



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 04:44 pm BST

PDB ID : 6UH4  
Title : B. theta Bile Salt Hydrolase with covalent inhibitor  
Authors : Seegar, T.C.M.  
Deposited on : 2019-09-26  
Resolution : 3.51 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

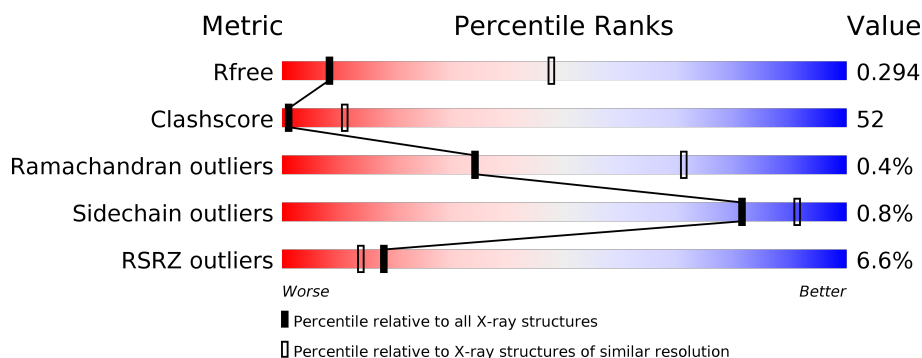
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.51 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))
$R_{free}$	130704	1161 (3.60-3.44)
Clashscore	141614	1244 (3.60-3.44)
Ramachandran outliers	138981	1206 (3.60-3.44)
Sidechain outliers	138945	1207 (3.60-3.44)
RSRZ outliers	127900	1080 (3.60-3.44)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	336	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 34%, green 63%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>34%</span> <span>63%</span> <span>••</span> </div> </div>
1	B	336	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 30%, green 66%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>30%</span> <span>66%</span> <span>••</span> </div> </div>
1	C	336	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 12%, orange 1%, yellow 32%, green 62%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>12%</span> <span>32%</span> <span>62%</span> <span>• 5%</span> </div> </div>
1	D	336	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 10%, orange 1%, yellow 29%, green 66%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>10%</span> <span>29%</span> <span>66%</span> <span>5%</span> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10290 atoms, of which 41 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 Choloylglycine hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	0	0
			2597	1653	437	491	16			
1	B	326	Total	C	N	O	S	0	0	0
			2574	1637	434	488	15			
1	C	319	Total	C	N	O	S	0	0	0
			2525	1608	423	480	14			
1	D	319	Total	C	N	O	S	0	0	0
			2525	1608	423	480	14			

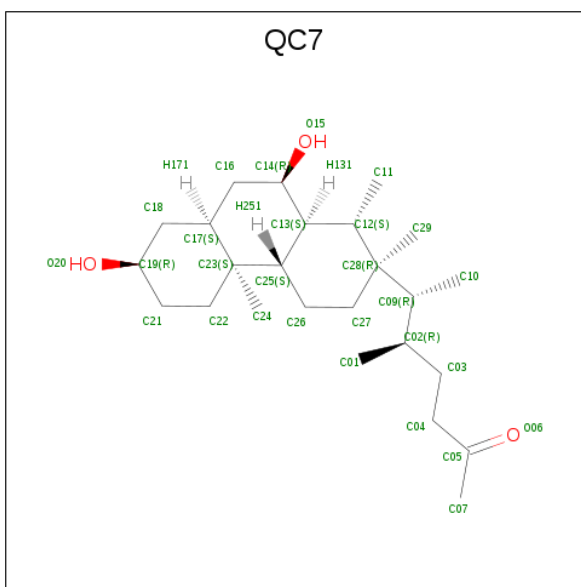
There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A0P0ENF5
A	329	LEU	-	expression tag	UNP A0A0P0ENF5
A	330	GLU	-	expression tag	UNP A0A0P0ENF5
A	331	HIS	-	expression tag	UNP A0A0P0ENF5
A	332	HIS	-	expression tag	UNP A0A0P0ENF5
A	333	HIS	-	expression tag	UNP A0A0P0ENF5
A	334	HIS	-	expression tag	UNP A0A0P0ENF5
A	335	HIS	-	expression tag	UNP A0A0P0ENF5
A	336	HIS	-	expression tag	UNP A0A0P0ENF5
B	1	MET	-	initiating methionine	UNP A0A0P0ENF5
B	329	LEU	-	expression tag	UNP A0A0P0ENF5
B	330	GLU	-	expression tag	UNP A0A0P0ENF5
B	331	HIS	-	expression tag	UNP A0A0P0ENF5
B	332	HIS	-	expression tag	UNP A0A0P0ENF5
B	333	HIS	-	expression tag	UNP A0A0P0ENF5
B	334	HIS	-	expression tag	UNP A0A0P0ENF5
B	335	HIS	-	expression tag	UNP A0A0P0ENF5
B	336	HIS	-	expression tag	UNP A0A0P0ENF5
C	1	MET	-	initiating methionine	UNP A0A0P0ENF5
C	329	LEU	-	expression tag	UNP A0A0P0ENF5
C	330	GLU	-	expression tag	UNP A0A0P0ENF5

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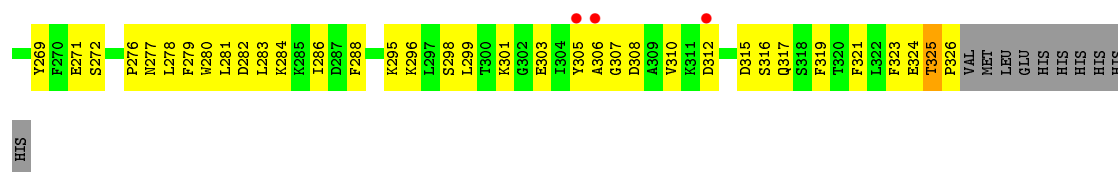
Chain	Residue	Modelled	Actual	Comment	Reference
C	331	HIS	-	expression tag	UNP A0A0P0ENF5
C	332	HIS	-	expression tag	UNP A0A0P0ENF5
C	333	HIS	-	expression tag	UNP A0A0P0ENF5
C	334	HIS	-	expression tag	UNP A0A0P0ENF5
C	335	HIS	-	expression tag	UNP A0A0P0ENF5
C	336	HIS	-	expression tag	UNP A0A0P0ENF5
D	1	MET	-	initiating methionine	UNP A0A0P0ENF5
D	329	LEU	-	expression tag	UNP A0A0P0ENF5
D	330	GLU	-	expression tag	UNP A0A0P0ENF5
D	331	HIS	-	expression tag	UNP A0A0P0ENF5
D	332	HIS	-	expression tag	UNP A0A0P0ENF5
D	333	HIS	-	expression tag	UNP A0A0P0ENF5
D	334	HIS	-	expression tag	UNP A0A0P0ENF5
D	335	HIS	-	expression tag	UNP A0A0P0ENF5
D	336	HIS	-	expression tag	UNP A0A0P0ENF5

- Molecule 2 is (5R,6R)-6-[(1S,2R,4aS,4bS,7R,8aS,10R,10aS)-7,10-dihydroxy-1,2,4b-trimethyl tetradecahydrophenanthren-2-yl]-5-methylheptan-2-one (three-letter code: QC7) (formula: C<sub>25</sub>H<sub>44</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by author).

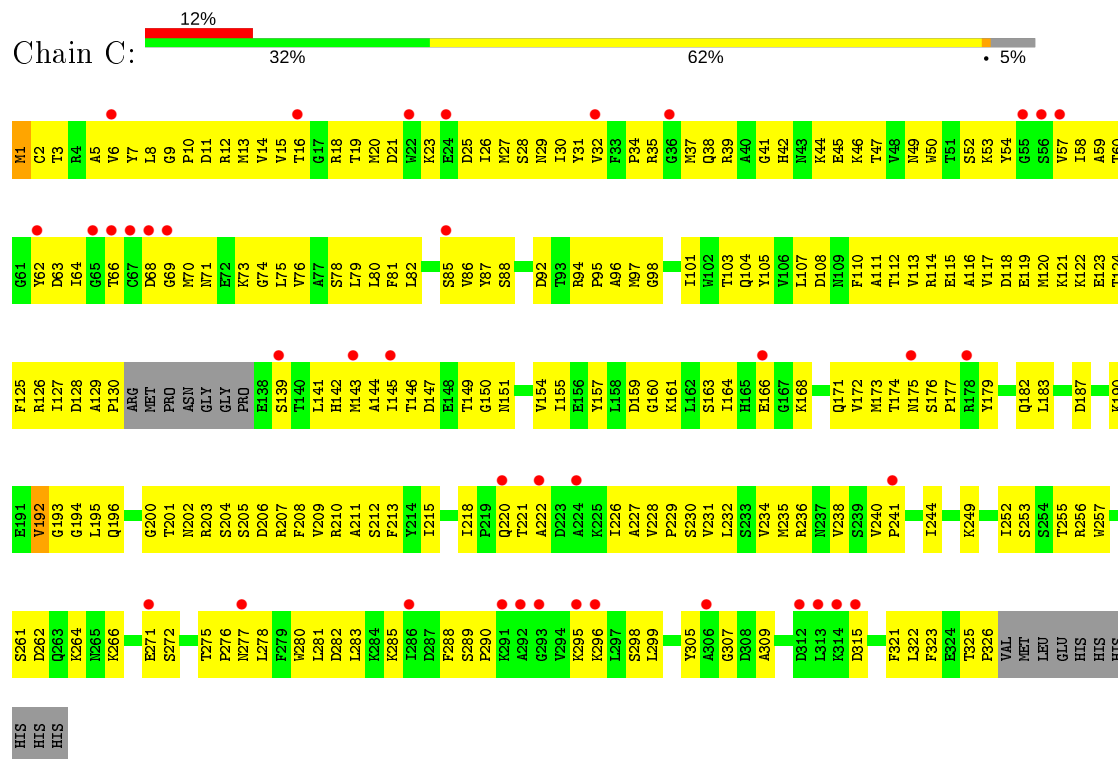


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	H	O	0	0
			69	25	41	3		





• Molecule 1: Cholylglycine hydrolase



• Molecule 1: Cholylglycine hydrolase



HIS  
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.58Å 99.52Å 162.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.29 – 3.51 49.29 – 3.51	Depositor EDS
% Data completeness (in resolution range)	97.0 (49.29-3.51) 94.8 (49.29-3.51)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.62 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, $R_{free}$	0.238 , 0.292 0.244 , 0.294	Depositor DCC
$R_{free}$ test set	1840 reflections (9.18%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	142.4	Xtriage
Anisotropy	0.563	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 163.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.35$ , $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	0.226 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10290	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	187.0	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.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 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: QC7

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	0.25	0/2658	0.41	0/3603
1	B	0.26	0/2635	0.43	0/3572
1	C	0.25	0/2583	0.44	2/3500 (0.1%)
1	D	0.24	0/2583	0.42	0/3500
All	All	0.25	0/10459	0.43	2/14175 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	203	ARG	NE-CZ-NH1	-5.35	117.62	120.30
1	C	203	ARG	NE-CZ-NH2	5.03	122.82	120.30

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2597	0	2581	244	2
1	B	2574	0	2551	314	2
1	C	2525	0	2503	245	0
1	D	2525	0	2503	277	0
2	B	28	41	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10249	41	10138	1054	2

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 52.

