:151:LEU:HD11	1.90	0.53
1:A:125:ILE:O	1:A:128:TYR:HB3	2.08	0.53
1:A:196:SER:HB2	2:B:143:GLY:O	2.07	0.53
1:A:16:LEU:CD1	1:A:106:GLU:HG2	2.36	0.53
1:A:267:VAL:HG23	2:B:87:ARG:CD	2.38	0.53
1:A:170:ASN:HA	1:A:259:TRP:CE3	2.43	0.53
3:C:112:ALA:O	3:C:113:SER:C	2.46	0.53
1:A:54:VAL:HG23	1:A:55:LEU:N	2.24	0.53
2:B:222:THR:O	2:B:223:ILE:C	2.45	0.53
3:C:17:ILE:O	3:C:21:TRP:CD1	2.62	0.53
1:A:129:LEU:O	1:A:130:THR:C	2.47	0.53
2:B:37:THR:O	2:B:41:TRP:NE1	2.41	0.53
1:A:80:LEU:HA	1:A:84:GLY:HA3	1.89	0.53
1:A:170:ASN:ND2	1:A:259:TRP:CZ2	2.76	0.53
2:B:171:TRP:CE3	2:B:171:TRP:HA	2.44	0.53
2:B:286:LEU:HD22	2:B:290:VAL:HB	1.89	0.53
2:B:38:LEU:C	2:B:40:GLY:N	2.62	0.53
1:A:35:GLY:O	8:B:856:U10:H353	2.08	0.53
3:C:111:PRO:HG2	3:C:243:TYR:CE2	2.44	0.53
1:A:239:SER:O	1:A:240:ALA:C	2.47	0.53
2:B:229:PHE:CE1	3:C:238:ALA:HB2	2.44	0.53
2:B:253:ARG:HH11	2:B:259:ASN:HD21	1.57	0.53
1:A:60:ASN:HB3	1:A:63:LEU:HD12	1.91	0.53
6:A:851:BCL:HAA2	6:B:853:BCL:HBC1	1.91	0.52
2:B:192:VAL:O	2:B:192:VAL:HG12	2.09	0.52
1:A:141:ALA:HB3	1:A:144:TYR:CE2	2.45	0.52
6:A:850:BCL:H191	2:B:70:ILE:HG21	1.91	0.52
2:B:277:THR:HG21	7:B:854:BPH:HAC2	1.91	0.52
1:A:172:ALA:HB3	1:A:247:CYS:HB3	1.91	0.52
7:A:855:BPH:HED3	2:B:218:MET:HE3	1.90	0.52
3:C:178:PHE:HD1	3:C:191:LEU:O	1.92	0.52
1:A:272:TRP:CZ3	2:B:86:LEU:HB2	2.44	0.52
2:B:4:GLN:O	2:B:6:ILE:N	2.43	0.52
3:C:140:PHE:HD2	3:C:169:VAL:HG21	1.75	0.52
1:A:207:ARG:HG3	1:A:211:HIS:CG	2.45	0.52
3:C:234:CYS:O	3:C:237:VAL:HB	2.10	0.52
1:A:272:TRP:O	1:A:275:ILE:HG12	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:PHE:O	1:A:218:ASP:N	2.43	0.52
2:B:261:THR:HG23	3:C:35:ASN:HA	1.92	0.52
2:B:182:HIS:O	2:B:183:LEU:C	2.49	0.52
2:B:265:ILE:HG22	2:B:266:HIS:ND1	2.25	0.52
1:A:116:HIS:CD2	2:B:224:LEU:CB	2.89	0.51
2:B:271:TRP:O	2:B:272:MET:C	2.47	0.51
2:B:155:TRP:CE3	2:B:155:TRP:HA	2.46	0.51
2:B:155:TRP:HE3	2:B:155:TRP:HA	1.75	0.51
3:C:17:ILE:O	3:C:21:TRP:HD1	1.94	0.51
2:B:72:ILE:O	2:B:75:TRP:HB2	2.10	0.51
1:A:121:PHE:N	7:A:855:BPH:HMD3	2.25	0.51
2:B:228:ARG:NH1	3:C:241:LEU:HD11	2.26	0.51
1:A:187:LEU:N	2:B:216:PHE:CE2	2.78	0.51
2:B:183:LEU:O	2:B:186:THR:HB	2.09	0.51
2:B:203:GLY:O	2:B:206:ILE:HB	2.10	0.51
2:B:208:PHE:CE2	2:B:275:LEU:HB3	2.46	0.51
1:A:144:TYR:O	1:A:156:TRP:HZ2	1.93	0.51
1:A:228:GLY:O	1:A:229:ILE:C	2.48	0.51
2:B:3:TYR:CE1	2:B:9:GLN:CG	2.93	0.51
1:A:267:VAL:HG23	2:B:87:ARG:CG	2.41	0.51
2:B:164:TYR:OH	2:B:288:ASP:CB	2.58	0.51
3:C:18:TYR:O	3:C:21:TRP:HB2	2.11	0.51
3:C:181:VAL:O	3:C:188:THR:HA	2.11	0.51
1:A:205:GLU:O	1:A:206:MET:C	2.49	0.51
1:A:54:VAL:HG12	1:A:59:TRP:CZ2	2.46	0.51
3:C:189:ARG:HH11	3:C:189:ARG:HG2	1.76	0.51
1:A:75:LEU:HD21	1:A:140:GLY:C	2.31	0.51
2:B:255:THR:HG22	2:B:256:MET:N	2.26	0.51
1:A:172:ALA:CB	1:A:247:CYS:HB3	2.40	0.51
3:C:156:CYS:HB3	3:C:206:ASN:O	2.11	0.51
1:A:36:VAL:O	1:A:39:PHE:HB3	2.11	0.51
2:B:175:VAL:CG1	2:B:176:PRO:HD2	2.40	0.51
3:C:233:ILE:C	3:C:237:VAL:HG23	2.30	0.51
2:B:74:PHE:CZ	2:B:92:PHE:HB2	2.45	0.51
2:B:258:PHE:O	2:B:259:ASN:HB3	2.11	0.51
1:A:15:THR:HG21	1:A:19:GLY:O	2.11	0.51
1:A:186:ALA:O	1:A:187:LEU:C	2.48	0.51
1:A:36:VAL:O	1:A:39:PHE:N	2.39	0.51
1:A:49:ILE:CD1	1:A:89:ILE:HD13	2.40	0.51
3:C:29:TYR:HD1	3:C:56:PHE:CE1	2.20	0.51
1:A:2:LEU:HB3	1:A:6:GLU:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:TRP:HZ2	2:B:254:TRP:CZ3	2.28	0.51
2:B:239:ALA:HA	3:C:73:LEU:CD2	2.41	0.50
2:B:206:ILE:HG13	6:B:852:BCL:HMB3	1.93	0.50
2:B:299:GLN:CA	2:B:299:GLN:HE21	2.08	0.50
2:B:24:VAL:HG22	2:B:139:ALA:HB1	1.92	0.50
2:B:270:ILE:C	2:B:270:ILE:HD13	2.31	0.50
1:A:52:SER:OG	1:A:66:VAL:HG22	2.11	0.50
2:B:260:ALA:CB	2:B:265:ILE:HD13	2.41	0.50
3:C:115:VAL:CG1	3:C:116:ALA:H	2.24	0.50
1:A:123:PHE:CG	1:A:238:LEU:HD22	2.46	0.50
1:A:186:ALA:CB	2:B:216:PHE:HE2	2.25	0.50
1:A:118:PRO:O	1:A:119:PHE:C	2.50	0.50
7:A:855:BPH:HBD	7:A:855:BPH:HAA2	1.94	0.50
1:A:214:THR:O	1:A:215:PHE:O	2.29	0.50
1:A:244:SER:HB3	6:A:851:BCL:O1D	2.12	0.50
2:B:186:THR:HG23	6:B:852:BCL:HMD2	1.93	0.50
2:B:250:LEU:HD22	2:B:254:TRP:NE1	2.26	0.50
1:A:18:GLY:O	1:A:21:LEU:HB2	2.11	0.50
1:A:206:MET:CE	2:B:235:LEU:HD22	2.42	0.49
3:C:193:MET:C	3:C:195:MET:H	2.15	0.49
2:B:16:ALA:O	2:B:18:LEU:HD22	2.12	0.49
1:A:187:LEU:N	2:B:216:PHE:HE2	2.09	0.49
