



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:18 AM UTC

PDB ID : 9BA2 / pdb_00009ba2
Title : Crystal structure of the binary complex of DCAF1 and WDR5
Authors : Mabanglo, M.F.; Wilson, B.J.; Srivastava, S.; Al-awar, R.; Vedadi, M.
Deposited on : 2024-04-03
Resolution : 2.97 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

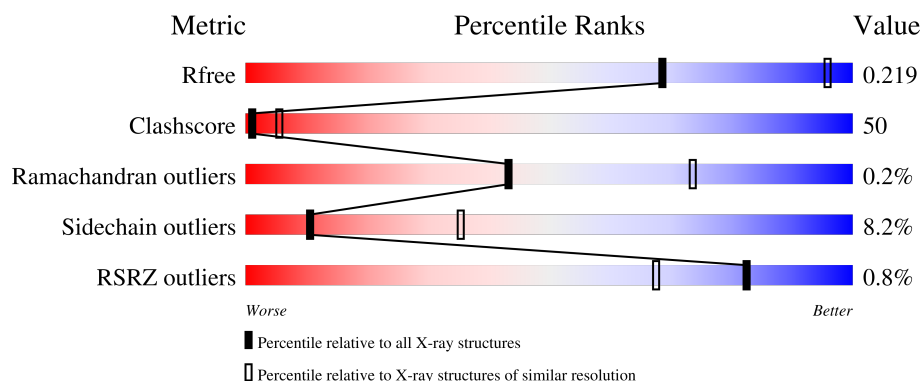
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

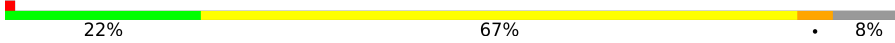
The reported resolution of this entry is 2.97 Å.

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}	180053	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	338	
2	B	329	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4891 atoms, of which 4 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 DDB1- and CUL4-associated factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2438	1537	417	465	19			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1053	MET	-	initiating methionine	UNP Q9Y4B6
A	1054	GLY	-	expression tag	UNP Q9Y4B6
A	1055	SER	-	expression tag	UNP Q9Y4B6
A	1056	SER	-	expression tag	UNP Q9Y4B6
A	1057	HIS	-	expression tag	UNP Q9Y4B6
A	1058	HIS	-	expression tag	UNP Q9Y4B6
A	1059	HIS	-	expression tag	UNP Q9Y4B6
A	1060	HIS	-	expression tag	UNP Q9Y4B6
A	1061	HIS	-	expression tag	UNP Q9Y4B6
A	1062	HIS	-	expression tag	UNP Q9Y4B6
A	1063	SER	-	expression tag	UNP Q9Y4B6
A	1064	SER	-	expression tag	UNP Q9Y4B6
A	1065	GLY	-	expression tag	UNP Q9Y4B6
A	1066	ARG	-	expression tag	UNP Q9Y4B6
A	1067	GLU	-	expression tag	UNP Q9Y4B6
A	1068	ASN	-	expression tag	UNP Q9Y4B6
A	1069	LEU	-	expression tag	UNP Q9Y4B6
A	1070	TYR	-	expression tag	UNP Q9Y4B6
A	1071	PHE	-	expression tag	UNP Q9Y4B6
A	1072	GLN	-	expression tag	UNP Q9Y4B6
A	1073	GLY	-	expression tag	UNP Q9Y4B6
A	1074	SER	-	expression tag	UNP Q9Y4B6
A	1075	SER	-	expression tag	UNP Q9Y4B6
A	1076	ARG	-	expression tag	UNP Q9Y4B6
A	1077	ALA	-	expression tag	UNP Q9Y4B6
A	1078	SER	-	expression tag	UNP Q9Y4B6
A	1079	ALA	-	expression tag	UNP Q9Y4B6

- Molecule 2 is a protein called WD repeat-containing protein 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	304	Total	C	N	O	S	0	2	0
			2360	1505	393	452	10			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	6	MET	-	initiating methionine	UNP P61964
B	7	HIS	-	expression tag	UNP P61964
B	8	HIS	-	expression tag	UNP P61964
B	9	HIS	-	expression tag	UNP P61964
B	10	HIS	-	expression tag	UNP P61964
B	11	HIS	-	expression tag	UNP P61964
B	12	HIS	-	expression tag	UNP P61964
B	13	SER	-	expression tag	UNP P61964
B	14	SER	-	expression tag	UNP P61964
B	15	GLY	-	expression tag	UNP P61964
B	16	ARG	-	expression tag	UNP P61964
B	17	GLU	-	expression tag	UNP P61964
B	18	ASN	-	expression tag	UNP P61964
B	19	LEU	-	expression tag	UNP P61964
B	20	TYR	-	expression tag	UNP P61964
B	21	PHE	-	expression tag	UNP P61964
B	22	GLN	-	expression tag	UNP P61964
B	23	GLY	-	expression tag	UNP P61964

- Molecule 3 is IMIDAZOLE (CCD ID: IMD) (formula: C₃H₅N₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	N	0	0
			9	3	4	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	68	Total	O	0	0
			68	68		
4	B	16	Total	O	0	0
			16	16		

I327
K328
L329
W330
K331
S332
D333
C334

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	47.60Å 83.19Å 158.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.58 – 2.97 45.58 – 2.97	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.58-2.97) 100.0 (45.58-2.97)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.230 , 0.266 (Not available) , 0.219	Depositor DCC
R_{free} test set	664 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	84.3	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 72.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4891	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.91% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: IMD

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	0.47	0/2492	0.66	0/3372
2	B	0.32	0/2419	0.53	1/3280 (0.0%)
All	All	0.41	0/4911	0.60	1/6652 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	35	TYR	CB-CA-C	5.14	117.98	110.26

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	2438	0	2340	148	0
2	B	2360	0	2344	334	0
3	A	5	4	5	3	0
4	A	68	0	0	10	0
4	B	16	0	0	10	0
All	All	4887	4	4689	473	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 50.