All (1054) 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:C:241:PRO:HB2	1:C:244:ILE:HD11	1.29	1.15
1:B:86:VAL:HB	1:B:159:ASP:HA	1.28	1.14
1:B:42:HIS:HB3	1:B:47:THR:HG21	1.29	1.12
1:B:241:PRO:HB2	1:B:244:ILE:HD11	1.23	1.09
1:B:94:ARG:HD2	1:B:95:PRO:HD2	1.36	1.07
1:D:130:PRO:HB2	1:D:325:THR:HG23	1.34	1.05
1:B:236:ARG:HG2	1:B:258:ARG:HH22	1.13	1.02
1:D:85:SER:HB3	1:D:140:THR:HB	1.37	1.02
1:B:58:ILE:HG22	1:B:69:GLY:HA3	1.45	0.98
1:A:236:ARG:HD3	1:B:236:ARG:HD3	1.42	0.95
1:B:42:HIS:HB3	1:B:47:THR:CG2	1.96	0.95
1:C:42:HIS:H	1:C:47:THR:HG21	1.31	0.94
1:D:103:THR:HA	1:D:143:MET:HE1	1.50	0.93
1:D:77:ALA:HA	1:D:145:ILE:HG13	1.48	0.93
1:A:3:THR:HG23	1:A:174:THR:HG22	1.48	0.92
1:A:202:ASN:O	1:A:207:ARG:NH1	2.06	0.89
1:D:151:ASN:HA	1:D:168:LYS:HG2	1.55	0.88
1:B:70:MET:HE3	1:B:74:GLY:HA2	1.54	0.88
1:C:211:ALA:HB2	1:C:238:VAL:HG11	1.55	0.88
1:B:283:LEU:HA	1:B:286:ILE:HD12	1.55	0.88
1:A:241:PRO:HB2	1:A:244:ILE:HD11	1.55	0.88
1:B:92:ASP:HB3	1:B:126:ARG:HD3	1.53	0.88
1:C:30:ILE:HD13	1:C:59:ALA:HA	1.55	0.87
1:C:172:VAL:HG11	1:C:212:SER:HB2	1.57	0.87
1:C:58:ILE:HG22	1:C:69:GLY:HA3	1.54	0.87
1:D:241:PRO:HB2	1:D:244:ILE:HD11	1.56	0.87
1:B:198:LEU:HD11	1:B:210:ARG:HG2	1.58	0.86
1:A:131:ARG:O	1:A:325:THR:HG21	1.76	0.86
1:C:46:LYS:H	1:C:46:LYS:HD2	1.42	0.85
1:C:117:VAL:HG12	1:C:121:LYS:HE2	1.57	0.85
1:B:71:ASN:HD21	1:B:75:LEU:HB3	1.39	0.85
1:B:130:PRO:HG2	1:B:325:THR:HG22	1.58	0.84
1:A:42:HIS:HB2	1:A:47:THR:HG21	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:LYS:HE2	1:D:252:ILE:HG12	1.61	0.83
1:D:58:ILE:HG22	1:D:69:GLY:HA3	1.60	0.83
1:C:66:THR:HG21	1:C:104:GLN:HB2	1.57	0.83
1:B:228:VAL:HB	1:B:229:PRO:HD3	1.61	0.82
1:A:58:ILE:HD13	1:A:66:THR:HG22	1.62	0.82
1:D:97:MET:O	1:D:128:ASP:N	2.13	0.82
1:D:38:GLN:HA	1:D:51:THR:HA	1.62	0.81
1:A:60:THR:HG21	1:A:63:ASP:HA	1.63	0.81
1:B:130:PRO:HG2	1:B:325:THR:CG2	2.11	0.81
1:B:10:PRO:HB2	1:B:222:ALA:HB2	1.62	0.80
1:A:192:VAL:HG11	1:A:197:MET:HB3	1.64	0.79
1:D:70:MET:HE1	1:D:266:LYS:HA	1.65	0.79
1:B:26:ILE:HD13	1:B:257:TRP:HE1	1.47	0.78
1:C:155:ILE:HG12	1:C:164:ILE:HG12	1.64	0.78
1:A:228:VAL:HB	1:A:229:PRO:HD3	1.66	0.78
1:A:271:GLU:HB2	1:A:278:LEU:HD13	1.66	0.78
1:A:130:PRO:HB2	1:A:325:THR:HG22	1.66	0.77
1:D:35:ARG:HH11	1:D:288:PHE:HB2	1.50	0.77
1:B:199:PRO:HB2	1:B:206:ASP:OD1	1.84	0.77
1:B:174:THR:HG22	1:B:175:ASN:H	1.50	0.77
1:A:276:PRO:HB2	1:B:278:LEU:HB3	1.67	0.76
1:B:56:SER:HB3	1:B:71:ASN:HA	1.66	0.76
1:B:236:ARG:HG2	1:B:258:ARG:NH2	1.97	0.76
1:C:95:PRO:HD2	1:C:124:THR:O	1.86	0.76
1:B:79:LEU:HD12	1:B:143:MET:HG3	1.67	0.76
1:D:26:ILE:HD13	1:D:257:TRP:HE1	1.50	0.76
1:B:42:HIS:CB	1:B:47:THR:HG21	2.13	0.75
1:B:174:THR:H	1:B:182:GLN:HE22	1.34	0.75
1:A:70:MET:CE	1:A:74:GLY:HA2	2.17	0.74
1:C:120:MET:HE2	1:C:120:MET:HA	1.69	0.74
1:D:228:VAL:HB	1:D:229:PRO:HD3	1.69	0.74
1:D:20:MET:HE1	1:D:22:TRP:HB2	1.69	0.74
1:C:114:ARG:HD2	1:C:166:GLU:OE2	1.88	0.74
1:A:75:LEU:HG	1:A:145:ILE:HD11	1.69	0.74
1:B:74:GLY:HA3	1:B:148:GLU:HB3	1.71	0.73
1:D:113:VAL:HG21	1:D:151:ASN:HB3	1.68	0.73
1:A:283:LEU:HA	1:A:286:ILE:HD12	1.71	0.73
1:D:36:GLY:N	1:D:52:SER:O	2.19	0.73
1:D:151:ASN:CA	1:D:168:LYS:HG2	2.18	0.73
1:D:71:ASN:ND2	1:D:75:LEU:HB3	2.03	0.73
1:A:20:MET:HE2	1:A:26:ILE:HD12	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:ILE:HG12	1:D:164:ILE:HG12	1.71	0.73
1:C:325:THR:HB	1:C:326:PRO:HD2	1.71	0.72
1:C:42:HIS:N	1:C:47:THR:HG21	2.04	0.72
1:C:60:THR:HG21	1:C:63:ASP:HA	1.71	0.72
1:D:89:LEU:HG	1:D:160:GLY:HA3	1.71	0.72
1:B:87:TYR:HB2	1:B:128:ASP:OD1	1.89	0.72
1:B:45:GLU:O	1:B:47:THR:HG23	1.89	0.72
1:A:70:MET:HE3	1:A:74:GLY:HA2	1.72	0.72
1:A:117:VAL:HG12	1:A:121:LYS:HE2	1.71	0.72
1:A:59:ALA:HB3	1:A:68:ASP:OD1	1.90	0.72
1:C:80:LEU:O	1:C:142:HIS:N	2.21	0.72
1:C:88:SER:HB2	1:C:92:ASP:CB	2.20	0.72
1:D:71:ASN:HD21	1:D:75:LEU:HB3	1.54	0.72
1:B:73:LYS:HG3	1:B:111:ALA:HB1	1.71	0.72
1:B:71:ASN:ND2	1:B:75:LEU:HB3	2.04	0.71
1:B:18:ARG:HD2	1:B:78:SER:HB3	1.73	0.71
1:D:174:THR:HG21	1:D:208:PHE:HB2	1.71	0.71
1:B:70:MET:CE	1:B:263:GLN:HA	2.20	0.71
1:D:154:VAL:HG11	1:D:179:TYR:CD2	2.26	0.71
1:B:23:LYS:HA	1:B:253:SER:HA	1.73	0.71
1:B:70:MET:HB2	1:B:76:VAL:HG22	1.72	0.71
1:C:151:ASN:HA	1:C:168:LYS:HG2	1.73	0.71
1:C:195:LEU:HA	1:C:213:PHE:CZ	2.26	0.71
1:D:201:THR:HG22	1:D:202:ASN:H	1.55	0.71
1:B:70:MET:HE1	1:B:266:LYS:HA	1.71	0.70
1:C:46:LYS:O	1:C:96:ALA:N	2.24	0.70
1:D:64:ILE:HG23	1:D:320:THR:O	1.92	0.70
1:C:282:ASP:HB3	1:C:285:LYS:HE2	1.74	0.70
1:C:98:GLY:HA3	1:C:323:PHE:CD1	2.27	0.70
1:A:192:VAL:CG1	1:A:197:MET:HB3	2.21	0.69
1:B:172:VAL:HG13	1:B:208:PHE:CE2	2.27	0.69
1:B:70:MET:CE	1:B:74:GLY:HA2	2.22	0.69
1:A:194:GLY:HA2	1:A:198:LEU:HD21	1.74	0.69
1:B:235:MET:HA	1:B:235:MET:HE2	1.73	0.69
1:A:71:ASN:ND2	1:A:110:PHE:O	2.25	0.69
1:A:276:PRO:HB3	1:B:278:LEU:HD23	1.74	0.69
1:C:35:ARG:CZ	1:C:290:PRO:HD3	2.22	0.69
1:A:64:ILE:O	1:A:321:PHE:HA	1.92	0.69
1:B:325:THR:N	1:B:326:PRO:HD3	2.07	0.69
1:A:126:ARG:HG2	1:A:127:ILE:H	1.57	0.69
1:D:271:GLU:HB2	1:D:278:LEU:HD13	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:VAL:O	1:A:234:VAL:HG22	1.91	0.69
1:B:110:PHE:CE1	1:B:116:ALA:HA	2.28	0.69
1:B:87:TYR:C	1:B:160:GLY:HA2	2.12	0.69
1:A:132:MET:SD	1:A:136:GLY:HA3	2.32	0.69
1:B:1:MET:HB3	1:B:175:ASN:OD1	1.93	0.69
1:B:64:ILE:O	1:B:321:PHE:HA	1.92	0.69
1:B:76:VAL:HG21	1:B:261:SER:HB2	1.74	0.69
1:B:80:LEU:HB2	1:B:173:MET:HE3	1.74	0.68
1:B:174:THR:HG21	1:B:204:SER:O	1.93	0.68
1:B:239:SER:OG	1:B:255:THR:HG21	1.93	0.68
1:D:155:ILE:HG12	1:D:164:ILE:HG23	1.74	0.68
1:D:152:THR:HB	1:D:170:TYR:O	1.93	0.68
1:A:71:ASN:OD1	1:A:75:LEU:HB3	1.93	0.68
1:A:232:LEU:HD12	1:A:235:MET:HB2	1.75	0.68
1:B:246:THR:HB	1:B:247:PRO:HD2	1.74	0.68
1:B:98:GLY:HA3	1:B:323:PHE:CD1	2.28	0.68
1:C:70:MET:CE	1:C:74:GLY:HA2	2.24	0.68
1:D:296:LYS:HB3	1:D:316:SER:HB3	1.74	0.68
1:C:95:PRO:HB2	1:C:125:PHE:HB3	1.75	0.68
1:A:174:THR:HG23	1:A:208:PHE:HD1	1.59	0.67
1:D:156:GLU:O	1:D:163:SER:HB3	1.93	0.67
1:D:98:GLY:HA3	1:D:323:PHE:CD1	2.29	0.67
1:A:80:LEU:O	1:A:141:LEU:HB3	1.94	0.67
1:C:41:GLY:HA2	1:C:101:ILE:HG21	1.76	0.67
1:B:70:MET:CE	1:B:266:LYS:HA	2.24	0.67
1:D:98:GLY:HA3	1:D:323:PHE:HD1	1.59	0.67
1:C:42:HIS:CD2	1:C:45:GLU:HB2	2.30	0.67
1:D:110:PHE:CE1	1:D:116:ALA:HA	2.30	0.67
1:A:201:THR:CG2	1:A:203:ARG:HG3	2.25	0.67
1:D:39:ARG:NH1	1:D:52:SER:OG	2.28	0.66
1:B:156:GLU:O	1:B:163:SER:N	2.27	0.66
1:A:86:VAL:HB	1:A:159:ASP:HA	1.77	0.66
1:A:38:GLN:HA	1:A:50:TRP:O	1.94	0.66
1:A:203:ARG:HH21	1:B:196:GLN:HA	1.60	0.66
1:D:155:ILE:HG23	1:D:164:ILE:HG12	1.77	0.66
1:A:249:LYS:HE2	1:A:252:ILE:HG12	1.77	0.66
1:B:92:ASP:CB	1:B:126:ARG:HD3	2.23	0.66
1:C:2:CYS:SG	1:C:20:MET:HA	2.36	0.66
1:C:15:VAL:HG22	1:C:262:ASP:HA	1.77	0.66
1:D:20:MET:CE	1:D:22:TRP:HB2	2.26	0.66
1:A:296:LYS:HE2	1:A:298:SER:HB2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:GLU:O	1:D:171:GLN:HG3	1.94	0.66
1:D:7:TYR:HB2	1:D:215:ILE:HD11	1.77	0.66
1:D:103:THR:CA	1:D:143:MET:HE1	2.25	0.66
1:C:64:ILE:O	1:C:321:PHE:HA	1.96	0.66
1:C:82:LEU:HB2	1:C:142:HIS:CD2	2.31	0.66
1:A:35:ARG:O	1:A:290:PRO:HA	1.96	0.66
1:D:117:VAL:HG11	1:D:166:GLU:OE1	1.96	0.66
1:D:189:TRP:CD1	1:D:209:VAL:HG21	2.32	0.65
1:A:120:MET:HA	1:A:120:MET:CE	2.26	0.65
1:A:82:LEU:HD22	1:A:142:HIS:HD2	1.61	0.65
1:A:35:ARG:HG2	1:A:288:PHE:O	1.95	0.65
1:C:13:MET:HG2	1:C:222:ALA:HA	1.78	0.65
1:C:232:LEU:HG	1:C:236:ARG:HE	1.62	0.65
1:C:70:MET:HB2	1:C:76:VAL:HG22	1.78	0.65
1:A:227:ALA:O	1:A:231:VAL:HG23	1.95	0.65
1:B:56:SER:CB	1:B:71:ASN:HA	2.26	0.65
1:D:308:ASP:OD1	1:D:310:VAL:HG23	1.97	0.65
1:B:66:THR:OG1	1:B:103:THR:HB	1.97	0.65
