



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:58 PM GMT

PDB ID : 1Z9K
Title : Photosynthetic Reaction Center from Rhodobacter sphaeroides
Authors : Camara-Artigas, A.; Allen, J.P.
Deposited on : 2005-04-02
Resolution : 4.60 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

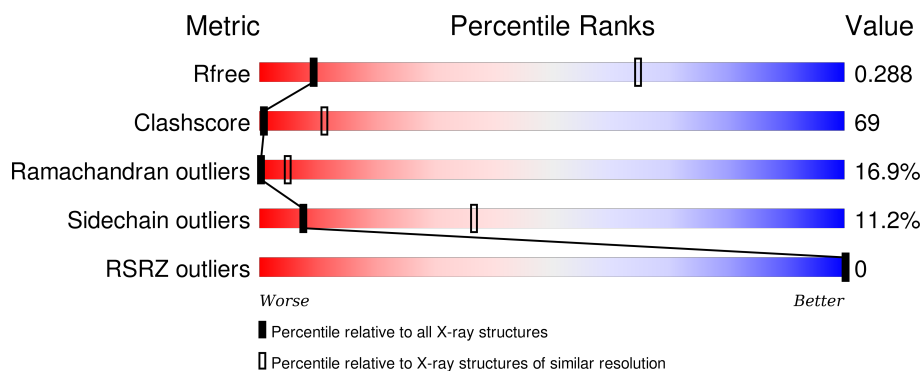
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.60 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	1089 (5.52-3.60)
Clashscore	102246	1004 (5.52-3.64)
Ramachandran outliers	100387	1131 (5.52-3.60)
Sidechain outliers	100360	1112 (5.50-3.60)
RSRZ outliers	91569	1092 (5.52-3.60)

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	 21% 58% 20% •
2	B	307	 22% 55% 19% ••
3	C	260	 28% 49% 12% • 8%

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 [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6946 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
			2232	1507	355	362	8			

- 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
			2408	1607	394	397	10			

- 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			

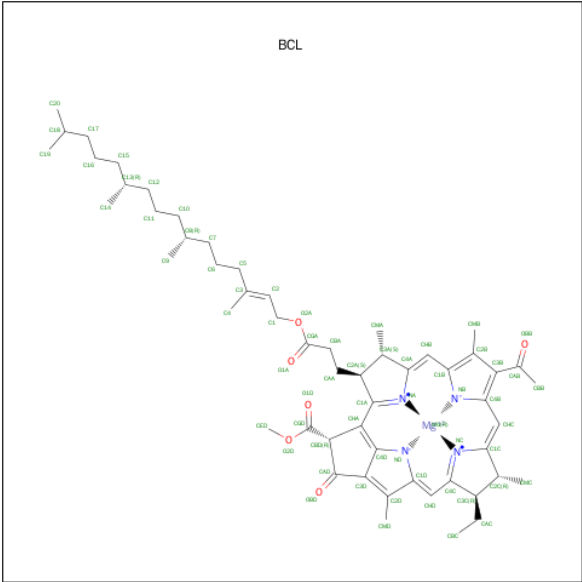
- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

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

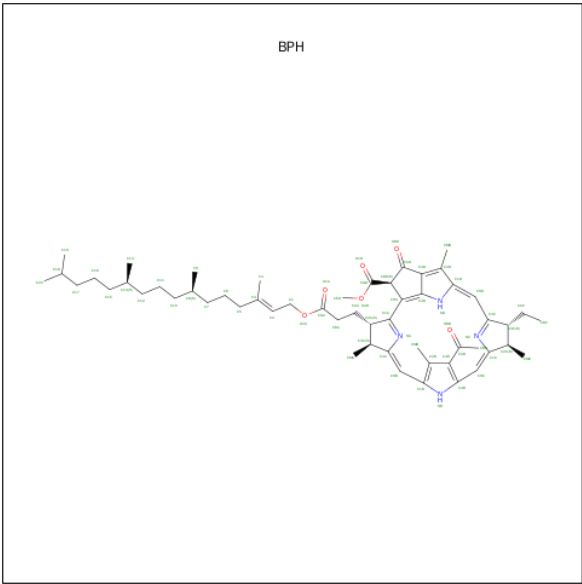
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Mn	0	0
			1	1		

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
6	A	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
6	B	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
6	B	1	Total 66	C 55	Mg 1	N 4	O 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: $C_{59}H_{90}O_4$).

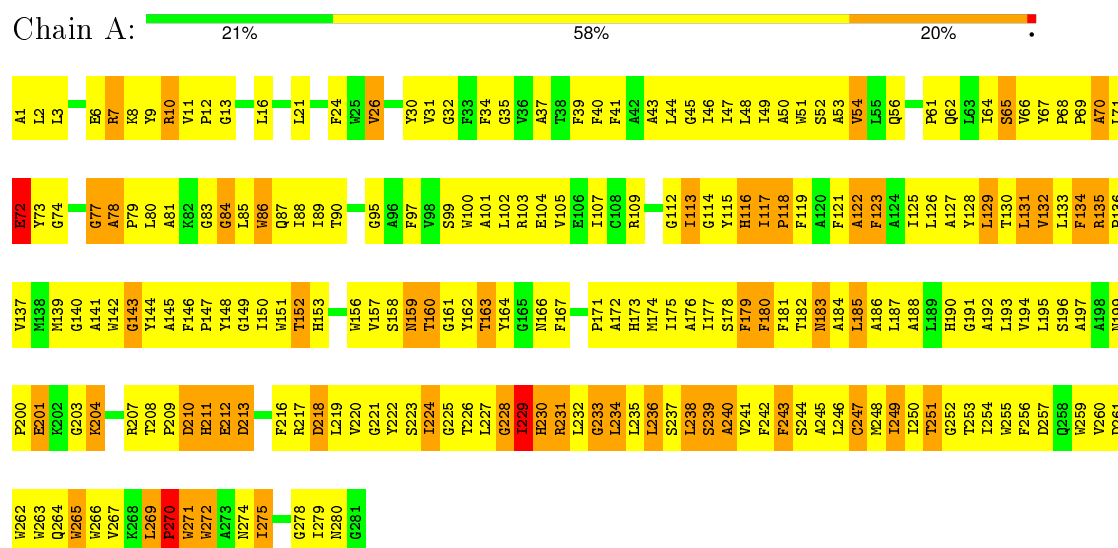


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			48	44	4		
8	A	1	Total	C	O	0	0
			48	44	4		

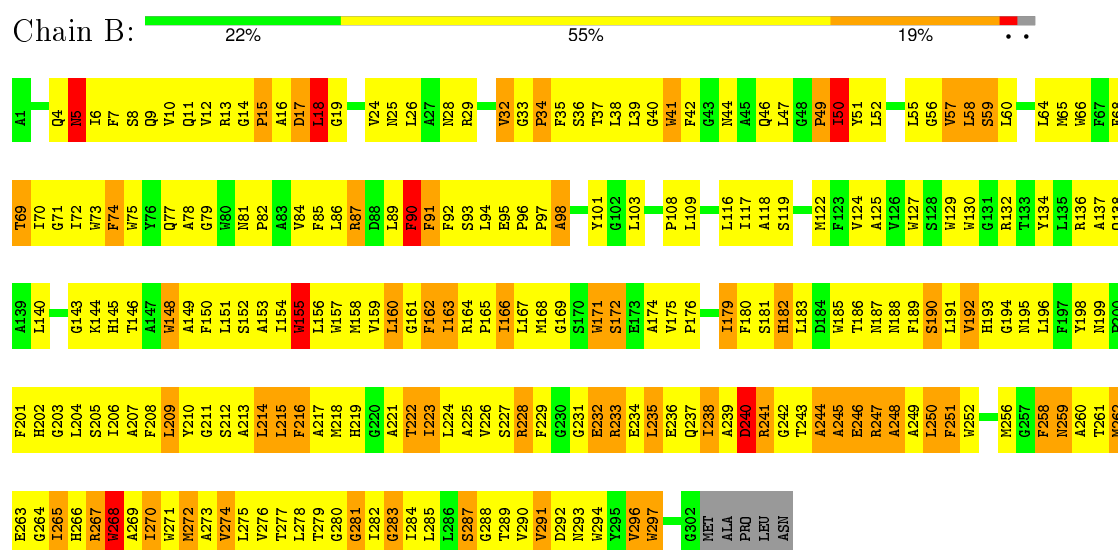
3 Residue-property plots

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.

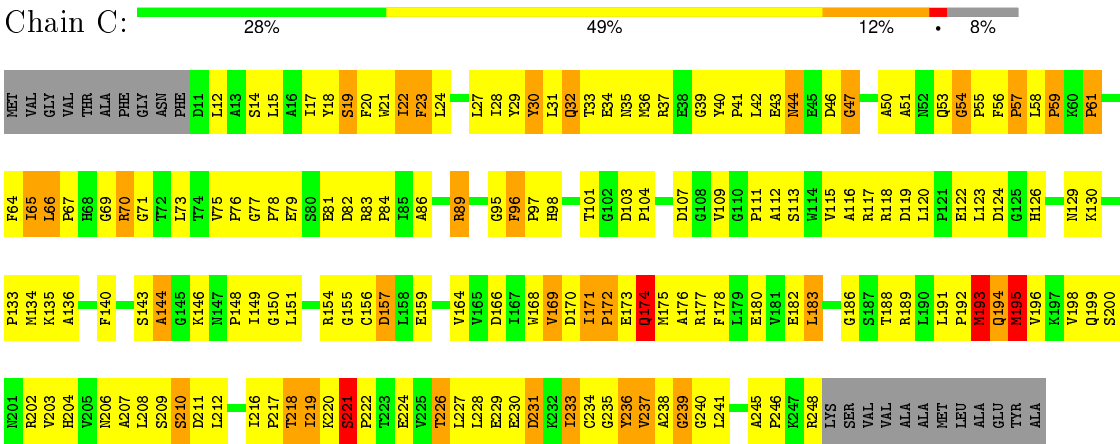
• Molecule 1: Reaction center protein L chain



• Molecule 2: Reaction center protein M chain



• Molecule 3: Reaction center protein H chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 ₂ 2 ₂	Depositor
Cell constants a, b, c, α , β , γ	207.80 Å 207.80 Å 107.50 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 4.60 24.90 – 4.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-4.60) 91.4 (24.90-4.30)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	0.22	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 4.24 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.330 , 0.330 0.247 , 0.288	Depositor DCC
R_{free} test set	1039 reflections (8.99%)	DCC
Wilson B-factor (Å ²)	174.1	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.19 , -10.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 24177 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6946	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 3.13% 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	0.52	0/2320	0.71	1/3175 (0.0%)
2	B	0.52	0/2500	0.75	1/3413 (0.0%)
3	C	0.55	0/1862	0.75	0/2534
All	All	0.53	0/6682	0.74	2/9122 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	52	LEU	CA-CB-CG	5.58	128.15	115.30
1	A	231	ARG	N-CA-C	-5.07	97.31	111.00

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	2232	0	2187	370	0
2	B	2408	0	2321	435	0
3	C	1814	0	1818	229	0
4	B	1	0	0	0	0
5	C	1	0	0	0	0
6	A	132	0	148	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	132	0	148	16	0
7	A	65	0	76	11	0
7	B	65	0	76	13	0
8	A	48	0	63	4	0
8	B	48	0	63	15	0
All	All	6946	0	6900	951	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 69.