All (473) 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)
1:A:1196:LYS:HE2	4:B:401:HOH:O	1.30	1.24
1:A:1204:ASP:HB2	1:A:1211:LEU:HD21	1.35	1.08
2:B:186:ILE:HB	2:B:198:TRP:HB2	1.39	1.03
2:B:197:ILE:HD11	2:B:229:ILE:HD11	1.43	0.98
2:B:55:PRO:HD2	2:B:99:SER:HB3	1.46	0.98
1:A:1151:LEU:HD13	1:A:1182:VAL:HG12	1.46	0.98
1:A:1207:THR:HG23	1:A:1209:ASN:H	1.31	0.96
2:B:182:ASP:OD1	2:B:183:GLY:N	1.98	0.95
2:B:144:ILE:HB	2:B:156:TRP:HB2	1.48	0.94
2:B:105:ALA:HB1	2:B:132:VAL:HG23	1.46	0.94
1:A:1136:SER:OG	1:A:1156:TRP:O	1.83	0.93
1:A:1298:ARG:HG3	3:A:1401:IMD:H4	1.50	0.92
2:B:265:ASN:ND2	2:B:308:ALA:HA	1.86	0.90
1:A:1294:LEU:HD11	1:A:1308:MET:HE1	1.53	0.89
2:B:97:SER:N	2:B:141:SER:OG	2.04	0.88
2:B:80:GLU:HG3	2:B:81:LYS:H	1.38	0.88
1:A:1109:MET:HE2	1:A:1117:LEU:HD21	1.52	0.87
1:A:1150:LEU:HD21	1:A:1152:THR:HG23	1.55	0.87
1:A:1085:VAL:HG13	1:A:1385:ARG:HG3	1.56	0.86
2:B:80:GLU:HG3	2:B:81:LYS:HG2	1.58	0.86
2:B:245:LYS:O	4:B:401:HOH:O	1.92	0.85
1:A:1151:LEU:HD22	1:A:1182:VAL:HG11	1.57	0.84
2:B:57:GLY:HA3	2:B:310:HIS:CE1	2.12	0.84
2:B:282:LEU:HD13	2:B:296:LYS:HE3	1.60	0.84
1:A:1274:ILE:HG23	1:A:1279:ILE:HD13	1.59	0.84
2:B:257:ASN:OD1	2:B:262:ILE:HD13	1.76	0.83
2:B:226:GLY:O	2:B:243:TYR:OH	1.95	0.83
2:B:180:ASN:ND2	2:B:182:ASP:OD1	2.12	0.83
2:B:275:VAL:HG23	2:B:285:ILE:HG13	1.61	0.83
2:B:249:LEU:O	2:B:250:LYS:HG3	1.78	0.83
2:B:265:ASN:HD22	2:B:308:ALA:HA	1.43	0.83
1:A:1230:PHE:HB2	4:A:1522:HOH:O	1.78	0.82
2:B:131:TYR:O	2:B:148:SER:OG	1.97	0.81
1:A:1196:LYS:O	1:A:1196:LYS:HD3	1.81	0.80
2:B:303:VAL:HB	2:B:321:LEU:HD23	1.63	0.80
2:B:97:SER:OG	2:B:139:PRO:O	1.98	0.79
2:B:267:SER:HG	2:B:273:TRP:CD1	2.00	0.79
2:B:271:GLY:HA3	2:B:273:TRP:CH2	2.17	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:148:SER:HB3	2:B:150:ASP:OD1	1.82	0.79
2:B:138:ASN:ND2	2:B:143:LEU:HB2	1.97	0.79
1:A:1320:ASP:O	1:A:1321:LEU:HD13	1.80	0.79
2:B:242:ASP:OD1	2:B:245:LYS:HB2	1.82	0.78
2:B:223:SER:HA	2:B:266:PHE:CE2	2.19	0.78
2:B:137:PHE:HE1	2:B:144:ILE:HG12	1.49	0.76
1:A:1150:LEU:CD2	1:A:1152:THR:HG23	2.16	0.76
2:B:285:ILE:HG22	2:B:294:VAL:CG1	2.16	0.76
1:A:1374:SER:C	1:A:1375:MET:HE3	2.11	0.75
2:B:230:LEU:HD12	2:B:231:ALA:H	1.51	0.75
2:B:252:TYR:CD2	2:B:291:LYS:HA	2.22	0.75
2:B:303:VAL:HB	2:B:321:LEU:CD2	2.17	0.75
1:A:1196:LYS:HD3	1:A:1196:LYS:C	2.10	0.74
2:B:69:ILE:HD11	2:B:104:SER:HB3	1.70	0.74
2:B:287:ASN:OD1	2:B:290:THR:HG22	1.88	0.74
2:B:271:GLY:HA3	2:B:273:TRP:CZ2	2.21	0.74
2:B:97:SER:H	2:B:141:SER:HG	1.33	0.74
1:A:1109:MET:HE3	1:A:1119:LEU:HD21	1.69	0.74
1:A:1190:ASP:O	1:A:1191:ARG:HG3	1.87	0.74
1:A:1134:HIS:CD2	1:A:1138:ILE:HD11	2.22	0.74
2:B:52:LYS:O	2:B:60:LEU:HD22	1.87	0.73
1:A:1158:GLN:HE22	2:B:207:LYS:HD3	1.53	0.73
2:B:234:LEU:HD23	2:B:257:ASN:ND2	2.03	0.73
2:B:185:LEU:HD21	2:B:206:LEU:HD12	1.71	0.73
2:B:185:LEU:HA	2:B:198:TRP:O	1.88	0.73
2:B:283:VAL:CG1	2:B:297:LEU:HB2	2.18	0.72
2:B:283:VAL:HG13	2:B:297:LEU:HB2	1.72	0.71
2:B:73:GLY:O	2:B:77:GLY:N	2.22	0.71
1:A:1325:ARG:HG2	4:A:1510:HOH:O	1.89	0.71
2:B:100:ASN:O	2:B:116:VAL:HG12	1.90	0.71
2:B:293:ILE:H	2:B:293:ILE:HD12	1.54	0.71
2:B:236:ASN:OD1	2:B:256:LYS:HA	1.89	0.70
2:B:251:THR:O	2:B:291:LYS:HD3	1.90	0.70
1:A:1134:HIS:HD2	1:A:1138:ILE:HD11	1.56	0.70
2:B:149:PHE:HA	2:B:173:PRO:HB3	1.73	0.70
1:A:1156:TRP:O	1:A:1157:SER:HB3	1.92	0.69
2:B:170:HIS:HB3	2:B:192:ASP:OD2	1.91	0.69
2:B:55:PRO:HD2	2:B:99:SER:CB	2.21	0.69
2:B:167:LEU:O	2:B:169:ALA:N	2.25	0.69
2:B:53:PHE:CD1	2:B:60:LEU:HD23	2.28	0.69
1:A:1211:LEU:O	1:A:1212:LEU:HD23	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:HIS:O	4:B:402:HOH:O	2.11	0.68
2:B:142:ASN:HA	2:B:158:VAL:CG2	2.24	0.68
2:B:285:ILE:HG21	4:B:413:HOH:O	1.93	0.68
2:B:287:ASN:CG	2:B:290:THR:HG22	2.18	0.68
2:B:112:LYS:NZ	2:B:124:THR:OG1	2.26	0.68
1:A:1274:ILE:HG23	1:A:1279:ILE:CD1	2.23	0.68
2:B:322:GLU:N	2:B:322:GLU:OE1	2.27	0.68
1:A:1298:ARG:HG3	3:A:1401:IMD:C4	2.22	0.67
2:B:122:LEU:O	2:B:123:LYS:HG3	1.94	0.67
2:B:216:PRO:HG2	2:B:234:LEU:HD12	1.75	0.67
1:A:1355:PHE:HE1	1:A:1371:ASN:HB2	1.59	0.67
2:B:196:ARG:HG2	2:B:198:TRP:CZ2	2.29	0.67
2:B:41:LEU:HB3	2:B:72:TRP:CE3	2.30	0.67
2:B:70:LYS:HE3	2:B:72:TRP:CZ2	2.30	0.66
2:B:73:GLY:HA3	2:B:78:LYS:H	1.60	0.66
2:B:255:HIS:HD2	2:B:286:TRP:CH2	2.13	0.66