1:B:189:TRP:O	1:B:192:VAL:HG12	1.97	0.65
1:B:97:MET:O	1:B:127:ILE:HA	1.96	0.65
1:A:203:ARG:HB2	1:A:206:ASP:OD1	1.96	0.65
1:B:98:GLY:HA3	1:B:323:PHE:CE1	2.32	0.65
1:C:86:VAL:O	1:C:157:TYR:HB3	1.96	0.65
1:C:231:VAL:O	1:C:235:MET:HG2	1.96	0.65
1:D:30:ILE:HD13	1:D:59:ALA:HA	1.78	0.64
1:D:81:PHE:HA	1:D:141:LEU:HG	1.77	0.64
1:C:95:PRO:HB2	1:C:125:PHE:CB	2.26	0.64
1:C:94:ARG:NH1	1:C:123:GLU:HB3	2.13	0.64
1:D:53:LYS:N	1:D:108:ASP:O	2.28	0.64
1:D:255:THR:HG23	1:D:273:THR:HG21	1.79	0.64
1:C:129:ALA:HB1	1:C:139:SER:HB2	1.79	0.64
1:A:211:ALA:HB2	1:A:238:VAL:HG11	1.77	0.64
1:B:2:CYS:H	1:B:175:ASN:HD21	1.45	0.64
1:B:236:ARG:CG	1:B:258:ARG:HH22	2.01	0.64
1:D:172:VAL:HG13	1:D:208:PHE:CE1	2.32	0.64
1:C:5:ALA:HA	1:C:171:GLN:O	1.98	0.64
1:C:34:PRO:HB3	1:C:289:SER:O	1.97	0.64
1:A:283:LEU:HA	1:A:286:ILE:CD1	2.27	0.64
1:B:37:MET:H	1:B:52:SER:HB3	1.63	0.64
1:D:20:MET:CE	1:D:26:ILE:HD12	2.28	0.64
1:A:130:PRO:HB2	1:A:325:THR:CG2	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:ARG:CD	1:B:95:PRO:HD2	2.21	0.63
1:C:7:TYR:OH	1:C:220:GLN:HA	1.98	0.63
1:D:204:SER:HA	1:D:207:ARG:NH2	2.13	0.63
1:A:113:VAL:O	1:A:117:VAL:HG23	1.99	0.63
1:C:280:TRP:CZ3	1:C:307:GLY:HA2	2.32	0.63
1:A:20:MET:HE1	1:A:22:TRP:HB2	1.81	0.63
1:C:80:LEU:HD22	1:C:173:MET:HE2	1.78	0.63
1:A:197:MET:HA	1:B:201:THR:CG2	2.28	0.63
1:D:82:LEU:HB2	1:D:142:HIS:CD2	2.33	0.63
1:D:244:ILE:HG22	1:D:252:ILE:HD12	1.80	0.63
1:B:61:GLY:O	1:B:64:ILE:HG12	1.98	0.63
1:B:186:ASN:OD1	1:B:190:LYS:HG3	1.99	0.63
1:B:296:LYS:CB	1:B:316:SER:HB2	2.28	0.63
1:B:20:MET:HG2	1:B:257:TRP:NE1	2.13	0.63
1:A:94:ARG:HH11	1:A:123:GLU:HG2	1.64	0.62
1:B:70:MET:SD	1:B:261:SER:HB3	2.39	0.62
1:D:18:ARG:HB3	1:D:259:SER:OG	1.98	0.62
1:A:211:ALA:O	1:A:215:ILE:HG22	1.99	0.62
1:A:221:THR:HG21	1:A:226:ILE:HD13	1.82	0.62
1:A:75:LEU:CD2	1:A:145:ILE:HD11	2.29	0.62
1:A:79:LEU:HD13	1:A:143:MET:HE2	1.81	0.62
1:A:272:SER:HB2	1:A:275:THR:HG23	1.81	0.62
1:A:75:LEU:CG	1:A:145:ILE:HD11	2.30	0.62
1:B:324:GLU:C	1:B:326:PRO:HD3	2.20	0.62
1:D:46:LYS:O	1:D:95:PRO:HA	1.99	0.62
1:B:39:ARG:HB2	1:B:50:TRP:CZ2	2.34	0.62
1:B:94:ARG:HD2	1:B:95:PRO:CD	2.24	0.62
1:A:131:ARG:N	1:A:325:THR:CG2	2.62	0.62
1:B:324:GLU:CB	1:B:326:PRO:HD3	2.30	0.62
1:A:94:ARG:NH1	1:A:123:GLU:HG2	2.15	0.61
1:B:242:PHE:HA	1:B:254:SER:HB3	1.82	0.61
1:C:95:PRO:O	1:C:125:PHE:HB2	2.00	0.61
1:C:71:ASN:ND2	1:C:110:PHE:O	2.32	0.61
1:A:308:ASP:OD1	1:A:310:VAL:HG23	1.99	0.61
1:A:102:TRP:O	1:A:106:VAL:HG23	2.00	0.61
1:A:58:ILE:HD12	1:A:58:ILE:O	2.00	0.61
1:D:199:PRO:O	1:D:210:ARG:HD2	2.00	0.61
1:C:175:ASN:HB3	1:C:204:SER:OG	2.00	0.61
1:D:26:ILE:CG2	1:D:256:ARG:HG2	2.31	0.61
1:A:11:ASP:O	1:A:264:LYS:HE2	2.00	0.61
1:A:29:ASN:HB2	1:A:63:ASP:OD1	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:MET:SD	1:B:145:ILE:HD11	2.41	0.61
1:B:82:LEU:HD22	1:B:156:GLU:OE1	2.01	0.61
1:D:262:ASP:OD2	1:D:265:ASN:HB2	2.01	0.61
1:B:123:GLU:OE2	1:B:162:LEU:HD22	2.00	0.61
1:B:18:ARG:HD2	1:B:78:SER:CB	2.31	0.61
1:C:113:VAL:O	1:C:117:VAL:HG23	2.00	0.61
1:C:53:LYS:N	1:C:108:ASP:O	2.34	0.61
1:D:56:SER:CB	1:D:71:ASN:HA	2.31	0.61
1:D:82:LEU:N	1:D:141:LEU:HA	2.16	0.61
1:B:179:TYR:HA	1:B:182:GLN:HB3	1.80	0.60
1:B:202:ASN:OD1	1:B:240:VAL:HG11	2.01	0.60
1:C:66:THR:OG1	1:C:103:THR:HB	2.00	0.60
1:D:70:MET:CE	1:D:74:GLY:HA2	2.31	0.60
1:A:199:PRO:HB2	1:A:206:ASP:OD2	2.00	0.60
1:D:241:PRO:O	1:D:244:ILE:HG12	2.01	0.60
1:B:234:VAL:O	1:B:238:VAL:HG22	2.01	0.60
1:C:88:SER:HB2	1:C:92:ASP:HB3	1.82	0.60
1:D:27:MET:HB2	1:D:62:TYR:CE1	2.35	0.60
1:D:4:ARG:HD2	1:D:78:SER:HB2	1.82	0.60
1:A:198:LEU:O	1:B:200:GLY:N	2.32	0.60
1:C:70:MET:HE2	1:C:74:GLY:HA2	1.82	0.60
1:C:46:LYS:O	1:C:95:PRO:HA	2.01	0.60
1:B:10:PRO:HD2	1:B:221:THR:C	2.21	0.60
1:C:8:LEU:HD23	1:C:14:VAL:HG13	1.84	0.60
1:B:81:PHE:CZ	1:B:138:GLU:HB3	2.36	0.60
1:B:113:VAL:HG21	1:B:151:ASN:O	2.01	0.60
1:C:272:SER:HB2	1:C:275:THR:HG23	1.84	0.60
1:D:70:MET:CE	1:D:266:LYS:HA	2.30	0.60
1:D:187:ASP:HA	1:D:190:LYS:NZ	2.17	0.60
1:D:32:VAL:HG22	1:D:57:VAL:HG22	1.84	0.60
1:A:110:PHE:CE1	1:A:116:ALA:HA	2.37	0.59
1:A:88:SER:OG	1:A:126:ARG:HD2	2.02	0.59
1:A:234:VAL:O	1:A:238:VAL:HG22	2.02	0.59
1:A:277:ASN:OD1	1:B:277:ASN:HB3	2.01	0.59
1:B:151:ASN:HA	1:B:168:LYS:HG2	1.83	0.59
1:B:47:THR:HA	1:B:95:PRO:HB2	1.83	0.59
1:D:52:SER:CB	1:D:108:ASP:HB2	2.32	0.59
1:A:20:MET:HG2	1:A:257:TRP:NE1	2.16	0.59
1:C:41:GLY:HA2	1:C:101:ILE:CG2	2.32	0.59
1:D:3:THR:HG23	1:D:174:THR:HG22	1.84	0.59
1:A:53:LYS:HB2	1:A:108:ASP:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:326:PRO:HA	1:D:324:GLU:HB2	1.83	0.59
1:D:145:ILE:O	1:D:152:THR:HG23	2.03	0.59
1:D:113:VAL:HG21	1:D:151:ASN:CB	2.30	0.59
1:D:283:LEU:HA	1:D:286:ILE:HD12	1.84	0.59
1:A:7:TYR:OH	1:A:220:GLN:HA	2.02	0.59
1:D:154:VAL:HG21	1:D:179:TYR:CE2	2.38	0.59
1:C:1:MET:N	1:C:1:MET:SD	2.74	0.59
1:D:158:LEU:O	1:D:158:LEU:HD12	2.02	0.59
1:D:256:ARG:HH12	1:D:274:LEU:HD12	1.68	0.59
1:B:144:ALA:HB2	1:B:173:MET:SD	2.41	0.59
1:B:70:MET:HE1	1:B:263:GLN:HA	1.84	0.59
1:C:68:ASP:OD1	1:C:69:GLY:N	2.36	0.59
1:B:42:HIS:HA	1:B:323:PHE:CE2	2.37	0.58
1:D:95:PRO:HD2	1:D:125:PHE:HA	1.85	0.58
1:B:235:MET:CA	1:B:235:MET:HE2	2.33	0.58
1:B:68:ASP:OD1	1:B:69:GLY:N	2.36	0.58
1:C:21:ASP:OD2	1:C:240:VAL:HG22	2.03	0.58
1:C:231:VAL:O	1:C:234:VAL:HG22	2.03	0.58
1:C:20:MET:HG2	1:C:257:TRP:NE1	2.18	0.58
1:A:214:TYR:CD2	1:B:241:PRO:HG2	2.38	0.58
1:B:21:ASP:OD1	1:B:255:THR:HA	2.03	0.58
1:C:112:THR:HG22	1:C:115:GLU:HG3	1.85	0.58
1:D:1:MET:HB2	1:D:175:ASN:ND2	2.19	0.58
1:D:176:SER:HB2	1:D:177:PRO:HA	1.86	0.58
1:D:35:ARG:O	1:D:290:PRO:HA	2.04	0.58
1:D:47:THR:HG22	1:D:48:VAL:H	1.68	0.58
1:B:214:TYR:O	1:B:218:ILE:HG23	2.04	0.58
1:D:241:PRO:HB2	1:D:244:ILE:CD1	2.32	0.58
1:C:176:SER:HB2	1:C:177:PRO:HA	1.85	0.58
1:C:235:MET:CE	1:C:235:MET:HA	2.34	0.58
1:C:60:THR:CG2	1:C:63:ASP:HA	2.33	0.58
1:A:85:SER:HB2	1:A:140:THR:HB	1.85	0.57
1:A:198:LEU:HD13	1:A:214:TYR:HE1	1.68	0.57
1:A:214:TYR:O	1:A:218:ILE:HG23	2.04	0.57
1:A:22:TRP:NE1	1:A:24:GLU:HG2	2.19	0.57
1:B:247:PRO:HG2	1:B:248:GLU:OE2	2.04	0.57
1:C:117:VAL:O	1:C:121:LYS:HG3	2.04	0.57
1:C:113:VAL:HG23	1:C:147:ASP:OD2	2.03	0.57
1:D:70:MET:HE3	1:D:74:GLY:HA2	1.85	0.57
1:B:99:ILE:HG22	1:B:129:ALA:HB2	1.84	0.57
1:B:82:LEU:HB2	1:B:142:HIS:ND1	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:HIS:HA	1:B:323:PHE:CD2	2.40	0.57
1:A:269:TYR:CD2	1:A:280:TRP:HB3	2.39	0.57
1:C:18:ARG:HD3	1:C:68:ASP:OD2	2.05	0.57
1:A:176:SER:HB2	1:A:177:PRO:HA	1.86	0.57
1:A:199:PRO:O	1:A:206:ASP:HB3	2.05	0.57
1:B:77:ALA:HA	1:B:145:ILE:HG13	1.86	0.57
1:B:158:LEU:N	1:B:161:LYS:O	2.35	0.57
1:D:130:PRO:HB2	1:D:325:THR:CG2	2.22	0.57
1:A:241:PRO:HB2	1:A:244:ILE:CD1	2.33	0.57
1:B:16:THR:O	1:B:260:VAL:HA	2.04	0.57
1:B:70:MET:CB	1:B:76:VAL:HG22	2.34	0.57
1:C:179:TYR:O	1:C:183:LEU:HG	2.04	0.57
1:B:266:LYS:HE2	1:B:284:LYS:HG2	1.86	0.57
1:B:276:PRO:HG2	1:B:277:ASN:ND2	2.20	0.57
1:C:7:TYR:O	1:C:14:VAL:HA	2.04	0.57
1:C:204:SER:HA	1:C:207:ARG:CZ	2.34	0.57
1:D:26:ILE:HG22	1:D:256:ARG:HG2	1.84	0.57
1:A:271:GLU:HB2	1:A:278:LEU:CD1	2.34	0.57
1:B:79:LEU:HD23	1:B:141:LEU:HD11	1.86	0.57
1:B:81:PHE:HZ	1:B:138:GLU:HB3	1.69	0.57
1:D:77:ALA:H	1:D:107:LEU:HD21	1.68	0.57
1:D:2:CYS:N	1:D:175:ASN:HD21	2.03	0.57
1:B:13:MET:HA	1:B:264:LYS:HD2	1.85	0.57
1:D:26:ILE:O	1:D:62:TYR:HD1	1.86	0.57
1:D:97:MET:O	1:D:127:ILE:HA	2.05	0.57
1:A:124:THR:HG23	1:A:125:PHE:HD2	1.70	0.57
1:C:105:TYR:HE2	1:C:120:MET:HE1	1.69	0.57
1:D:76:VAL:HG23	1:D:263:GLN:HE21	1.69	0.57
1:A:276:PRO:CB	1:B:278:LEU:HD23	2.33	0.56
1:B:70:MET:HE3	1:B:263:GLN:HA	1.86	0.56
1:C:105:TYR:CE2	1:C:120:MET:HE1	2.41	0.56