All (951) 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:50:ILE:HD13	2:B:51:TYR:H	1.08	1.08
1:A:187:LEU:HD21	2:B:269:ALA:HB1	1.31	1.06
1:A:179:PHE:O	1:A:240:ALA:HB2	1.57	1.05
3:C:170:ASP:HB2	3:C:177:ARG:HE	1.22	1.03
2:B:159:VAL:HA	2:B:163:ILE:HB	1.36	1.03
1:A:227:LEU:HD13	2:B:232:GLU:HB3	1.42	1.00
1:A:52:SER:HB2	1:A:85:LEU:HD13	1.43	1.00
3:C:156:CYS:HB2	3:C:248:ARG:HD3	1.41	1.00
1:A:180:PHE:CD2	1:A:240:ALA:HB1	1.97	0.99
2:B:32:VAL:HG12	2:B:33:GLY:H	1.27	0.97
2:B:50:ILE:HD13	2:B:51:TYR:N	1.78	0.97
2:B:265:ILE:O	2:B:268:TRP:HB2	1.65	0.96
2:B:90:PHE:HA	2:B:179:ILE:HD12	1.46	0.94
1:A:149:GLY:HA3	1:A:152:THR:HG1	1.30	0.94
1:A:269:LEU:HD13	1:A:270:PRO:HD2	1.49	0.93
1:A:264:GLN:HA	1:A:267:VAL:HG12	1.49	0.93
2:B:208:PHE:HB3	2:B:276:VAL:HG22	1.49	0.92
3:C:86:ALA:HB1	3:C:101:THR:OG1	1.72	0.89
1:A:16:LEU:HD21	1:A:109:ARG:HD2	1.53	0.89
3:C:148:PRO:HA	3:C:151:LEU:HG	1.53	0.89
2:B:155:TRP:CD1	2:B:278:LEU:HD12	2.08	0.89
2:B:4:GLN:O	2:B:6:ILE:HG12	1.72	0.88
2:B:95:GLU:HA	2:B:176:PRO:HB3	1.54	0.87
3:C:115:VAL:HG12	3:C:116:ALA:N	1.90	0.87
3:C:70:ARG:NH2	3:C:120:LEU:HD13	1.89	0.87
1:A:44:LEU:HA	1:A:47:ILE:HD12	1.57	0.86
1:A:149:GLY:HA3	1:A:152:THR:OG1	1.73	0.86
1:A:100:TRP:O	1:A:104:GLU:HG3	1.74	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:170:ASP:HB2	3:C:177:ARG:NE	1.90	0.85
2:B:193:HIS:CD2	2:B:287:SER:HB3	2.12	0.85
1:A:185:LEU:O	1:A:188:ALA:HB3	1.76	0.85
6:A:850:BCL:H2	6:A:850:BCL:H71	1.59	0.84
2:B:155:TRP:HD1	2:B:278:LEU:HA	1.43	0.83
6:A:850:BCL:HED1	2:B:183:LEU:HD11	1.59	0.82
1:A:12:PRO:HG3	3:C:97:PRO:HB3	1.60	0.82
3:C:18:TYR:C	3:C:20:PHE:H	1.79	0.81
2:B:36:SER:HB3	2:B:39:LEU:HD12	1.63	0.80
1:A:122:ALA:HA	1:A:125:ILE:HB	1.62	0.80
2:B:213:ALA:O	2:B:217:ALA:HB3	1.81	0.80
1:A:196:SER:HB3	2:B:145:HIS:HB2	1.63	0.79
2:B:154:ILE:HG22	2:B:158:MET:HG2	1.63	0.79
1:A:187:LEU:HD13	2:B:216:PHE:HB2	1.62	0.79
1:A:239:SER:O	1:A:241:VAL:N	2.16	0.78
2:B:159:VAL:HG21	2:B:281:GLY:O	1.84	0.78
2:B:12:VAL:HG12	2:B:13:ARG:H	1.48	0.78
2:B:93:SER:HB2	2:B:181:SER:HB3	1.66	0.78
2:B:243:THR:N	3:C:115:VAL:HG21	1.99	0.78
3:C:29:TYR:O	3:C:31:LEU:N	2.17	0.78
1:A:244:SER:C	1:A:246:LEU:H	1.85	0.77
1:A:173:HIS:ND1	1:A:177:ILE:HD11	1.99	0.77
3:C:170:ASP:CB	3:C:177:ARG:HE	1.97	0.77
2:B:90:PHE:CA	2:B:179:ILE:HD12	2.14	0.77
2:B:208:PHE:CB	2:B:276:VAL:HG22	2.15	0.77
2:B:228:ARG:HG3	2:B:229:PHE:CE1	2.20	0.77
3:C:220:LYS:O	3:C:221:SER:HB2	1.84	0.77
3:C:57:PRO:O	3:C:58:LEU:HD23	1.83	0.77
2:B:273:ALA:O	2:B:276:VAL:HG23	1.85	0.76
2:B:36:SER:H	2:B:47:LEU:HD11	1.49	0.76
3:C:115:VAL:HG12	3:C:116:ALA:H	1.48	0.76
3:C:75:VAL:HA	3:C:76:PRO:O	1.84	0.76
2:B:149:ALA:O	2:B:152:SER:HB3	1.85	0.76
2:B:95:GLU:HB3	2:B:96:PRO:HD2	1.66	0.76
3:C:83:ARG:HB2	3:C:84:PRO:HD2	1.66	0.76
1:A:224:ILE:O	1:A:228:GLY:HA3	1.86	0.75
2:B:14:GLY:HA3	3:C:140:PHE:CE1	2.20	0.75
1:A:116:HIS:HB2	2:B:221:ALA:O	1.86	0.75
2:B:46:GLN:O	2:B:47:LEU:HD23	1.86	0.75
3:C:171:ILE:HB	3:C:172:PRO:CD	2.17	0.75
1:A:50:ALA:O	1:A:54:VAL:HG22	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:ILE:O	1:A:180:PHE:HB2	1.87	0.74
6:A:850:BCL:HMD2	6:A:851:BCL:HBB3	1.68	0.74
1:A:12:PRO:HG3	3:C:97:PRO:CB	2.17	0.74
1:A:222:TYR:CG	1:A:223:SER:N	2.56	0.73
1:A:177:ILE:HG22	1:A:181:PHE:CE2	2.24	0.72
1:A:210:ASP:OD1	3:C:172:PRO:HG3	1.89	0.72
3:C:156:CYS:CB	3:C:248:ARG:HD3	2.17	0.72
2:B:261:THR:OG1	2:B:262:MET:N	2.20	0.72
2:B:32:VAL:HG12	2:B:33:GLY:N	2.03	0.72
1:A:113:ILE:CG2	2:B:226:VAL:HG12	2.20	0.72
2:B:25:ASN:HD22	2:B:28:ASN:HD22	1.37	0.72
3:C:148:PRO:HB2	3:C:164:VAL:HG21	1.72	0.72
1:A:223:SER:C	1:A:225:GLY:H	1.94	0.72
1:A:185:LEU:N	7:B:854:BPH:HMC2	2.04	0.71
2:B:229:PHE:CZ	3:C:238:ALA:HB2	2.25	0.71
3:C:195:MET:HA	3:C:195:MET:CE	2.20	0.71
3:C:115:VAL:CG1	3:C:116:ALA:H	2.02	0.71
1:A:35:GLY:HA2	1:A:103:ARG:HD2	1.72	0.71
1:A:173:HIS:HD1	1:A:177:ILE:HD11	1.55	0.70
2:B:214:LEU:HD11	2:B:218:MET:SD	2.31	0.70
3:C:70:ARG:HH22	3:C:120:LEU:HD13	1.55	0.70
1:A:219:LEU:HD11	2:B:129:TRP:CZ2	2.26	0.70
1:A:160:THR:O	1:A:163:THR:HB	1.92	0.70
1:A:117:ILE:C	1:A:119:PHE:H	1.95	0.70
2:B:103:LEU:HD21	2:B:169:GLY:HA2	1.74	0.70
2:B:175:VAL:CG1	2:B:182:HIS:HB2	2.21	0.70
1:A:187:LEU:HD13	2:B:216:PHE:CB	2.21	0.70
2:B:90:PHE:HA	2:B:179:ILE:CD1	2.21	0.70
2:B:215:LEU:O	2:B:218:MET:HB2	1.91	0.69
1:A:254:ILE:HD12	1:A:255:TRP:HB2	1.74	0.69
1:A:173:HIS:O	1:A:177:ILE:HG13	1.91	0.69
1:A:183:ASN:O	1:A:186:ALA:HB3	1.92	0.69
2:B:264:GLY:HA3	3:C:35:ASN:OD1	1.92	0.69
2:B:36:SER:CB	2:B:39:LEU:HD12	2.22	0.69
2:B:293:ASN:OD1	2:B:296:VAL:HG23	1.93	0.69
3:C:115:VAL:CG1	3:C:116:ALA:N	2.56	0.69
2:B:268:TRP:HE1	8:B:856:U10:C10	2.05	0.69
3:C:14:SER:O	3:C:17:ILE:HG22	1.92	0.69
2:B:16:ALA:O	2:B:18:LEU:N	2.25	0.68
2:B:229:PHE:O	2:B:244:ALA:HB2	1.93	0.68
2:B:82:PRO:O	2:B:86:LEU:HD23	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:ALA:O	1:A:2:LEU:HG	1.93	0.68
1:A:172:ALA:C	1:A:247:CYS:HB3	2.13	0.68
2:B:134:TYR:CE2	2:B:144:LYS:HD2	2.27	0.68
2:B:17:ASP:O	2:B:19:GLY:N	2.26	0.68
3:C:22:ILE:HG22	3:C:23:PHE:N	2.08	0.67
1:A:236:LEU:O	1:A:236:LEU:HD23	1.94	0.67
2:B:265:ILE:HG21	8:B:856:U10:H3M2	1.75	0.67
3:C:29:TYR:OH	3:C:57:PRO:HG3	1.94	0.67
2:B:237:GLN:O	2:B:241:ARG:N	2.28	0.67
2:B:211:GLY:O	2:B:215:LEU:N	2.27	0.67
1:A:72:GLU:O	1:A:74:GLY:N	2.28	0.67
1:A:248:MET:C	1:A:250:ILE:H	1.96	0.67
2:B:247:ARG:NH2	3:C:111:PRO:O	2.27	0.66
1:A:190:HIS:CE1	1:A:194:VAL:HG21	2.29	0.66
2:B:26:LEU:C	2:B:28:ASN:H	1.98	0.66
1:A:220:VAL:HG23	1:A:221:GLY:N	2.11	0.66
2:B:258:PHE:HD1	3:C:32:GLN:HE22	1.43	0.66
2:B:38:LEU:C	2:B:40:GLY:H	1.97	0.66
3:C:18:TYR:C	3:C:20:PHE:N	2.49	0.66
3:C:178:PHE:HD1	3:C:191:LEU:O	1.78	0.66
1:A:190:HIS:CE1	1:A:230:HIS:HE1	2.14	0.66
2:B:215:LEU:CD2	2:B:269:ALA:HB2	2.25	0.66
1:A:230:HIS:CD2	2:B:223:ILE:HG13	2.30	0.65
2:B:269:ALA:HA	2:B:272:MET:HB3	1.77	0.65
2:B:213:ALA:O	2:B:217:ALA:CB	2.45	0.65
2:B:159:VAL:HG12	2:B:160:LEU:HD23	1.78	0.65
1:A:217:ARG:HH21	2:B:44:ASN:ND2	1.95	0.65
1:A:250:ILE:HG13	1:A:251:THR:N	2.11	0.65
2:B:90:PHE:H	2:B:90:PHE:HD1	1.44	0.65
1:A:172:ALA:CB	1:A:247:CYS:HB3	2.27	0.65
6:B:852:BCL:HBB3	6:B:853:BCL:HMD2	1.79	0.65
1:A:177:ILE:HD12	6:A:850:BCL:OBD	1.97	0.65
1:A:135:ARG:HB3	1:A:136:PRO:HD3	1.79	0.65
3:C:171:ILE:HB	3:C:172:PRO:HD2	1.77	0.65
1:A:116:HIS:ND1	2:B:225:ALA:HA	2.11	0.65
2:B:268:TRP:HE1	8:B:856:U10:H101	1.60	0.64
2:B:152:SER:OG	2:B:274:VAL:HG13	1.98	0.64
2:B:242:GLY:C	2:B:244:ALA:N	2.50	0.64
1:A:224:ILE:HG23	1:A:229:ILE:H	1.63	0.64
1:A:246:LEU:C	1:A:248:MET:H	2.00	0.64
1:A:187:LEU:CD2	2:B:269:ALA:HB1	2.17	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:TYR:O	1:A:11:VAL:HG13	1.97	0.64
1:A:196:SER:CB	2:B:145:HIS:HB2	2.26	0.64
1:A:52:SER:OG	1:A:66:VAL:HG22	1.98	0.64
1:A:100:TRP:HE1	7:A:855:BPH:HBD	1.63	0.63
3:C:89:ARG:HG3	3:C:98:HIS:CE1	2.33	0.63
1:A:232:LEU:O	1:A:236:LEU:HB2	1.99	0.63
3:C:64:PHE:HB2	3:C:73:LEU:O	1.98	0.63
1:A:244:SER:C	1:A:246:LEU:N	2.52	0.63
1:A:167:PHE:HB3	6:A:851:BCL:HMC3	1.81	0.63
1:A:231:ARG:NH2	2:B:5:ASN:HD21	1.96	0.63
3:C:112:ALA:HB2	3:C:239:GLY:HA3	1.79	0.63
1:A:265:TRP:CD1	1:A:266:TRP:N	2.67	0.63
2:B:243:THR:O	2:B:247:ARG:HG3	1.99	0.63
1:A:43:ALA:C	1:A:45:GLY:N	2.51	0.63
1:A:233:GLY:HA3	2:B:216:PHE:CE1	2.34	0.63
3:C:61:PRO:HG3	3:C:76:PRO:HD2	1.81	0.63
3:C:182:GLU:CG	3:C:186:GLY:HA2	2.29	0.63
1:A:246:LEU:O	1:A:250:ILE:HG23	1.99	0.62
3:C:61:PRO:HG3	3:C:76:PRO:HG2	1.81	0.62
1:A:247:CYS:HA	1:A:250:ILE:CD1	2.29	0.62
2:B:228:ARG:HG3	2:B:229:PHE:CZ	2.34	0.62
3:C:77:GLY:O	3:C:79:GLU:HG3	1.98	0.62
2:B:270:ILE:HG23	2:B:271:TRP:N	2.13	0.62
3:C:156:CYS:HB2	3:C:248:ARG:CD	2.24	0.62
1:A:163:THR:HG22	1:A:163:THR:O	1.98	0.62
1:A:254:ILE:HD12	1:A:254:ILE:C	2.19	0.62
2:B:164:ARG:HB3	2:B:165:PRO:HD3	1.80	0.62
3:C:219:ILE:HD12	3:C:222:PRO:HB3	1.81	0.62
2:B:201:PHE:O	2:B:205:SER:CB	2.48	0.62
3:C:81:GLU:O	3:C:83:ARG:N	2.27	0.62
7:A:855:BPH:C1D	2:B:214:LEU:HD13	2.29	0.62
2:B:214:LEU:CD1	2:B:218:MET:SD	2.88	0.62
2:B:271:TRP:O	2:B:275:LEU:HG	1.99	0.62
1:A:114:GLY:HA3	2:B:225:ALA:HA	1.82	0.62
1:A:114:GLY:N	2:B:225:ALA:O	2.33	0.62
1:A:176:ALA:CB	1:A:243:PHE:HB3	2.30	0.61
2:B:153:ALA:HA	2:B:277:THR:HG21	1.82	0.61
3:C:148:PRO:HA	3:C:151:LEU:CG	2.28	0.61
2:B:10:VAL:HG12	2:B:11:GLN:N	2.15	0.61
2:B:127:TRP:CZ2	2:B:154:ILE:HG21	2.35	0.61
2:B:199:ASN:HA	2:B:294:TRP:CZ3	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:59:PRO:O	3:C:61:PRO:HD3	2.01	0.61
3:C:41:PRO:HG3	3:C:58:LEU:HD11	1.82	0.61
1:A:146:PHE:HA	1:A:156:TRP:CD1	2.35	0.61
2:B:134:TYR:O	2:B:137:ALA:N	2.33	0.61
2:B:152:SER:CB	2:B:274:VAL:HG13	2.30	0.61
2:B:89:LEU:HA	2:B:92:PHE:CE2	2.36	0.61
1:A:248:MET:C	1:A:250:ILE:N	2.54	0.61
2:B:199:ASN:OD1	2:B:201:PHE:HB2	2.00	0.61
2:B:214:LEU:HD12	2:B:214:LEU:O	2.00	0.61
2:B:266:HIS:C	2:B:268:TRP:N	2.54	0.61
3:C:146:LYS:HE2	3:C:200:SER:O	2.00	0.61
2:B:37:THR:HG22	2:B:37:THR:O	2.01	0.61
3:C:86:ALA:C	3:C:101:THR:HG23	2.22	0.60
3:C:148:PRO:CA	3:C:151:LEU:HG	2.28	0.60
1:A:43:ALA:C	1:A:45:GLY:H	2.04	0.60
1:A:278:GLY:O	1:A:279:ILE:HD13	2.01	0.60
2:B:64:LEU:C	2:B:66:TRP:H	2.04	0.60
2:B:164:ARG:O	2:B:168:MET:HG2	2.02	0.60
2:B:214:LEU:C	2:B:214:LEU:HD12	2.22	0.60
1:A:222:TYR:OH	1:A:224:ILE:HA	2.01	0.60
2:B:215:LEU:O	2:B:216:PHE:C	2.40	0.60
2:B:264:GLY:O	2:B:266:HIS:N	2.34	0.60
1:A:77:GLY:O	1:A:78:ALA:HB2	2.02	0.60
1:A:178:SER:C	1:A:180:PHE:H	2.04	0.60
2:B:270:ILE:HD13	2:B:270:ILE:O	2.02	0.60
2:B:124:VAL:HG12	2:B:124:VAL:O	2.00	0.60
2:B:216:PHE:HD1	2:B:216:PHE:O	1.85	0.60
2:B:193:HIS:HD2	2:B:287:SER:HB3	1.66	0.60
2:B:211:GLY:C	2:B:213:ALA:H	2.02	0.60
2:B:101:TYR:CZ	2:B:108:PRO:HD2	2.37	0.60
1:A:117:ILE:H	1:A:118:PRO:HD2	1.66	0.60
2:B:26:LEU:C	2:B:28:ASN:N	2.55	0.60
1:A:184:ALA:HB3	7:B:854:BPH:CMC	2.32	0.59
1:A:239:SER:O	1:A:240:ALA:C	2.40	0.59
1:A:244:SER:O	1:A:246:LEU:N	2.34	0.59
6:A:850:BCL:H52	8:A:857:U10:H302	1.84	0.59
1:A:231:ARG:HH21	2:B:5:ASN:HD21	1.50	0.59
3:C:193:MET:O	3:C:196:VAL:HG22	2.02	0.59
2:B:273:ALA:O	2:B:275:LEU:N	2.36	0.59
2:B:239:ALA:O	2:B:240:ASP:HB2	2.01	0.59
3:C:143:SER:O	3:C:144:ALA:HB3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:CYS:HA	1:A:250:ILE:HD11	1.84	0.59
2:B:211:GLY:HA3	2:B:272:MET:CE	2.32	0.59
2:B:5:ASN:C	2:B:6:ILE:HD13	2.22	0.59
1:A:185:LEU:HG	7:B:854:BPH:NC	2.16	0.59
1:A:219:LEU:HD12	2:B:132:ARG:HH12	1.67	0.59
2:B:262:MET:O	2:B:265:ILE:HG22	2.01	0.59
2:B:12:VAL:HG12	2:B:13:ARG:N	2.17	0.59
2:B:208:PHE:C	2:B:210:TYR:H	2.06	0.59
3:C:168:TRP:HB2	3:C:178:PHE:HB2	1.84	0.59
1:A:126:LEU:HD12	1:A:129:LEU:HD12	1.83	0.59
2:B:215:LEU:O	2:B:218:MET:N	2.35	0.59
1:A:174:MET:HA	1:A:177:ILE:HD12	1.83	0.59
2:B:232:GLU:O	2:B:233:ARG:C	2.41	0.59
7:A:855:BPH:HED3	2:B:252:TRP:HZ3	1.67	0.59
2:B:280:GLY:HA2	6:B:852:BCL:HED2	1.83	0.59
1:A:89:ILE:HG23	1:A:90:THR:N	2.17	0.59
3:C:192:PRO:O	3:C:193:MET:C	2.40	0.59
2:B:150:PHE:HA	7:B:854:BPH:HMD3	1.83	0.59
2:B:266:HIS:O	2:B:268:TRP:N	2.36	0.59
3:C:36:MET:HG2	3:C:40:TYR:CE1	2.38	0.59
2:B:156:LEU:O	2:B:160:LEU:HG	2.03	0.58
2:B:85:PHE:O	2:B:89:LEU:HB2	2.03	0.58
1:A:62:GLN:HG2	1:A:151:TRP:CD1	2.38	0.58
1:A:52:SER:HB2	1:A:85:LEU:CD1	2.27	0.58
2:B:229:PHE:CE1	3:C:238:ALA:HB2	2.38	0.58
2:B:122:MET:SD	2:B:157:TRP:HZ2	2.25	0.58
2:B:50:ILE:CD1	2:B:51:TYR:N	2.61	0.58
2:B:207:ALA:O	2:B:210:TYR:HB2	2.04	0.58
1:A:30:TYR:CG	1:A:31:VAL:N	2.71	0.58
2:B:49:PRO:O	2:B:50:ILE:HB	2.02	0.58
2:B:265:ILE:HG23	2:B:266:HIS:N	2.17	0.58
1:A:142:TRP:O	1:A:144:TYR:N	2.35	0.58
1:A:216:PHE:HB3	1:A:220:VAL:HG22	1.85	0.58
2:B:205:SER:HA	2:B:279:THR:OG1	2.02	0.58
2:B:152:SER:HB2	2:B:274:VAL:HG13	1.84	0.58
3:C:18:TYR:O	3:C:20:PHE:N	2.36	0.58
3:C:32:GLN:HG2	3:C:56:PHE:CE2	2.38	0.58
3:C:178:PHE:CE1	3:C:192:PRO:HA	2.38	0.58
1:A:176:ALA:HB2	1:A:243:PHE:HB3	1.86	0.58
6:A:850:BCL:CMD	6:A:851:BCL:HBB3	2.33	0.58
6:A:850:BCL:HBD	6:A:850:BCL:HAA2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:55:LEU:HD23	2:B:132:ARG:HB2	1.84	0.58
3:C:35:ASN:O	3:C:36:MET:HG3	2.04	0.58
1:A:239:SER:O	1:A:242:PHE:N	2.37	0.58
1:A:266:TRP:HE1	2:B:87:ARG:HA	1.69	0.58
2:B:245:ALA:O	2:B:248:ALA:HB3	2.04	0.58
2:B:129:TRP:HD1	2:B:150:PHE:HE2	1.51	0.57
2:B:201:PHE:O	2:B:205:SER:HB3	2.04	0.57
2:B:243:THR:H	3:C:115:VAL:HG21	1.67	0.57
1:A:191:GLY:O	1:A:195:LEU:HB2	2.03	0.57
1:A:190:HIS:NE2	2:B:266:HIS:NE2	2.50	0.57
2:B:38:LEU:C	2:B:40:GLY:N	2.56	0.57
2:B:234:GLU:O	2:B:237:GLN:HB2	2.05	0.57
2:B:180:PHE:HD1	2:B:183:LEU:HD12	1.70	0.57
2:B:78:ALA:HB2	2:B:92:PHE:CZ	2.39	0.57
1:A:97:PHE:HB3	1:A:125:ILE:HD11	1.87	0.57
2:B:74:PHE:N	2:B:74:PHE:HD1	2.03	0.57
2:B:166:ILE:HG22	2:B:167:LEU:HD23	1.86	0.57
1:A:187:LEU:HB2	2:B:216:PHE:HD2	1.68	0.57
2:B:163:ILE:HG22	2:B:285:LEU:HD13	1.86	0.57
2:B:73:TRP:CD1	2:B:94:LEU:HB2	2.40	0.57
1:A:174:MET:HG3	1:A:175:ILE:N	2.19	0.57
3:C:31:LEU:O	3:C:33:THR:N	2.38	0.57
2:B:261:THR:HG23	3:C:35:ASN:HA	1.85	0.57
1:A:244:SER:HA	1:A:247:CYS:SG	2.44	0.57
3:C:54:GLY:O	3:C:56:PHE:N	2.36	0.57
3:C:17:ILE:O	3:C:21:TRP:HD1	1.88	0.57
1:A:54:VAL:C	1:A:56:GLN:H	2.07	0.57
1:A:226:THR:OG1	1:A:227:LEU:N	2.37	0.56
2:B:269:ALA:O	2:B:272:MET:HB3	2.04	0.56
2:B:116:LEU:C	2:B:118:ALA:H	2.09	0.56
2:B:258:PHE:HD1	3:C:32:GLN:NE2	2.04	0.56
2:B:237:GLN:NE2	3:C:117:ARG:NH2	2.52	0.56
3:C:219:ILE:CD1	3:C:222:PRO:HB3	2.35	0.56
2:B:192:VAL:O	2:B:192:VAL:HG12	2.05	0.56
2:B:270:ILE:CG2	2:B:271:TRP:N	2.68	0.56
3:C:27:LEU:C	3:C:29:TYR:N	2.56	0.56
3:C:54:GLY:C	3:C:56:PHE:H	2.07	0.56
3:C:65:ILE:N	3:C:65:ILE:HD12	2.21	0.56
1:A:180:PHE:CE2	1:A:240:ALA:HB1	2.39	0.56
2:B:215:LEU:HD23	2:B:269:ALA:HB2	1.86	0.56
1:A:173:HIS:C	1:A:177:ILE:HG13	2.26	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:857:U10:H122	8:A:857:U10:H303	1.87	0.56