2:B:235:LEU:O	2:B:238:ILE:HB	2.12	0.49
2:B:269:ALA:O	2:B:270:ILE:C	2.50	0.49
1:A:175:ILE:HG22	1:A:176:ALA:N	2.27	0.49
1:A:208:THR:C	1:A:210:ASP:N	2.64	0.49
3:C:83:ARG:CB	3:C:84:PRO:HD2	2.38	0.49
2:B:117:ILE:O	2:B:120:PHE:HB3	2.13	0.49
1:A:102:LEU:O	1:A:105:VAL:HB	2.12	0.49
1:A:20:ASN:O	1:A:21:LEU:C	2.50	0.49
1:A:89:ILE:HG22	1:A:148:TYR:HE2	1.77	0.49
2:B:4:GLN:O	2:B:6:ILE:HD13	2.11	0.49
1:A:2:LEU:HA	1:A:6:GLU:OE1	2.13	0.49
1:A:79:PRO:O	1:A:80:LEU:O	2.29	0.49
1:A:254:ILE:HD12	1:A:254:ILE:C	2.32	0.49
1:A:96:ALA:HB1	7:A:855:BPH:C4	2.39	0.49
3:C:70:ARG:CZ	3:C:120:LEU:HD13	2.43	0.49
1:A:30:TYR:CD1	1:A:31:VAL:N	2.78	0.49
2:B:94:LEU:HD11	2:B:114:LEU:HB3	1.94	0.49
1:A:208:THR:HG23	1:A:211:HIS:CE1	2.47	0.49
6:A:850:BCL:HMD2	6:A:851:BCL:CBB	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:152:SER:HB2	2:B:274:VAL:HG13	1.95	0.49
2:B:152:SER:O	2:B:155:TRP:HB3	2.12	0.49
2:B:3:TYR:HD2	3:C:194:GLN:HA	1.73	0.49
3:C:18:TYR:O	3:C:20:PHE:N	2.46	0.49
2:B:99:PRO:HG3	2:B:172:SER:OG	2.12	0.49
1:A:186:ALA:HB3	2:B:216:PHE:HE2	1.77	0.49
1:A:9:TYR:OH	2:B:246:GLU:OE1	2.11	0.49
2:B:239:ALA:HA	3:C:73:LEU:HD22	1.94	0.49
3:C:226:THR:O	3:C:227:LEU:C	2.50	0.49
2:B:140:LEU:HB3	2:B:142:MET:HG3	1.94	0.49
1:A:27:GLY:C	1:A:29:PHE:H	2.16	0.49
2:B:192:VAL:O	2:B:192:VAL:CG1	2.61	0.49
1:A:243:PHE:O	1:A:246:LEU:HB3	2.12	0.49
2:B:151:LEU:HD12	2:B:151:LEU:HA	1.62	0.49
2:B:229:PHE:HE1	3:C:238:ALA:HB2	1.76	0.49
2:B:201:PHE:HB2	2:B:283:GLY:HA2	1.95	0.49
3:C:215:GLY:O	3:C:216:ILE:C	2.49	0.49
1:A:243:PHE:O	1:A:244:SER:C	2.50	0.48
2:B:222:THR:O	2:B:224:LEU:N	2.46	0.48
3:C:183:LEU:HD11	3:C:189:ARG:HG3	1.95	0.48
2:B:168:GLU:CG	2:B:173:GLU:HG3	2.42	0.48
1:A:235:LEU:O	1:A:236:LEU:C	2.49	0.48
1:A:179:PHE:CB	1:A:240:ALA:HB2	2.43	0.48
1:A:239:SER:C	1:A:241:VAL:N	2.65	0.48
3:C:189:ARG:NH1	3:C:189:ARG:HG2	2.28	0.48
3:C:40:TYR:HB3	3:C:58:LEU:HD21	1.94	0.48
2:B:189:PHE:CD1	2:B:189:PHE:O	2.66	0.48
2:B:58:LEU:O	2:B:61:PHE:N	2.46	0.48
1:A:187:LEU:HB2	2:B:216:PHE:HD2	1.78	0.48
1:A:217:ARG:HH21	2:B:44:ASN:ND2	2.09	0.48
1:A:249:ILE:CD1	1:A:249:ILE:O	2.62	0.48
1:A:178:SER:O	1:A:181:PHE:HB2	2.14	0.48
6:B:853:BCL:HMA1	6:B:853:BCL:H142	1.96	0.48
1:A:177:ILE:CD1	6:A:850:BCL:HMD1	2.44	0.48
2:B:228:ARG:O	2:B:229:PHE:CD1	2.67	0.48
1:A:53:ALA:CB	1:A:64:ILE:HD12	2.43	0.48
1:A:179:PHE:C	1:A:181:PHE:N	2.66	0.48
1:A:181:PHE:CD2	7:B:854:BPH:HBB1	2.49	0.48
1:A:100:TRP:CZ3	8:B:856:U10:H321	2.42	0.48
1:A:146:PHE:HA	1:A:156:TRP:NE1	2.29	0.48
1:A:114:GLY:HA3	2:B:225:ALA:CB	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:263:GLU:O	2:B:266:HIS:HB2	2.12	0.48
3:C:83:ARG:HB2	3:C:84:PRO:CD	2.41	0.48
1:A:30:TYR:HB2	2:B:254:TRP:HB3	1.96	0.48
2:B:148:TRP:HA	2:B:148:TRP:CE3	2.49	0.48
3:C:81:GLU:HA	3:C:81:GLU:OE2	2.12	0.48
1:A:173:HIS:CG	1:A:173:HIS:O	2.66	0.48
2:B:150:PHE:N	7:B:854:BPH:HMD3	2.29	0.48
2:B:199:ASN:HB2	2:B:294:TRP:CD2	2.49	0.48
1:A:217:ARG:NH2	2:B:44:ASN:HD22	2.10	0.48
1:A:219:LEU:HD11	2:B:133:THR:HG22	1.96	0.48
1:A:229:ILE:HD11	8:A:857:U10:O4	2.14	0.48
3:C:82:ASP:O	3:C:83:ARG:HB3	2.14	0.48
1:A:25:TRP:O	1:A:26:VAL:HG23	2.14	0.48
1:A:89:ILE:HG22	1:A:148:TYR:CE2	2.49	0.47
2:B:164:TYR:OH	2:B:288:ASP:HB3	2.13	0.47
2:B:235:LEU:HA	2:B:235:LEU:HD23	1.67	0.47
1:A:228:GLY:O	1:A:231:ARG:HB2	2.14	0.47
3:C:83:ARG:NH2	3:C:107:ASP:O	2.47	0.47
1:A:28:PRO:CB	2:B:253:ARG:HE	2.26	0.47
2:B:66:TRP:CZ2	2:B:122:MET:HE1	2.49	0.47
1:A:173:HIS:HB2	1:A:247:CYS:SG	2.54	0.47
2:B:260:ALA:O	8:B:856:U10:H4M3	2.14	0.47
3:C:118:ARG:C	3:C:120:LEU:H	2.18	0.47
3:C:111:PRO:CG	3:C:243:TYR:CE2	2.97	0.47
2:B:123:PHE:HA	2:B:157:TRP:CH2	2.46	0.47
3:C:177:ARG:HG2	3:C:177:ARG:HH11	1.79	0.47
3:C:226:THR:O	3:C:229:GLU:HB2	2.14	0.47
3:C:148:PRO:HA	3:C:151:LEU:CD1	2.42	0.47
1:A:79:PRO:O	1:A:80:LEU:C	2.53	0.47
2:B:73:TRP:O	2:B:77:GLN:HG3	2.15	0.47
2:B:134:TYR:O	2:B:137:ALA:N	2.48	0.47
2:B:215:LEU:O	2:B:218:MET:HB2	2.15	0.47
2:B:20:MET:HE2	3:C:125:GLY:HA3	1.97	0.47
1:A:210:ASP:HB3	2:B:20:MET:SD	2.55	0.47
2:B:241:ARG:O	3:C:117:ARG:HG2	2.14	0.47
1:A:102:LEU:HD23	1:A:102:LEU:HA	1.74	0.47
1:A:54:VAL:CG2	1:A:55:LEU:N	2.78	0.47
1:A:28:PRO:O	2:B:253:ARG:O	2.33	0.47
1:A:26:VAL:O	1:A:29:PHE:HB2	2.14	0.47