1:C:155:ILE:HA	1:C:163:SER:O	2.05	0.56
1:D:189:TRP:CG	1:D:209:VAL:HG11	2.39	0.56
1:D:95:PRO:HD2	1:D:124:THR:O	2.04	0.56
1:A:201:THR:HB	1:A:206:ASP:OD2	2.05	0.56
1:B:176:SER:HB2	1:B:177:PRO:HA	1.88	0.56
1:C:15:VAL:HG13	1:C:261:SER:O	2.05	0.56
1:D:70:MET:SD	1:D:261:SER:HB3	2.45	0.56
1:A:2:CYS:SG	1:A:20:MET:HA	2.46	0.56
1:B:215:ILE:HD12	1:B:218:ILE:HD13	1.86	0.56
1:B:282:ASP:O	1:B:286:ILE:HG13	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:LEU:HD13	1:C:213:PHE:HZ	1.70	0.56
1:D:174:THR:HG23	1:D:208:PHE:HD1	1.71	0.56
1:B:296:LYS:HB3	1:B:316:SER:HB2	1.87	0.56
1:B:95:PRO:O	1:B:125:PHE:HB2	2.06	0.56
1:A:5:ALA:HA	1:A:171:GLN:O	2.06	0.56
1:B:174:THR:H	1:B:182:GLN:NE2	2.03	0.56
1:C:280:TRP:O	1:C:281:LEU:HD23	2.05	0.56
1:C:35:ARG:NH2	1:C:289:SER:HA	2.21	0.56
1:D:96:ALA:HB2	1:D:126:ARG:CZ	2.36	0.56
1:D:146:THR:HG23	1:D:263:GLN:HE22	1.70	0.56
1:A:197:MET:HA	1:B:201:THR:HG22	1.88	0.56
1:D:296:LYS:HB3	1:D:316:SER:CB	2.36	0.56
1:A:243:GLY:H	1:A:254:SER:CB	2.19	0.56
1:C:112:THR:CG2	1:C:115:GLU:HG3	2.36	0.56
1:C:96:ALA:HB2	1:C:126:ARG:CZ	2.36	0.56
1:D:26:ILE:HG22	1:D:256:ARG:HE	1.71	0.56
1:D:77:ALA:HB1	1:D:143:MET:SD	2.46	0.56
1:D:80:LEU:O	1:D:141:LEU:HB3	2.05	0.56
1:C:272:SER:HB2	1:C:275:THR:CG2	2.36	0.55
1:A:34:PRO:CG	1:A:292:ALA:HB3	2.36	0.55
1:B:202:ASN:OD1	1:B:207:ARG:NE	2.32	0.55
1:B:211:ALA:O	1:B:215:ILE:HG22	2.07	0.55
1:B:25:ASP:OD2	1:B:27:MET:HG2	2.06	0.55
1:A:32:VAL:N	1:A:295:LYS:O	2.36	0.55
1:B:280:TRP:CZ3	1:B:307:GLY:HA2	2.42	0.55
1:D:113:VAL:O	1:D:117:VAL:HG23	2.06	0.55
1:D:76:VAL:CG2	1:D:263:GLN:HE21	2.19	0.55
1:D:74:GLY:O	1:D:263:GLN:HG2	2.07	0.55
1:A:297:LEU:HB2	1:A:313:LEU:CD2	2.37	0.55
1:A:30:ILE:HB	1:A:297:LEU:HB3	1.88	0.55
1:B:30:ILE:HD13	1:B:59:ALA:HA	1.89	0.55
1:B:80:LEU:HD22	1:B:173:MET:HE3	1.87	0.55
1:C:13:MET:CB	1:C:222:ALA:HA	2.37	0.55
1:D:76:VAL:O	1:D:145:ILE:HG23	2.06	0.55
1:A:194:GLY:HA2	1:A:198:LEU:CD2	2.36	0.55
1:B:235:MET:HA	1:B:238:VAL:HG22	1.89	0.55
1:D:245:ASN:HB2	1:D:250:PRO:O	2.06	0.55
1:A:55:GLY:O	1:A:72:GLU:HG3	2.06	0.55
1:C:80:LEU:O	1:C:141:LEU:HB3	2.07	0.55
1:B:97:MET:SD	1:B:127:ILE:HD12	2.46	0.55
1:D:58:ILE:HA	1:D:69:GLY:CA	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:THR:CG2	1:A:63:ASP:HA	2.35	0.55
1:B:73:LYS:CG	1:B:111:ALA:HB1	2.36	0.55
1:B:227:ALA:O	1:B:231:VAL:HG23	2.07	0.55
1:B:76:VAL:HG21	1:B:261:SER:CB	2.36	0.55
1:C:10:PRO:HD3	1:C:220:GLN:HG2	1.88	0.55
1:C:87:TYR:CD1	1:C:127:ILE:HB	2.42	0.55
1:C:2:CYS:HB3	1:C:19:THR:O	2.07	0.55
1:D:227:ALA:O	1:D:231:VAL:HG23	2.06	0.55
1:A:20:MET:CE	1:A:22:TRP:HB2	2.37	0.54
1:B:79:LEU:HD11	1:B:143:MET:HE2	1.89	0.54
1:C:112:THR:HG22	1:C:115:GLU:CD	2.28	0.54
1:C:18:ARG:HD2	1:C:78:SER:HB3	1.88	0.54
1:D:58:ILE:HA	1:D:69:GLY:HA2	1.89	0.54
1:D:54:TYR:HB3	1:D:72:GLU:HG3	1.89	0.54
1:A:92:ASP:CG	1:A:126:ARG:HD3	2.27	0.54
1:B:189:TRP:HE3	1:B:192:VAL:HG11	1.72	0.54
1:B:81:PHE:HA	1:B:141:LEU:HA	1.89	0.54
1:A:126:ARG:HG2	1:A:127:ILE:N	2.20	0.54
1:A:56:SER:HB2	1:A:70:MET:O	2.08	0.54
1:B:69:GLY:O	1:B:76:VAL:HG13	2.07	0.54
1:D:18:ARG:HD2	1:D:78:SER:HB3	1.89	0.54
1:A:214:TYR:HD2	1:B:241:PRO:HG2	1.72	0.54
1:A:61:GLY:O	1:A:64:ILE:HG12	2.07	0.54
1:B:324:GLU:HB3	1:B:326:PRO:HD3	1.88	0.54
1:C:204:SER:HA	1:C:207:ARG:NH2	2.23	0.54
1:A:224:ALA:O	1:A:228:VAL:HG23	2.07	0.54
1:B:144:ALA:C	1:B:145:ILE:HD12	2.28	0.54
1:B:47:THR:HG22	1:B:96:ALA:O	2.07	0.54
1:C:249:LYS:HB3	1:C:252:ILE:HD11	1.89	0.54
1:A:24:GLU:O	1:A:256:ARG:NH1	2.40	0.54
1:B:102:TRP:HB2	1:B:127:ILE:HD13	1.89	0.54
1:B:189:TRP:CD1	1:B:209:VAL:HG21	2.42	0.54
1:C:5:ALA:O	1:C:16:THR:HG23	2.07	0.54
1:C:80:LEU:HD22	1:C:173:MET:CE	2.38	0.54
1:C:249:LYS:HG3	1:C:252:ILE:CG1	2.38	0.54
1:B:198:LEU:HD11	1:B:210:ARG:CG	2.32	0.54
1:B:73:LYS:CB	1:B:111:ALA:HB1	2.37	0.54
1:C:14:VAL:HG11	1:C:150:GLY:HA2	1.89	0.54
1:D:4:ARG:HD3	1:D:144:ALA:HB3	1.89	0.54
1:A:75:LEU:CD2	1:A:107:LEU:HD23	2.38	0.54
1:B:5:ALA:N	1:B:17:GLY:O	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MET:O	1:C:21:ASP:HB2	2.08	0.54
1:C:157:TYR:HA	1:C:161:LYS:O	2.08	0.54
1:D:174:THR:CG2	1:D:208:PHE:HB2	2.37	0.54
1:D:203:ARG:HB2	1:D:206:ASP:OD1	2.08	0.54
1:D:41:GLY:CA	1:D:47:THR:HG21	2.38	0.54
1:A:124:THR:HG23	1:A:125:PHE:CD2	2.43	0.53
1:B:72:GLU:OE2	1:B:288:PHE:HB2	2.07	0.53
1:B:215:ILE:HD12	1:B:218:ILE:CD1	2.37	0.53
1:C:179:TYR:CE2	1:C:183:LEU:HD11	2.43	0.53
1:B:102:TRP:CG	1:B:127:ILE:HD13	2.43	0.53
1:C:35:ARG:NH1	1:C:290:PRO:HD3	2.23	0.53
1:D:81:PHE:HA	1:D:141:LEU:CG	2.38	0.53
1:B:296:LYS:HB2	1:B:316:SER:HB2	1.89	0.53
1:B:82:LEU:HD23	1:B:85:SER:OG	2.08	0.53
1:C:42:HIS:CE1	1:C:44:LYS:HB2	2.43	0.53
1:B:231:VAL:O	1:B:235:MET:HG2	2.08	0.53
1:D:113:VAL:HG21	1:D:151:ASN:CG	2.29	0.53
1:A:201:THR:HG22	1:A:203:ARG:HG3	1.89	0.53
1:A:42:HIS:NE2	1:A:323:PHE:HB3	2.23	0.53
1:A:30:ILE:HD13	1:A:59:ALA:HA	1.91	0.53
1:B:258:ARG:NH1	1:B:271:GLU:OE2	2.35	0.53
1:C:1:MET:HB3	1:C:175:ASN:HB2	1.91	0.53
1:C:232:LEU:CD2	1:C:236:ARG:HH21	2.21	0.53
1:D:56:SER:HB3	1:D:71:ASN:HA	1.91	0.53
1:D:75:LEU:CD2	1:D:107:LEU:HD23	2.38	0.53
1:D:80:LEU:O	1:D:142:HIS:N	2.40	0.53
1:A:92:ASP:HB3	1:A:126:ARG:HD3	1.90	0.53
1:A:79:LEU:HD12	1:A:142:HIS:O	2.08	0.53
1:A:186:ASN:O	1:A:190:LYS:HG2	2.07	0.53
1:B:73:LYS:HG3	1:B:111:ALA:CB	2.37	0.53
1:D:298:SER:O	1:D:299:LEU:HD23	2.08	0.53
1:A:79:LEU:HD13	1:A:143:MET:CE	2.39	0.53
1:B:189:TRP:HD1	1:B:209:VAL:HG21	1.73	0.53
1:D:113:VAL:HG11	1:D:151:ASN:O	2.09	0.53
1:A:142:HIS:HB2	1:A:155:ILE:O	2.09	0.53
1:A:201:THR:HG21	1:A:203:ARG:HG3	1.89	0.53
1:B:102:TRP:HB2	1:B:127:ILE:CD1	2.38	0.53
1:B:143:MET:HG2	1:B:145:ILE:HD11	1.91	0.53
1:B:298:SER:O	1:B:299:LEU:HD23	2.09	0.53
1:C:96:ALA:HB2	1:C:126:ARG:NH2	2.23	0.53
1:C:86:VAL:HB	1:C:159:ASP:CA	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:LYS:CE	1:D:252:ILE:HG12	2.38	0.53
1:B:66:THR:HG21	1:B:104:GLN:NE2	2.23	0.53
1:B:232:LEU:O	1:B:236:ARG:HG3	2.09	0.53
1:D:321:PHE:O	1:D:322:LEU:HD23	2.08	0.53
1:D:116:ALA:O	1:D:120:MET:HG3	2.09	0.52
1:D:78:SER:O	1:D:143:MET:HA	2.09	0.52
1:C:277:ASN:HB2	1:C:305:TYR:O	2.09	0.52
1:C:281:LEU:HD21	1:C:309:ALA:HB3	1.91	0.52
1:D:75:LEU:HD22	1:D:107:LEU:HD23	1.89	0.52
1:A:112:THR:HG22	1:A:114:ARG:H	1.73	0.52
1:C:298:SER:O	1:C:299:LEU:HD23	2.10	0.52
1:D:41:GLY:C	1:D:47:THR:HG21	2.29	0.52
1:C:94:ARG:HH11	1:C:123:GLU:HB3	1.74	0.52
1:C:187:ASP:HA	1:C:190:LYS:HZ1	1.74	0.52
1:D:112:THR:HG23	1:D:147:ASP:OD2	2.10	0.52
1:D:149:THR:HG22	1:D:149:THR:O	2.08	0.52
1:A:157:TYR:HA	1:A:162:LEU:HA	1.92	0.52
1:A:235:MET:HA	1:A:235:MET:HE2	1.90	0.52
1:D:25:ASP:OD1	1:D:27:MET:HG2	2.09	0.52
1:A:223:ASP:HB3	1:A:226:ILE:HG22	1.91	0.52
1:C:112:THR:HG22	1:C:115:GLU:CG	2.40	0.52
1:C:249:LYS:HG3	1:C:252:ILE:HG12	1.91	0.52
1:D:82:LEU:HD12	1:D:175:ASN:O	2.09	0.52
1:B:55:GLY:HA3	1:B:288:PHE:CD1	2.44	0.52
1:B:76:VAL:O	1:B:145:ILE:HG23	2.09	0.52
1:A:280:TRP:O	1:A:281:LEU:HD23	2.09	0.52
1:B:58:ILE:CG2	1:B:69:GLY:HA3	2.30	0.52
1:C:70:MET:HE3	1:C:74:GLY:HA2	1.90	0.52
1:D:95:PRO:O	1:D:125:PHE:HB2	2.09	0.52
1:A:241:PRO:CB	1:A:244:ILE:HD11	2.34	0.52
1:B:79:LEU:HD11	1:B:143:MET:CE	2.40	0.52
1:D:72:GLU:O	1:D:266:LYS:HD2	2.09	0.52
1:A:297:LEU:HB2	1:A:313:LEU:HD21	1.91	0.52
1:B:58:ILE:HD12	1:B:58:ILE:O	2.10	0.52
1:B:74:GLY:O	1:B:263:GLN:HB3	2.10	0.52
1:D:74:GLY:O	1:D:76:VAL:HG23	2.10	0.52
1:B:97:MET:N	1:B:126:ARG:O	2.43	0.51
1:D:82:LEU:HD22	1:D:142:HIS:HD2	1.74	0.51
1:D:154:VAL:HG13	1:D:173:MET:SD	2.50	0.51
1:D:181:LEU:O	1:D:185:VAL:HG23	2.10	0.51
1:D:235:MET:HA	1:D:235:MET:CE	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:MET:CE	1:A:300:THR:HG23	2.39	0.51