8:B:856:U10:H4M2	8:B:856:U10:H3M3	1.88	0.56
2:B:90:PHE:CD1	2:B:90:PHE:N	2.72	0.56
2:B:74:PHE:N	2:B:74:PHE:CD1	2.73	0.56
1:A:3:LEU:HD22	3:C:39:GLY:C	2.26	0.56
3:C:208:LEU:CD2	3:C:240:GLY:HA3	2.35	0.56
1:A:117:ILE:O	1:A:119:PHE:N	2.39	0.56
3:C:119:ASP:OD1	3:C:228:LEU:HD23	2.05	0.56
2:B:211:GLY:C	2:B:213:ALA:N	2.59	0.56
2:B:155:TRP:CD1	2:B:278:LEU:HA	2.33	0.56
1:A:171:PRO:HD2	1:A:259:TRP:CZ3	2.41	0.56
3:C:32:GLN:O	3:C:32:GLN:HG3	2.06	0.56
3:C:104:PRO:O	3:C:109:VAL:HG22	2.05	0.56
1:A:241:VAL:HG12	1:A:242:PHE:N	2.21	0.55
3:C:29:TYR:C	3:C:31:LEU:N	2.59	0.55
1:A:166:ASN:ND2	2:B:187:ASN:HB2	2.20	0.55
2:B:273:ALA:O	2:B:276:VAL:N	2.36	0.55
1:A:113:ILE:HG21	2:B:226:VAL:HG12	1.87	0.55
2:B:243:THR:OG1	2:B:247:ARG:NE	2.39	0.55
2:B:46:GLN:C	2:B:47:LEU:HG	2.27	0.55
3:C:61:PRO:HG3	3:C:76:PRO:CG	2.36	0.55
1:A:109:ARG:HH11	1:A:109:ARG:HG2	1.72	0.55
3:C:43:GLU:O	3:C:44:ASN:O	2.25	0.55
3:C:69:GLY:C	3:C:71:GLY:H	2.10	0.54
1:A:107:ILE:HG22	1:A:107:ILE:O	2.08	0.54
1:A:37:ALA:C	1:A:39:PHE:H	2.11	0.54
1:A:166:ASN:HD21	2:B:187:ASN:HB2	1.73	0.54
2:B:4:GLN:O	2:B:6:ILE:N	2.40	0.54
2:B:246:GLU:O	2:B:248:ALA:N	2.40	0.54
2:B:237:GLN:NE2	3:C:117:ARG:HH22	2.05	0.54
3:C:148:PRO:O	3:C:164:VAL:HB	2.08	0.54
2:B:77:GLN:C	2:B:79:GLY:H	2.10	0.54
1:A:16:LEU:CD2	1:A:109:ARG:HD2	2.32	0.54
2:B:243:THR:N	3:C:115:VAL:CG2	2.68	0.54
3:C:238:ALA:O	3:C:240:GLY:N	2.41	0.54
3:C:61:PRO:HG3	3:C:76:PRO:CD	2.37	0.54
2:B:201:PHE:O	2:B:205:SER:HB2	2.07	0.54
3:C:170:ASP:HB2	3:C:177:ARG:CD	2.38	0.54
1:A:65:SER:OG	1:A:149:GLY:HA3	2.08	0.54
3:C:148:PRO:O	3:C:150:GLY:N	2.40	0.54
3:C:217:PRO:HD3	3:C:236:TYR:CD2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:174:ALA:O	2:B:185:TRP:NE1	2.40	0.54
3:C:15:LEU:CD1	3:C:19:SER:HB3	2.37	0.54
1:A:65:SER:CB	1:A:149:GLY:HA3	2.38	0.54
3:C:95:GLY:O	3:C:96:PHE:O	2.26	0.54
1:A:9:TYR:CE1	3:C:113:SER:HB2	2.43	0.54
2:B:275:LEU:O	2:B:279:THR:HG23	2.08	0.54
1:A:147:PRO:CD	1:A:156:TRP:HB2	2.37	0.54
1:A:183:ASN:HB2	1:A:236:LEU:HD22	1.90	0.54
2:B:191:LEU:C	2:B:193:HIS:H	2.11	0.54
3:C:178:PHE:CD1	3:C:191:LEU:O	2.61	0.54
1:A:41:PHE:CD2	1:A:95:GLY:HA3	2.42	0.54
1:A:235:LEU:O	1:A:236:LEU:C	2.46	0.53
1:A:241:VAL:O	1:A:244:SER:N	2.37	0.53
1:A:116:HIS:CD2	2:B:224:LEU:HB2	2.43	0.53
3:C:189:ARG:HD2	3:C:216:ILE:HB	1.90	0.53
1:A:156:TRP:HE3	1:A:157:VAL:HG23	1.74	0.53
2:B:116:LEU:O	2:B:118:ALA:N	2.42	0.53
3:C:203:VAL:HG12	3:C:204:HIS:H	1.72	0.53
2:B:40:GLY:C	2:B:42:PHE:H	2.12	0.53
1:A:83:GLY:O	1:A:85:LEU:N	2.41	0.53
1:A:43:ALA:O	1:A:47:ILE:HG13	2.09	0.53
2:B:90:PHE:CG	2:B:179:ILE:HD12	2.44	0.53
3:C:171:ILE:CB	3:C:172:PRO:CD	2.84	0.53
3:C:169:VAL:HG23	3:C:170:ASP:N	2.24	0.53
3:C:43:GLU:HB3	3:C:47:GLY:HA2	1.91	0.53
3:C:129:ASN:ND2	3:C:224:GLU:HB2	2.24	0.53
3:C:83:ARG:HB2	3:C:84:PRO:CD	2.36	0.53
1:A:230:HIS:CD2	2:B:223:ILE:HG21	2.44	0.53
1:A:192:ALA:O	1:A:196:SER:HB3	2.08	0.53
1:A:255:TRP:CZ2	1:A:262:TRP:HB2	2.44	0.53
6:A:851:BCL:HAA2	6:A:851:BCL:HBD	1.91	0.53
2:B:89:LEU:HA	2:B:92:PHE:CD2	2.44	0.53
3:C:171:ILE:O	3:C:173:GLU:N	2.41	0.53
2:B:25:ASN:ND2	2:B:28:ASN:HD22	2.06	0.53
3:C:182:GLU:HG3	3:C:186:GLY:HA2	1.90	0.53
1:A:130:THR:HA	1:A:134:PHE:HB2	1.91	0.53
1:A:250:ILE:HG13	1:A:251:THR:H	1.74	0.52
2:B:265:ILE:C	2:B:268:TRP:HB2	2.29	0.52
1:A:217:ARG:NH2	2:B:44:ASN:ND2	2.57	0.52
1:A:220:VAL:CG2	1:A:221:GLY:N	2.73	0.52
1:A:226:THR:C	1:A:228:GLY:N	2.61	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:212:SER:OG	2:B:272:MET:HG3	2.08	0.52
2:B:91:PHE:O	2:B:92:PHE:C	2.47	0.52
1:A:185:LEU:C	1:A:188:ALA:HB3	2.29	0.52
1:A:182:THR:O	1:A:185:LEU:N	2.42	0.52
1:A:263:TRP:CE3	2:B:180:PHE:HZ	2.26	0.52
3:C:156:CYS:SG	3:C:209:SER:HB3	2.48	0.52
3:C:66:LEU:HD22	3:C:67:PRO:HD2	1.92	0.52
1:A:210:ASP:O	1:A:211:HIS:C	2.46	0.52
2:B:246:GLU:O	2:B:247:ARG:C	2.48	0.52
2:B:66:TRP:CD1	2:B:122:MET:HB2	2.43	0.52
1:A:208:THR:OG1	1:A:210:ASP:HB2	2.09	0.52
1:A:211:HIS:O	1:A:212:GLU:C	2.47	0.52
2:B:103:LEU:CD2	2:B:169:GLY:HA2	2.40	0.52
2:B:46:GLN:HG2	2:B:47:LEU:N	2.25	0.52
2:B:210:TYR:HD2	6:B:853:BCL:H11	1.75	0.52
3:C:134:MET:C	3:C:136:ALA:H	2.13	0.52
2:B:155:TRP:CE3	2:B:155:TRP:HA	2.45	0.52
2:B:260:ALA:HB1	3:C:35:ASN:OD1	2.09	0.52
1:A:85:LEU:O	1:A:87:GLN:N	2.43	0.52
1:A:113:ILE:HB	2:B:226:VAL:HG12	1.91	0.52
1:A:116:HIS:CD2	2:B:224:LEU:CB	2.92	0.52
6:B:853:BCL:HAA2	6:B:853:BCL:HBD	1.91	0.52
3:C:207:ALA:HA	3:C:241:LEU:HD23	1.92	0.52
1:A:159:ASN:O	1:A:161:GLY:N	2.43	0.52
2:B:143:GLY:C	2:B:145:HIS:H	2.12	0.52
2:B:60:LEU:HD12	7:B:854:BPH:H5C2	1.92	0.52
2:B:78:ALA:HB2	2:B:92:PHE:HZ	1.75	0.52
2:B:243:THR:H	3:C:115:VAL:CG2	2.24	0.51
1:A:190:HIS:CE1	1:A:230:HIS:CE1	2.98	0.51
2:B:26:LEU:HD22	2:B:29:ARG:CD	2.40	0.51
1:A:237:SER:O	1:A:239:SER:N	2.43	0.51
2:B:256:MET:HE2	2:B:258:PHE:CE2	2.45	0.51
2:B:242:GLY:C	2:B:244:ALA:H	2.12	0.51
3:C:122:GLU:O	3:C:123:LEU:HD23	2.10	0.51
1:A:44:LEU:O	1:A:48:LEU:HG	2.10	0.51
2:B:155:TRP:HA	2:B:155:TRP:HE3	1.76	0.51
2:B:154:ILE:CG2	2:B:158:MET:HG2	2.39	0.51
2:B:187:ASN:O	2:B:191:LEU:HG	2.09	0.51
2:B:266:HIS:C	2:B:268:TRP:H	2.11	0.51
2:B:55:LEU:O	2:B:56:GLY:C	2.48	0.51
3:C:236:TYR:O	3:C:237:VAL:C	2.49	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:THR:C	2:B:70:ILE:HD13	2.30	0.51
1:A:217:ARG:O	2:B:50:ILE:HA	2.10	0.51
1:A:223:SER:C	1:A:225:GLY:N	2.63	0.51
1:A:166:ASN:OD1	1:A:167:PHE:N	2.44	0.51
1:A:226:THR:O	1:A:228:GLY:N	2.44	0.51
1:A:235:LEU:O	1:A:237:SER:N	2.44	0.51
2:B:206:ILE:HA	6:B:852:BCL:HMA1	1.93	0.51
1:A:87:GLN:O	1:A:90:THR:N	2.44	0.51
1:A:89:ILE:CG2	1:A:90:THR:N	2.74	0.51
1:A:51:TRP:HD1	1:A:51:TRP:O	1.94	0.51
2:B:64:LEU:O	2:B:66:TRP:N	2.44	0.51
3:C:159:GLU:HB3	3:C:210:SER:HB3	1.92	0.51
2:B:256:MET:HE1	8:B:856:U10:H161	1.92	0.50
1:A:216:PHE:HA	1:A:219:LEU:HB3	1.94	0.50
1:A:237:SER:O	1:A:238:LEU:C	2.49	0.50
2:B:265:ILE:CG2	2:B:266:HIS:N	2.74	0.50
2:B:265:ILE:HD12	2:B:268:TRP:HD1	1.76	0.50
3:C:23:PHE:O	3:C:27:LEU:HB2	2.11	0.50
3:C:86:ALA:O	3:C:101:THR:HG23	2.11	0.50
1:A:173:HIS:O	1:A:176:ALA:N	2.44	0.50
1:A:184:ALA:HB3	7:B:854:BPH:HMC3	1.93	0.50
2:B:95:GLU:HA	2:B:176:PRO:CB	2.34	0.50
2:B:64:LEU:C	2:B:66:TRP:N	2.62	0.50
2:B:78:ALA:O	2:B:81:ASN:HB3	2.12	0.50
2:B:77:GLN:C	2:B:79:GLY:N	2.65	0.50
1:A:61:PRO:HB3	1:A:150:ILE:HD12	1.93	0.50
1:A:123:PHE:CG	1:A:238:LEU:HD22	2.46	0.50
3:C:29:TYR:C	3:C:31:LEU:H	2.15	0.50
3:C:31:LEU:C	3:C:33:THR:N	2.64	0.50
1:A:56:GLN:HE22	1:A:64:ILE:HA	1.76	0.50
2:B:93:SER:CB	2:B:181:SER:HB3	2.39	0.50
3:C:220:LYS:HG3	3:C:220:LYS:O	2.12	0.50
1:A:218:ASP:OD2	2:B:29:ARG:NH2	2.44	0.50
2:B:10:VAL:CG1	2:B:11:GLN:N	2.74	0.50
1:A:176:ALA:O	1:A:180:PHE:HD2	1.95	0.50
2:B:40:GLY:O	2:B:42:PHE:N	2.44	0.50
7:A:855:BPH:HED3	2:B:252:TRP:CZ3	2.46	0.50
1:A:65:SER:HB2	1:A:149:GLY:HA3	1.92	0.50
1:A:132:VAL:HG23	1:A:133:LEU:N	2.27	0.50
1:A:116:HIS:HB3	2:B:221:ALA:HA	1.92	0.50
1:A:216:PHE:O	1:A:220:VAL:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:267:ARG:O	2:B:270:ILE:HG22	2.12	0.50
3:C:148:PRO:HG2	3:C:164:VAL:HG11	1.94	0.50
1:A:190:HIS:CG	1:A:229:ILE:HD11	2.47	0.49
1:A:179:PHE:C	1:A:240:ALA:HB2	2.27	0.49
2:B:190:SER:O	2:B:194:GLY:O	2.29	0.49
2:B:231:GLY:O	2:B:232:GLU:O	2.29	0.49
3:C:169:VAL:HG23	3:C:170:ASP:O	2.12	0.49
1:A:269:LEU:CD1	1:A:270:PRO:HD2	2.33	0.49
1:A:34:PHE:CZ	1:A:102:LEU:HD13	2.47	0.49
1:A:208:THR:C	1:A:210:ASP:H	2.15	0.49
6:A:850:BCL:H3A	6:A:850:BCL:H152	1.95	0.49
1:A:117:ILE:C	1:A:119:PHE:N	2.63	0.49
1:A:193:LEU:HD22	1:A:216:PHE:HE2	1.77	0.49
6:A:850:BCL:H171	6:A:850:BCL:CHB	2.42	0.49
3:C:31:LEU:C	3:C:33:THR:H	2.15	0.49
1:A:101:ALA:O	1:A:104:GLU:N	2.45	0.49
1:A:233:GLY:O	1:A:234:LEU:C	2.50	0.49
1:A:190:HIS:CE1	2:B:266:HIS:HE2	2.30	0.49
2:B:265:ILE:HG21	8:B:856:U10:C3M	2.41	0.49
3:C:180:GLU:OE2	3:C:188:THR:HG21	2.12	0.49
2:B:259:ASN:HA	8:B:856:U10:H8	1.95	0.49
2:B:96:PRO:CG	2:B:172:SER:HA	2.42	0.49
2:B:242:GLY:CA	3:C:117:ARG:HD2	2.43	0.49
3:C:233:ILE:O	3:C:234:CYS:C	2.51	0.49
2:B:265:ILE:HD12	2:B:268:TRP:CD1	2.48	0.49
2:B:150:PHE:O	2:B:151:LEU:C	2.50	0.49
2:B:40:GLY:C	2:B:42:PHE:N	2.65	0.49
3:C:192:PRO:O	3:C:194:GLN:N	2.45	0.49
3:C:183:LEU:HD11	3:C:189:ARG:HG3	1.94	0.49
1:A:173:HIS:CE1	1:A:177:ILE:HD11	2.48	0.49
2:B:210:TYR:O	2:B:213:ALA:HB3	2.13	0.49
2:B:264:GLY:O	2:B:265:ILE:C	2.49	0.49
3:C:53:GLN:O	3:C:54:GLY:O	2.30	0.49
1:A:200:PRO:O	1:A:201:GLU:C	2.50	0.49
2:B:270:ILE:HD13	2:B:270:ILE:C	2.32	0.49
1:A:39:PHE:O	1:A:40:PHE:C	2.51	0.49
1:A:246:LEU:C	1:A:248:MET:N	2.65	0.49
1:A:250:ILE:O	1:A:252:GLY:N	2.46	0.49
6:A:850:BCL:H71	6:A:850:BCL:C2	2.33	0.49
1:A:229:ILE:HD12	8:A:857:U10:H4M1	1.95	0.49
2:B:204:LEU:O	2:B:207:ALA:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:PRO:CA	2:B:235:LEU:HD12	2.43	0.49
1:A:69:PRO:HG2	1:A:87:GLN:HE21	1.78	0.49
1:A:208:THR:C	1:A:210:ASP:N	2.66	0.48
2:B:265:ILE:O	2:B:268:TRP:CB	2.49	0.48
2:B:239:ALA:O	2:B:240:ASP:CB	2.61	0.48
1:A:2:LEU:HD22	1:A:6:GLU:HB3	1.95	0.48
1:A:44:LEU:HA	1:A:47:ILE:CD1	2.38	0.48
1:A:187:LEU:HB2	2:B:216:PHE:CD2	2.46	0.48
1:A:172:ALA:HB3	1:A:247:CYS:HB3	1.94	0.48
3:C:29:TYR:CD1	3:C:56:PHE:HE1	2.31	0.48
2:B:246:GLU:C	2:B:248:ALA:N	2.66	0.48
1:A:128:TYR:O	1:A:129:LEU:C	2.51	0.48
2:B:14:GLY:O	2:B:15:PRO:O	2.32	0.48
3:C:245:ALA:N	3:C:246:PRO:CD	2.76	0.48
1:A:231:ARG:O	1:A:232:LEU:C	2.52	0.48
2:B:159:VAL:HA	2:B:163:ILE:CB	2.26	0.48
2:B:186:THR:HG23	6:B:852:BCL:HMD2	1.95	0.48
2:B:202:HIS:O	2:B:206:ILE:HD12	2.14	0.48
2:B:271:TRP:O	2:B:272:MET:C	2.52	0.48
2:B:175:VAL:HG22	2:B:185:TRP:CD2	2.49	0.48
1:A:186:ALA:O	1:A:187:LEU:C	2.52	0.48
2:B:127:TRP:HZ2	2:B:154:ILE:HG21	1.78	0.48
2:B:159:VAL:CA	2:B:163:ILE:HB	2.25	0.48
2:B:204:LEU:O	2:B:205:SER:C	2.51	0.48
1:A:131:LEU:O	1:A:132:VAL:HG13	2.14	0.48
1:A:34:PHE:HA	1:A:37:ALA:HB3	1.95	0.48
1:A:234:LEU:O	1:A:237:SER:HB2	2.14	0.48
3:C:120:LEU:N	3:C:226:THR:HB	2.29	0.48
1:A:224:ILE:HG23	1:A:229:ILE:N	2.26	0.48
1:A:67:TYR:O	1:A:86:TRP:HB2	2.14	0.48
2:B:71:GLY:O	2:B:75:TRP:HD1	1.97	0.48
2:B:195:ASN:HB3	2:B:198:TYR:HD2	1.78	0.47
2:B:198:TYR:O	2:B:294:TRP:HE3	1.97	0.47
3:C:111:PRO:HB2	3:C:239:GLY:HA2	1.95	0.47
2:B:4:GLN:HA	2:B:4:GLN:OE1	2.14	0.47
3:C:22:ILE:C	3:C:24:LEU:H	2.17	0.47
2:B:90:PHE:CB	2:B:179:ILE:HD12	2.44	0.47
1:A:209:PRO:N	2:B:235:LEU:HD12	2.29	0.47
3:C:169:VAL:HG23	3:C:170:ASP:C	2.35	0.47
2:B:228:ARG:HG3	2:B:229:PHE:CD1	2.48	0.47
3:C:65:ILE:H	3:C:65:ILE:HD12	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:161:GLY:O	2:B:162:PHE:HB2	2.14	0.47
2:B:155:TRP:O	2:B:156:LEU:C	2.52	0.47
1:A:227:LEU:HD23	3:C:175:MET:SD	2.55	0.47
2:B:248:ALA:O	2:B:250:LEU:N	2.47	0.47
3:C:65:ILE:O	3:C:66:LEU:O	2.33	0.47
2:B:116:LEU:C	2:B:118:ALA:N	2.68	0.47
3:C:103:ASP:O	3:C:107:ASP:OD2	2.31	0.47
1:A:172:ALA:O	1:A:247:CYS:HB3	2.13	0.47
1:A:163:THR:O	1:A:163:THR:CG2	2.61	0.47
2:B:242:GLY:O	2:B:244:ALA:N	2.47	0.47
1:A:46:ILE:HA	1:A:49:ILE:HB	1.96	0.47
1:A:208:THR:HB	1:A:209:PRO:HD2	1.96	0.47
2:B:199:ASN:HA	2:B:294:TRP:HZ3	1.80	0.47
3:C:17:ILE:O	3:C:17:ILE:HG13	2.14	0.47
3:C:104:PRO:HA	3:C:109:VAL:HG22	1.97	0.47
1:A:127:ALA:HB1	6:A:851:BCL:H12	1.96	0.47
1:A:187:LEU:HD13	2:B:216:PHE:CG	2.49	0.47
2:B:269:ALA:HA	2:B:272:MET:CB	2.44	0.47
2:B:90:PHE:O	2:B:92:PHE:N	2.47	0.47
3:C:17:ILE:HG23	3:C:18:TYR:CD1	2.50	0.47
2:B:256:MET:CE	2:B:258:PHE:HE2	2.28	0.47
2:B:32:VAL:CG1	2:B:33:GLY:H	2.11	0.47
3:C:66:LEU:HB3	3:C:67:PRO:HD2	1.96	0.47
3:C:37:ARG:HG2	3:C:76:PRO:HD3	1.96	0.47
3:C:143:SER:O	3:C:144:ALA:CB	2.63	0.47
1:A:141:ALA:O	1:A:142:TRP:C	2.53	0.47
3:C:134:MET:C	3:C:136:ALA:N	2.68	0.47
1:A:100:TRP:NE1	7:A:855:BPH:HAA2	2.30	0.47
1:A:123:PHE:CE2	1:A:238:LEU:HB3	2.49	0.47
2:B:208:PHE:C	2:B:210:TYR:N	2.68	0.47
7:A:855:BPH:HMB2	6:B:853:BCL:H2	1.97	0.47
3:C:75:VAL:HA	3:C:76:PRO:C	2.30	0.47
1:A:279:ILE:HG22	1:A:279:ILE:O	2.15	0.47
2:B:171:TRP:CE3	2:B:171:TRP:HA	2.50	0.47
1:A:195:LEU:HD11	2:B:267:ARG:N	2.29	0.47
1:A:117:ILE:HG12	2:B:221:ALA:HB1	1.96	0.47
2:B:153:ALA:O	2:B:154:ILE:C	2.52	0.47
2:B:273:ALA:C	2:B:275:LEU:N	2.68	0.47
2:B:291:VAL:HG12	2:B:293:ASN:O	2.15	0.47
1:A:41:PHE:CE2	1:A:95:GLY:HA3	2.50	0.47
3:C:245:ALA:N	3:C:246:PRO:HD3	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:268:TRP:CE3	2:B:268:TRP:HA	2.50	0.46
2:B:280:GLY:HA2	6:B:852:BCL:CED	2.45	0.46
2:B:282:ILE:O	2:B:284:ILE:N	2.48	0.46
2:B:150:PHE:CA	7:B:854:BPH:HMD3	2.44	0.46
1:A:12:PRO:HG3	3:C:97:PRO:HB2	1.96	0.46
2:B:251:PHE:C	2:B:251:PHE:CD1	2.88	0.46
2:B:256:MET:HE1	8:B:856:U10:C16	2.46	0.46
2:B:36:SER:C	2:B:38:LEU:H	2.18	0.46
3:C:156:CYS:SG	3:C:248:ARG:NH1	2.88	0.46
1:A:267:VAL:HG23	2:B:87:ARG:HG2	1.97	0.46
2:B:25:ASN:ND2	2:B:28:ASN:ND2	2.64	0.46
1:A:271:TRP:HD1	1:A:271:TRP:H	1.56	0.46
1:A:187:LEU:N	2:B:216:PHE:CE2	2.83	0.46
1:A:54:VAL:C	1:A:56:GLN:N	2.68	0.46
3:C:195:MET:HA	3:C:195:MET:HE2	1.96	0.46
1:A:70:ALA:O	1:A:72:GLU:N	2.48	0.46
3:C:203:VAL:HG12	3:C:204:HIS:N	2.30	0.46
2:B:129:TRP:HD1	2:B:150:PHE:CE2	2.31	0.46
2:B:90:PHE:HA	2:B:179:ILE:CG1	2.44	0.46
2:B:190:SER:CB	6:B:852:BCL:HBC3	2.45	0.46
2:B:38:LEU:HD12	2:B:41:TRP:CD1	2.51	0.46
1:A:209:PRO:HG2	3:C:130:LYS:HE2	1.97	0.46
1:A:156:TRP:CE3	1:A:157:VAL:HG23	2.50	0.46
2:B:229:PHE:HB3	2:B:243:THR:CG2	2.45	0.46
2:B:237:GLN:HE22	3:C:117:ARG:NH1	2.13	0.46
2:B:242:GLY:HA2	3:C:117:ARG:HD2	1.97	0.46
1:A:137:VAL:O	1:A:137:VAL:HG12	2.15	0.46
1:A:175:ILE:HG22	1:A:243:PHE:CD1	2.51	0.46
2:B:34:PRO:C	2:B:47:LEU:HD12	2.36	0.46
2:B:34:PRO:O	2:B:47:LEU:HD12	2.15	0.46
3:C:37:ARG:HH11	3:C:37:ARG:HG2	1.79	0.46
2:B:125:ALA:O	7:B:854:BPH:H1C2	2.15	0.46
3:C:36:MET:HG2	3:C:40:TYR:CD1	2.51	0.46
3:C:233:ILE:O	3:C:237:VAL:HG23	2.15	0.46
1:A:178:SER:HA	1:A:181:PHE:HD2	1.79	0.46