1:A:68:PRO:HB2	1:A:143:GLY:HA2	1.97	0.47
3:C:23:PHE:C	3:C:23:PHE:CD2	2.88	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:ARG:HG3	1:A:211:HIS:CD2	2.48	0.47
1:A:187:LEU:HD13	2:B:216:PHE:CB	2.45	0.47
2:B:30:SER:OG	2:B:50:ILE:HG22	2.13	0.47
3:C:240:GLY:O	3:C:244:ALA:HB3	2.14	0.47
1:A:211:HIS:O	1:A:212:GLU:C	2.53	0.47
1:A:52:SER:HB2	1:A:85:LEU:HD12	1.97	0.47
7:A:855:BPH:HBB1	2:B:210:TYR:CD2	2.50	0.47
2:B:271:TRP:O	2:B:274:VAL:N	2.47	0.47
1:A:185:LEU:HG	7:B:854:BPH:NC	2.30	0.47
2:B:261:THR:CG2	3:C:35:ASN:HA	2.45	0.47
1:A:179:PHE:C	1:A:181:PHE:H	2.18	0.46
2:B:240:ASP:O	3:C:117:ARG:NE	2.46	0.46
3:C:66:LEU:HD13	3:C:118:ARG:HH12	1.79	0.46
1:A:131:HIS:HB3	1:A:146:PHE:HE2	1.79	0.46
3:C:153:VAL:HG21	3:C:181:VAL:CG1	2.45	0.46
1:A:190:HIS:CE1	1:A:230:HIS:CE1	3.03	0.46
2:B:293:ASN:OD1	2:B:295:TYR:N	2.45	0.46
3:C:171:ILE:N	3:C:171:ILE:HD13	2.30	0.46
2:B:64:LEU:O	2:B:68:PHE:N	2.40	0.46
3:C:170:ASP:OD1	3:C:172:PRO:CG	2.63	0.46
2:B:106:ALA:O	2:B:107:ALA:C	2.53	0.46
3:C:96:PHE:HB3	3:C:97:PRO:HD2	1.96	0.46
2:B:97:PRO:HG2	2:B:171:TRP:CB	2.45	0.46
3:C:195:MET:HA	3:C:195:MET:HE2	1.97	0.46
2:B:24:VAL:CG2	2:B:139:ALA:HB1	2.45	0.46
1:A:217:ARG:O	1:A:221:GLY:HA2	2.16	0.46
1:A:217:ARG:NH2	2:B:44:ASN:ND2	2.63	0.46
3:C:147:ASN:OD1	3:C:149:ILE:HG13	2.15	0.46
3:C:44:ASN:ND2	3:C:49:PRO:O	2.48	0.46
2:B:57:VAL:O	2:B:58:LEU:C	2.54	0.46
3:C:61:PRO:HG3	3:C:76:PRO:CG	2.44	0.46
2:B:256:MET:O	2:B:256:MET:HG3	2.15	0.46
1:A:50:ALA:O	1:A:54:VAL:HG13	2.16	0.46
3:C:33:THR:O	3:C:34:GLU:C	2.55	0.46
1:A:31:VAL:HG12	1:A:32:GLY:N	2.31	0.46
2:B:285:LEU:O	2:B:285:LEU:HG	2.16	0.46
2:B:64:LEU:O	2:B:67:PHE:N	2.49	0.46
1:A:279:ILE:HG22	1:A:279:ILE:O	2.15	0.46
3:C:24:LEU:O	3:C:28:ILE:HG12	2.15	0.46
1:A:126:LEU:O	1:A:127:ALA:C	2.54	0.45
2:B:59:SER:OG	2:B:129:TRP:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:182:HIS:O	2:B:185:TRP:HB3	2.16	0.45
1:A:151:TRP:O	1:A:154:LEU:HB2	2.16	0.45
1:A:212:GLU:O	1:A:213:ASP:C	2.55	0.45
2:B:199:ASN:O	2:B:202:HIS:HB3	2.16	0.45
2:B:215:LEU:HD23	2:B:269:ALA:HA	1.98	0.45
3:C:233:ILE:O	3:C:234:CYS:C	2.53	0.45
3:C:37:ARG:HG2	3:C:37:ARG:HH11	1.81	0.45
3:C:14:SER:O	3:C:15:LEU:C	2.54	0.45
1:A:183:ASN:O	1:A:186:ALA:CB	2.60	0.45
1:A:230:HIS:HE1	2:B:234:GLU:OE1	1.99	0.45
2:B:280:GLY:O	2:B:281:GLY:C	2.53	0.45
2:B:253:ARG:HA	2:B:258:PHE:O	2.16	0.45
3:C:146:LYS:HG2	3:C:199:GLN:O	2.17	0.45
3:C:185:ASP:OD1	3:C:187:SER:OG	2.32	0.45
1:A:148:TYR:CD2	7:A:855:BPH:H143	2.51	0.45
2:B:206:ILE:CG2	2:B:210:TYR:CE2	2.99	0.45
7:A:855:BPH:CMC	2:B:213:ALA:HB3	2.47	0.45
2:B:206:ILE:HG21	6:B:853:BCL:CAD	2.46	0.45
1:A:28:PRO:CB	2:B:253:ARG:NE	2.79	0.45
2:B:81:ASN:HB3	2:B:84:VAL:CG2	2.45	0.45
1:A:114:GLY:CA	2:B:225:ALA:CB	2.94	0.45
1:A:146:PHE:HB2	1:A:147:PRO:CD	2.47	0.45
3:C:134:MET:HB2	3:C:167:ILE:O	2.17	0.45
3:C:37:ARG:CZ	3:C:62:LYS:CD	2.93	0.45
3:C:37:ARG:HB3	3:C:75:VAL:HB	1.99	0.45
1:A:54:VAL:CG1	1:A:59:TRP:HZ2	2.29	0.45
2:B:78:ALA:HB2	2:B:92:PHE:CZ	2.52	0.45
1:A:267:VAL:HG23	2:B:87:ARG:HG2	1.99	0.45
2:B:290:VAL:HG12	2:B:290:VAL:O	2.16	0.45
2:B:116:LEU:O	2:B:117:ILE:C	2.55	0.45
1:A:166:ASN:HB3	1:A:169:TYR:CD2	2.52	0.45
2:B:227:SER:C	2:B:229:PHE:N	2.54	0.45
2:B:273:ALA:C	2:B:275:LEU:N	2.70	0.45
2:B:190:SER:O	2:B:194:GLY:O	2.35	0.45
3:C:65:ILE:N	3:C:65:ILE:HD12	2.29	0.45
1:A:187:LEU:HG	2:B:269:ALA:HB1	1.98	0.45
1:A:186:ALA:C	1:A:188:ALA:N	2.70	0.45
2:B:264:GLY:C	2:B:266:HIS:N	2.69	0.45
2:B:3:TYR:CE1	2:B:9:GLN:HG3	2.51	0.45
1:A:178:SER:HA	6:A:850:BCL:O1A	2.16	0.45
2:B:240:ASP:O	2:B:241:ARG:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:264:GLY:O	2:B:265:ILE:C	2.55	0.45
2:B:280:GLY:C	2:B:282:ILE:H	2.21	0.45
1:A:267:VAL:HA	2:B:87:ARG:HG3	1.98	0.45
3:C:122:GLU:OE2	3:C:130:LYS:HE2	2.17	0.45
2:B:108:PRO:O	2:B:109:LEU:C	2.55	0.45
1:A:169:TYR:O	1:A:170:ASN:C	2.52	0.44
2:B:270:ILE:C	2:B:270:ILE:CD1	2.86	0.44
6:B:853:BCL:HBD	6:B:853:BCL:HAA2	1.99	0.44
3:C:37:ARG:NH1	3:C:37:ARG:HG2	2.32	0.44
8:A:857:U10:H1M1	8:A:857:U10:H72	1.80	0.44
2:B:215:LEU:O	2:B:218:MET:N	2.46	0.44
3:C:29:TYR:HB3	3:C:30:TYR:H	1.62	0.44
1:A:279:ILE:CG2	1:A:279:ILE:O	2.65	0.44
2:B:185:TRP:CE3	2:B:185:TRP:C	2.90	0.44
1:A:230:HIS:CE1	2:B:234:GLU:CD	2.91	0.44
1:A:100:TRP:CZ2	8:B:856:U10:H253	2.52	0.44
