Full wwPDB X-ray Structure Validation Report (i)

Oct 16, 2023 – 01:51 PM EDT

PDB ID	:	1XC1
Title	:	Oxo Zirconium(IV) Cluster in the Ferric Binding Protein (FBP)
Authors	:	Zhong, W.; Alexeev, D.; Harvey, I.; Guo, M.; Hunter, D.J.B.; Zhu, H.; Campopiano, D.J.; Sadler, P.J.
Deposited on	:	2004-08-31
Resolution	:	1.51 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

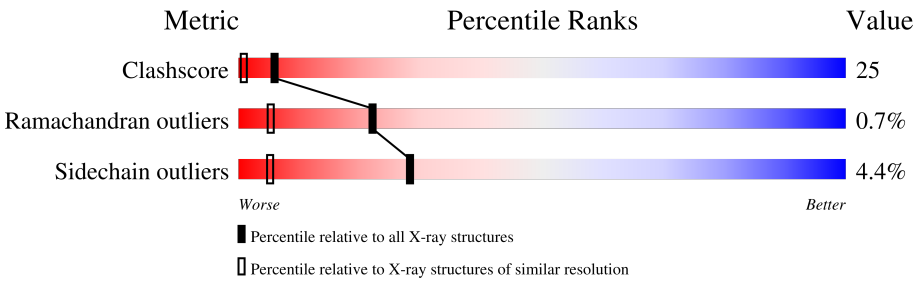
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.51 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))
Clashscore	141614	4249 (1.54-1.50)
Ramachandran outliers	138981	4148 (1.54-1.50)
Sidechain outliers	138945	4146 (1.54-1.50)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	309	66% 32% •
1	B	309	63% 35% •
1	C	309	52% 45% •
1	D	309	54% 42% •
1	E	309	70% 29% •
1	F	309	66% 30% •
1	G	309	57% 41% •
1	H	309	55% 42% •

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Mol	Chain	Length	Quality of chain
1	I	309	58% 39%

2 Entry composition (i)

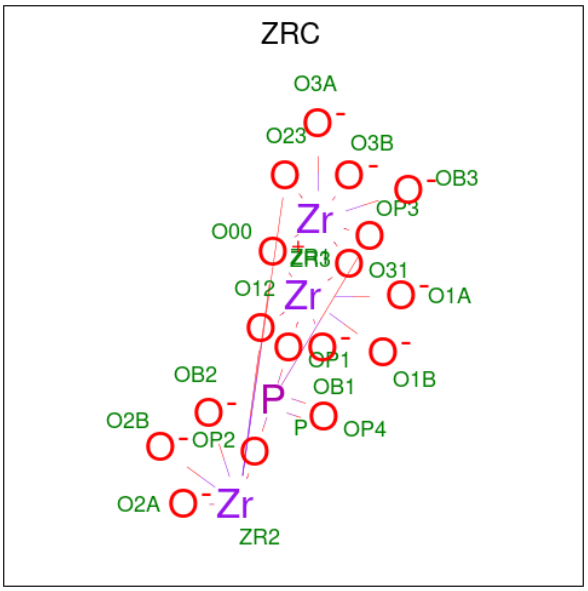
There are 3 unique types of molecules in this entry. The entry contains 22547 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called periplasmic iron-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	309	2378	1508	423	446	1	0	0	0
1	B	309	2378	1508	423	446	1	0	0	0
1	C	309	2378	1508	423	446	1	0	0	0
1	D	309	2378	1508	423	446	1	0	0	0
1	E	309	2378	1508	423	446	1	0	0	0
1	F	309	2378	1508	423	446	1	0	0	0
1	G	309	2378	1508	423	446	1	0	0	0
1	H	309	2378	1508	423	446	1	0	0	0
1	I	309	2378	1508	423	446	1	0	0	0

- Molecule 2 is OXO ZIRCONIUM(IV) CLUSTER (three-letter code: ZRC) (formula: $O_{17}PZr_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	P	Zr		
2	A	1	19	15	1	3	0	0
2	B	1	19	15	1	3	0	0
2	C	1	19	15	1	3	0	0
2	D	1	19	15	1	3	0	0
2	E	1	19	15	1	3	0	0
2	F	1	19	15	1	3	0	0
2	G	1	19	15	1	3	0	0
2	H	1	19	15	1	3	0	0
2	I	1	19	15	1	3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	142	142	142	0	0
3	B	103	103	103	0	0
3	C	111	111	111	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	D	113	113	113	0	0
			Total	O		
3	E	136	136	136	0	0
			Total	O		
3	F	124	124	124	0	0
			Total	O		
3	G	79	79	79	0	0
			Total	O		
3	H	81	81	81	0	0
			Total	O		
3	I	85	85	85	0	0