1:A:171:PRO:HD2	1:A:259:TRP:CE3	2.51	0.46
2:B:268:TRP:NE1	8:B:856:U10:H101	2.29	0.46
3:C:173:GLU:O	3:C:175:MET:N	2.48	0.46
1:A:113:ILE:CB	2:B:226:VAL:HG12	2.44	0.46
1:A:226:THR:O	1:A:229:ILE:HG23	2.15	0.46
1:A:246:LEU:O	1:A:248:MET:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:198:VAL:HG12	3:C:199:GLN:N	2.31	0.46
2:B:219:HIS:NE2	2:B:223:ILE:HG13	2.30	0.46
2:B:122:MET:SD	2:B:157:TRP:CZ2	3.07	0.46
3:C:129:ASN:HD22	3:C:224:GLU:HB2	1.80	0.46
2:B:171:TRP:HE3	2:B:171:TRP:HA	1.80	0.46
3:C:22:ILE:C	3:C:24:LEU:N	2.70	0.46
1:A:125:ILE:HG22	1:A:126:LEU:HD12	1.98	0.46
2:B:280:GLY:O	2:B:281:GLY:C	2.54	0.45
2:B:5:ASN:HD22	2:B:5:ASN:C	2.18	0.45
1:A:56:GLN:NE2	1:A:64:ILE:HA	2.31	0.45
3:C:235:GLY:O	3:C:236:TYR:C	2.53	0.45
2:B:258:PHE:N	2:B:258:PHE:CD2	2.83	0.45
1:A:34:PHE:CE2	1:A:102:LEU:HB3	2.51	0.45
1:A:255:TRP:NE1	1:A:257:ASP:O	2.50	0.45
6:B:852:BCL:HAA2	6:B:852:BCL:HBD	1.98	0.45
1:A:175:ILE:HG22	1:A:243:PHE:CE1	2.51	0.45
2:B:203:GLY:HA2	6:B:853:BCL:O1D	2.17	0.45
1:A:230:HIS:HD2	2:B:223:ILE:HG13	1.81	0.45
2:B:242:GLY:HA2	3:C:115:VAL:HG21	1.98	0.45
1:A:2:LEU:HD21	1:A:10:ARG:CZ	2.46	0.45
1:A:271:TRP:CD1	1:A:271:TRP:N	2.79	0.45
7:A:855:BPH:H112	7:A:855:BPH:H7C1	1.77	0.45
2:B:190:SER:HB3	6:B:852:BCL:HBC3	1.99	0.45
1:A:90:THR:HG23	1:A:148:TYR:OH	2.16	0.45
1:A:51:TRP:CD1	1:A:51:TRP:C	2.90	0.45
1:A:264:GLN:C	1:A:266:TRP:N	2.66	0.45
3:C:37:ARG:NH1	3:C:37:ARG:HG2	2.32	0.45
1:A:229:ILE:C	1:A:231:ARG:H	2.20	0.45
7:A:855:BPH:HBB2	7:A:855:BPH:HH C	1.98	0.45
2:B:55:LEU:HB3	2:B:132:ARG:HD2	1.99	0.45
2:B:60:LEU:HD12	7:B:854:BPH:C5	2.46	0.45
3:C:173:GLU:O	3:C:174:GLN:C	2.55	0.45
2:B:240:ASP:O	2:B:241:ARG:O	2.34	0.45
1:A:116:HIS:CB	2:B:221:ALA:O	2.61	0.45
1:A:121:PHE:C	1:A:123:PHE:H	2.20	0.45
1:A:139:MET:CE	1:A:252:GLY:HA3	2.46	0.45
2:B:260:ALA:O	8:B:856:U10:H4M3	2.15	0.45
2:B:264:GLY:O	2:B:267:ARG:N	2.50	0.45
8:B:856:U10:H1M1	8:B:856:U10:H71	1.76	0.45
2:B:91:PHE:HD1	2:B:91:PHE:H	1.60	0.45
2:B:182:HIS:O	2:B:185:TRP:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:189:ARG:HD3	3:C:218:THR:HG23	1.98	0.45
1:A:162:TYR:C	1:A:164:TYR:H	2.20	0.45
1:A:172:ALA:HB3	1:A:247:CYS:CB	2.47	0.45
1:A:250:ILE:CG1	1:A:251:THR:N	2.78	0.45
2:B:17:ASP:OD2	3:C:172:PRO:HB3	2.17	0.45
1:A:113:ILE:HG22	2:B:229:PHE:HE2	1.82	0.45
1:A:274:ASN:O	1:A:275:ILE:O	2.35	0.45
2:B:265:ILE:HG12	8:B:856:U10:C2	2.47	0.45
1:A:126:LEU:C	1:A:128:TYR:N	2.68	0.45
1:A:117:ILE:N	1:A:118:PRO:HD2	2.31	0.45
1:A:26:VAL:HG12	1:A:26:VAL:O	2.16	0.45
2:B:215:LEU:HD23	2:B:269:ALA:CB	2.47	0.45
8:B:856:U10:H222	8:B:856:U10:H201	1.64	0.45
3:C:191:LEU:HA	3:C:192:PRO:HD3	1.57	0.45
1:A:116:HIS:CE1	2:B:225:ALA:HA	2.52	0.45
3:C:44:ASN:ND2	3:C:50:ALA:HA	2.32	0.45
3:C:14:SER:O	3:C:17:ILE:CG2	2.63	0.44
3:C:27:LEU:O	3:C:29:TYR:N	2.50	0.44
1:A:157:VAL:O	1:A:158:SER:C	2.55	0.44
3:C:115:VAL:CG1	3:C:117:ARG:HG3	2.47	0.44
1:A:266:TRP:C	1:A:266:TRP:CD1	2.89	0.44
1:A:199:ASN:N	1:A:200:PRO:CD	2.80	0.44
1:A:139:MET:HG3	1:A:253:THR:HG22	1.99	0.44
1:A:174:MET:HB2	6:A:850:BCL:CGD	2.48	0.44
1:A:244:SER:HB3	6:A:851:BCL:O1D	2.16	0.44
2:B:130:TRP:CD1	2:B:154:ILE:HD11	2.52	0.44
3:C:27:LEU:O	3:C:28:ILE:C	2.54	0.44
1:A:69:PRO:HG3	1:A:83:GLY:HA3	1.98	0.44
3:C:122:GLU:N	3:C:227:LEU:HD21	2.33	0.44
3:C:37:ARG:HA	3:C:76:PRO:HB3	1.99	0.44
1:A:203:GLY:O	1:A:204:LYS:O	2.36	0.44
2:B:290:VAL:O	2:B:290:VAL:HG12	2.18	0.44
2:B:256:MET:HE3	2:B:258:PHE:HE2	1.82	0.44
1:A:85:LEU:O	1:A:86:TRP:C	2.55	0.44
3:C:171:ILE:O	3:C:174:GLN:N	2.51	0.44
2:B:248:ALA:C	2:B:250:LEU:N	2.70	0.44
3:C:69:GLY:O	3:C:71:GLY:N	2.45	0.44
2:B:258:PHE:O	2:B:259:ASN:HB3	2.18	0.44
6:A:850:BCL:H172	7:B:854:BPH:HMB3	2.00	0.44
1:A:83:GLY:O	1:A:84:GLY:C	2.56	0.44
1:A:128:TYR:O	1:A:131:LEU:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:PRO:O	1:A:150:ILE:HD12	2.18	0.44
2:B:256:MET:CE	2:B:258:PHE:CE2	3.00	0.44
2:B:229:PHE:HZ	3:C:238:ALA:HB2	1.75	0.44
3:C:212:LEU:N	3:C:212:LEU:HD23	2.33	0.44
1:A:185:LEU:HA	1:A:188:ALA:HB3	2.00	0.44
1:A:190:HIS:NE2	1:A:230:HIS:HE1	2.15	0.44
2:B:4:GLN:HB3	2:B:6:ILE:HD11	1.99	0.44
1:A:157:VAL:C	1:A:159:ASN:N	2.71	0.44
1:A:105:VAL:C	1:A:107:ILE:N	2.70	0.44
2:B:97:PRO:O	2:B:98:ALA:O	2.36	0.44
2:B:266:HIS:O	2:B:267:ARG:C	2.55	0.44
2:B:38:LEU:O	2:B:40:GLY:N	2.50	0.44
1:A:116:HIS:CD2	2:B:224:LEU:HB3	2.52	0.44
1:A:37:ALA:C	1:A:39:PHE:N	2.71	0.44
2:B:119:SER:O	2:B:122:MET:HB3	2.17	0.44
1:A:249:ILE:HD13	1:A:249:ILE:O	2.18	0.44
1:A:174:MET:HB2	6:A:850:BCL:O1D	2.18	0.43
2:B:232:GLU:HG3	3:C:177:ARG:HH12	1.82	0.43
1:A:153:HIS:O	1:A:156:TRP:HB3	2.18	0.43
3:C:115:VAL:CG2	3:C:231:ASP:OD2	2.66	0.43
1:A:187:LEU:N	2:B:216:PHE:HE2	2.16	0.43
2:B:222:THR:O	2:B:223:ILE:C	2.57	0.43
1:A:146:PHE:HB2	1:A:147:PRO:HD2	2.00	0.43
1:A:112:GLY:O	1:A:113:ILE:O	2.35	0.43
2:B:240:ASP:O	2:B:241:ARG:C	2.55	0.43
3:C:66:LEU:HD13	3:C:118:ARG:HH12	1.83	0.43
1:A:115:TYR:O	1:A:118:PRO:HD2	2.18	0.43
2:B:57:VAL:O	2:B:58:LEU:C	2.56	0.43
1:A:267:VAL:HG23	2:B:87:ARG:CG	2.48	0.43
2:B:227:SER:O	2:B:229:PHE:N	2.51	0.43
3:C:227:LEU:O	3:C:230:GLU:HB2	2.17	0.43
1:A:122:ALA:CA	1:A:125:ILE:HB	2.41	0.43
1:A:2:LEU:HD23	1:A:6:GLU:OE2	2.17	0.43
1:A:142:TRP:O	1:A:143:GLY:C	2.56	0.43
3:C:154:ARG:HG2	3:C:155:GLY:N	2.33	0.43
1:A:235:LEU:C	1:A:237:SER:N	2.69	0.43
2:B:282:ILE:O	2:B:283:GLY:C	2.57	0.43
1:A:209:PRO:CG	3:C:130:LYS:HE2	2.49	0.43
3:C:235:GLY:O	3:C:238:ALA:HB3	2.18	0.43
1:A:34:PHE:CE1	1:A:102:LEU:HD13	2.53	0.43
2:B:209:LEU:O	2:B:209:LEU:HD12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:206:ILE:HD12	6:B:853:BCL:OBD	2.18	0.43
2:B:273:ALA:O	2:B:274:VAL:C	2.57	0.43
2:B:291:VAL:CG1	2:B:293:ASN:O	2.67	0.43
6:A:850:BCL:HBC1	6:B:852:BCL:HAA2	1.99	0.43
3:C:29:TYR:O	3:C:30:TYR:C	2.57	0.43
2:B:238:ILE:HG22	2:B:239:ALA:N	2.33	0.43
1:A:196:SER:HB2	2:B:143:GLY:O	2.19	0.43
2:B:268:TRP:CE2	8:B:856:U10:H122	2.54	0.43
2:B:226:VAL:O	2:B:227:SER:C	2.56	0.43
3:C:120:LEU:O	3:C:227:LEU:HG	2.19	0.43
3:C:192:PRO:HG2	3:C:237:VAL:HG21	2.00	0.43
3:C:229:GLU:O	3:C:233:ILE:HG13	2.19	0.43
1:A:2:LEU:O	3:C:42:LEU:HA	2.19	0.43
1:A:41:PHE:HD2	1:A:95:GLY:C	2.22	0.43
3:C:245:ALA:H	3:C:246:PRO:HD3	1.82	0.43
1:A:219:LEU:HG	1:A:220:VAL:N	2.34	0.43
2:B:268:TRP:CZ2	8:B:856:U10:H122	2.53	0.43
2:B:293:ASN:OD1	2:B:294:TRP:N	2.52	0.43
3:C:230:GLU:O	3:C:234:CYS:SG	2.75	0.43
3:C:133:PRO:HG2	3:C:136:ALA:HB3	1.99	0.43
3:C:66:LEU:HB2	3:C:71:GLY:O	2.19	0.43
1:A:116:HIS:O	2:B:221:ALA:HB1	2.19	0.43
2:B:26:LEU:HD22	2:B:29:ARG:HG3	2.00	0.43
1:A:61:PRO:HB3	1:A:150:ILE:CD1	2.49	0.43
1:A:236:LEU:C	1:A:236:LEU:HD23	2.39	0.43
2:B:210:TYR:CD2	6:B:853:BCL:H11	2.54	0.43
3:C:20:PHE:C	3:C:22:ILE:H	2.18	0.43
1:A:65:SER:HB2	1:A:149:GLY:CA	2.49	0.43
2:B:240:ASP:O	3:C:117:ARG:HG2	2.18	0.43
1:A:255:TRP:CH2	1:A:262:TRP:HD1	2.37	0.43
1:A:255:TRP:CZ3	1:A:262:TRP:HD1	2.36	0.43
2:B:17:ASP:CG	3:C:126:HIS:HE1	2.22	0.42
2:B:204:LEU:O	2:B:207:ALA:N	2.52	0.42
1:A:68:PRO:HA	1:A:86:TRP:CG	2.54	0.42
2:B:242:GLY:C	3:C:115:VAL:HG21	2.39	0.42
2:B:25:ASN:HD22	2:B:28:ASN:ND2	2.09	0.42
1:A:49:ILE:O	1:A:53:ALA:HB2	2.19	0.42
2:B:7:PHE:HD1	2:B:41:TRP:HB3	1.84	0.42
3:C:202:ARG:HG2	3:C:202:ARG:HH11	1.84	0.42
2:B:136:ARG:HD3	2:B:136:ARG:HA	1.85	0.42
2:B:218:MET:HE3	2:B:252:TRP:CZ3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:MET:HE2	2:B:288:GLY:HA3	2.02	0.42
1:A:231:ARG:NH1	2:B:41:TRP:O	2.53	0.42
1:A:51:TRP:O	1:A:54:VAL:HG23	2.19	0.42
1:A:193:LEU:O	1:A:194:VAL:C	2.57	0.42
1:A:219:LEU:CD1	2:B:132:ARG:HH12	2.30	0.42
2:B:78:ALA:HA	2:B:84:VAL:HG11	2.01	0.42
3:C:171:ILE:C	3:C:173:GLU:H	2.22	0.42
3:C:96:PHE:HD2	3:C:97:PRO:HD2	1.84	0.42
1:A:171:PRO:HA	1:A:174:MET:HG2	2.00	0.42
1:A:219:LEU:HD12	2:B:132:ARG:NH1	2.35	0.42
2:B:206:ILE:HG21	6:B:853:BCL:CAD	2.50	0.42
7:A:855:BPH:HMC2	2:B:214:LEU:N	2.35	0.42
3:C:122:GLU:HB2	3:C:227:LEU:HD21	2.01	0.42
2:B:148:TRP:HA	2:B:148:TRP:HE3	1.85	0.42
1:A:99:SER:O	1:A:100:TRP:C	2.58	0.42
2:B:216:PHE:CD1	2:B:216:PHE:C	2.93	0.42
3:C:224:GLU:O	3:C:224:GLU:HG3	2.19	0.42
1:A:217:ARG:HH21	2:B:44:ASN:HD22	1.66	0.42
1:A:187:LEU:HD11	2:B:269:ALA:CB	2.50	0.42
1:A:226:THR:C	1:A:228:GLY:H	2.23	0.42
2:B:38:LEU:O	2:B:41:TRP:HD1	2.03	0.42
3:C:33:THR:OG1	3:C:34:GLU:N	2.52	0.42
1:A:64:ILE:O	1:A:65:SER:HB2	2.19	0.42
1:A:267:VAL:HA	2:B:87:ARG:HG3	2.01	0.42
3:C:69:GLY:C	3:C:71:GLY:N	2.73	0.42
1:A:114:GLY:HA3	2:B:225:ALA:CA	2.48	0.42
3:C:146:LYS:HG2	3:C:199:GLN:O	2.19	0.42
1:A:49:ILE:CG2	1:A:49:ILE:O	2.67	0.42
2:B:148:TRP:CE3	2:B:148:TRP:HA	2.55	0.42
2:B:191:LEU:C	2:B:193:HIS:N	2.72	0.42
2:B:211:GLY:O	2:B:213:ALA:N	2.52	0.42
2:B:268:TRP:CE3	3:C:31:LEU:HD13	2.55	0.42
1:A:65:SER:CB	1:A:149:GLY:CA	2.98	0.42
1:A:43:ALA:O	1:A:45:GLY:N	2.52	0.42
1:A:115:TYR:O	1:A:117:ILE:N	2.53	0.42
3:C:189:ARG:HH11	3:C:189:ARG:HG2	1.84	0.42
1:A:79:PRO:C	1:A:81:ALA:H	2.24	0.42
1:A:47:ILE:HG22	1:A:48:LEU:HD23	2.02	0.42
2:B:8:SER:C	2:B:10:VAL:N	2.73	0.42
1:A:174:MET:HA	1:A:177:ILE:CD1	2.50	0.41
1:A:229:ILE:O	1:A:232:LEU:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:233:ARG:HG3	2:B:233:ARG:H	1.54	0.41
2:B:268:TRP:HB3	2:B:269:ALA:H	1.59	0.41
2:B:280:GLY:O	2:B:282:ILE:N	2.53	0.41
3:C:174:GLN:H	3:C:174:GLN:HG2	1.56	0.41
3:C:103:ASP:HA	3:C:104:PRO:HD2	1.80	0.41
1:A:229:ILE:O	1:A:231:ARG:N	2.54	0.41
2:B:41:TRP:N	2:B:41:TRP:CD1	2.84	0.41
3:C:157:ASP:OD1	3:C:209:SER:HB2	2.20	0.41
1:A:56:GLN:HE22	1:A:65:SER:N	2.18	0.41
3:C:70:ARG:HE	3:C:123:LEU:HD11	1.84	0.41
2:B:24:VAL:HG12	2:B:25:ASN:N	2.34	0.41
1:A:7:ARG:O	1:A:9:TYR:N	2.47	0.41
1:A:185:LEU:CA	1:A:188:ALA:HB3	2.50	0.41
2:B:132:ARG:C	2:B:134:TYR:N	2.74	0.41
2:B:189:PHE:C	2:B:191:LEU:N	2.72	0.41
1:A:263:TRP:HZ3	2:B:90:PHE:CE2	2.37	0.41
1:A:159:ASN:O	1:A:160:THR:C	2.59	0.41
1:A:265:TRP:CD1	1:A:266:TRP:HB2	2.55	0.41
2:B:13:ARG:HG2	2:B:14:GLY:N	2.35	0.41
1:A:9:TYR:CE1	3:C:113:SER:CB	3.03	0.41
1:A:9:TYR:HE1	3:C:113:SER:HB2	1.84	0.41
1:A:220:VAL:HG23	1:A:222:TYR:N	2.34	0.41
2:B:163:ILE:HG22	2:B:164:ARG:N	2.35	0.41
2:B:59:SER:OG	2:B:129:TRP:HE3	2.03	0.41
3:C:175:MET:O	3:C:177:ARG:HG3	2.20	0.41
2:B:154:ILE:HG22	2:B:158:MET:CG	2.42	0.41
7:A:855:BPH:ND	2:B:214:LEU:HD13	2.35	0.41
2:B:232:GLU:HG2	2:B:233:ARG:HG3	2.02	0.41
2:B:258:PHE:N	2:B:258:PHE:HD2	2.18	0.41
2:B:46:GLN:HG2	2:B:47:LEU:H	1.85	0.41
1:A:87:GLN:O	1:A:89:ILE:N	2.54	0.41
2:B:239:ALA:HB1	3:C:66:LEU:HD21	2.02	0.41
3:C:176:ALA:HB1	3:C:193:MET:SD	2.60	0.41
1:A:196:SER:CA	2:B:145:HIS:HB2	2.50	0.41
2:B:94:LEU:HG	2:B:94:LEU:O	2.21	0.41
1:A:227:LEU:HD13	2:B:232:GLU:CB	2.31	0.41
1:A:180:PHE:CG	1:A:240:ALA:HB1	2.51	0.41
3:C:20:PHE:C	3:C:22:ILE:N	2.72	0.41
1:A:147:PRO:C	1:A:149:GLY:H	2.24	0.41
1:A:147:PRO:O	1:A:153:HIS:HB3	2.20	0.41
2:B:229:PHE:CZ	3:C:238:ALA:CB	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:66:LEU:HD13	3:C:118:ARG:HH22	1.85	0.41
2:B:175:VAL:HG22	2:B:185:TRP:CE2	2.55	0.41
2:B:158:MET:O	2:B:163:ILE:HG12	2.21	0.41
2:B:208:PHE:HB3	2:B:276:VAL:CG2	2.35	0.41
2:B:287:SER:HG	2:B:294:TRP:HE1	1.67	0.41
3:C:17:ILE:O	3:C:17:ILE:CG1	2.68	0.41
1:A:85:LEU:C	1:A:87:GLN:N	2.72	0.41
1:A:147:PRO:O	1:A:149:GLY:N	2.46	0.41
2:B:8:SER:O	2:B:10:VAL:N	2.54	0.41
6:A:850:BCL:H11	7:B:854:BPH:HBB2	2.03	0.41
2:B:285:LEU:O	2:B:285:LEU:HD12	2.21	0.41
3:C:124:ASP:N	3:C:130:LYS:HB2	2.36	0.41
2:B:229:PHE:HZ	3:C:238:ALA:CB	2.34	0.41
1:A:254:ILE:HD12	1:A:255:TRP:N	2.36	0.41
1:A:62:GLN:HG2	1:A:151:TRP:NE1	2.36	0.41
1:A:173:HIS:O	1:A:177:ILE:N	2.51	0.41
2:B:57:VAL:O	2:B:59:SER:N	2.54	0.41
1:A:212:GLU:O	1:A:213:ASP:C	2.59	0.41
7:B:854:BPH:HMB1	7:B:854:BPH:HHB	1.78	0.41
2:B:238:ILE:HD11	2:B:263:GLU:HA	2.02	0.41
3:C:70:ARG:HE	3:C:123:LEU:CD1	2.34	0.41
3:C:238:ALA:O	3:C:239:GLY:C	2.60	0.41
3:C:96:PHE:CD2	3:C:97:PRO:HD2	2.56	0.41
1:A:192:ALA:HB1	2:B:146:THR:HA	2.01	0.41
1:A:34:PHE:HB2	1:A:103:ARG:HB2	2.02	0.41
3:C:182:GLU:CD	3:C:186:GLY:HA2	2.41	0.41
2:B:138:GLN:C	2:B:140:LEU:N	2.74	0.41
1:A:208:THR:OG1	1:A:210:ASP:CB	2.69	0.41
1:A:164:TYR:CE2	1:A:251:THR:HG22	2.56	0.41
1:A:100:TRP:CG	7:A:855:BPH:O1A	2.74	0.41
2:B:216:PHE:HD1	2:B:216:PHE:C	2.24	0.41
1:A:147:PRO:HD2	1:A:156:TRP:HB2	2.02	0.41
2:B:13:ARG:CG	2:B:14:GLY:N	2.83	0.41
3:C:135:LYS:NZ	3:C:166:ASP:CB	2.84	0.41
2:B:216:PHE:C	2:B:218:MET:H	2.25	0.40
2:B:13:ARG:HD3	2:B:35:PHE:CD2	2.56	0.40
1:A:31:VAL:HG12	1:A:32:GLY:O	2.21	0.40
1:A:178:SER:C	1:A:180:PHE:N	2.73	0.40
2:B:6:ILE:HD13	2:B:6:ILE:N	2.36	0.40
1:A:24:PHE:CD1	1:A:24:PHE:C	2.94	0.40
1:A:184:ALA:CB	7:B:854:BPH:HMC3	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:THR:O	1:A:227:LEU:C	2.60	0.40
2:B:90:PHE:CD2	2:B:179:ILE:HD13	2.57	0.40
2:B:187:ASN:C	2:B:189:PHE:H	2.25	0.40
2:B:101:TYR:OH	2:B:108:PRO:HD2	2.21	0.40
1:A:121:PHE:O	1:A:123:PHE:N	2.55	0.40
1:A:195:LEU:O	1:A:197:ALA:N	2.55	0.40
2:B:151:LEU:HA	2:B:154:ILE:HD12	2.04	0.40
2:B:293:ASN:C	2:B:293:ASN:OD1	2.59	0.40
1:A:86:TRP:O	1:A:89:ILE:HG22	2.21	0.40
1:A:64:ILE:HD13	1:A:64:ILE:HA	1.95	0.40
1:A:109:ARG:HG2	1:A:109:ARG:NH1	2.34	0.40
1:A:133:LEU:O	1:A:137:VAL:HG23	2.21	0.40
1:A:117:ILE:HA	2:B:221:ALA:HB1	2.03	0.40
2:B:66:TRP:NE1	2:B:122:MET:HB2	2.37	0.40
1:A:213:ASP:OD1	1:A:213:ASP:N	2.46	0.40
1:A:223:SER:OG	8:A:857:U10:H3M3	2.22	0.40
1:A:190:HIS:CG	1:A:229:ILE:CD1	3.04	0.40
2:B:153:ALA:O	2:B:155:TRP:N	2.55	0.40
2:B:201:PHE:HB3	2:B:283:GLY:HA3	2.04	0.40
2:B:235:LEU:HA	2:B:235:LEU:HD23	1.79	0.40
3:C:148:PRO:O	3:C:151:LEU:HG	2.22	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	A	279/281 (99%)	149 (53%)	76 (27%)	54 (19%)	0	3
2	B	300/307 (98%)	164 (55%)	84 (28%)	52 (17%)	0	4
3	C	236/260 (91%)	144 (61%)	60 (25%)	32 (14%)	0	7
All	All	815/848 (96%)	457 (56%)	220 (27%)	138 (17%)	0	5