1:A:1150:LEU:HD21	1:A:1152:THR:CG2	2.25	0.66
2:B:142:ASN:O	2:B:158:VAL:HG13	1.96	0.66
2:B:157:ASP:O	2:B:161:GLY:N	2.27	0.66
2:B:86:HIS:HE1	2:B:110:THR:HB	1.62	0.65
1:A:1163:LEU:HD21	1:A:1205:ILE:HG23	1.79	0.65
1:A:1191:ARG:N	1:A:1205:ILE:HD11	2.11	0.65
1:A:1385:ARG:HD2	1:A:1387:TYR:OH	1.97	0.65
2:B:157:ASP:OD2	2:B:160:THR:OG1	2.11	0.65
1:A:1225:ARG:HH12	1:A:1298:ARG:HD3	1.60	0.65
1:A:1187:HIS:HB3	1:A:1234:ASP:OD2	1.97	0.64
2:B:143:LEU:HD23	2:B:155:ILE:HG23	1.79	0.64
2:B:180:ASN:OD1	2:B:185:LEU:HB2	1.97	0.64
2:B:64:SER:HB3	2:B:66:ASP:OD1	1.97	0.64
2:B:217:VAL:HG22	2:B:233:THR:HG22	1.80	0.64
2:B:227:LYS:NZ	4:B:403:HOH:O	2.30	0.64
1:A:1151:LEU:HD22	1:A:1182:VAL:CG1	2.26	0.64
2:B:227:LYS:HB3	2:B:228:TYR:CE2	2.33	0.64
2:B:111:LEU:HD11	2:B:146:SER:HB3	1.78	0.64
1:A:1158:GLN:NE2	2:B:207:LYS:HD3	2.13	0.63
2:B:184:SER:O	2:B:185:LEU:HD23	1.98	0.63
2:B:55:PRO:CD	2:B:99:SER:HB3	2.26	0.63
2:B:248:CYS:SG	2:B:251:THR:HG22	2.38	0.63
1:A:1091:GLU:HA	4:A:1506:HOH:O	1.97	0.63
1:A:1135:ASN:HD21	1:A:1157:SER:HB2	1.63	0.63
2:B:41:LEU:HD13	2:B:327:ILE:HB	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:PRO:HG2	4:B:413:HOH:O	1.98	0.63
1:A:1215:PHE:CE2	1:A:1217:PRO:HD3	2.34	0.63
2:B:67:LYS:HE2	4:B:406:HOH:O	1.99	0.63
2:B:96:SER:HB3	2:B:137:PHE:CD2	2.34	0.63
2:B:104:SER:O	2:B:111:LEU:HD23	1.99	0.62
2:B:279:GLU:HA	2:B:303:VAL:HG22	1.81	0.62
1:A:1122:VAL:HG21	1:A:1386:LEU:HD13	1.81	0.62
2:B:54:SER:HB2	2:B:57:GLY:H	1.63	0.62
2:B:173:PRO:HG2	2:B:191:TYR:CD2	2.34	0.62
2:B:296:LYS:O	2:B:297:LEU:HD23	1.99	0.62
2:B:184:SER:C	2:B:200:THR:HG23	2.25	0.62
2:B:252:TYR:HD2	2:B:291:LYS:HA	1.61	0.62
2:B:270:GLY:HA3	2:B:334:CYS:OXT	1.99	0.62
1:A:1352:ARG:NH2	1:A:1370:GLU:OE1	2.29	0.62
2:B:151:GLU:HG2	2:B:172:ASP:C	2.25	0.62
1:A:1156:TRP:O	1:A:1157:SER:CB	2.49	0.61
2:B:230:LEU:HD12	2:B:231:ALA:N	2.14	0.61
2:B:331:LYS:HD2	2:B:332:SER:N	2.16	0.61
2:B:210:ILE:HG22	2:B:211:ASP:O	2.01	0.61
1:A:1190:ASP:C	1:A:1205:ILE:HD11	2.26	0.60
2:B:236:ASN:OD1	2:B:256:LYS:HD3	2.01	0.60
2:B:59:TRP:HB2	4:B:409:HOH:O	1.99	0.60
1:A:1135:ASN:ND2	1:A:1157:SER:HB2	2.16	0.60
2:B:144:ILE:HG13	2:B:158:VAL:HG12	1.82	0.60
2:B:176:ALA:HB3	2:B:220:VAL:HG12	1.81	0.60
2:B:185:LEU:HD21	2:B:206:LEU:CD1	2.31	0.60
2:B:190:SER:HB3	2:B:192:ASP:OD1	2.00	0.60
1:A:1109:MET:CE	1:A:1117:LEU:HD21	2.30	0.60
1:A:1322:MET:HG3	2:B:272:LYS:HE3	1.84	0.60
1:A:1332:SER:OG	1:A:1349:ASP:OD1	2.19	0.60
2:B:216:PRO:CG	2:B:234:LEU:HD12	2.32	0.60
2:B:86:HIS:CE1	2:B:110:THR:HB	2.36	0.59
1:A:1322:MET:HG2	1:A:1323:GLU:N	2.18	0.59
2:B:137:PHE:CE1	2:B:144:ILE:HG12	2.36	0.59
2:B:41:LEU:HB3	2:B:72:TRP:CZ3	2.37	0.59
2:B:108:ASP:OD1	2:B:110:THR:HB	2.02	0.59
2:B:275:VAL:HG23	2:B:285:ILE:CG1	2.32	0.59
2:B:72:TRP:HA	2:B:78:LYS:O	2.02	0.59
2:B:142:ASN:HA	2:B:158:VAL:HG21	1.83	0.59
1:A:1158:GLN:HE22	2:B:207:LYS:CD	2.15	0.58
2:B:96:SER:HB2	2:B:141:SER:OG	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:213:ASP:HB3	2:B:215:PRO:HD3	1.85	0.58
2:B:322:GLU:O	2:B:325:LYS:HG3	2.01	0.58
2:B:192:ASP:OD1	2:B:194:LEU:HB2	2.03	0.58
1:A:1326:MET:HG2	1:A:1380:MET:HE2	1.84	0.58
2:B:33:PRO:HA	2:B:334:CYS:SG	2.43	0.58
2:B:240:LEU:HD23	2:B:241:TRP:N	2.18	0.58
1:A:1322:MET:HE1	1:A:1325:ARG:HE	1.68	0.58
2:B:58:GLU:C	2:B:74:ALA:HB3	2.29	0.57
2:B:178:HIS:HB3	2:B:187:VAL:CG1	2.34	0.57
2:B:35:TYR:H	2:B:295:GLN:NE2	2.02	0.57
2:B:128:HIS:ND1	2:B:150:ASP:OD2	2.26	0.57
1:A:1163:LEU:CD2	1:A:1205:ILE:HG23	2.34	0.57
2:B:46:LYS:HA	2:B:325:LYS:HD3	1.85	0.57
2:B:157:ASP:HB2	2:B:164:LEU:HD21	1.85	0.57
2:B:113:ILE:O	2:B:122:LEU:N	2.37	0.57
2:B:125:LEU:HB3	2:B:156:TRP:CE3	2.40	0.57
2:B:153:VAL:HG22	2:B:174:VAL:HG11	1.86	0.57
2:B:303:VAL:O	2:B:321:LEU:HD22	2.05	0.57
2:B:76:ASP:C	2:B:78:LYS:HE3	2.30	0.57
1:A:1324:GLU:HG3	2:B:225:ASN:ND2	2.19	0.57
2:B:67:LYS:C	2:B:68:LEU:HD23	2.30	0.57
2:B:316:ILE:HG22	2:B:330:TRP:HD1	1.70	0.57
2:B:57:GLY:HA3	2:B:310:HIS:NE2	2.18	0.56
2:B:300:HIS:CE1	2:B:328:LYS:HE3	2.40	0.56
2:B:293:ILE:HD12	2:B:293:ILE:N	2.19	0.56
2:B:69:ILE:HD11	2:B:104:SER:CB	2.35	0.56
2:B:69:ILE:CD1	2:B:104:SER:HB3	2.35	0.56
2:B:111:LEU:HD21	2:B:135:CYS:HB3	1.87	0.56
2:B:145:VAL:HG22	2:B:177:VAL:HB	1.87	0.56
1:A:1148:SER:O	1:A:1149:LEU:HD23	2.05	0.56