1:B:280:TRP:CH2	1:B:307:GLY:HA2	2.45	0.51
1:B:296:LYS:HB3	1:B:316:SER:CB	2.40	0.51
1:A:131:ARG:H	1:A:325:THR:CG2	2.22	0.51
1:A:215:ILE:O	1:A:218:ILE:HG12	2.10	0.51
1:A:235:MET:CA	1:A:235:MET:HE2	2.40	0.51
1:A:232:LEU:O	1:A:236:ARG:HG3	2.10	0.51
1:B:20:MET:HB3	1:B:257:TRP:O	2.10	0.51
1:C:112:THR:HA	1:C:147:ASP:HB3	1.93	0.51
1:D:80:LEU:HD13	1:D:173:MET:CE	2.40	0.51
1:B:18:ARG:NH2	2:B:401:QC7:C04	2.73	0.51
1:C:272:SER:HB2	1:C:275:THR:OG1	2.11	0.51
1:C:42:HIS:HA	1:C:323:PHE:CD2	2.44	0.51
1:A:234:VAL:HG23	1:A:235:MET:HE2	1.92	0.51
1:C:144:ALA:C	1:C:145:ILE:HD12	2.31	0.51
1:C:255:THR:C	1:C:256:ARG:HD2	2.31	0.51
1:A:101:ILE:O	1:A:101:ILE:HG12	2.11	0.51
1:B:147:ASP:OD1	1:B:149:THR:HB	2.10	0.51
1:B:130:PRO:HG2	1:B:325:THR:HG21	1.91	0.51
1:B:4:ARG:HD2	1:B:78:SER:CB	2.41	0.51
1:D:231:VAL:O	1:D:234:VAL:HG22	2.10	0.51
1:C:98:GLY:HA3	1:C:323:PHE:HD1	1.76	0.51
1:D:193:GLY:HA3	1:D:196:GLN:NE2	2.25	0.51
1:B:46:LYS:O	1:B:95:PRO:HA	2.11	0.51
1:B:75:LEU:HA	1:B:146:THR:O	2.11	0.51
1:A:147:ASP:OD2	1:A:151:ASN:HB3	2.11	0.51
1:A:271:GLU:HG2	1:A:272:SER:N	2.24	0.51
1:A:277:ASN:HA	1:B:277:ASN:HA	1.92	0.51
1:B:79:LEU:CD1	1:B:143:MET:HG3	2.39	0.51
1:C:96:ALA:HB1	1:C:128:ASP:HB2	1.92	0.51
1:A:77:ALA:HB2	1:A:145:ILE:HD13	1.93	0.51
1:A:233:SER:HB2	1:B:241:PRO:HA	1.93	0.51
1:B:231:VAL:O	1:B:234:VAL:HG22	2.10	0.51
1:B:79:LEU:HD23	1:B:141:LEU:CD1	2.41	0.50
1:A:201:THR:OG1	1:B:198:LEU:N	2.43	0.50
1:B:200:GLY:HA2	1:B:210:ARG:NH2	2.27	0.50
1:C:174:THR:HG21	1:C:208:PHE:N	2.26	0.50
1:D:20:MET:HE2	1:D:26:ILE:HD12	1.93	0.50
1:D:35:ARG:NH1	1:D:288:PHE:HB2	2.24	0.50
1:A:117:VAL:O	1:A:121:LYS:HE2	2.11	0.50
1:C:201:THR:HG22	1:C:202:ASN:H	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:LYS:HG2	1:A:315:ASP:OD1	2.11	0.50
1:B:137:PRO:HB2	1:B:138:GLU:OE1	2.12	0.50
1:B:147:ASP:O	1:B:263:GLN:NE2	2.44	0.50
1:C:116:ALA:O	1:C:120:MET:HG2	2.11	0.50
1:C:3:THR:H	1:C:19:THR:HB	1.76	0.50
1:C:7:TYR:CD1	1:C:218:ILE:HD11	2.45	0.50
1:B:295:LYS:HA	1:B:315:ASP:HA	1.92	0.50
1:B:43:ASN:OD1	1:B:323:PHE:HB2	2.12	0.50
1:D:42:HIS:HB2	1:D:96:ALA:O	2.11	0.50
1:A:272:SER:HB2	1:A:275:THR:CG2	2.40	0.50
1:A:217:ALA:HB1	1:B:244:ILE:HG23	1.94	0.50
1:B:29:ASN:OD1	1:B:299:LEU:N	2.40	0.50
1:A:94:ARG:NH2	1:A:126:ARG:HA	2.27	0.50
1:B:325:THR:OG1	1:B:325:THR:O	2.27	0.50
1:C:295:LYS:HG2	1:C:315:ASP:OD1	2.11	0.50
1:C:34:PRO:O	1:C:37:MET:HG3	2.12	0.50
1:D:86:VAL:HB	1:D:159:ASP:HA	1.94	0.50
1:A:279:PHE:HA	1:A:307:GLY:O	2.12	0.50
1:B:75:LEU:HD21	1:B:145:ILE:CG2	2.42	0.50
1:B:36:GLY:N	1:B:52:SER:O	2.34	0.50
1:C:9:GLY:N	1:C:13:MET:O	2.44	0.50
1:D:20:MET:HG2	1:D:257:TRP:NE1	2.27	0.50
1:D:296:LYS:CB	1:D:316:SER:HB3	2.39	0.50
1:D:27:MET:CE	1:D:300:THR:HG23	2.41	0.50
1:A:84:GLU:CD	1:A:84:GLU:H	2.15	0.50
1:B:41:GLY:O	1:B:97:MET:HG3	2.11	0.50
1:B:55:GLY:O	1:B:72:GLU:HG3	2.12	0.50
1:C:25:ASP:OD1	1:C:26:ILE:N	2.45	0.50
1:D:155:ILE:CG1	1:D:164:ILE:HG12	2.42	0.50
1:C:26:ILE:HG12	1:C:26:ILE:O	2.12	0.49
1:D:201:THR:HB	1:D:206:ASP:OD2	2.12	0.49
1:D:301:LYS:HB2	1:D:303:GLU:OE2	2.12	0.49
1:D:64:ILE:HG21	1:D:322:LEU:HG	1.94	0.49
1:B:80:LEU:N	1:B:142:HIS:O	2.34	0.49
1:C:176:SER:O	1:C:182:GLN:NE2	2.44	0.49
1:C:13:MET:CG	1:C:222:ALA:HA	2.42	0.49
1:C:92:ASP:OD1	1:C:94:ARG:HG3	2.12	0.49
1:D:186:ASN:HA	1:D:209:VAL:HG22	1.94	0.49
1:D:189:TRP:CZ3	1:D:199:PRO:HD3	2.46	0.49
1:A:189:TRP:CD1	1:A:209:VAL:HG21	2.48	0.49
1:A:21:ASP:OD1	1:A:255:THR:HA	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ILE:HG13	1:A:65:GLY:N	2.28	0.49
1:B:102:TRP:CB	1:B:127:ILE:HD13	2.43	0.49
1:C:75:LEU:CD2	1:C:107:LEU:HD23	2.42	0.49
1:A:22:TRP:HE1	1:A:24:GLU:HG2	1.76	0.49
1:B:15:VAL:HG22	1:B:262:ASP:HA	1.93	0.49
1:C:205:SER:O	1:C:209:VAL:HG23	2.13	0.49
1:D:145:ILE:N	1:D:145:ILE:HD12	2.27	0.49
1:D:157:TYR:HA	1:D:161:LYS:O	2.12	0.49
1:A:172:VAL:HG13	1:A:208:PHE:CZ	2.47	0.49
1:A:28:SER:HB2	1:A:60:THR:O	2.12	0.49
1:C:228:VAL:HB	1:C:229:PRO:HD3	1.94	0.49
1:A:8:LEU:HD11	1:A:168:LYS:O	2.12	0.49
1:A:301:LYS:N	1:A:301:LYS:HD2	2.27	0.49
1:A:46:LYS:O	1:A:95:PRO:HA	2.13	0.49
1:B:179:TYR:CD2	1:B:183:LEU:HD23	2.47	0.49
1:A:174:THR:HG23	1:A:208:PHE:CD1	2.45	0.49
1:A:242:PHE:HE2	1:A:274:LEU:HD21	1.78	0.49
1:B:101:ILE:O	1:B:101:ILE:HG12	2.13	0.49
1:C:121:LYS:HG2	1:C:164:ILE:HD12	1.94	0.49
1:C:255:THR:O	1:C:256:ARG:HD2	2.13	0.49
1:C:70:MET:HE1	1:C:266:LYS:HA	1.95	0.49
1:C:79:LEU:HG	1:C:141:LEU:HD22	1.94	0.49
1:C:146:THR:HG23	1:C:151:ASN:O	2.13	0.49
1:D:77:ALA:CA	1:D:145:ILE:HG13	2.33	0.49
1:D:255:THR:O	1:D:255:THR:HG23	2.13	0.49
1:A:171:GLN:HE21	1:A:215:ILE:HG21	1.77	0.49
1:A:232:LEU:HG	1:A:236:ARG:HE	1.78	0.49
1:A:131:ARG:N	1:A:325:THR:HG21	2.27	0.49
1:B:145:ILE:O	1:B:152:THR:HG23	2.13	0.49
1:C:130:PRO:HB2	1:C:325:THR:HG23	1.93	0.49
1:C:52:SER:CB	1:C:108:ASP:HB2	2.42	0.49
1:C:32:VAL:HG22	1:C:57:VAL:HG22	1.95	0.49
1:D:144:ALA:HB2	1:D:173:MET:SD	2.53	0.49
1:B:80:LEU:HD22	1:B:173:MET:CE	2.42	0.49
1:B:202:ASN:ND2	1:B:207:ARG:HH21	2.11	0.49
1:B:220:GLN:OE1	1:B:220:GLN:HA	2.12	0.49
1:B:262:ASP:O	1:B:266:LYS:N	2.46	0.49
1:B:79:LEU:HB3	1:B:141:LEU:HD13	1.94	0.49
1:C:52:SER:HA	1:C:108:ASP:HB2	1.94	0.49
1:A:21:ASP:HA	1:A:254:SER:O	2.13	0.48
1:C:110:PHE:CZ	1:C:116:ALA:HA	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:MET:HB2	1:C:39:ARG:HH12	1.77	0.48
1:D:33:PHE:HB3	1:D:37:MET:SD	2.52	0.48
1:A:132:MET:CE	1:A:136:GLY:HA3	2.43	0.48
1:A:56:SER:HA	1:A:71:ASN:HA	1.96	0.48
1:A:81:PHE:HB3	1:A:175:ASN:OD1	2.12	0.48
1:B:74:GLY:O	1:B:148:GLU:N	2.47	0.48
1:B:18:ARG:HH22	2:B:401:QC7:C04	2.26	0.48
1:B:189:TRP:CE3	1:B:192:VAL:HG11	2.47	0.48
1:B:20:MET:HE1	1:B:22:TRP:HB2	1.94	0.48
1:B:283:LEU:HA	1:B:286:ILE:CD1	2.36	0.48
1:B:4:ARG:HD2	1:B:78:SER:OG	2.13	0.48
1:C:39:ARG:HB3	1:C:101:ILE:HD11	1.94	0.48
1:D:4:ARG:O	1:D:172:VAL:HG23	2.13	0.48
1:A:87:TYR:OH	1:A:140:THR:HA	2.13	0.48
1:B:171:GLN:HE21	1:B:215:ILE:CG2	2.26	0.48
1:C:42:HIS:HD2	1:C:45:GLU:HB2	1.75	0.48
1:B:127:ILE:O	1:B:127:ILE:HG23	2.14	0.48
1:B:63:ASP:O	1:B:319:PHE:HB2	2.13	0.48
1:D:110:PHE:CD1	1:D:116:ALA:HA	2.49	0.48
1:D:98:GLY:HA2	1:D:128:ASP:O	2.13	0.48
1:D:154:VAL:HG11	1:D:179:TYR:CE2	2.49	0.48
1:D:155:ILE:CG2	1:D:162:LEU:HD11	2.43	0.48
1:A:249:LYS:HD3	1:A:252:ILE:HD11	1.94	0.48
1:A:120:MET:HE3	1:A:120:MET:HA	1.94	0.48
1:C:54:TYR:O	1:C:108:ASP:HA	2.13	0.48
1:C:271:GLU:HB2	1:C:278:LEU:HD13	1.96	0.48
1:C:42:HIS:ND1	1:C:323:PHE:HB2	2.28	0.48
1:D:82:LEU:H	1:D:141:LEU:HA	1.78	0.48
1:A:75:LEU:O	1:A:75:LEU:HD23	2.13	0.48
1:C:281:LEU:O	1:C:283:LEU:HD12	2.14	0.48
1:D:153:ALA:HA	1:D:166:GLU:HA	1.96	0.48
1:B:18:ARG:HB3	1:B:259:SER:OG	2.14	0.48
1:B:308:ASP:OD1	1:B:310:VAL:HG23	2.14	0.48
1:B:4:ARG:HA	1:B:17:GLY:O	2.13	0.48
1:A:86:VAL:HB	1:A:159:ASP:CA	2.44	0.48
1:B:20:MET:HG2	1:B:257:TRP:CE2	2.48	0.48
1:B:18:ARG:CD	1:B:78:SER:HB3	2.42	0.48
1:D:64:ILE:CG2	1:D:322:LEU:HG	2.44	0.48
1:A:140:THR:C	1:A:141:LEU:HD12	2.34	0.47
1:D:29:ASN:ND2	1:D:63:ASP:HB2	2.29	0.47
1:C:326:PRO:HB3	1:D:326:PRO:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:MET:HB2	1:D:76:VAL:HG22	1.96	0.47
1:B:158:LEU:HD23	1:B:158:LEU:O	2.13	0.47
1:C:41:GLY:O	1:C:98:GLY:N	2.43	0.47
1:C:86:VAL:HB	1:C:159:ASP:HA	1.95	0.47
1:D:29:ASN:HD22	1:D:63:ASP:HB2	1.79	0.47
1:A:94:ARG:HB3	1:A:95:PRO:HD2	1.97	0.47
1:C:87:TYR:C	1:C:160:GLY:HA2	2.34	0.47
1:C:226:ILE:C	1:C:229:PRO:HD2	2.34	0.47
1:C:280:TRP:CH2	1:C:307:GLY:HA2	2.49	0.47
1:C:52:SER:HB2	1:C:108:ASP:HB2	1.95	0.47
1:D:113:VAL:HG13	1:D:147:ASP:HB2	1.96	0.47
1:D:37:MET:HB2	1:D:39:ARG:HH12	1.78	0.47
1:B:215:ILE:HG23	1:B:216:HIS:CD2	2.50	0.47
1:C:187:ASP:HA	1:C:190:LYS:NZ	2.28	0.47