All (138) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	LYS
1	A	21	LEU
1	A	73	TYR
1	A	113	ILE
1	A	143	GLY
1	A	145	ALA
1	A	160	THR
1	A	204	LYS
1	A	212	GLU
1	A	239	SER
1	A	240	ALA
1	A	251	THR
1	A	275	ILE
2	B	5	ASN
2	B	15	PRO
2	B	17	ASP
2	B	18	LEU
2	B	49	PRO
2	B	57	VAL
2	B	98	ALA
2	B	109	LEU
2	B	223	ILE
2	B	232	GLU
2	B	240	ASP
2	B	241	ARG
2	B	244	ALA
2	B	248	ALA
2	B	268	TRP
3	C	30	TYR
3	C	44	ASN
3	C	51	ALA
3	C	54	GLY
3	C	59	PRO
3	C	66	LEU
3	C	78	PRO
3	C	82	ASP
3	C	89	ARG
3	C	96	PHE
3	C	149	ILE
3	C	171	ILE
3	C	219	ILE
3	C	221	SER

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Mol	Chain	Res	Type
1	A	10	ARG
1	A	65	SER
1	A	71	LEU
1	A	72	GLU
1	A	80	LEU
1	A	84	GLY
1	A	86	TRP
1	A	116	HIS
1	A	159	ASN
1	A	230	HIS
1	A	238	LEU
1	A	245	ALA
1	A	247	CYS
1	A	280	ASN
2	B	32	VAL
2	B	50	ILE
2	B	58	LEU
2	B	59	SER
2	B	87	ARG
2	B	91	PHE
2	B	117	ILE
2	B	155	TRP
2	B	162	PHE
2	B	163	ILE
2	B	215	LEU
2	B	228	ARG
2	B	265	ILE
2	B	274	VAL
2	B	283	GLY
3	C	19	SER
3	C	144	ALA
3	C	174	GLN
3	C	193	MET
3	C	239	GLY
1	A	26	VAL
1	A	77	GLY
1	A	122	ALA
1	A	131	LEU
1	A	132	VAL
1	A	233	GLY
2	B	34	PRO
2	B	65	MET