1:A:1206:GLN:HB2	4:A:1502:HOH:O	2.05	0.56
2:B:179:PHE:HE1	2:B:200:THR:CG2	2.18	0.56
2:B:128:HIS:HD1	2:B:150:ASP:CG	2.12	0.56
2:B:296:LYS:HE2	2:B:298:GLN:HB3	1.88	0.56
1:A:1324:GLU:HB2	2:B:225:ASN:HB2	1.86	0.56
2:B:53:PHE:CE1	2:B:60:LEU:HD23	2.39	0.56
2:B:291:LYS:HD2	2:B:291:LYS:O	2.05	0.56
2:B:290:THR:O	2:B:290:THR:OG1	2.24	0.55
2:B:86:HIS:CD2	2:B:106:SER:HB2	2.40	0.55
2:B:142:ASN:HA	2:B:158:VAL:HG22	1.88	0.55
2:B:224:PRO:HD3	2:B:266:PHE:CD2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1098:CYS:SG	1:A:1138:ILE:HG22	2.47	0.55
1:A:1328:SER:OG	1:A:1353:ASN:HB3	2.07	0.55
1:A:1209:ASN:O	1:A:1211:LEU:HD22	2.06	0.55
2:B:125:LEU:CD1	2:B:161:GLY:HA2	2.37	0.55
2:B:185:LEU:CD2	2:B:206:LEU:HD12	2.36	0.55
1:A:1222:ASN:O	4:A:1501:HOH:O	2.18	0.55
2:B:187:VAL:CG2	2:B:220:VAL:HG21	2.36	0.55
1:A:1105:GLU:OE1	1:A:1362:LYS:NZ	2.28	0.54
1:A:1190:ASP:C	1:A:1205:ILE:CD1	2.81	0.54
1:A:1211:LEU:HD22	1:A:1211:LEU:H	1.73	0.54
2:B:76:ASP:OD1	2:B:76:ASP:N	2.38	0.54
2:B:78:LYS:HE2	2:B:78:LYS:HA	1.90	0.54
2:B:133:PHE:HE1	2:B:263:PHE:CZ	2.25	0.54
1:A:1279:ILE:HB	1:A:1289:HIS:HB2	1.90	0.54
1:A:1294:LEU:HD11	1:A:1308:MET:CE	2.34	0.54
2:B:73:GLY:H	2:B:78:LYS:N	2.06	0.54
2:B:172:ASP:HB3	2:B:173:PRO:HD2	1.88	0.54
1:A:1087:ARG:NH2	1:A:1381:ASP:OD1	2.41	0.54
2:B:100:ASN:O	2:B:101:LEU:HD23	2.08	0.54
2:B:40:THR:OG1	2:B:328:LYS:HG2	2.07	0.54
2:B:96:SER:HB2	2:B:141:SER:CB	2.38	0.54
2:B:179:PHE:CE1	2:B:200:THR:HG21	2.43	0.53
2:B:324:ASP:OD1	2:B:326:THR:HG23	2.08	0.53
2:B:197:ILE:HD11	2:B:229:ILE:CD1	2.29	0.53
2:B:242:ASP:HB3	2:B:249:LEU:CD1	2.39	0.53
2:B:155:ILE:HD12	2:B:167:LEU:HD11	1.89	0.53
2:B:232:ALA:HB2	2:B:238:LEU:CD1	2.38	0.53
2:B:76:ASP:HB2	2:B:78:LYS:HE3	1.90	0.53
2:B:105:ALA:CB	2:B:132:VAL:HG23	2.29	0.53
1:A:1174:HIS:CD2	1:A:1208:GLY:HA3	2.44	0.53
2:B:312:THR:OG1	2:B:313:GLU:N	2.41	0.53
2:B:186:ILE:HG13	2:B:200:THR:HG22	1.90	0.53
2:B:302:ASP:OD1	2:B:303:VAL:N	2.36	0.53
2:B:214:ASN:N	2:B:215:PRO:HD3	2.23	0.53
1:A:1204:ASP:CB	1:A:1211:LEU:HD21	2.25	0.53
1:A:1158:GLN:HE22	2:B:207:LYS:CE	2.21	0.52
2:B:50[A]:SER:CB	2:B:92:ASP:HA	2.39	0.52
2:B:140:GLN:HG2	2:B:142:ASN:OD1	2.09	0.52
2:B:103:VAL:HG13	2:B:137:PHE:CZ	2.44	0.52
1:A:1276:ASN:ND2	1:A:1277:THR:HG23	2.24	0.52
1:A:1294:LEU:CD1	1:A:1308:MET:HE1	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1322:MET:CG	1:A:1323:GLU:N	2.72	0.52
2:B:218:SER:HB2	2:B:261:CYS:SG	2.49	0.52
2:B:262:ILE:HD12	2:B:262:ILE:N	2.23	0.52
2:B:316:ILE:HG22	2:B:330:TRP:CD1	2.44	0.52
2:B:76:ASP:HB2	2:B:78:LYS:CE	2.39	0.52
2:B:137:PHE:HE1	2:B:144:ILE:CG1	2.19	0.52
2:B:149:PHE:CD1	2:B:149:PHE:O	2.62	0.52
1:A:1312:MET:HG2	1:A:1313:LEU:O	2.10	0.52
2:B:324:ASP:O	2:B:326:THR:HG23	2.10	0.52
1:A:1151:LEU:CD1	1:A:1182:VAL:HG12	2.30	0.52
1:A:1115:GLY:HA3	1:A:1134:HIS:O	2.10	0.52
1:A:1279:ILE:HD12	1:A:1342:TYR:CE1	2.45	0.52
2:B:80:GLU:HG3	2:B:81:LYS:N	2.16	0.52
2:B:125:LEU:HB3	2:B:156:TRP:CZ3	2.45	0.51
1:A:1314:GLN:O	1:A:1315:ALA:HB2	2.09	0.51
2:B:145:VAL:CG2	2:B:177:VAL:HB	2.41	0.51
2:B:88:LEU:HB2	2:B:108:ASP:HB3	1.93	0.51
2:B:186:ILE:O	2:B:198:TRP:N	2.43	0.51
2:B:130:ASN:OD1	2:B:131:TYR:N	2.34	0.51
1:A:1322:MET:HE1	1:A:1325:ARG:NE	2.25	0.51
1:A:1205:ILE:HD12	1:A:1205:ILE:H	1.74	0.51
2:B:44:HIS:CE1	2:B:70:LYS:HG3	2.46	0.51
2:B:63:SER:HB2	2:B:90:ILE:CG2	2.40	0.51
1:A:1107:PHE:HE2	1:A:1128:GLU:HG3	1.75	0.51
1:A:1204:ASP:HB3	1:A:1207:THR:HG22	1.91	0.51
2:B:179:PHE:HE1	2:B:200:THR:HG21	1.75	0.51
2:B:301:THR:OG1	2:B:323:ASN:O	2.27	0.51
1:A:1225:ARG:NH1	1:A:1298:ARG:HD3	2.26	0.50
2:B:111:LEU:HD11	2:B:146:SER:CB	2.40	0.50
2:B:207:LYS:HE3	2:B:243:TYR:O	2.10	0.50
2:B:227:LYS:HB3	2:B:228:TYR:CD2	2.47	0.50
2:B:285:ILE:HG22	2:B:294:VAL:HG13	1.90	0.50
1:A:1228:ALA:HB2	1:A:1239:ASN:HD22	1.76	0.49
1:A:1284:THR:O	1:A:1285:PHE:HB2	2.12	0.49
2:B:96:SER:HB2	2:B:141:SER:HB3	1.93	0.49
2:B:142:ASN:C	2:B:158:VAL:HG13	2.37	0.49
2:B:204:GLN:HG2	2:B:205:CYS:N	2.25	0.49
2:B:233:THR:OG1	2:B:235:ASP:OD1	2.29	0.49
2:B:287:ASN:HA	4:B:407:HOH:O	2.12	0.49
2:B:310:HIS:CD2	2:B:315:ILE:HD12	2.46	0.49
2:B:37:LEU:HD12	2:B:329:LEU:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1109:MET:SD	1:A:1150:LEU:HD12	2.52	0.49
2:B:133:PHE:HD1	2:B:133:PHE:O	1.96	0.49