1:A:123:PHE:CD2	1:A:238:LEU:HD22	2.52	0.44
1:A:199:ASN:O	1:A:200:PRO:O	2.36	0.44
1:A:183:ASN:HB2	1:A:236:LEU:HB3	2.00	0.44
2:B:222:THR:O	2:B:225:ALA:N	2.48	0.44
2:B:38:LEU:C	2:B:40:GLY:H	2.20	0.44
2:B:115:TRP:CZ3	2:B:116:LEU:HD23	2.52	0.44
1:A:175:ILE:CG2	1:A:243:PHE:CD2	3.00	0.44
2:B:38:LEU:O	2:B:39:LEU:C	2.54	0.44
3:C:120:LEU:O	3:C:227:LEU:N	2.43	0.44
1:A:105:VAL:O	1:A:106:GLU:C	2.55	0.44
2:B:4:GLN:O	2:B:5:ASN:C	2.55	0.44
1:A:26:VAL:C	1:A:27:GLY:O	2.52	0.44
2:B:135:LEU:N	2:B:135:LEU:HD23	2.32	0.44
1:A:162:TYR:HA	1:A:165:GLY:O	2.18	0.44
3:C:89:ARG:HG3	3:C:98:HIS:HE1	1.82	0.44
2:B:97:PRO:HD2	2:B:171:TRP:HB3	1.99	0.44
1:A:35:GLY:O	8:B:856:U10:H351	2.18	0.44
1:A:49:ILE:HD13	1:A:89:ILE:HD13	2.00	0.44
3:C:99:ALA:HA	3:C:100:PRO:HD3	1.78	0.44
1:A:85:LEU:O	1:A:86:TRP:C	2.54	0.44
1:A:177:ILE:HD13	6:A:850:BCL:HMD1	1.99	0.44
1:A:216:PHE:O	1:A:220:VAL:N	2.44	0.44
1:A:237:SER:O	1:A:238:LEU:C	2.55	0.44
1:A:127:ALA:HB1	6:A:851:BCL:H12	1.99	0.44
2:B:208:PHE:O	2:B:209:LEU:C	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:133:PRO:HA	3:C:168:TRP:HA	2.00	0.44
2:B:300:ASN:C	2:B:301:HIS:ND1	2.71	0.44
1:A:122:ALA:O	1:A:125:ILE:HB	2.18	0.43
1:A:222:TYR:CG	1:A:223:SER:N	2.85	0.43
1:A:148:TYR:HA	7:A:855:BPH:H193	2.00	0.43
2:B:17:ASP:C	2:B:19:GLY:H	2.22	0.43
2:B:264:GLY:O	2:B:267:ARG:N	2.37	0.43
2:B:273:ALA:O	2:B:274:VAL:C	2.52	0.43
2:B:282:ILE:O	2:B:283:GLY:C	2.56	0.43
3:C:193:MET:CE	3:C:193:MET:HA	2.48	0.43
1:A:94:THR:HG22	1:A:95:GLY:N	2.32	0.43
1:A:185:LEU:N	7:B:854:BPH:HMC2	2.33	0.43
2:B:271:TRP:C	2:B:273:ALA:H	2.20	0.43
1:A:16:LEU:O	1:A:17:VAL:HG22	2.18	0.43
1:A:256:PHE:N	1:A:256:PHE:CD1	2.87	0.43
2:B:25:ASN:OD1	2:B:27:ALA:HB3	2.19	0.43
1:A:193:LEU:O	1:A:195:LEU:N	2.52	0.43
1:A:213:ASP:O	1:A:214:THR:C	2.57	0.43
3:C:238:ALA:O	3:C:239:GLY:C	2.57	0.43
2:B:268:TRP:CE3	3:C:31:LEU:HD13	2.53	0.43
3:C:87:LEU:HA	3:C:99:ALA:O	2.19	0.43
1:A:34:PHE:CZ	1:A:102:LEU:HD13	2.53	0.43
2:B:227:SER:HB2	2:B:232:GLU:OE1	2.18	0.43
2:B:200:PRO:HD2	2:B:294:TRP:CZ3	2.53	0.43
3:C:134:MET:C	3:C:136:ALA:N	2.71	0.43
1:A:121:PHE:CA	7:A:855:BPH:HMD3	2.49	0.43
2:B:228:ARG:O	3:C:234:CYS:HB3	2.18	0.43
2:B:296:VAL:O	2:B:299:GLN:N	2.41	0.43
2:B:97:PRO:CA	2:B:112:GLY:HA3	2.49	0.43
3:C:183:LEU:HD11	3:C:189:ARG:CG	2.48	0.43
1:A:193:LEU:HB3	1:A:194:VAL:H	1.69	0.43
2:B:176:PRO:HD3	2:B:185:TRP:CD1	2.53	0.43
2:B:199:ASN:HB2	2:B:294:TRP:CG	2.54	0.43
2:B:4:GLN:O	2:B:6:ILE:CD1	2.66	0.43
2:B:3:TYR:HE2	3:C:194:GLN:HA	1.80	0.43
3:C:157:ASP:O	3:C:158:LEU:HB2	2.18	0.43
2:B:59:SER:HB2	2:B:128:SER:OG	2.18	0.43
3:C:170:ASP:C	3:C:172:PRO:HD2	2.39	0.43
3:C:134:MET:O	3:C:137:ALA:N	2.38	0.43
1:A:249:ILE:HD12	1:A:249:ILE:O	2.19	0.43
1:A:268:LYS:HA	1:A:268:LYS:HD3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:ASN:HA	1:A:236:LEU:CD1	2.45	0.43
1:A:244:SER:O	1:A:246:LEU:N	2.52	0.43
2:B:159:VAL:HG13	2:B:285:LEU:HD12	2.01	0.43
1:A:183:ASN:O	1:A:186:ALA:N	2.52	0.43
1:A:48:LEU:O	1:A:89:ILE:HD11	2.18	0.43
2:B:222:THR:CG2	2:B:223:ILE:N	2.81	0.43
2:B:240:ASP:O	2:B:241:ARG:O	2.36	0.43
1:A:16:LEU:C	1:A:17:VAL:CG2	2.87	0.43
1:A:28:PRO:HB3	2:B:253:ARG:NE	2.28	0.43
2:B:32:VAL:HG12	2:B:33:GLY:N	2.33	0.43
1:A:169:TYR:CD2	1:A:260:VAL:HB	2.53	0.42
3:C:20:PHE:O	3:C:21:TRP:C	2.57	0.42
2:B:81:ASN:O	2:B:84:VAL:HB	2.19	0.42
1:A:208:THR:HB	1:A:209:PRO:HD2	2.01	0.42
1:A:206:MET:HE2	2:B:235:LEU:HD22	2.01	0.42
2:B:273:ALA:O	2:B:275:LEU:N	2.53	0.42
3:C:129:ASN:ND2	3:C:224:GLU:HB3	2.35	0.42
7:A:855:BPH:HMC3	2:B:213:ALA:CB	2.49	0.42
1:A:181:PHE:CE1	6:B:852:BCL:O1A	2.71	0.42
2:B:296:VAL:HG12	2:B:297:TRP:N	2.33	0.42
1:A:272:TRP:HZ3	2:B:86:LEU:CB	2.33	0.42
2:B:123:PHE:O	2:B:126:VAL:N	2.43	0.42
2:B:286:LEU:HD23	2:B:286:LEU:HA	1.79	0.42
8:B:856:U10:H101	8:B:856:U10:H122	1.90	0.42
3:C:85:ILE:O	3:C:87:LEU:N	2.48	0.42
1:A:107:ILE:HG21	2:B:251:PHE:CD2	2.54	0.42
2:B:208:PHE:CE2	2:B:279:THR:HG21	2.54	0.42
1:A:264:GLN:O	1:A:266:TRP:N	2.52	0.42
3:C:25:ALA:O	3:C:28:ILE:HB	2.20	0.42
1:A:166:ASN:HB3	1:A:169:TYR:HD2	1.85	0.42
1:A:215:PHE:O	1:A:216:PHE:C	2.56	0.42
3:C:168:TRP:NE1	3:C:190:LEU:HD21	2.33	0.42
3:C:134:MET:C	3:C:136:ALA:H	2.22	0.42
3:C:48:THR:O	3:C:49:PRO:O	2.37	0.42
1:A:262:TRP:HE3	1:A:263:TRP:CD1	2.38	0.42