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Mol	Chain	Res	Type
2	B	69	THR
2	B	90	PHE
2	B	247	ARG
2	B	297	TRP
3	C	12	LEU
3	C	32	GLN
3	C	55	PRO
3	C	61	PRO
3	C	70	ARG
3	C	172	PRO
3	C	195	MET
1	A	118	PRO
1	A	129	LEU
1	A	179	PHE
1	A	201	GLU
1	A	234	LEU
1	A	272	TRP
2	B	41	TRP
2	B	222	THR
2	B	235	LEU
2	B	246	GLU
2	B	249	ALA
2	B	267	ARG
2	B	287	SER
3	C	194	GLN
1	A	70	ALA
1	A	134	PHE
1	A	163	THR
1	A	236	LEU
1	A	270	PRO
2	B	9	GLN
2	B	179	ILE
2	B	245	ALA
2	B	259	ASN
2	B	296	VAL
3	C	47	GLY
3	C	183	LEU
1	A	117	ILE
1	A	211	HIS
1	A	224	ILE
2	B	272	MET
3	C	57	PRO

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Mol	Chain	Res	Type
3	C	210	SER
1	A	13	GLY
1	A	140	GLY
1	A	228	GLY
1	A	229	ILE
1	A	78	ALA
1	A	88	ILE
2	B	291	VAL
3	C	237	VAL
2	B	192	VAL
2	B	281	GLY
1	A	135	ARG