1:A:1264:GLY:HA3	1:A:1275:ILE:HG12	1.94	0.49
2:B:199:ASP:O	2:B:203:GLY:N	2.41	0.49
1:A:1294:LEU:HD21	1:A:1308:MET:HE3	1.95	0.49
2:B:149:PHE:C	2:B:151:GLU:H	2.20	0.48
1:A:1139:THR:CG2	1:A:1155:THR:HG22	2.43	0.48
1:A:1155:THR:OG1	1:A:1156:TRP:N	2.46	0.48
2:B:271:GLY:CA	2:B:273:TRP:CZ2	2.93	0.48
1:A:1276:ASN:ND2	1:A:1277:THR:H	2.11	0.48
2:B:313:GLU:HB2	2:B:315:ILE:HD11	1.94	0.48
2:B:35:TYR:H	2:B:295:GLN:HE21	1.61	0.48
2:B:140:GLN:CG	2:B:142:ASN:OD1	2.61	0.48
2:B:298:GLN:HG3	2:B:299:GLY:N	2.29	0.48
1:A:1150:LEU:HD23	1:A:1150:LEU:C	2.39	0.48
2:B:187:VAL:HG22	2:B:220:VAL:HG21	1.96	0.48
2:B:296:LYS:NZ	2:B:298:GLN:HB3	2.29	0.48
2:B:59:TRP:C	2:B:74:ALA:HB2	2.38	0.48
2:B:167:LEU:N	2:B:167:LEU:HD12	2.29	0.48
2:B:138:ASN:HD21	2:B:143:LEU:HD13	1.79	0.48
2:B:287:ASN:HB3	2:B:290:THR:HG23	1.96	0.48
1:A:1213:THR:O	1:A:1213:THR:HG22	2.14	0.48
2:B:142:ASN:O	2:B:158:VAL:HG22	2.14	0.48
2:B:67:LYS:HD3	2:B:87:LYS:O	2.14	0.47
2:B:149:PHE:C	2:B:151:GLU:N	2.68	0.47
1:A:1117:LEU:CD1	1:A:1141:LEU:HD21	2.45	0.47
1:A:1160:LEU:HD13	1:A:1180:HIS:HB3	1.97	0.47
1:A:1332:SER:HA	1:A:1352:ARG:O	2.14	0.47
2:B:132:VAL:HG23	2:B:132:VAL:O	2.14	0.47
2:B:208:THR:O	2:B:210:ILE:HD12	2.14	0.47
2:B:258:GLU:H	2:B:279:GLU:CD	2.22	0.47
1:A:1182:VAL:HG13	1:A:1192:VAL:CG1	2.44	0.47
2:B:103:VAL:HG11	2:B:137:PHE:CE1	2.49	0.47
2:B:313:GLU:HB3	2:B:315:ILE:CG1	2.44	0.47
2:B:86:HIS:HE1	2:B:110:THR:CB	2.27	0.47
2:B:310:HIS:HD2	2:B:315:ILE:HD12	1.78	0.47
2:B:70:LYS:HE3	2:B:72:TRP:HZ2	1.77	0.47
1:A:1181:TYR:HB2	4:A:1535:HOH:O	2.14	0.47
2:B:68:LEU:HD23	2:B:68:LEU:N	2.29	0.47
2:B:92:ASP:OD1	2:B:93:VAL:N	2.47	0.47
2:B:96:SER:HB3	2:B:137:PHE:HD2	1.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:193:GLY:HA2	2:B:215:PRO:O	2.15	0.47
2:B:236:ASN:HD21	2:B:258:GLU:CG	2.28	0.47
1:A:1156:TRP:HB2	2:B:244:SER:OG	2.15	0.47
2:B:76:ASP:CG	2:B:78:LYS:HG2	2.40	0.46
2:B:164:LEU:N	2:B:164:LEU:HD22	2.30	0.46
2:B:230:LEU:HD11	2:B:238:LEU:HG	1.97	0.46
1:A:1137:ALA:O	1:A:1155:THR:HG23	2.15	0.46
1:A:1149:LEU:CD1	1:A:1205:ILE:HG21	2.45	0.46
1:A:1163:LEU:HD12	1:A:1164:TRP:N	2.31	0.46
2:B:285:ILE:HG22	2:B:294:VAL:HG11	1.95	0.46
2:B:96:SER:HB3	2:B:137:PHE:CE2	2.50	0.46
2:B:111:LEU:HD21	2:B:135:CYS:CB	2.45	0.46
2:B:232:ALA:HA	2:B:238:LEU:HD12	1.97	0.46
2:B:296:LYS:HG2	2:B:297:LEU:N	2.31	0.46
2:B:296:LYS:C	2:B:297:LEU:HD23	2.41	0.46
2:B:331:LYS:HD2	2:B:331:LYS:C	2.41	0.46
2:B:67:LYS:HG2	2:B:88:LEU:O	2.15	0.46
1:A:1308:MET:HB3	1:A:1337:PHE:HB2	1.97	0.46
2:B:290:THR:HG23	2:B:292:GLU:HG2	1.98	0.46
2:B:296:LYS:CE	2:B:298:GLN:HB3	2.45	0.46
2:B:300:HIS:HA	2:B:328:LYS:HZ2	1.81	0.46
2:B:242:ASP:HB3	2:B:249:LEU:HD11	1.98	0.46
2:B:258:GLU:N	2:B:279:GLU:OE1	2.46	0.46
1:A:1161:SER:OG	1:A:1179:ASP:O	2.21	0.46
2:B:110:THR:CG2	2:B:124:THR:HG23	2.46	0.46
2:B:245:LYS:HE3	4:B:403:HOH:O	2.16	0.46
1:A:1207:THR:N	4:A:1502:HOH:O	2.24	0.45
1:A:1371:ASN:HA	1:A:1382:THR:HG22	1.98	0.45
2:B:125:LEU:HD11	2:B:161:GLY:HA2	1.98	0.45
1:A:1114:THR:O	1:A:1114:THR:OG1	2.31	0.45
2:B:196:ARG:CD	2:B:208:THR:HG23	2.47	0.45
2:B:41:LEU:N	2:B:41:LEU:HD12	2.31	0.45
2:B:133:PHE:HE1	2:B:263:PHE:HZ	1.63	0.45
1:A:1117:LEU:HD11	1:A:1141:LEU:CD2	2.46	0.45
1:A:1158:GLN:NE2	2:B:206:LEU:O	2.49	0.45
1:A:1207:THR:HG22	4:A:1502:HOH:O	2.15	0.45
1:A:1098:CYS:O	1:A:1110:LEU:HA	2.17	0.45
1:A:1320:ASP:C	1:A:1321:LEU:HD22	2.41	0.45
2:B:133:PHE:O	2:B:133:PHE:CD1	2.70	0.45
2:B:178:HIS:CD2	2:B:221:LYS:HB2	2.52	0.45
2:B:331:LYS:NZ	2:B:333:ASP:OD1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:267:SER:OG	2:B:273:TRP:CD1	2.68	0.45
1:A:1243:LEU:HA	1:A:1243:LEU:HD12	1.80	0.44
2:B:63:SER:HB2	2:B:90:ILE:HG21	1.99	0.44
2:B:138:ASN:HD21	2:B:143:LEU:HB2	1.79	0.44
2:B:287:ASN:CG	2:B:290:THR:CG2	2.88	0.44
2:B:186:ILE:HG22	2:B:198:TRP:HD1	1.81	0.44
2:B:199:ASP:HB2	2:B:206:LEU:HD21	1.99	0.44
2:B:290:THR:OG1	2:B:292:GLU:OE1	2.32	0.44
1:A:1322:MET:CG	1:A:1323:GLU:H	2.29	0.44
2:B:44:HIS:NE2	2:B:70:LYS:HG3	2.32	0.44
2:B:73:GLY:CA	2:B:78:LYS:H	2.28	0.44
2:B:106:SER:O	2:B:132:VAL:HG22	2.17	0.44
2:B:153:VAL:HG12	2:B:154:ARG:N	2.32	0.44
1:A:1160:LEU:HB3	1:A:1179:ASP:O	2.17	0.44
1:A:1300:VAL:HG22	1:A:1309:TYR:HB2	2.00	0.44
2:B:149:PHE:O	2:B:149:PHE:HD1	2.00	0.44
1:A:1077:ALA:HB2	1:A:1307:VAL:HG21	2.00	0.44