1:D:119:GLU:O	1:D:122:LYS:HG2	2.14	0.47
1:A:78:SER:O	1:A:143:MET:HG3	2.13	0.47
1:C:196:GLN:OE1	1:C:196:GLN:HA	2.14	0.47
1:D:194:GLY:HA3	1:D:213:PHE:CZ	2.49	0.47
1:D:55:GLY:HA3	1:D:288:PHE:CD1	2.50	0.47
1:D:3:THR:C	1:D:80:LEU:HD21	2.35	0.47
1:A:131:ARG:H	1:A:325:THR:HG21	1.79	0.47
1:B:112:THR:HG22	1:B:114:ARG:H	1.79	0.47
1:C:130:PRO:HG3	1:C:323:PHE:C	2.35	0.47
1:D:16:THR:O	1:D:260:VAL:HA	2.15	0.47
1:A:153:ALA:HA	1:A:165:HIS:O	2.14	0.47
1:C:6:VAL:HG22	1:C:16:THR:HG23	1.97	0.47
1:C:81:PHE:HA	1:C:141:LEU:HA	1.96	0.47
1:D:269:TYR:CD2	1:D:280:TRP:HB3	2.50	0.47
1:D:155:ILE:HG12	1:D:164:ILE:CG1	2.43	0.47
1:D:189:TRP:CB	1:D:209:VAL:HG11	2.45	0.47
1:D:262:ASP:O	1:D:266:LYS:N	2.48	0.47
1:A:194:GLY:CA	1:A:198:LEU:HD21	2.42	0.47
1:A:7:TYR:HB2	1:A:215:ILE:HD11	1.97	0.47
1:B:202:ASN:ND2	1:B:240:VAL:HG11	2.29	0.47
1:C:149:THR:HG22	1:C:149:THR:O	2.15	0.47
1:D:3:THR:HG22	1:D:4:ARG:N	2.30	0.47
1:A:154:VAL:O	1:A:164:ILE:HA	2.14	0.47
1:A:328:MET:CE	1:A:329:LEU:HG	2.45	0.47
1:A:61:GLY:O	1:A:62:TYR:HB2	2.15	0.47
1:B:96:ALA:HA	1:B:126:ARG:O	2.14	0.47
1:A:91:GLY:O	1:A:93:THR:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:TRP:CB	1:B:109:ASN:HD21	2.26	0.47
1:B:146:THR:HG22	1:B:263:GLN:HE22	1.80	0.47
1:B:120:MET:SD	1:B:155:ILE:HD13	2.55	0.47
1:B:226:ILE:O	1:B:229:PRO:HD2	2.15	0.47
1:C:73:LYS:CB	1:C:111:ALA:HB1	2.45	0.47
1:C:321:PHE:O	1:C:322:LEU:HD23	2.15	0.47
1:D:28:SER:O	1:D:299:LEU:HB2	2.15	0.47
1:A:210:ARG:O	1:A:214:TYR:HD1	1.98	0.46
1:B:86:VAL:CB	1:B:159:ASP:HA	2.19	0.46
1:B:186:ASN:HD21	1:B:212:SER:HB3	1.80	0.46
1:B:186:ASN:OD1	1:B:190:LYS:HE3	2.15	0.46
1:B:244:ILE:HB	1:B:252:ILE:HG21	1.98	0.46
1:B:174:THR:N	1:B:182:GLN:HE22	2.06	0.46
1:B:299:LEU:HD23	1:B:305:TYR:HE2	1.80	0.46
1:C:252:ILE:HG22	1:C:253:SER:N	2.30	0.46
1:D:38:GLN:HA	1:D:50:TRP:O	2.16	0.46
1:B:2:CYS:H	1:B:175:ASN:ND2	2.11	0.46
1:B:66:THR:HG21	1:B:104:GLN:HE21	1.80	0.46
1:C:114:ARG:HA	1:C:114:ARG:HE	1.79	0.46
1:D:101:ILE:HG12	1:D:101:ILE:O	2.15	0.46
1:D:296:LYS:HG2	1:D:297:LEU:N	2.31	0.46
1:D:29:ASN:O	1:D:60:THR:HG23	2.15	0.46
1:D:39:ARG:N	1:D:50:TRP:O	2.40	0.46
1:D:41:GLY:O	1:D:97:MET:HA	2.16	0.46
1:B:131:ARG:HG2	1:B:132:MET:N	2.30	0.46
1:D:140:THR:C	1:D:141:LEU:HD12	2.36	0.46
1:D:79:LEU:C	1:D:80:LEU:HD12	2.36	0.46
1:B:114:ARG:NE	1:B:114:ARG:HA	2.31	0.46
1:B:202:ASN:CG	1:B:240:VAL:HG11	2.36	0.46
1:B:32:VAL:HG22	1:B:57:VAL:HG22	1.97	0.46
1:C:141:LEU:N	1:C:141:LEU:HD12	2.31	0.46
1:C:82:LEU:HB3	1:C:85:SER:OG	2.16	0.46
1:D:155:ILE:HG23	1:D:162:LEU:HD11	1.98	0.46
1:D:204:SER:HA	1:D:207:ARG:CZ	2.46	0.46
1:D:66:THR:HG1	1:D:321:PHE:HE2	1.63	0.46
1:D:7:TYR:CD1	1:D:218:ILE:HD11	2.51	0.46
1:A:232:LEU:HD11	1:A:258:ARG:HD2	1.97	0.46
1:A:36:GLY:HA2	1:A:51:THR:HG22	1.98	0.46
1:A:74:GLY:N	1:A:266:LYS:HE3	2.31	0.46
1:B:110:PHE:CD1	1:B:116:ALA:HA	2.51	0.46
1:C:46:LYS:N	1:C:46:LYS:HD2	2.20	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:187:ASP:HA	1:D:190:LYS:HZ1	1.79	0.46
1:D:12:ARG:O	1:D:264:LYS:HD2	2.16	0.46
1:D:194:GLY:HA2	1:D:198:LEU:HD21	1.98	0.46
1:D:92:ASP:OD1	1:D:94:ARG:HG3	2.16	0.46
1:A:306:ALA:HB1	1:B:277:ASN:OD1	2.16	0.46
1:B:82:LEU:HD13	1:B:175:ASN:O	2.16	0.46
1:D:178:ARG:H	1:D:181:LEU:HD12	1.80	0.46
1:D:23:LYS:HA	1:D:253:SER:HA	1.98	0.46
1:B:76:VAL:O	1:B:145:ILE:HA	2.16	0.45
1:C:201:THR:HG22	1:C:202:ASN:N	2.30	0.45
1:D:56:SER:HA	1:D:71:ASN:HA	1.99	0.45
1:A:117:VAL:HG12	1:A:121:LYS:CE	2.43	0.45
1:A:60:THR:HG22	1:A:61:GLY:N	2.32	0.45
1:A:4:ARG:HD2	1:A:78:SER:HB2	1.97	0.45
1:B:212:SER:O	1:B:215:ILE:HG22	2.16	0.45
1:C:120:MET:CE	1:C:120:MET:HA	2.45	0.45
1:C:6:VAL:HG13	1:C:16:THR:OG1	2.16	0.45
1:A:92:ASP:CB	1:A:126:ARG:HD3	2.46	0.45
1:B:174:THR:HG22	1:B:175:ASN:N	2.25	0.45
1:A:219:PRO:HG3	1:B:243:GLY:HA3	1.97	0.45
1:B:280:TRP:O	1:B:281:LEU:HD23	2.16	0.45
1:B:41:GLY:O	1:B:42:HIS:HB2	2.15	0.45
1:C:49:ASN:O	1:C:50:TRP:HB3	2.16	0.45
1:C:66:THR:HG23	1:C:321:PHE:CZ	2.51	0.45
1:C:94:ARG:HD2	1:C:123:GLU:O	2.16	0.45
1:D:271:GLU:HG2	1:D:272:SER:N	2.32	0.45
1:A:328:MET:HE3	1:A:329:LEU:HG	1.98	0.45
1:A:75:LEU:HD21	1:A:145:ILE:HD11	1.98	0.45
1:A:95:PRO:HD2	1:A:124:THR:O	2.16	0.45
1:A:13:MET:HE2	1:A:224:ALA:HA	1.98	0.45
1:C:122:LYS:HB3	1:C:124:THR:HG23	1.99	0.45
1:C:326:PRO:C	1:D:324:GLU:HB2	2.37	0.45
1:C:73:LYS:HG3	1:C:111:ALA:HB1	1.98	0.45
1:A:171:GLN:NE2	1:A:215:ILE:HG21	2.31	0.45
1:A:200:GLY:N	1:B:198:LEU:O	2.50	0.45
1:D:55:GLY:O	1:D:72:GLU:HG2	2.16	0.45
1:B:143:MET:CG	1:B:145:ILE:HD11	2.47	0.45
1:B:260:VAL:O	1:B:269:TYR:N	2.48	0.45
1:D:75:LEU:HD21	1:D:145:ILE:HG21	1.99	0.45
1:D:162:LEU:HD21	1:D:164:ILE:HD11	1.98	0.45
1:D:272:SER:HB2	1:D:275:THR:OG1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ARG:HB3	1:A:259:SER:OG	2.17	0.44
1:B:47:THR:HA	1:B:95:PRO:CB	2.45	0.44
1:C:3:THR:HG23	1:C:174:THR:HG22	1.99	0.44
1:D:27:MET:HE2	1:D:300:THR:HG23	1.98	0.44
1:A:39:ARG:HB2	1:A:50:TRP:CE2	2.52	0.44
1:A:72:GLU:OE2	1:A:288:PHE:HB2	2.17	0.44
1:B:64:ILE:HG13	1:B:65:GLY:N	2.32	0.44
1:B:81:PHE:CZ	1:B:138:GLU:CB	3.01	0.44
1:C:18:ARG:HD2	1:C:78:SER:CB	2.46	0.44
1:D:94:ARG:HB3	1:D:95:PRO:HD2	1.98	0.44
1:A:280:TRP:CZ3	1:A:307:GLY:HA2	2.52	0.44
1:B:20:MET:CE	1:B:22:TRP:HB2	2.47	0.44
1:B:232:LEU:HG	1:B:236:ARG:HE	1.82	0.44
1:C:30:ILE:HD13	1:C:59:ALA:CA	2.37	0.44
1:A:70:MET:HE2	1:A:74:GLY:HA2	1.96	0.44
1:B:79:LEU:HA	1:B:143:MET:HA	1.99	0.44
1:C:103:THR:HA	1:C:143:MET:HE1	2.00	0.44
1:D:1:MET:HB2	1:D:175:ASN:HD21	1.81	0.44
1:A:143:MET:HG2	1:A:144:ALA:N	2.32	0.44
1:B:132:MET:N	1:B:133:PRO:HD3	2.32	0.44
1:C:154:VAL:O	1:C:164:ILE:HA	2.18	0.44
1:C:38:GLN:HA	1:C:50:TRP:O	2.17	0.44
1:A:236:ARG:HB3	1:B:236:ARG:HB3	1.99	0.44
1:A:296:LYS:HE2	1:A:298:SER:CB	2.44	0.44
1:C:195:LEU:CD1	1:C:213:PHE:HZ	2.31	0.44
1:D:114:ARG:HA	1:D:114:ARG:NE	2.32	0.44
1:D:113:VAL:HG23	1:D:114:ARG:N	2.33	0.44
1:D:266:LYS:HE3	1:D:284:LYS:HG2	2.00	0.44
1:D:86:VAL:HB	1:D:159:ASP:CA	2.47	0.44
1:A:255:THR:O	1:A:256:ARG:HD2	2.18	0.44
1:A:130:PRO:CB	1:A:325:THR:CG2	2.96	0.44
1:C:52:SER:CA	1:C:108:ASP:HB2	2.48	0.44
1:D:46:LYS:O	1:D:96:ALA:N	2.49	0.44
1:B:75:LEU:HA	1:B:147:ASP:HA	2.00	0.44
1:B:232:LEU:O	1:B:235:MET:HB2	2.18	0.44
1:C:79:LEU:C	1:C:80:LEU:HD12	2.38	0.44
1:D:20:MET:HE3	1:D:26:ILE:HD12	2.00	0.44
1:D:42:HIS:HB3	1:D:47:THR:OG1	2.18	0.44
1:B:79:LEU:CG	1:B:143:MET:HE2	2.48	0.43
1:C:32:VAL:HG22	1:C:57:VAL:HG13	2.00	0.43
1:D:114:ARG:HA	1:D:114:ARG:HE	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:PHE:HA	1:D:141:LEU:CB	2.48	0.43
1:A:198:LEU:HD13	1:A:214:TYR:CE1	2.50	0.43
1:B:18:ARG:HD3	1:B:68:ASP:HB2	1.99	0.43
1:B:79:LEU:CD1	1:B:143:MET:HE2	2.47	0.43
1:C:218:ILE:HB	1:C:230:SER:HB3	2.00	0.43
1:C:70:MET:CB	1:C:76:VAL:HG22	2.47	0.43
1:D:85:SER:HB3	1:D:140:THR:CB	2.26	0.43
1:A:235:MET:N	1:A:235:MET:HE2	2.33	0.43
1:C:194:GLY:O	1:C:195:LEU:HB3	2.19	0.43
1:D:193:GLY:HA3	1:D:196:GLN:HE21	1.83	0.43
1:D:60:THR:HG22	1:D:319:PHE:CE2	2.54	0.43
1:A:36:GLY:HA2	1:A:51:THR:CG2	2.49	0.43
1:B:13:MET:HE2	1:B:224:ALA:HA	2.00	0.43
1:B:232:LEU:CD2	1:B:236:ARG:HH21	2.32	0.43
1:B:241:PRO:HB2	1:B:244:ILE:CD1	2.17	0.43
1:D:112:THR:HA	1:D:147:ASP:CG	2.39	0.43
1:B:235:MET:HB3	1:B:258:ARG:HD2	2.01	0.43
1:C:66:THR:HG21	1:C:104:GLN:HE21	1.84	0.43
1:C:147:ASP:OD1	1:C:149:THR:HB	2.17	0.43
1:B:79:LEU:CD1	1:B:103:THR:HG23	2.49	0.43
1:B:232:LEU:HD21	1:B:236:ARG:HH21	1.83	0.43
1:B:301:LYS:HB2	1:B:303:GLU:OE2	2.18	0.43
1:B:31:TYR:CD1	1:B:60:THR:HG21	2.53	0.43
1:C:114:ARG:HA	1:C:114:ARG:NE	2.33	0.43
1:C:221:THR:HG23	1:C:227:ALA:HB2	2.01	0.43
1:C:28:SER:HA	1:C:60:THR:O	2.18	0.43
1:D:141:LEU:N	1:D:141:LEU:HD12	2.33	0.43