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%)	197 (90%)	23 (10%)	8	39
2	B	236/240 (98%)	203 (86%)	33 (14%)	4	28
3	C	193/208 (93%)	176 (91%)	17 (9%)	12	48
All	All	649/668 (97%)	576 (89%)	73 (11%)	7	37

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	54	VAL
1	A	72	GLU
1	A	123	PHE
1	A	152	THR
1	A	180	PHE
1	A	183	ASN
1	A	185	LEU
1	A	207	ARG
1	A	210	ASP

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Mol	Chain	Res	Type
1	A	213	ASP
1	A	218	ASP
1	A	229	ILE
1	A	243	PHE
1	A	249	ILE
1	A	256	PHE
1	A	260	VAL
1	A	261	ASP
1	A	265	TRP
1	A	269	LEU
1	A	270	PRO
1	A	271	TRP
1	A	272	TRP
2	B	5	ASN
2	B	18	LEU
2	B	50	ILE
2	B	68	PHE
2	B	72	ILE
2	B	74	PHE
2	B	90	PHE
2	B	148	TRP
2	B	155	TRP
2	B	160	LEU
2	B	166	ILE
2	B	171	TRP
2	B	172	SER
2	B	182	HIS
2	B	188	ASN
2	B	190	SER
2	B	196	LEU
2	B	209	LEU
2	B	214	LEU
2	B	216	PHE
2	B	233	ARG
2	B	236	GLU
2	B	238	ILE
2	B	240	ASP
2	B	250	LEU
2	B	251	PHE
2	B	258	PHE
2	B	262	MET
2	B	268	TRP

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Mol	Chain	Res	Type
2	B	270	ILE
2	B	289	THR
2	B	292	ASP
2	B	297	TRP
3	C	22	ILE
3	C	23	PHE
3	C	46	ASP
3	C	65	ILE
3	C	157	ASP
3	C	169	VAL
3	C	174	GLN
3	C	193	MET
3	C	195	MET
3	C	206	ASN
3	C	211	ASP
3	C	218	THR
3	C	221	SER
3	C	226	THR
3	C	231	ASP
3	C	233	ILE
3	C	236	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	87	GLN
1	A	280	ASN
2	B	5	ASN
2	B	11	GLN
2	B	28	ASN
2	B	44	ASN
2	B	145	HIS
2	B	188	ASN
3	C	126	HIS
3	C	204	HIS
3	C	206	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 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	2	53,74,74	1.75	9 (16%)	57,115,115	2.13	17 (29%)
6	BCL	A	851	1	53,74,74	1.40	9 (16%)	57,115,115	1.72	10 (17%)
7	BPH	A	855	-	64,70,70	1.32	8 (12%)	73,101,101	1.75	14 (19%)
8	U10	A	857	-	48,48,63	2.63	16 (33%)	58,61,79	2.09	19 (32%)
6	BCL	B	852	2	53,74,74	1.36	5 (9%)	57,115,115	1.71	10 (17%)
6	BCL	B	853	1	53,74,74	1.42	9 (16%)	57,115,115	1.90	11 (19%)
7	BPH	B	854	-	64,70,70	1.44	6 (9%)	73,101,101	1.69	12 (16%)
8	U10	B	856	-	48,48,63	2.26	14 (29%)	58,61,79	2.21	21 (36%)