1:A:1163:LEU:HD21	1:A:1205:ILE:CG2	2.45	0.44
2:B:34:ASN:OD1	2:B:34:ASN:N	2.51	0.43
2:B:185:LEU:HD13	2:B:197:ILE:CG2	2.47	0.43
2:B:196:ARG:HD3	2:B:208:THR:HG23	1.99	0.43
1:A:1088:GLU:HA	1:A:1096:PHE:CZ	2.53	0.43
1:A:1248:SER:HB2	1:A:1250:GLN:HG3	2.01	0.43
2:B:235:ASP:OD1	2:B:235:ASP:N	2.50	0.43
2:B:73:GLY:O	2:B:77:GLY:CA	2.66	0.43
1:A:1151:LEU:CD2	1:A:1182:VAL:HG11	2.38	0.43
2:B:146:SER:O	2:B:153:VAL:HA	2.18	0.43
1:A:1207:THR:HG23	1:A:1208:GLY:N	2.34	0.43
1:A:1225:ARG:HH22	3:A:1401:IMD:H4	1.82	0.43
2:B:186:ILE:O	2:B:197:ILE:HA	2.18	0.43
1:A:1098:CYS:HB2	1:A:1356:ASP:OD2	2.18	0.43
2:B:300:HIS:HA	2:B:328:LYS:NZ	2.34	0.43
1:A:1185:SER:HA	1:A:1230:PHE:CD2	2.54	0.43
1:A:1228:ALA:CB	1:A:1239:ASN:HB2	2.49	0.43
2:B:35:TYR:CZ	2:B:316:ILE:HG13	2.54	0.43
2:B:149:PHE:CE1	2:B:173:PRO:HG3	2.54	0.43
2:B:291:LYS:O	2:B:291:LYS:CG	2.66	0.43
1:A:1276:ASN:HD22	1:A:1277:THR:H	1.66	0.42
2:B:94:ALA:O	2:B:102:LEU:HA	2.19	0.42
2:B:110:THR:HG21	2:B:124:THR:HG23	2.01	0.42
2:B:228:TYR:HB3	2:B:240:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:250:LYS:HE3	2:B:289:GLN:HA	2.01	0.42
2:B:210:ILE:HD12	2:B:210:ILE:N	2.34	0.42
2:B:280:ASP:OD2	2:B:284:TYR:OH	2.38	0.42
2:B:331:LYS:HD2	2:B:332:SER:C	2.45	0.42
1:A:1214:LEU:HD22	1:A:1244:TRP:CE3	2.55	0.42
1:A:1335:ARG:HD2	4:A:1553:HOH:O	2.19	0.42
2:B:101:LEU:HA	2:B:114:TRP:O	2.18	0.42
2:B:35:TYR:CE1	2:B:316:ILE:HG13	2.54	0.42
2:B:132:VAL:O	2:B:132:VAL:CG2	2.67	0.42
1:A:1161:SER:HB3	1:A:1182:VAL:HG21	2.02	0.42
1:A:1262:ILE:CD1	1:A:1262:ILE:N	2.82	0.42
2:B:185:LEU:HD13	2:B:197:ILE:HG21	2.02	0.42
2:B:234:LEU:O	2:B:258:GLU:HA	2.20	0.42
1:A:1304:THR:OG1	1:A:1306:THR:HG23	2.20	0.42
1:A:1190:ASP:HA	1:A:1205:ILE:CD1	2.50	0.42
1:A:1321:LEU:HD22	1:A:1321:LEU:N	2.35	0.42
2:B:170:HIS:CG	2:B:190:SER:HB2	2.54	0.42
2:B:187:VAL:HG21	2:B:220:VAL:CG2	2.50	0.42
2:B:284:TYR:C	2:B:285:ILE:HD12	2.44	0.42
2:B:286:TRP:HA	2:B:294:VAL:HG12	2.02	0.42
1:A:1321:LEU:O	1:A:1322:MET:HB3	2.19	0.42
1:A:1158:GLN:N	1:A:1158:GLN:OE1	2.53	0.42
2:B:257:ASN:HA	2:B:279:GLU:CD	2.44	0.42
2:B:257:ASN:HA	2:B:279:GLU:OE1	2.19	0.42
2:B:306:SER:O	2:B:307:THR:HG23	2.20	0.42
2:B:179:PHE:CE1	2:B:186:ILE:HG12	2.55	0.41
2:B:281:ASN:OD1	2:B:281:ASN:C	2.63	0.41
2:B:51:VAL:O	2:B:52:LYS:HD3	2.19	0.41
2:B:142:ASN:ND2	2:B:143:LEU:HD12	2.35	0.41
1:A:1122:VAL:CG2	1:A:1386:LEU:HD13	2.49	0.41
1:A:1173:LYS:HD2	4:A:1551:HOH:O	2.19	0.41
1:A:1375:MET:SD	1:A:1375:MET:N	2.93	0.41
2:B:81:LYS:H	2:B:81:LYS:HG2	1.48	0.41
2:B:207:LYS:NZ	2:B:244:SER:HA	2.35	0.41
2:B:225:ASN:C	2:B:225:ASN:OD1	2.63	0.41
2:B:42:ALA:O	2:B:72:TRP:HH2	2.03	0.41
2:B:78:LYS:HE2	2:B:78:LYS:CA	2.50	0.41
2:B:187:VAL:CG2	2:B:220:VAL:CG2	2.98	0.41
2:B:314:ASN:HB2	2:B:332:SER:O	2.20	0.41
1:A:1134:HIS:CD2	1:A:1138:ILE:CD1	2.98	0.41
1:A:1182:VAL:HG13	1:A:1192:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1228:ALA:HB2	1:A:1239:ASN:HB2	2.02	0.41
1:A:1118:LYS:HE2	1:A:1130:SER:OG	2.21	0.41
2:B:86:HIS:HE1	2:B:110:THR:CG2	2.34	0.41
2:B:145:VAL:HG22	2:B:177:VAL:CG2	2.51	0.41
1:A:1207:THR:HG23	1:A:1209:ASN:N	2.14	0.41
2:B:227:LYS:HG2	2:B:228:TYR:CZ	2.56	0.41
1:A:1083:ILE:HB	1:A:1386:LEU:O	2.21	0.41
2:B:255:HIS:HD2	2:B:286:TRP:CZ2	2.39	0.41
2:B:280:ASP:O	2:B:282:LEU:HG	2.21	0.41
2:B:286:TRP:CA	2:B:294:VAL:HG12	2.51	0.41
2:B:44:HIS:CE1	2:B:64:SER:HB2	2.56	0.41
2:B:71:ILE:O	2:B:80:GLU:HB3	2.20	0.41
2:B:71:ILE:HB	2:B:80:GLU:HB3	2.03	0.40
2:B:145:VAL:HG22	2:B:177:VAL:CB	2.50	0.40
2:B:223:SER:HA	2:B:266:PHE:HE2	1.77	0.40
2:B:35:TYR:CD1	2:B:332:SER:HB3	2.57	0.40
2:B:313:GLU:CB	2:B:315:ILE:HD11	2.51	0.40
1:A:1099:CYS:HB3	1:A:1369:ILE:HD11	2.02	0.40
1:A:1117:LEU:HD11	1:A:1141:LEU:HD21	2.04	0.40
2:B:86:HIS:CE1	2:B:106:SER:HB3	2.56	0.40
2:B:180:ASN:ND2	2:B:183:GLY:H	2.19	0.40
2:B:219:PHE:CG	2:B:220:VAL:N	2.89	0.40
1:A:1161:SER:CB	1:A:1182:VAL:HG21	2.51	0.40
2:B:191:TYR:O	2:B:216:PRO:HB3	2.22	0.40
2:B:331:LYS:C	2:B:331:LYS:CD	2.95	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	301/338 (89%)	275 (91%)	25 (8%)	1 (0%)	36 67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	303/329 (92%)	273 (90%)	30 (10%)	0	100	100
All	All	604/667 (91%)	548 (91%)	55 (9%)	1 (0%)	43	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1157	SER