3:C:245:ALA:N	3:C:246:PRO:CD	2.82	0.42
1:A:128:TYR:CZ	1:A:132:VAL:HG21	2.55	0.42
2:B:282:ILE:HG22	2:B:283:GLY:N	2.35	0.42
3:C:112:ALA:HB2	3:C:239:GLY:HA3	2.00	0.42
1:A:141:ALA:O	1:A:142:TRP:C	2.57	0.42
1:A:215:PHE:HB3	1:A:216:PHE:H	1.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:253:ARG:O	2:B:253:ARG:HG2	2.19	0.42
1:A:244:SER:C	1:A:246:LEU:N	2.73	0.42
2:B:150:PHE:O	2:B:151:LEU:C	2.57	0.42
2:B:293:ASN:OD1	2:B:294:TRP:N	2.53	0.42
1:A:61:PRO:HA	1:A:64:ILE:HG12	2.02	0.42
2:B:81:ASN:HA	2:B:82:PRO:HD3	1.77	0.42
2:B:247:ARG:O	2:B:248:ALA:C	2.56	0.41
1:A:194:VAL:HG21	2:B:266:HIS:NE2	2.35	0.41
2:B:134:TYR:O	2:B:135:LEU:C	2.59	0.41
2:B:51:TYR:CE2	2:B:136:ARG:CZ	3.03	0.41
1:A:217:ARG:HA	1:A:222:TYR:N	2.35	0.41
1:A:116:HIS:NE2	2:B:224:LEU:HB3	2.35	0.41
2:B:239:ALA:O	3:C:73:LEU:HD22	2.20	0.41
3:C:32:GLN:OE1	3:C:32:GLN:HA	2.20	0.41
2:B:245:ALA:HB2	2:B:262:MET:CE	2.51	0.41
1:A:35:GLY:CA	1:A:103:ARG:HD2	2.45	0.41
2:B:143:GLY:C	2:B:145:HIS:N	2.72	0.41
2:B:19:GLY:C	2:B:20:MET:O	2.56	0.41
2:B:38:LEU:HA	2:B:38:LEU:HD12	1.80	0.41
1:A:221:GLY:HA3	2:B:50:ILE:HG12	2.02	0.41
2:B:66:TRP:HD1	2:B:118:ALA:O	2.03	0.41
1:A:192:ALA:HB1	2:B:146:THR:N	2.36	0.41
2:B:199:ASN:HA	2:B:200:PRO:HD2	1.90	0.41
2:B:264:GLY:O	2:B:266:HIS:N	2.54	0.41
1:A:144:TYR:O	1:A:156:TRP:CZ2	2.73	0.41
1:A:59:TRP:HA	1:A:64:ILE:HD11	2.02	0.41
1:A:274:ASN:O	1:A:275:ILE:C	2.58	0.41
3:C:82:ASP:O	3:C:83:ARG:CB	2.69	0.41
3:C:171:ILE:N	3:C:172:PRO:HD2	2.35	0.41
3:C:248:ARG:HG2	3:C:248:ARG:O	2.20	0.41
7:A:855:BPH:HMC3	2:B:213:ALA:HB3	2.00	0.41
2:B:280:GLY:O	2:B:283:GLY:N	2.53	0.41
2:B:148:TRP:HA	2:B:148:TRP:HE3	1.84	0.41
1:A:170:ASN:HB2	1:A:259:TRP:CE2	2.56	0.41
1:A:229:ILE:CD1	8:A:857:U10:O4	2.69	0.41
3:C:100:PRO:O	3:C:101:THR:C	2.59	0.41
2:B:84:VAL:O	2:B:87:ARG:N	2.51	0.41
1:A:107:ILE:CG2	2:B:251:PHE:CD2	3.04	0.41
2:B:37:THR:CG2	2:B:37:THR:O	2.67	0.41
1:A:216:PHE:HB3	1:A:222:TYR:O	2.20	0.41
2:B:155:TRP:O	2:B:158:MET:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:248:ALA:HB1	8:B:856:U10:O3	2.20	0.41
2:B:247:ARG:CZ	3:C:111:PRO:O	2.68	0.41
1:A:125:ILE:O	1:A:126:LEU:C	2.58	0.41
1:A:185:LEU:O	1:A:185:LEU:CD2	2.69	0.41
1:A:97:PHE:CZ	6:A:851:BCL:H91	2.55	0.41
2:B:70:ILE:HD11	2:B:177:TYR:CD2	2.56	0.41
3:C:120:LEU:N	3:C:226:THR:HB	2.35	0.41
3:C:33:THR:O	3:C:36:MET:N	2.54	0.41
1:A:2:LEU:O	3:C:42:LEU:HA	2.21	0.41
2:B:250:LEU:HD22	2:B:254:TRP:HE1	1.84	0.41
2:B:136:ARG:NE	2:B:136:ARG:HA	2.32	0.41
3:C:103:ASP:HA	3:C:104:PRO:HD2	1.66	0.41
1:A:96:ALA:CB	7:A:855:BPH:H4C2	2.48	0.40
2:B:218:MET:O	2:B:219:HIS:C	2.58	0.40
2:B:260:ALA:O	8:B:856:U10:C4M	2.70	0.40
1:A:227:LEU:O	1:A:227:LEU:HD12	2.21	0.40
2:B:14:GLY:HA3	3:C:140:PHE:CD1	2.55	0.40
3:C:191:LEU:HD23	3:C:192:PRO:HD3	2.03	0.40
2:B:135:LEU:O	2:B:138:GLN:N	2.54	0.40
1:A:259:TRP:O	1:A:261:ASP:N	2.54	0.40
6:A:850:BCL:HMD2	6:A:851:BCL:HBB3	2.02	0.40
2:B:206:ILE:CG2	2:B:210:TYR:CD2	3.05	0.40
1:A:16:LEU:HD12	1:A:106:GLU:HG3	2.00	0.40
3:C:17:ILE:O	3:C:17:ILE:HG13	2.21	0.40
1:A:248:MET:HG3	6:A:851:BCL:OBD	2.22	0.40
2:B:239:ALA:HB1	3:C:66:LEU:HD21	2.03	0.40
2:B:297:TRP:O	2:B:297:TRP:CE3	2.74	0.40
3:C:173:GLU:O	3:C:174:GLN:O	2.39	0.40
2:B:140:LEU:CB	2:B:142:MET:HG3	2.51	0.40
3:C:104:PRO:HA	3:C:109:VAL:HG22	2.03	0.40
2:B:60:LEU:HD12	2:B:60:LEU:HA	1.89	0.40
1:A:205:GLU:C	1:A:206:MET:O	2.58	0.40
1:A:121:PHE:HA	7:A:855:BPH:HMD3	2.04	0.40
2:B:260:ALA:HB2	8:B:856:U10:H103	2.03	0.40
2:B:265:ILE:HA	2:B:265:ILE:HD12	1.72	0.40
2:B:18:LEU:N	2:B:18:LEU:CD2	2.79	0.40
1:A:129:LEU:O	1:A:133:LEU:N	2.54	0.40
2:B:105:PHE:CD2	2:B:116:LEU:HD13	2.57	0.40
1:A:260:VAL:O	1:A:260:VAL:HG22	2.21	0.40
2:B:144:LYS:O	2:B:145:HIS:C	2.58	0.40
8:B:856:U10:H201	8:B:856:U10:H222	1.66	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:128:HIS:NE2	3:C:128:HIS:NE2[5_656]	2.18	0.02

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	A	279/281 (99%)	199 (71%)	51 (18%)	29 (10%)	1	12
2	B	300/307 (98%)	202 (67%)	69 (23%)	29 (10%)	1	14
3	C	236/260 (91%)	175 (74%)	45 (19%)	16 (7%)	1	24
All	All	815/848 (96%)	576 (71%)	165 (20%)	74 (9%)	1	16

All (74) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	80	LEU
1	A	186	ALA
1	A	200	PRO
1	A	215	PHE
1	A	262	TRP