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	2	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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 (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	856	U10	C7-C8	-4.08	1.44	1.50
7	A	855	BPH	C3D-CAD	-2.82	1.41	1.46
8	A	857	U10	C7-C8	-2.60	1.46	1.50
7	B	854	BPH	C3D-CAD	-2.47	1.41	1.46
6	B	853	BCL	C3C-C4C	-2.42	1.48	1.51
6	A	850	BCL	O2D-CGD	-2.39	1.27	1.33
6	B	853	BCL	O2D-CGD	-2.23	1.27	1.33
6	B	853	BCL	CHD-C4C	-2.23	1.34	1.41
6	B	853	BCL	C3D-CAD	-2.12	1.39	1.45
6	B	852	BCL	CHD-C4C	-2.11	1.35	1.41
6	A	851	BCL	O2D-CGD	-2.05	1.27	1.33
8	B	856	U10	C22-C23	-2.01	1.44	1.50
8	A	857	U10	C30-C29	2.01	1.55	1.50
8	A	857	U10	O3-C3	2.02	1.42	1.37
7	A	855	BPH	CBB-CAB	2.04	1.54	1.50
6	A	851	BCL	CBB-CAB	2.11	1.56	1.49
7	A	855	BPH	C3B-CAB	2.30	1.54	1.46
8	B	856	U10	C8-C9	2.35	1.37	1.33
6	A	850	BCL	C3D-C2D	2.36	1.45	1.40
6	A	851	BCL	OBD-CAD	2.38	1.26	1.22
7	A	855	BPH	CMD-C2D	2.40	1.56	1.51
8	A	857	U10	C1M-C1	2.43	1.56	1.50
6	B	852	BCL	CMB-C2B	2.47	1.56	1.51
8	B	856	U10	O4-C4	2.47	1.43	1.37
6	A	851	BCL	CMB-C2B	2.50	1.56	1.51
6	B	852	BCL	C3B-C2B	2.56	1.46	1.40
7	B	854	BPH	C3B-CAB	2.60	1.55	1.46
6	A	851	BCL	CMD-C2D	2.63	1.57	1.51
6	B	853	BCL	CMB-C2B	2.70	1.57	1.51
7	A	855	BPH	C3D-C2D	2.75	1.46	1.40
8	B	856	U10	C38-C39	2.77	1.40	1.32
6	A	850	BCL	CMB-C2B	2.80	1.57	1.51
6	A	850	BCL	CBA-CGA	2.81	1.59	1.50
8	A	857	U10	O4-C4	2.88	1.44	1.37
6	B	853	BCL	C3D-C2D	2.95	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	856	U10	C6-C5	3.07	1.55	1.46
7	A	855	BPH	C3B-C2B	3.08	1.47	1.38
7	B	854	BPH	CMB-C2B	3.10	1.57	1.50
6	A	850	BCL	C3B-C2B	3.18	1.47	1.40
8	B	856	U10	C13-C14	3.23	1.39	1.33
6	A	850	BCL	C3B-CAB	3.26	1.57	1.49
8	A	857	U10	C38-C39	3.26	1.42	1.32
6	A	851	BCL	C3B-C2B	3.29	1.48	1.40
6	B	853	BCL	C3B-CAB	3.32	1.58	1.49
8	A	857	U10	C6-C5	3.33	1.56	1.46
6	A	851	BCL	C3D-C2D	3.35	1.48	1.40
8	B	856	U10	C7-C6	3.36	1.57	1.51
8	A	857	U10	C8-C9	3.37	1.39	1.33
6	A	851	BCL	C3B-CAB	3.37	1.58	1.49
7	B	854	BPH	C3B-C2B	3.37	1.48	1.38
7	B	854	BPH	C3D-C2D	3.38	1.48	1.40
6	B	853	BCL	C2-C3	3.50	1.39	1.33
6	B	853	BCL	C3B-C2B	3.66	1.48	1.40
8	B	856	U10	C18-C19	3.66	1.40	1.33
7	A	855	BPH	CMB-C2B	3.69	1.58	1.50
8	B	856	U10	C23-C24	3.69	1.40	1.33
8	B	856	U10	C4-C3	3.78	1.52	1.35
7	A	855	BPH	C2-C3	3.91	1.40	1.33
6	A	850	BCL	CAA-C2A	3.96	1.62	1.54
6	B	852	BCL	C3D-C2D	3.97	1.49	1.40
8	A	857	U10	C33-C34	3.97	1.40	1.33
6	A	850	BCL	C5-C3	4.15	1.60	1.51
8	B	856	U10	C33-C34	4.18	1.41	1.33
8	A	857	U10	C4-C3	4.19	1.53	1.35
8	A	857	U10	C23-C24	4.31	1.41	1.33
8	A	857	U10	C13-C14	4.49	1.41	1.33
6	A	851	BCL	C2-C3	4.51	1.41	1.33
6	B	852	BCL	C2-C3	4.53	1.41	1.33
7	B	854	BPH	C2-C3	4.66	1.42	1.33
8	A	857	U10	C7-C6	4.76	1.60	1.51
8	A	857	U10	C18-C19	4.77	1.42	1.33
8	B	856	U10	C28-C29	4.87	1.42	1.33
8	A	857	U10	C28-C29	5.34	1.43	1.33
6	A	850	BCL	C2-C3	6.34	1.45	1.33
8	B	856	U10	C6-C1	7.14	1.52	1.35
8	A	857	U10	C6-C1	9.03	1.56	1.35

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	853	BCL	CMB-C2B-C1B	-6.33	117.90	128.36
6	A	851	BCL	CMB-C2B-C1B	-6.16	118.17	128.36
6	B	852	BCL	CMB-C2B-C1B	-5.91	118.58	128.36
6	A	850	BCL	CMB-C2B-C1B	-5.76	118.83	128.36
8	A	857	U10	C15-C14-C13	-5.44	112.83	123.50
8	B	856	U10	C10-C9-C8	-5.21	113.27	123.50
6	B	853	BCL	CAA-C2A-C1A	-5.20	94.15	112.47
8	B	856	U10	C15-C14-C13	-5.00	113.68	123.50
8	A	857	U10	C10-C9-C8	-4.68	114.31	123.50
8	B	856	U10	C25-C24-C23	-4.38	114.90	123.50
8	A	857	U10	C35-C34-C33	-4.28	115.10	123.50
7	B	854	BPH	O1D-CGD-CBD	-4.26	118.51	124.62
6	A	850	BCL	CAA-C2A-C1A	-4.24	97.50	112.47
7	A	855	BPH	C4D-C3D-C2D	-4.10	101.79	107.08
8	B	856	U10	C35-C34-C33	-4.08	115.48	123.50
8	A	857	U10	C25-C24-C23	-4.04	115.57	123.50
7	B	854	BPH	C4D-C3D-C2D	-3.96	101.97	107.08
7	A	855	BPH	O1D-CGD-CBD	-3.96	118.95	124.62
7	A	855	BPH	CHC-C4B-NB	-3.90	117.49	124.91
7	B	854	BPH	CMB-C2B-C1B	-3.86	118.78	125.06
6	A	851	BCL	OBD-CAD-C3D	-3.76	120.69	128.35
7	A	855	BPH	CMB-C2B-C1B	-3.56	119.26	125.06
8	A	857	U10	C20-C19-C18	-3.48	116.68	123.50
7	B	854	BPH	CHC-C4B-NB	-3.38	118.47	124.91
8	B	856	U10	C20-C19-C18	-3.21	117.21	123.50
6	A	850	BCL	CMD-C2D-C3D	-3.13	118.97	125.09
7	A	855	BPH	C5-C3-C2	-3.12	115.13	121.05
6	B	852	BCL	OBD-CAD-C3D	-3.09	122.04	128.35
6	A	850	BCL	OBD-CAD-C3D	-3.09	122.05	128.35
6	B	853	BCL	OBD-CAD-C3D	-2.93	122.37	128.35
6	A	850	BCL	C10-C8-C7	-2.93	94.80	112.27
6	A	850	BCL	O1D-CGD-CBD	-2.90	120.46	124.62
8	A	857	U10	C30-C29-C28	-2.83	117.95	123.50
7	B	854	BPH	CBB-CAB-C3B	-2.79	114.33	120.52
6	B	853	BCL	O1D-CGD-CBD	-2.77	120.65	124.62
6	B	852	BCL	CHA-C1A-NA	-2.66	119.51	126.06
6	A	851	BCL	CHA-C1A-NA	-2.66	119.52	126.06
8	A	857	U10	C1-C6-C5	-2.61	117.14	120.12
8	B	856	U10	C30-C29-C28	-2.56	118.47	123.50
6	A	850	BCL	C7-C6-C5	-2.50	105.67	113.06
7	A	855	BPH	C1C-NC-C4C	-2.49	107.89	110.44
7	A	855	BPH	CAC-C3C-C2C	-2.31	108.32	114.13
6	A	851	BCL	O1D-CGD-CBD	-2.26	121.38	124.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	850	BCL	CHA-C1A-NA	-2.26	120.51	126.06
8	B	856	U10	C21-C22-C23	-2.25	105.81	111.69
6	B	852	BCL	O1D-CGD-CBD	-2.24	121.41	124.62
8	B	856	U10	C1-C6-C5	-2.22	117.59	120.12
6	A	850	BCL	C12-C11-C10	-2.15	102.32	112.99
6	B	853	BCL	CHA-C1A-NA	-2.15	120.78	126.06
8	B	856	U10	O5-C5-C4	-2.10	116.25	120.79
6	A	850	BCL	C15-C13-C12	-2.06	99.95	112.27
8	A	857	U10	O5-C5-C4	-2.05	116.36	120.79
6	A	851	BCL	C2A-C1A-CHA	2.03	127.62	123.89
8	B	856	U10	C21-C19-C18	2.09	125.02	121.05
6	A	851	BCL	O2A-CGA-CBA	2.13	118.39	111.90
6	A	850	BCL	C11-C12-C13	2.13	122.57	115.49
6	B	852	BCL	C3D-CAD-CBD	2.15	110.64	107.60
6	B	852	BCL	C2A-C1A-CHA	2.17	127.88	123.89
8	A	857	U10	C10-C9-C11	2.32	118.95	115.41
8	B	856	U10	C36-C34-C33	2.33	125.46	121.05
6	B	853	BCL	C2A-C1A-CHA	2.37	128.26	123.89
7	B	854	BPH	C3D-CAD-CBD	2.38	110.96	107.60
6	B	852	BCL	O2A-CGA-CBA	2.38	119.16	111.90
8	A	857	U10	C35-C34-C36	2.38	119.05	115.41
6	A	850	BCL	O2D-CGD-CBD	2.39	114.57	111.30
8	B	856	U10	C35-C34-C36	2.39	119.06	115.41
8	B	856	U10	C30-C29-C31	2.39	119.06	115.41
6	A	851	BCL	C3D-CAD-CBD	2.40	111.00	107.60
8	B	856	U10	C10-C9-C11	2.47	119.19	115.41
7	A	855	BPH	CMB-C2B-C3B	2.52	133.92	128.04
8	A	857	U10	C36-C34-C33	2.53	125.85	121.05
8	A	857	U10	C4M-O4-C4	2.55	125.68	116.61
7	B	854	BPH	CMB-C2B-C3B	2.55	133.98	128.04
7	A	855	BPH	C3D-CAD-CBD	2.55	111.20	107.60
8	B	856	U10	C11-C12-C13	2.55	118.38	111.69
7	B	854	BPH	CED-O2D-CGD	2.56	121.99	115.99
8	B	856	U10	C7-C8-C9	2.60	131.11	126.70
8	B	856	U10	C4M-O4-C4	2.60	125.87	116.61
7	A	855	BPH	CED-O2D-CGD	2.78	122.51	115.99
8	A	857	U10	C11-C12-C13	2.81	119.05	111.69
8	A	857	U10	C30-C29-C31	2.83	119.73	115.41
8	A	857	U10	C21-C19-C18	2.84	126.44	121.05
8	A	857	U10	C7-C6-C5	2.94	122.02	118.56
6	B	853	BCL	C6-C5-C3	3.00	119.06	112.48
8	A	857	U10	C11-C9-C8	3.00	126.74	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	853	BCL	O2D-CGD-CBD	3.13	115.59	111.30
7	A	855	BPH	O2D-CGD-CBD	3.27	115.79	111.30
8	B	856	U10	C25-C24-C26	3.29	120.43	115.41
8	B	856	U10	C11-C9-C8	3.42	127.54	121.05
6	A	850	BCL	CED-O2D-CGD	3.45	124.08	115.99
8	A	857	U10	C25-C24-C26	3.47	120.71	115.41
6	B	853	BCL	CED-O2D-CGD	3.48	124.16	115.99
7	B	854	BPH	O2D-CGD-CBD	3.76	116.46	111.30
6	A	851	BCL	CED-O2D-CGD	3.78	124.86	115.99
6	B	852	BCL	CED-O2D-CGD	3.90	125.14	115.99
6	A	850	BCL	CMB-C2B-C3B	4.03	132.98	125.09
7	B	854	BPH	C6-C5-C3	4.10	121.48	112.48
7	B	854	BPH	C4-C3-C5	4.14	121.72	115.41
6	B	853	BCL	CBA-CAA-C2A	4.14	125.40	113.73
6	A	850	BCL	CBA-CAA-C2A	4.21	125.60	113.73
7	A	855	BPH	C6-C5-C3	4.35	122.03	112.48
6	B	852	BCL	CMB-C2B-C3B	4.40	133.70	125.09
6	A	851	BCL	CMB-C2B-C3B	4.43	133.76	125.09
6	A	851	BCL	C6-C5-C3	4.46	122.28	112.48
7	B	854	BPH	C3C-C4C-NC	4.56	112.50	107.93
6	A	850	BCL	C6-C7-C8	4.58	130.69	115.49
6	B	852	BCL	C6-C5-C3	4.70	122.80	112.48
8	A	857	U10	C15-C14-C16	4.79	122.72	115.41
6	B	853	BCL	CMB-C2B-C3B	4.81	134.49	125.09
7	A	855	BPH	C4-C3-C5	5.14	123.26	115.41
7	A	855	BPH	C3C-C4C-NC	5.21	113.15	107.93
8	B	856	U10	C15-C14-C16	5.29	123.49	115.41
8	B	856	U10	C7-C6-C5	5.41	124.92	118.56
6	A	850	BCL	C6-C5-C3	6.41	126.55	112.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 73 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	850	BCL	15	0
6	A	851	BCL	6	0
7	A	855	BPH	11	0
8	A	857	U10	4	0
6	B	852	BCL	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	853	BCL	8	0
7	B	854	BPH	13	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%)	-0.69	0 100 100	90, 90, 90, 90	0
2	B	302/307 (98%)	-0.69	0 100 100	90, 90, 90, 90	0
3	C	238/260 (91%)	-0.56	0 100 100	90, 90, 90, 90	0
All	All	821/848 (96%)	-0.65	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
7	BPH	B	854	65/65	0.69	0.47	7.86	90,90,90,90	0
8	U10	B	856	48/63	0.80	0.42	3.61	90,90,90,90	0
8	U10	A	857	48/63	0.80	0.45	2.63	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	851	66/66	0.89	0.28	2.17	90,90,90,90	0
6	BCL	A	850	66/66	0.86	0.33	2.10	90,90,90,90	0
6	BCL	B	852	66/66	0.93	0.24	0.88	90,90,90,90	0
6	BCL	B	853	66/66	0.93	0.22	0.56	90,90,90,90	0
7	BPH	A	855	65/65	0.93	0.22	0.41	90,90,90,90	0
4	FE	B	858	1/1	0.99	0.13	-0.57	90,90,90,90	0
5	MN	C	860	1/1	0.79	0.08	-	181,181,181,181	1

6.5 Other polymers [i](#)

There are no such residues in this entry.