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	270/297 (91%)	245 (91%)	25 (9%)	8	30
2	B	267/289 (92%)	247 (92%)	20 (8%)	12	39
All	All	537/586 (92%)	492 (92%)	45 (8%)	10	35

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1085	VAL
1	A	1114	THR
1	A	1136	SER
1	A	1158	GLN
1	A	1167	LYS
1	A	1168	SER
1	A	1169	VAL
1	A	1171	ASP
1	A	1177	THR
1	A	1183	GLU
1	A	1213	THR
1	A	1222	ASN
1	A	1239	ASN
1	A	1247	ARG
1	A	1272	GLU

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Mol	Chain	Res	Type
1	A	1291	VAL
1	A	1300	VAL
1	A	1306	THR
1	A	1321	LEU
1	A	1323	GLU
1	A	1332	SER
1	A	1357	LEU
1	A	1361	THR
1	A	1363	ASP
1	A	1369	ILE
2	B	34	ASN
2	B	41	LEU
2	B	44	HIS
2	B	48	VAL
2	B	54	SER
2	B	84	SER
2	B	86	HIS
2	B	88	LEU
2	B	91[A]	SER
2	B	91[B]	SER
2	B	98	ASP
2	B	129	SER
2	B	134	CYS
2	B	202	SER
2	B	213	ASP
2	B	237	THR
2	B	242	ASP
2	B	298	GLN
2	B	301	THR
2	B	315	ILE