1:D:189:TRP:CH2	1:D:199:PRO:HD3	2.54	0.43
1:D:81:PHE:HA	1:D:141:LEU:HA	2.01	0.43
1:A:86:VAL:HB	1:A:160:GLY:N	2.34	0.43
1:A:34:PRO:HB3	1:A:288:PHE:C	2.38	0.43
1:B:76:VAL:HG23	1:B:263:GLN:HG2	2.01	0.43
1:C:82:LEU:HD13	1:C:142:HIS:CD2	2.54	0.43
1:D:289:SER:OG	1:D:292:ALA:HB2	2.19	0.43
1:A:86:VAL:HB	1:A:160:GLY:H	1.83	0.43
1:C:173:MET:HA	1:C:208:PHE:HE1	1.83	0.43
1:D:144:ALA:C	1:D:145:ILE:HD12	2.39	0.43
1:D:185:VAL:HG11	1:D:205:SER:HB3	2.01	0.43
1:D:87:TYR:CD1	1:D:88:SER:N	2.87	0.43
1:C:113:VAL:HG12	1:C:166:GLU:OE2	2.19	0.43
1:C:232:LEU:O	1:C:236:ARG:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:THR:HG22	1:A:153:ALA:N	2.34	0.43
1:A:246:THR:HG21	1:B:195:LEU:HD11	2.00	0.43
1:B:55:GLY:HA3	1:B:288:PHE:CG	2.53	0.43
1:B:58:ILE:HD13	1:B:66:THR:HG22	1.99	0.43
1:B:4:ARG:CD	1:B:78:SER:HB2	2.49	0.43
1:B:87:TYR:O	1:B:88:SER:HB3	2.18	0.43
1:C:75:LEU:HG	1:C:145:ILE:CG2	2.49	0.43
1:D:172:VAL:HG11	1:D:212:SER:OG	2.19	0.43
1:A:197:MET:HA	1:B:201:THR:HG21	2.01	0.42
1:A:94:ARG:HB3	1:A:95:PRO:CD	2.49	0.42
1:C:11:ASP:O	1:C:264:LYS:HE2	2.19	0.42
1:C:201:THR:HB	1:C:206:ASP:OD2	2.19	0.42
1:C:23:LYS:HA	1:C:253:SER:HA	2.01	0.42
1:D:155:ILE:CG2	1:D:164:ILE:HG12	2.48	0.42
1:A:75:LEU:HD23	1:A:107:LEU:HD23	2.00	0.42
1:C:182:GLN:HG3	1:C:208:PHE:CD2	2.54	0.42
1:D:40:ALA:HB2	1:D:49:ASN:ND2	2.34	0.42
1:D:58:ILE:C	1:D:58:ILE:HD12	2.40	0.42
1:A:153:ALA:HA	1:A:166:GLU:HA	2.00	0.42
1:A:18:ARG:HD2	1:A:78:SER:HB3	2.00	0.42
1:A:235:MET:HA	1:A:235:MET:CE	2.49	0.42
1:C:145:ILE:HD12	1:C:145:ILE:N	2.34	0.42
1:D:262:ASP:HB3	1:D:267:VAL:H	1.85	0.42
1:A:64:ILE:HD12	1:A:322:LEU:HD12	2.00	0.42
1:B:31:TYR:OH	1:B:296:LYS:HD2	2.19	0.42
1:C:172:VAL:HG21	1:C:211:ALA:HB3	2.00	0.42
1:C:211:ALA:O	1:C:215:ILE:HG22	2.19	0.42
1:C:326:PRO:HB3	1:D:325:THR:O	2.20	0.42
1:D:153:ALA:HA	1:D:165:HIS:O	2.20	0.42
1:D:172:VAL:HG13	1:D:208:PHE:CZ	2.54	0.42
1:D:26:ILE:HG22	1:D:256:ARG:CG	2.49	0.42
1:A:26:ILE:HD13	1:A:28:SER:HB3	2.01	0.42
1:A:298:SER:O	1:A:299:LEU:HD23	2.19	0.42
1:A:38:GLN:HA	1:A:51:THR:HA	2.01	0.42
1:B:257:TRP:HB2	1:B:271:GLU:O	2.19	0.42
1:C:20:MET:CE	1:C:26:ILE:HD12	2.49	0.42
1:D:54:TYR:HE2	1:D:109:ASN:O	2.02	0.42
1:B:73:LYS:HB2	1:B:111:ALA:HB1	2.02	0.42
1:C:79:LEU:CD2	1:C:141:LEU:HD22	2.49	0.42
1:C:173:MET:HA	1:C:208:PHE:CE1	2.55	0.42
1:C:232:LEU:O	1:C:235:MET:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:ILE:HG12	1:D:164:ILE:CG2	2.45	0.42
1:A:141:LEU:N	1:A:141:LEU:HD12	2.34	0.42
1:D:225:LYS:O	1:D:229:PRO:HG2	2.19	0.42
1:A:34:PRO:O	1:A:37:MET:HG3	2.20	0.42
1:A:83:PRO:HD2	1:A:84:GLU:OE2	2.20	0.42
1:C:70:MET:CG	1:C:76:VAL:HG22	2.50	0.42
1:D:86:VAL:HB	1:D:159:ASP:N	2.35	0.42
1:B:45:GLU:HB3	1:B:96:ALA:HB3	2.01	0.42
1:C:97:MET:HB3	1:C:127:ILE:HD13	2.01	0.42
1:D:147:ASP:CG	1:D:148:GLU:H	2.22	0.42
1:D:20:MET:HG2	1:D:257:TRP:CE2	2.55	0.42
1:D:78:SER:C	1:D:143:MET:HG3	2.41	0.42
1:A:7:TYR:CD1	1:A:218:ILE:HD11	2.54	0.42
1:B:202:ASN:CG	1:B:207:ARG:HH21	2.23	0.42
1:B:94:ARG:HA	1:B:94:ARG:HD3	1.72	0.42
1:C:95:PRO:HD2	1:C:125:PHE:HA	2.02	0.42
1:D:151:ASN:HA	1:D:168:LYS:CG	2.39	0.42
1:A:178:ARG:NH1	1:A:180:GLU:OE1	2.53	0.41
1:B:87:TYR:O	1:B:160:GLY:HA2	2.19	0.41
1:B:325:THR:N	1:B:326:PRO:CD	2.80	0.41
1:B:94:ARG:HB3	1:B:125:PHE:HA	2.01	0.41
1:C:192:VAL:HG13	1:C:193:GLY:N	2.35	0.41
1:B:235:MET:HA	1:B:238:VAL:CG2	2.49	0.41
1:C:7:TYR:OH	1:C:221:THR:N	2.46	0.41
1:D:145:ILE:HG22	1:D:146:THR:N	2.34	0.41
1:D:41:GLY:O	1:D:98:GLY:N	2.39	0.41
1:A:87:TYR:HB3	1:A:127:ILE:HB	2.02	0.41
1:B:78:SER:O	1:B:143:MET:HA	2.21	0.41
1:B:232:LEU:HD11	1:B:258:ARG:CZ	2.49	0.41
1:C:321:PHE:HB3	1:C:323:PHE:CZ	2.56	0.41
1:C:29:ASN:HB2	1:C:63:ASP:OD1	2.21	0.41
1:A:95:PRO:O	1:A:126:ARG:N	2.52	0.41
1:B:172:VAL:HG21	1:B:211:ALA:HB3	2.03	0.41
1:C:6:VAL:HG22	1:C:16:THR:CG2	2.50	0.41
1:C:20:MET:HG2	1:C:257:TRP:CE2	2.55	0.41
1:C:42:HIS:CE1	1:C:323:PHE:HB2	2.55	0.41
1:D:232:LEU:CD2	1:D:236:ARG:HH21	2.33	0.41
1:A:280:TRP:N	1:A:307:GLY:O	2.53	0.41
1:B:80:LEU:HB2	1:B:173:MET:CE	2.46	0.41
1:C:200:GLY:HA2	1:C:210:ARG:NH2	2.36	0.41
1:D:194:GLY:HA3	1:D:213:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:VAL:HG23	1:A:235:MET:CE	2.50	0.41
1:A:286:ILE:HG22	1:A:287:ASP:N	2.35	0.41
1:C:326:PRO:CA	1:D:324:GLU:HB2	2.50	0.41
1:C:76:VAL:O	1:C:145:ILE:HA	2.21	0.41
1:D:58:ILE:HG22	1:D:107:LEU:CD1	2.50	0.41
1:D:78:SER:O	1:D:143:MET:HG3	2.20	0.41
1:D:199:PRO:HB2	1:D:206:ASP:OD2	2.20	0.41
1:A:58:ILE:C	1:A:58:ILE:HD12	2.41	0.41
1:B:75:LEU:HD21	1:B:145:ILE:HG21	2.02	0.41
1:B:16:THR:O	1:B:260:VAL:HG13	2.20	0.41
1:C:215:ILE:O	1:C:218:ILE:HG12	2.21	0.41
1:C:23:LYS:HG2	1:C:253:SER:N	2.36	0.41
1:D:256:ARG:HG3	1:D:257:TRP:HD1	1.86	0.41
1:A:152:THR:HB	1:A:170:TYR:O	2.21	0.41
1:A:283:LEU:N	1:A:283:LEU:HD12	2.36	0.41
1:B:62:TYR:O	1:B:63:ASP:HB2	2.21	0.41
1:C:110:PHE:HZ	1:C:119:GLU:CB	2.34	0.41
1:D:113:VAL:CG2	1:D:151:ASN:HB3	2.44	0.41
1:D:21:ASP:HA	1:D:254:SER:O	2.20	0.41
1:D:297:LEU:O	1:D:299:LEU:HG	2.21	0.41
1:A:147:ASP:OD1	1:A:149:THR:HB	2.21	0.41
1:B:145:ILE:HD12	1:B:145:ILE:N	2.36	0.41
1:C:235:MET:HA	1:C:235:MET:HE2	2.02	0.41
1:C:58:ILE:C	1:C:58:ILE:HD12	2.41	0.41
1:D:76:VAL:O	1:D:145:ILE:HA	2.21	0.41
1:D:42:HIS:NE2	1:D:323:PHE:HB3	2.36	0.41
1:A:140:THR:N	1:A:141:LEU:HD12	2.35	0.41
1:A:74:GLY:CA	1:A:266:LYS:HE3	2.50	0.41
1:B:232:LEU:HD12	1:B:235:MET:HB2	2.03	0.41
1:B:58:ILE:HD12	1:B:58:ILE:C	2.42	0.41
1:D:172:VAL:HG22	1:D:173:MET:N	2.36	0.41
1:D:26:ILE:HG12	1:D:61:GLY:O	2.21	0.41
1:A:171:GLN:NE2	1:A:215:ILE:CG2	2.84	0.40
1:A:259:SER:HB2	1:A:268:TYR:OH	2.22	0.40
1:B:99:ILE:HD11	1:B:141:LEU:HD11	2.02	0.40
1:B:279:PHE:HB3	1:B:306:ALA:CA	2.51	0.40
1:B:79:LEU:HG	1:B:143:MET:HE2	2.03	0.40
1:C:26:ILE:HD13	1:C:257:TRP:HE1	1.86	0.40
1:C:82:LEU:HD23	1:C:85:SER:OG	2.21	0.40
1:D:115:GLU:HG3	1:D:115:GLU:H	1.67	0.40
1:D:96:ALA:HB2	1:D:126:ARG:NH2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ARG:HH11	1:A:237:ASN:HD21	1.69	0.40
1:A:262:ASP:O	1:A:266:LYS:N	2.54	0.40
1:A:39:ARG:HD3	1:A:101:ILE:HD11	2.03	0.40
1:B:122:LYS:CB	1:B:124:THR:HG23	2.50	0.40
1:B:30:ILE:HA	1:B:30:ILE:HD13	1.98	0.40
1:B:317:GLN:N	1:B:317:GLN:OE1	2.44	0.40
1:C:11:ASP:O	1:C:12:ARG:HB2	2.22	0.40
1:C:27:MET:HB2	1:C:62:TYR:HD1	1.86	0.40
1:D:201:THR:HG22	1:D:202:ASN:N	2.27	0.40
1:D:47:THR:HG22	1:D:48:VAL:N	2.34	0.40
1:A:19:THR:HG22	1:A:20:MET:N	2.36	0.40
1:B:228:VAL:HB	1:B:229:PRO:CD	2.40	0.40
1:B:305:TYR:HD1	1:B:312:ASP:OD2	2.04	0.40
1:C:271:GLU:HG2	1:C:272:SER:N	2.35	0.40
1:C:31:TYR:CE2	1:C:296:LYS:HB2	2.56	0.40
1:D:154:VAL:O	1:D:165:HIS:N	2.53	0.40
1:B:106:VAL:HG13	1:B:110:PHE:CD2	2.56	0.40
1:B:174:THR:HB	1:B:182:GLN:NE2	2.37	0.40
1:B:189:TRP:CH2	1:B:199:PRO:HG3	2.57	0.40
1:B:296:LYS:HE2	1:B:298:SER:HB2	2.04	0.40
1:B:75:LEU:C	1:B:75:LEU:HD23	2.41	0.40
1:C:172:VAL:HG11	1:C:212:SER:CB	2.38	0.40
1:D:112:THR:HA	1:D:147:ASP:OD1	2.21	0.40
1:D:149:THR:HG22	1:D:168:LYS:NZ	2.37	0.40
1:D:221:THR:HG21	1:D:226:ILE:CG2	2.52	0.40
1:D:232:LEU:HD23	1:D:236:ARG:HH21	1.87	0.40
1:A:5:ALA:HA	1:A:172:VAL:HA	2.02	0.40
1:B:152:THR:HG22	1:B:153:ALA:N	2.36	0.40
1:B:271:GLU:HG2	1:B:272:SER:N	2.36	0.40
1:B:31:TYR:HD1	1:B:60:THR:HG21	1.87	0.40
1:B:28:SER:HB2	1:B:60:THR:O	2.20	0.40
1:C:201:THR:HB	1:C:206:ASP:CG	2.42	0.40
1:C:35:ARG:HG2	1:C:288:PHE:O	2.22	0.40
1:C:62:TYR:O	1:C:63:ASP:HB2	2.21	0.40
1:D:112:THR:HG23	1:D:147:ASP:CG	2.42	0.40
1:D:226:ILE:C	1:D:229:PRO:HD2	2.42	0.40
1:D:32:VAL:HG13	1:D:57:VAL:HG22	2.03	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:LYS:NZ	1:B:324:GLU:OE1[3_555]	2.16	0.04
1:A:320:THR:OG1	1:B:132:MET:O[3_555]	2.18	0.02