2	B	5	ASN
2	B	20	MET
2	B	39	LEU
2	B	228	ARG
2	B	269	ALA
2	B	270	ILE
2	B	272	MET
3	C	113	SER
1	A	26	VAL
1	A	187	LEU

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Mol	Chain	Res	Type
1	A	194	VAL
1	A	226	THR
1	A	240	ALA
1	A	273	ALA
2	B	58	LEU
2	B	123	PHE
2	B	154	ILE
2	B	155	TRP
2	B	162	PHE
2	B	163	ILE
2	B	241	ARG
2	B	249	ALA
2	B	268	TRP
2	B	281	GLY
2	B	288	ASP
3	C	19	SER
3	C	29	TYR
3	C	34	GLU
3	C	135	LYS
3	C	194	GLN
3	C	233	ILE
3	C	239	GLY
1	A	180	PHE
1	A	263	TRP
1	A	265	TRP
1	A	270	PRO
2	B	15	PRO
2	B	18	LEU
2	B	124	VAL
2	B	222	THR
3	C	49	PRO
3	C	69	GLY
3	C	86	ALA
3	C	174	GLN
1	A	81	ALA
2	B	219	HIS
2	B	223	ILE
2	B	250	LEU
3	C	193	MET
1	A	21	LEU
1	A	175	ILE
1	A	183	ASN

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Mol	Chain	Res	Type
1	A	193	LEU
1	A	206	MET
1	A	275	ILE
2	B	22	GLU
3	C	144	ALA
2	B	117	ILE
2	B	283	GLY
2	B	296	VAL
3	C	83	ARG
1	A	260	VAL
1	A	84	GLY
1	A	225	GLY
3	C	66	LEU
1	A	31	VAL
1	A	113	ILE
1	A	117	ILE

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	A	220/220 (100%)	201 (91%)	19 (9%)	13	49
2	B	237/241 (98%)	223 (94%)	14 (6%)	24	63
3	C	193/208 (93%)	186 (96%)	7 (4%)	42	75
All	All	650/669 (97%)	610 (94%)	40 (6%)	23	62

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	21	LEU
1	A	38	THR
1	A	79	PRO
1	A	154	LEU
1	A	167	PHE

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Mol	Chain	Res	Type
1	A	170	ASN
1	A	178	SER
1	A	183	ASN
1	A	185	LEU
1	A	206	MET
1	A	207	ARG
1	A	210	ASP
1	A	241	VAL
1	A	249	ILE
1	A	256	PHE
1	A	270	PRO
1	A	271	TRP
1	A	272	TRP
2	B	18	LEU
2	B	42	PHE
2	B	50	ILE
2	B	86	LEU
2	B	90	PHE
2	B	93	SER
2	B	160	HIS
2	B	171	TRP
2	B	182	HIS
2	B	188	ASN
2	B	197	HIS
2	B	216	PHE
2	B	258	PHE
2	B	270	ILE
3	C	67	PRO
3	C	105	MET
3	C	169	VAL
3	C	185	ASP
3	C	206	ASN
3	C	222	PRO
3	C	225	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	HIS
2	B	5	ASN
2	B	44	ASN
2	B	188	ASN

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Mol	Chain	Res	Type
2	B	202	HIS
2	B	259	ASN
2	B	299	GLN
3	C	44	ASN
3	C	68	HIS
3	C	129	ASN
3	C	206	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	$\# Z > 2$
6	BCL	A	850	-	53,74,74	1.48	12 (22%)	57,115,115	1.85	10 (17%)
6	BCL	A	851	1	53,74,74	1.37	10 (18%)	57,115,115	1.60	7 (12%)
7	BPH	A	855	-	64,70,70	1.23	8 (12%)	73,101,101	1.63	13 (17%)
8	U10	A	857	-	48,48,63	2.69	16 (33%)	58,61,79	2.32	20 (34%)
6	BCL	B	852	2	53,74,74	1.38	8 (15%)	57,115,115	1.88	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	BCL	B	853	1	53,74,74	1.38	9 (16%)	57,115,115	2.05	14 (24%)
7	BPH	B	854	-	64,70,70	1.50	11 (17%)	73,101,101	1.80	16 (21%)
8	U10	B	856	-	48,48,63	2.36	15 (31%)	58,61,79	2.29	19 (32%)

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
6	BCL	A	850	-	-	0/37/137/137	0/0/9/9
6	BCL	A	851	1	-	0/37/137/137	0/0/9/9
7	BPH	A	855	-	-	0/54/105/105	0/1/6/6
8	U10	A	857	-	-	0/45/69/87	0/1/1/1
6	BCL	B	852	2	-	0/37/137/137	0/0/9/9
6	BCL	B	853	1	-	0/37/137/137	0/0/9/9
7	BPH	B	854	-	-	0/54/105/105	0/1/6/6
8	U10	B	856	-	-	0/45/69/87	0/1/1/1

All (89) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	854	BPH	C3D-CAD	-3.96	1.38	1.46
8	A	857	U10	C7-C8	-3.93	1.44	1.50
8	B	856	U10	C7-C8	-3.27	1.45	1.50
6	B	853	BCL	C3C-C4C	-3.00	1.47	1.51
6	A	850	BCL	C3C-C4C	-2.99	1.47	1.51
7	B	854	BPH	O2A-CGA	-2.97	1.24	1.33
6	A	850	BCL	O2D-CGD	-2.84	1.25	1.33
6	B	852	BCL	C3C-C4C	-2.62	1.48	1.51
6	A	850	BCL	O2A-CGA	-2.57	1.25	1.33
6	A	850	BCL	CHD-C4C	-2.52	1.33	1.41
6	A	851	BCL	C3A-C2A	-2.44	1.47	1.54
6	B	852	BCL	CHD-C4C	-2.39	1.34	1.41
7	A	855	BPH	O2A-CGA	-2.37	1.26	1.33
6	A	850	BCL	C3A-C2A	-2.37	1.47	1.54
6	A	851	BCL	O2D-CGD	-2.33	1.27	1.33
7	A	855	BPH	C1B-C2B	-2.33	1.40	1.45
8	B	856	U10	C22-C23	-2.31	1.44	1.50
6	B	852	BCL	C3D-CAD	-2.30	1.39	1.45
6	B	853	BCL	O2A-CGA	-2.23	1.26	1.33
6	B	853	BCL	C3A-C2A	-2.17	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	856	U10	C12-C13	-2.15	1.44	1.50
6	A	851	BCL	CHD-C4C	-2.13	1.35	1.41
6	A	851	BCL	O2A-CGA	-2.10	1.26	1.33
7	B	854	BPH	C1B-C2B	-2.09	1.41	1.45
6	A	850	BCL	C3D-CAD	-2.00	1.40	1.45
7	A	855	BPH	CMD-C2D	2.00	1.55	1.51
7	A	855	BPH	CBD-CGD	2.03	1.59	1.52
6	A	851	BCL	CMB-C2B	2.03	1.55	1.51
7	B	854	BPH	C6-C5	2.03	1.59	1.52