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

Mol	Chain	Res	Type
1	A	1121	ASN
1	A	1132	ASN
1	A	1135	ASN
1	A	1216	ASN
1	A	1239	ASN
1	A	1253	HIS
1	A	1314	GLN
1	A	1353	ASN

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Mol	Chain	Res	Type
2	B	86	HIS
2	B	255	HIS
2	B	295	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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	$\# Z > 2$
3	IMD	A	1401	-	5,5,5	0.82	0	5,5,5	0.49	0

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
3	IMD	A	1401	-	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

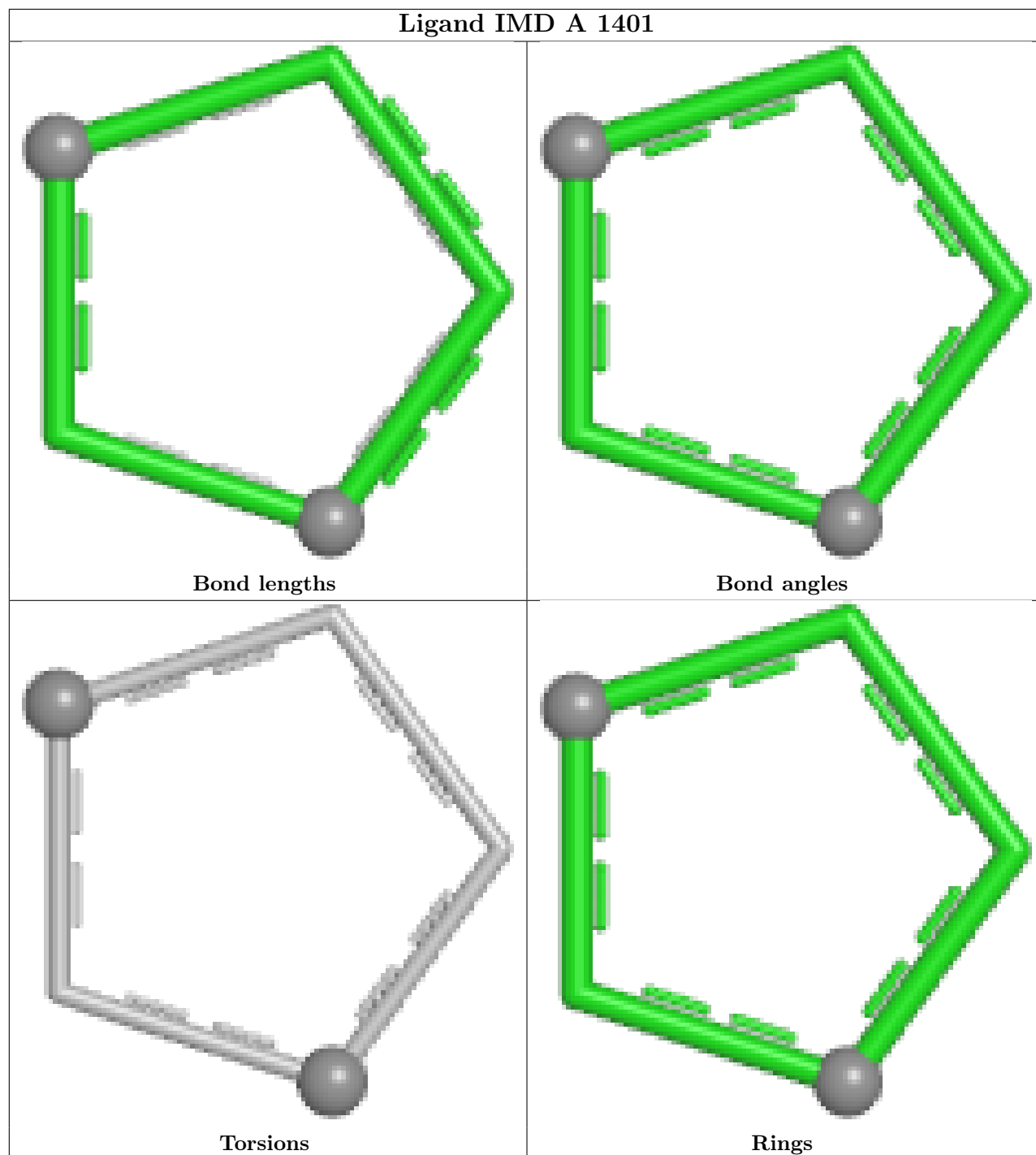
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1401	IMD	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	307/338 (90%)	-0.24	1 (0%) 90 82	50, 68, 96, 137	0
2	B	304/329 (92%)	0.14	4 (1%) 75 57	58, 113, 138, 155	1 (0%)
All	All	611/667 (91%)	-0.05	5 (0%) 82 67	50, 92, 135, 155	1 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	101	LEU	3.0
2	B	144	ILE	2.5
1	A	1321	LEU	2.3
2	B	316	ILE	2.2
2	B	186	ILE	2.1

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](#)

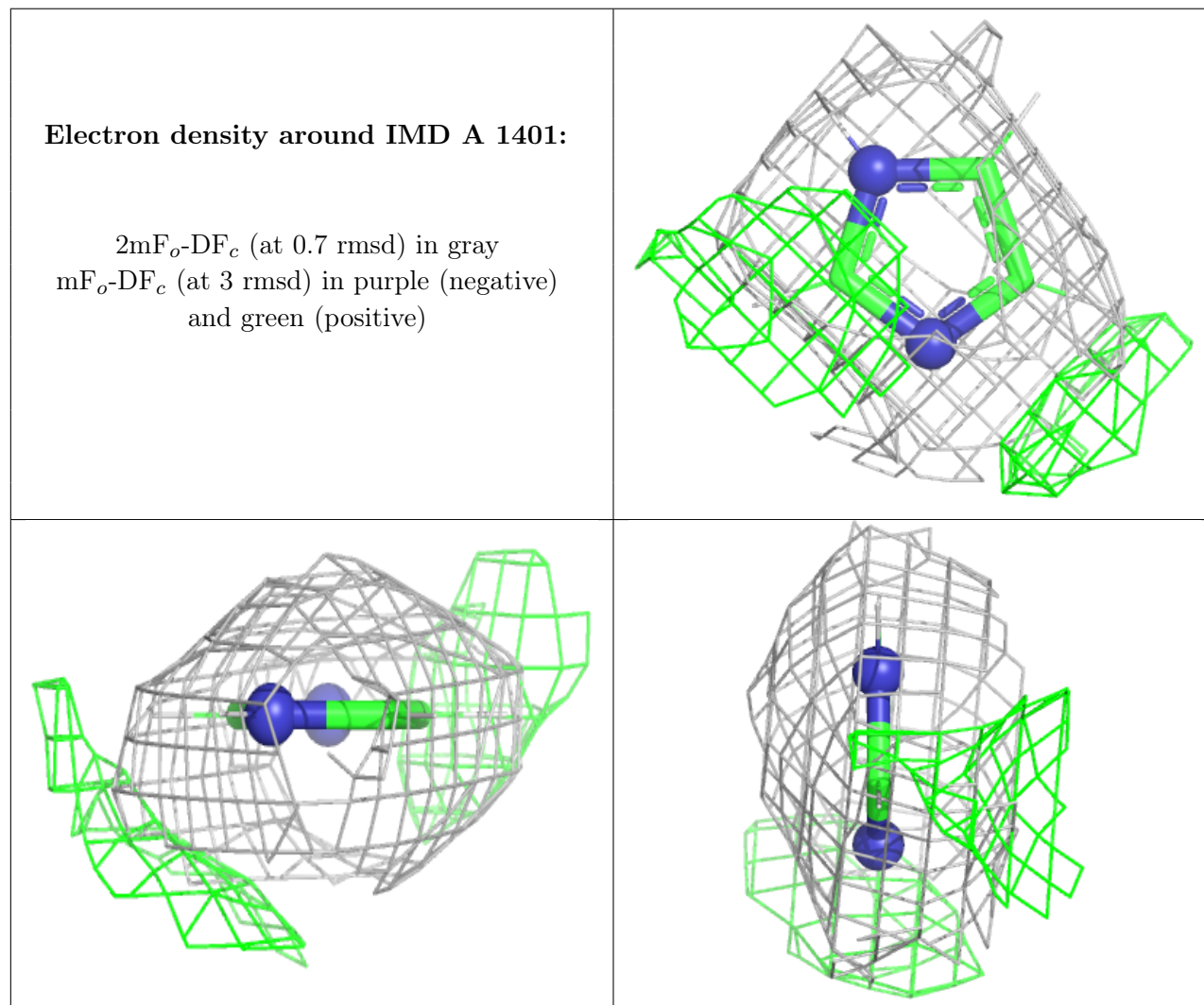
There are no oligosaccharides in this entry.

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. 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	B-factors($\text{\AA}^2$)	Q<0.9
3	IMD	A	1401	5/5	0.61	0.17	89,95,113,114	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers ⓘ

There are no such residues in this entry.