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	327/336 (97%)	297 (91%)	27 (8%)	3 (1%)	17	57
1	B	324/336 (96%)	285 (88%)	39 (12%)	0	100	100
1	C	315/336 (94%)	277 (88%)	37 (12%)	1 (0%)	41	75
1	D	315/336 (94%)	285 (90%)	29 (9%)	1 (0%)	41	75
All	All	1281/1344 (95%)	1144 (89%)	132 (10%)	5 (0%)	34	71

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	170	TYR
1	C	276	PRO
1	A	133	PRO
1	A	250	PRO
1	D	276	PRO

### 5.3.2 Protein sidechains [i](#)

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	287/294 (98%)	286 (100%)	1 (0%)	92	97
1	B	284/294 (97%)	281 (99%)	3 (1%)	73	87
1	C	279/294 (95%)	276 (99%)	3 (1%)	73	87
1	D	279/294 (95%)	277 (99%)	2 (1%)	84	93
All	All	1129/1176 (96%)	1120 (99%)	9 (1%)	81	91

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	GLU
1	B	3	THR
1	B	92	ASP
1	B	325	THR
1	C	1	MET
1	C	118	ASP
1	C	192	VAL
1	D	84	GLU
1	D	114	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	HIS
1	A	171	GLN
1	B	49	ASN
1	B	104	GLN
1	B	171	GLN
1	B	182	GLN
1	B	216	HIS
1	C	104	GLN
1	C	216	HIS
1	C	263	GLN
1	C	277	ASN
1	D	49	ASN
1	D	142	HIS
1	D	171	GLN
1	D	175	ASN
1	D	216	HIS
1	D	263	GLN
1	D	277	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 ⓘ

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$
2	QC7	B	401	1	28,30,30	2.77	8 (28%)	40,47,47	2.88	15 (37%)

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
2	QC7	B	401	1	-	4/15/65/65	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	QC7	C27-C26	7.74	1.69	1.53
2	B	401	QC7	C13-C25	6.69	1.66	1.53
2	B	401	QC7	C16-C14	5.48	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	QC7	C16-C17	4.85	1.61	1.53
2	B	401	QC7	C11-C12	3.95	1.61	1.53
2	B	401	QC7	C13-C14	-2.35	1.49	1.53
2	B	401	QC7	C10-C09	2.31	1.58	1.53
2	B	401	QC7	O15-C14	-2.18	1.38	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	QC7	C11-C12-C28	-9.87	102.96	114.62
2	B	401	QC7	C11-C12-C13	6.34	121.22	111.87
2	B	401	QC7	C18-C17-C16	-6.17	104.08	111.19
2	B	401	QC7	C28-C12-C13	5.77	118.03	111.81
2	B	401	QC7	C12-C13-C25	-4.64	103.32	109.72
2	B	401	QC7	C03-C04-C05	-4.35	110.09	114.57
2	B	401	QC7	C25-C13-C14	3.53	116.10	111.88
2	B	401	QC7	C04-C03-C02	2.84	119.70	114.52
2	B	401	QC7	C26-C27-C28	2.62	117.27	112.78
2	B	401	QC7	C23-C25-C13	2.59	114.60	111.82
2	B	401	QC7	C22-C23-C17	2.51	111.47	107.77
2	B	401	QC7	C17-C16-C14	-2.40	111.81	114.46
2	B	401	QC7	C22-C21-C19	2.11	113.18	110.47
2	B	401	QC7	C29-C28-C12	-2.05	107.59	110.94
2	B	401	QC7	C22-C23-C25	-2.02	108.18	111.35

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	QC7	C03-C04-C05-C07
2	B	401	QC7	C03-C04-C05-O06
2	B	401	QC7	C10-C09-C28-C29
2	B	401	QC7	C10-C09-C28-C12

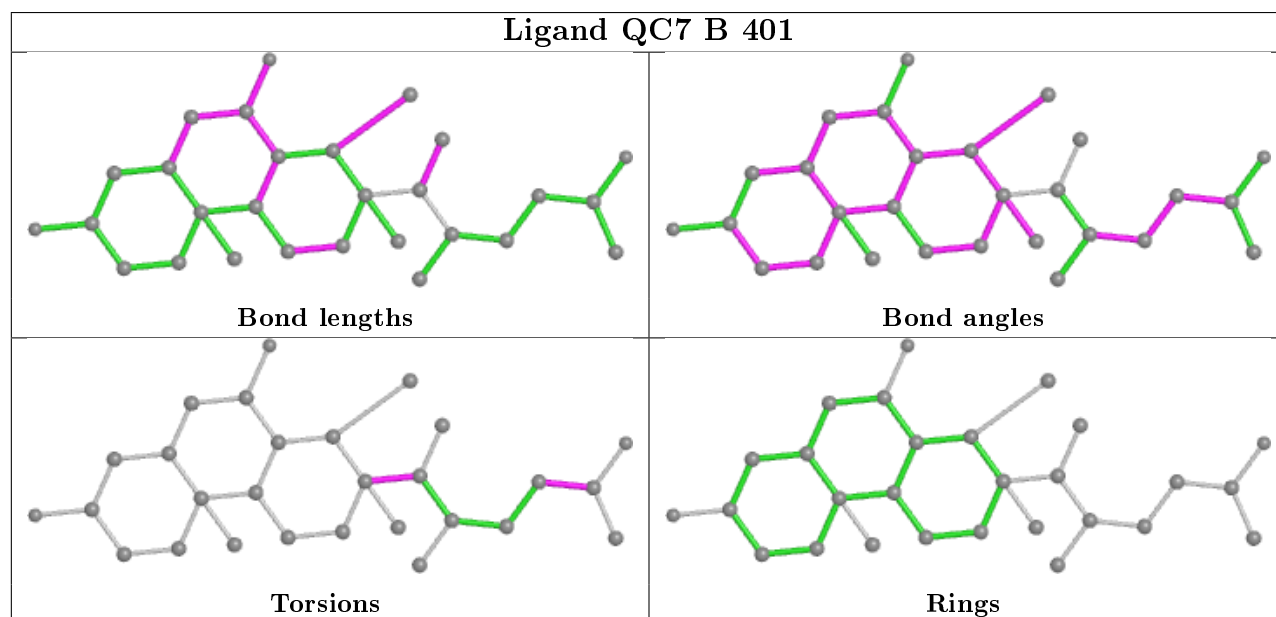
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	QC7	2	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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	329/336 (97%)	0.06	3 (0%) 84 73	107, 134, 173, 235	0
1	B	326/336 (97%)	0.16	11 (3%) 45 34	114, 152, 183, 205	0
1	C	319/336 (94%)	0.68	39 (12%) 4 4	196, 234, 255, 285	0
1	D	319/336 (94%)	0.60	32 (10%) 7 6	168, 222, 275, 336	0
All	All	1293/1344 (96%)	0.37	85 (6%) 18 14	107, 191, 254, 336	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	312	ASP	9.7
1	D	271	GLU	8.5
1	C	55	GLY	7.9
1	C	85	SER	7.7
1	C	56	SER	6.8
1	C	57	VAL	6.6
1	D	270	PHE	5.8
1	C	293	GLY	5.1
1	C	139	SER	4.7
1	D	287	ASP	4.7
1	C	292	ALA	4.6
1	C	222	ALA	4.4
1	C	68	ASP	4.3
1	D	214	TYR	4.1
1	D	210	ARG	3.9
1	D	263	GLN	3.8
1	C	241	PRO	3.8
1	C	175	ASN	3.7
1	C	143	MET	3.6
1	C	16	THR	3.5
1	B	156	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	68	ASP	3.5
1	C	271	GLU	3.4
1	D	278	LEU	3.4
1	B	113	VAL	3.4
1	C	24	GLU	3.3
1	D	25	ASP	3.3
1	C	67	CYS	3.2
1	C	65	GLY	3.2
1	D	120	MET	3.2
1	C	277	ASN	3.1
1	C	286	ILE	3.1
1	C	66	THR	3.1
1	D	192	VAL	3.0
1	D	283	LEU	3.0
1	D	292	ALA	3.0
1	D	296	LYS	2.9
1	D	258	ARG	2.9
1	D	156	GLU	2.9
1	C	224	ALA	2.9
1	D	105	TYR	2.8
1	B	163	SER	2.7
1	D	313	LEU	2.7
1	C	306	ALA	2.7
1	C	32	VAL	2.7
1	D	173	MET	2.7
1	D	272	SER	2.6
1	D	227	ALA	2.6
1	C	22	TRP	2.5
1	D	326	PRO	2.5
1	D	269	TYR	2.5
1	C	315	ASP	2.5
1	C	295	LYS	2.5
1	C	314	LYS	2.5
1	D	212	SER	2.5
1	B	164	ILE	2.5
1	D	87	TYR	2.4
1	C	313	LEU	2.4
1	D	211	ALA	2.4
1	C	166	GLU	2.4
1	B	312	ASP	2.4
1	C	220	GLN	2.4
1	C	62	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	305	TYR	2.4
1	D	310	VAL	2.3
1	C	296	LYS	2.3
1	B	227	ALA	2.3
1	D	222	ALA	2.3
1	D	216	HIS	2.3
1	D	322	LEU	2.3
1	C	6	VAL	2.3
1	C	178	ARG	2.3
1	A	67	CYS	2.2
1	D	290	PRO	2.2
1	C	291	LYS	2.2
1	D	231	VAL	2.2
1	A	276	PRO	2.2
1	B	14	VAL	2.2
1	B	306	ALA	2.2
1	C	36	GLY	2.2
1	B	254	SER	2.1
1	C	145	ILE	2.1
1	B	32	VAL	2.1
1	C	69	GLY	2.1
1	D	273	THR	2.0

## 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](#)

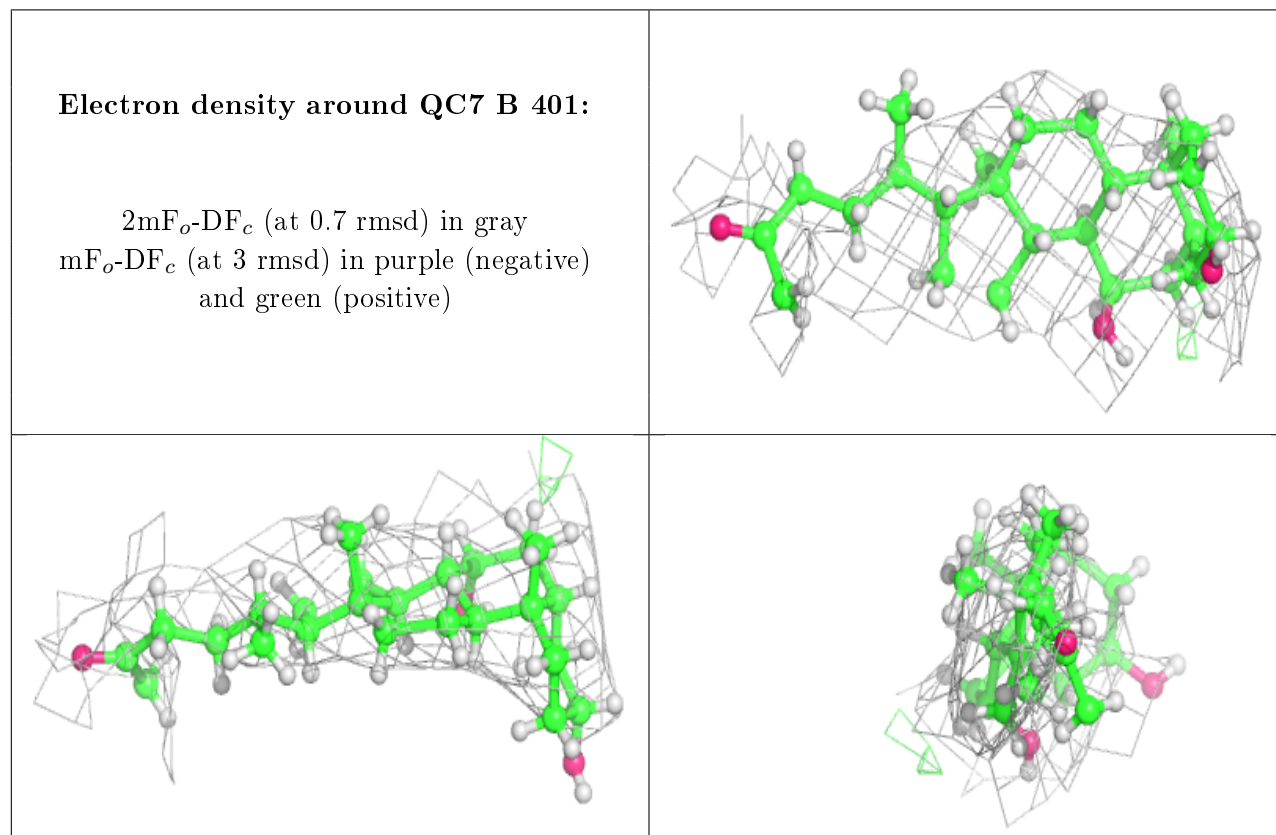
There are no carbohydrates in this entry.

## 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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	QC7	B	401	28/28	0.86	0.33	226,237,246,251	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 [i](#)

There are no such residues in this entry.