7	B	854	BPH	CMD-C2D	2.05	1.55	1.51
6	A	850	BCL	C2-C3	2.05	1.37	1.33
7	B	854	BPH	C4-C3	2.07	1.55	1.50
6	A	850	BCL	CBB-CAB	2.10	1.56	1.49
6	B	853	BCL	CBB-CAB	2.12	1.56	1.49
8	A	857	U10	C31-C29	2.16	1.56	1.51
6	A	851	BCL	CBB-CAB	2.18	1.56	1.49
6	B	852	BCL	CBB-CAB	2.19	1.56	1.49
6	A	851	BCL	C3B-C2B	2.29	1.45	1.40
8	B	856	U10	C26-C24	2.35	1.56	1.51
8	A	857	U10	C16-C14	2.36	1.56	1.51
6	B	852	BCL	CMD-C2D	2.39	1.56	1.51
6	A	850	BCL	CMB-C2B	2.40	1.56	1.51
6	B	853	BCL	CMB-C2B	2.44	1.56	1.51
6	A	851	BCL	C3B-CAB	2.46	1.55	1.49
8	B	856	U10	C38-C39	2.51	1.40	1.32
8	B	856	U10	C8-C9	2.51	1.37	1.33
6	A	850	BCL	C3D-C2D	2.57	1.46	1.40
6	B	852	BCL	CMB-C2B	2.70	1.57	1.51
6	B	853	BCL	C3D-C2D	2.71	1.46	1.40
7	B	854	BPH	C5-C3	2.74	1.57	1.51
7	B	854	BPH	C3B-CAB	2.77	1.55	1.46
6	B	853	BCL	C3B-CAB	2.85	1.56	1.49
6	B	853	BCL	C3B-C2B	2.91	1.47	1.40
8	B	856	U10	C13-C14	2.92	1.38	1.33
7	A	855	BPH	CMB-C2B	2.92	1.57	1.50
8	A	857	U10	C6-C5	2.93	1.54	1.46
8	A	857	U10	C36-C34	3.05	1.58	1.51
8	B	856	U10	C6-C5	3.07	1.55	1.46
7	A	855	BPH	C2-C3	3.16	1.39	1.33
7	A	855	BPH	C3D-C2D	3.19	1.47	1.40
7	B	854	BPH	CMB-C2B	3.23	1.57	1.50
7	B	854	BPH	C3B-C2B	3.26	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	857	U10	C8-C9	3.33	1.39	1.33
7	A	855	BPH	C3B-C2B	3.34	1.48	1.38
8	A	857	U10	C26-C24	3.41	1.59	1.51
6	A	850	BCL	C3B-C2B	3.46	1.48	1.40
8	A	857	U10	C4-C3	3.50	1.50	1.35
8	B	856	U10	C7-C6	3.52	1.57	1.51
8	B	856	U10	C23-C24	3.55	1.39	1.33
8	B	856	U10	C4-C3	3.67	1.51	1.35
8	A	857	U10	C7-C6	3.77	1.58	1.51
6	B	852	BCL	C3D-C2D	3.77	1.49	1.40
6	A	850	BCL	C3B-CAB	3.80	1.59	1.49
6	A	851	BCL	C3D-C2D	3.82	1.49	1.40
8	A	857	U10	C38-C39	3.83	1.44	1.32
6	B	853	BCL	C2-C3	3.86	1.40	1.33
6	A	851	BCL	C2-C3	3.94	1.40	1.33
6	B	852	BCL	C2-C3	4.12	1.41	1.33
8	A	857	U10	C23-C24	4.31	1.41	1.33
8	B	856	U10	C18-C19	4.37	1.41	1.33
8	B	856	U10	C33-C34	4.60	1.42	1.33
7	B	854	BPH	C2-C3	4.93	1.42	1.33
8	A	857	U10	C13-C14	4.98	1.42	1.33
8	A	857	U10	C18-C19	5.39	1.43	1.33
8	B	856	U10	C28-C29	5.79	1.44	1.33
8	A	857	U10	C33-C34	6.03	1.44	1.33
8	A	857	U10	C28-C29	6.08	1.44	1.33
8	A	857	U10	C6-C1	7.77	1.53	1.35
8	B	856	U10	C6-C1	8.03	1.54	1.35

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	853	BCL	CAA-C2A-C1A	-6.34	90.10	112.47
6	B	853	BCL	CMB-C2B-C1B	-6.34	117.88	128.36
6	A	850	BCL	CMB-C2B-C1B	-6.17	118.16	128.36
6	A	851	BCL	CMB-C2B-C1B	-6.11	118.25	128.36
6	B	852	BCL	CMB-C2B-C1B	-5.90	118.61	128.36
8	B	856	U10	C25-C24-C23	-5.66	112.39	123.50
8	B	856	U10	C15-C14-C13	-5.55	112.60	123.50
8	A	857	U10	C15-C14-C13	-5.31	113.07	123.50
8	B	856	U10	C10-C9-C8	-5.07	113.55	123.50
8	A	857	U10	C25-C24-C23	-4.93	113.81	123.50
6	A	850	BCL	CAA-C2A-C1A	-4.92	95.11	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	857	U10	C10-C9-C8	-4.75	114.18	123.50
7	B	854	BPH	C4D-C3D-C2D	-4.13	101.75	107.08
8	A	857	U10	C35-C34-C33	-4.09	115.46	123.50
7	A	855	BPH	C4D-C3D-C2D	-4.07	101.83	107.08
7	B	854	BPH	O1D-CGD-CBD	-3.96	118.95	124.62
8	B	856	U10	C35-C34-C33	-3.92	115.80	123.50
7	B	854	BPH	CMB-C2B-C1B	-3.80	118.88	125.06
7	A	855	BPH	CMB-C2B-C1B	-3.60	119.19	125.06
8	A	857	U10	C20-C19-C18	-3.60	116.43	123.50
7	A	855	BPH	O1D-CGD-CBD	-3.59	119.48	124.62
8	B	856	U10	C20-C19-C18	-3.41	116.81	123.50
6	B	852	BCL	CGD-CBD-CAD	-3.40	99.11	110.62
6	B	852	BCL	OBD-CAD-C3D	-3.33	121.55	128.35
7	B	854	BPH	CHC-C4B-NB	-3.28	118.66	124.91
6	B	853	BCL	O1D-CGD-CBD	-3.21	120.02	124.62
6	A	850	BCL	OBD-CAD-C3D	-3.20	121.81	128.35
7	A	855	BPH	CBB-CAB-C3B	-3.14	113.55	120.52
6	B	852	BCL	CHA-C1A-NA	-3.08	118.48	126.06
8	A	857	U10	C30-C29-C28	-3.05	117.51	123.50
6	A	850	BCL	O1D-CGD-CBD	-3.02	120.30	124.62
7	B	854	BPH	C1C-NC-C4C	-2.94	107.43	110.44
6	B	853	BCL	CAC-C3C-C2C	-2.93	106.76	114.13
6	B	853	BCL	OBD-CAD-C3D	-2.92	122.39	128.35
6	A	851	BCL	CHA-C1A-NA	-2.85	119.05	126.06
8	A	857	U10	C1-C6-C5	-2.70	117.04	120.12
6	A	851	BCL	OBD-CAD-C3D	-2.70	122.85	128.35
8	B	856	U10	C21-C22-C23	-2.59	104.91	111.69
8	B	856	U10	C1-C6-C5	-2.58	117.18	120.12
7	B	854	BPH	CBB-CAB-C3B	-2.52	114.91	120.52
6	B	853	BCL	CMD-C2D-C3D	-2.31	120.57	125.09
8	B	856	U10	C30-C29-C28	-2.29	119.00	123.50
6	B	853	BCL	CAA-C2A-C3A	-2.28	106.67	113.22
8	B	856	U10	O5-C5-C4	-2.27	115.88	120.79
6	B	852	BCL	O1D-CGD-CBD	-2.27	121.37	124.62
7	A	855	BPH	C4-C3-C2	-2.25	119.08	123.50
7	A	855	BPH	CHC-C4B-NB	-2.24	120.65	124.91
8	A	857	U10	O5-C5-C4	-2.18	116.07	120.79
6	B	853	BCL	CHA-C1A-NA	-2.15	120.78	126.06
7	B	854	BPH	OBD-CAD-C3D	-2.06	124.15	128.35
7	B	854	BPH	CAC-C3C-C2C	-2.06	108.96	114.13
6	B	852	BCL	O2D-CGD-CBD	2.03	114.08	111.30
8	A	857	U10	C35-C34-C36	2.06	118.56	115.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	852	BCL	O2A-CGA-CBA	2.14	118.42	111.90
8	A	857	U10	C26-C24-C23	2.16	125.16	121.05
7	B	854	BPH	O2D-CGD-CBD	2.20	114.31	111.30
8	A	857	U10	C17-C16-C14	2.23	119.98	112.71
6	A	850	BCL	C3D-CAD-CBD	2.31	110.87	107.60
8	B	856	U10	C21-C19-C18	2.37	125.54	121.05
6	B	853	BCL	C2A-C1A-CHA	2.43	128.37	123.89
8	B	856	U10	C10-C9-C11	2.49	119.21	115.41
8	A	857	U10	C10-C9-C11	2.52	119.25	115.41
8	A	857	U10	C11-C12-C13	2.52	118.30	111.69
8	B	856	U10	C11-C12-C13	2.56	118.39	111.69
8	A	857	U10	C36-C34-C33	2.60	125.97	121.05
6	B	853	BCL	C6-C5-C3	2.60	118.20	112.48
8	B	856	U10	C36-C34-C33	2.73	126.22	121.05
7	A	855	BPH	CED-O2D-CGD	2.79	122.53	115.99
6	B	853	BCL	O2D-CGD-CBD	2.80	115.14	111.30
7	A	855	BPH	CMB-C2B-C3B	2.81	134.58	128.04
8	A	857	U10	C11-C9-C8	2.91	126.56	121.05
7	A	855	BPH	C3D-CAD-CBD	2.91	111.71	107.60
7	B	854	BPH	CMB-C2B-C3B	2.94	134.88	128.04
7	A	855	BPH	C6-C5-C3	2.94	118.95	112.48
6	B	852	BCL	C3D-CAD-CBD	2.96	111.78	107.60
8	B	856	U10	C25-C24-C26	2.97	119.95	115.41
7	B	854	BPH	C3D-CAD-CBD	2.98	111.81	107.60
8	B	856	U10	C7-C8-C9	3.06	131.87	126.70
6	A	850	BCL	O2D-CGD-CBD	3.08	115.53	111.30
7	B	854	BPH	C7-C6-C5	3.11	122.24	113.06
8	A	857	U10	C16-C17-C18	3.12	119.86	111.69
7	B	854	BPH	CED-O2D-CGD	3.13	123.32	115.99
6	A	851	BCL	C2A-C1A-CHA	3.18	129.75	123.89
8	B	856	U10	C11-C9-C8	3.26	127.24	121.05
8	B	856	U10	C26-C24-C23	3.48	127.66	121.05
6	B	852	BCL	C2A-C1A-CHA	3.49	130.31	123.89
6	A	851	BCL	C6-C5-C3	3.56	120.29	112.48
7	A	855	BPH	O2D-CGD-CBD	3.59	116.22	111.30
8	A	857	U10	C25-C24-C26	3.68	121.03	115.41
6	A	850	BCL	CBA-CAA-C2A	3.69	124.15	113.73
6	A	851	BCL	CED-O2D-CGD	3.71	124.70	115.99
6	A	850	BCL	CED-O2D-CGD	3.77	124.83	115.99
8	A	857	U10	C21-C19-C18	3.86	128.37	121.05
6	A	850	BCL	C6-C5-C3	3.96	121.17	112.48
6	B	852	BCL	CED-O2D-CGD	4.11	125.64	115.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	853	BCL	CED-O2D-CGD	4.27	126.00	115.99
6	A	850	BCL	CMB-C2B-C3B	4.30	133.49	125.09
6	B	852	BCL	CMB-C2B-C3B	4.31	133.52	125.09
7	B	854	BPH	C6-C5-C3	4.40	122.15	112.48
6	A	851	BCL	CMB-C2B-C3B	4.42	133.74	125.09
7	A	855	BPH	C4-C3-C5	4.51	122.30	115.41
6	B	853	BCL	CMB-C2B-C3B	4.57	134.03	125.09
7	B	854	BPH	C4-C3-C5	4.69	122.57	115.41
6	B	853	BCL	CBA-CAA-C2A	4.77	127.20	113.73
7	A	855	BPH	C3C-C4C-NC	4.83	112.77	107.93
8	B	856	U10	C7-C6-C5	4.97	124.40	118.56
8	B	856	U10	C15-C14-C16	5.36	123.60	115.41
8	A	857	U10	C15-C14-C16	5.41	123.67	115.41
6	B	852	BCL	C6-C5-C3	5.46	124.47	112.48
7	B	854	BPH	C3C-C4C-NC	5.49	113.43	107.93
8	A	857	U10	C7-C6-C5	5.56	125.10	118.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 87 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	850	BCL	11	0
6	A	851	BCL	11	0
7	A	855	BPH	19	0
8	A	857	U10	7	0
6	B	852	BCL	9	0
6	B	853	BCL	11	0
7	B	854	BPH	14	0
8	B	856	U10	15	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	A	281/281 (100%)	-0.88	0 100 100	90, 90, 90, 90	0
2	B	302/307 (98%)	-0.83	0 100 100	90, 90, 90, 90	0
3	C	238/260 (91%)	-0.69	0 100 100	90, 90, 90, 90	0
All	All	821/848 (96%)	-0.81	0 100 100	90, 90, 90, 90	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
8	U10	A	857	48/63	0.81	0.39	4.98	90,90,90,90	13
7	BPH	B	854	65/65	0.89	0.30	3.67	90,90,90,90	0
8	U10	B	856	48/63	0.85	0.35	2.94	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	BCL	A	850	66/66	0.92	0.27	2.60	90,90,90,90	0
6	BCL	A	851	66/66	0.93	0.23	2.49	90,90,90,90	0
5	MN	B	900	1/1	0.98	0.18	1.92	90,90,90,90	0
6	BCL	B	853	66/66	0.92	0.24	1.59	90,90,90,90	0
7	BPH	A	855	65/65	0.95	0.19	0.52	90,90,90,90	0
6	BCL	B	852	66/66	0.95	0.18	0.39	90,90,90,90	0
4	FE	B	858	1/1	1.00	0.05	-2.85	90,90,90,90	0

6.5 Other polymers

There are no such residues in this entry.