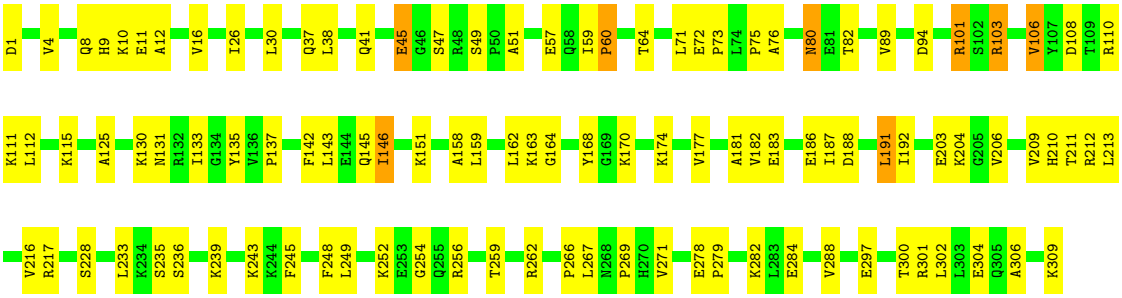
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

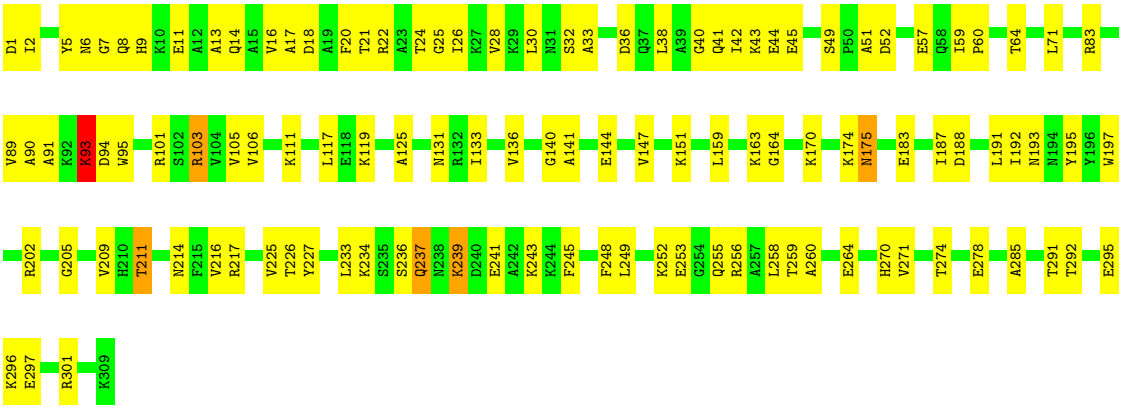
• Molecule 1: periplasmic iron-binding protein

Chain A:



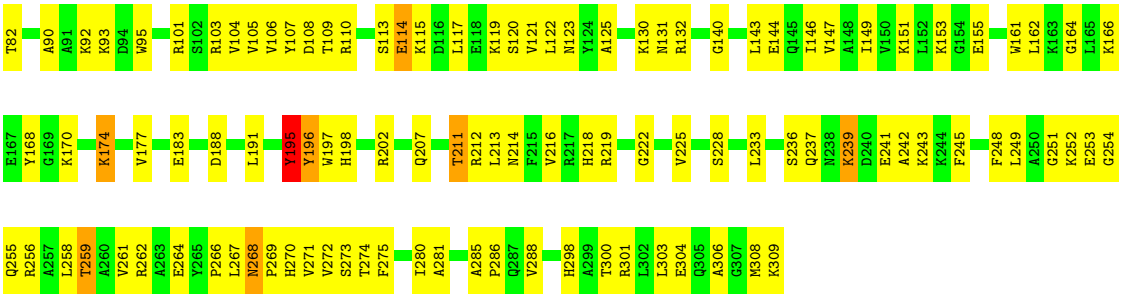
• Molecule 1: periplasmic iron-binding protein

Chain B:



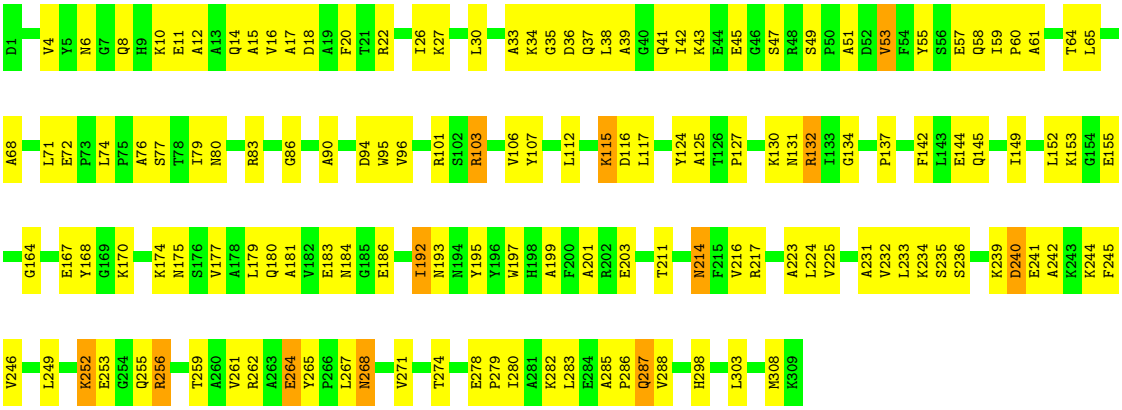
• Molecule 1: periplasmic iron-binding protein

Chain C:



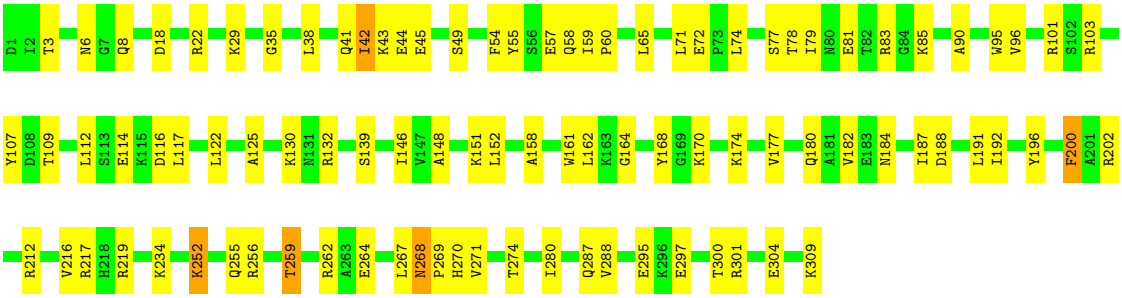
• Molecule 1: periplasmic iron-binding protein

Chain D:



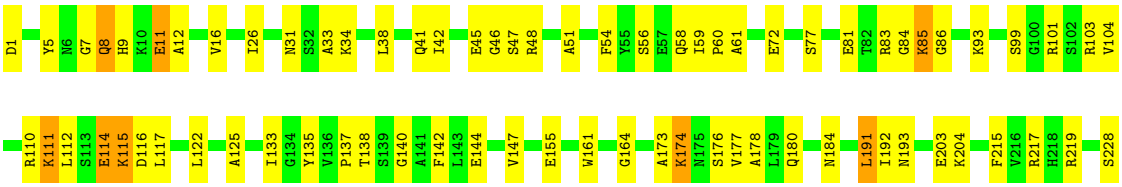
• Molecule 1: periplasmic iron-binding protein

Chain E:



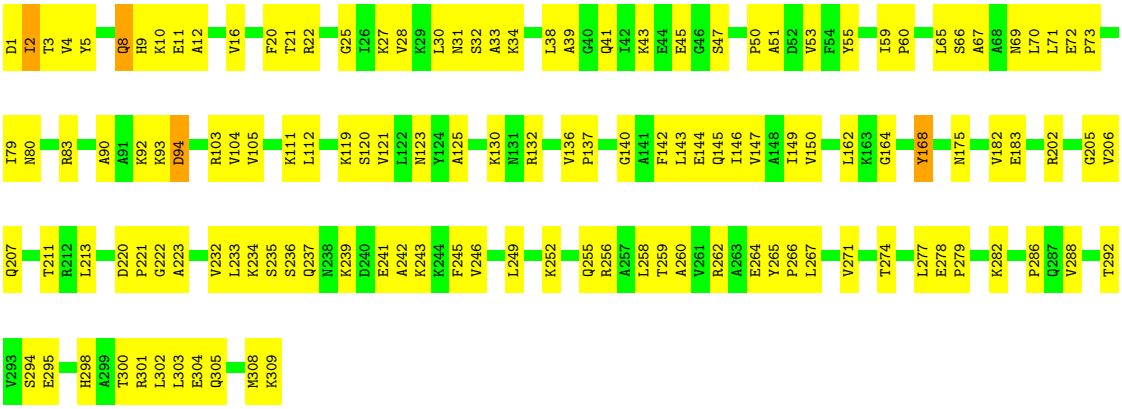
• Molecule 1: periplasmic iron-binding protein

Chain F:



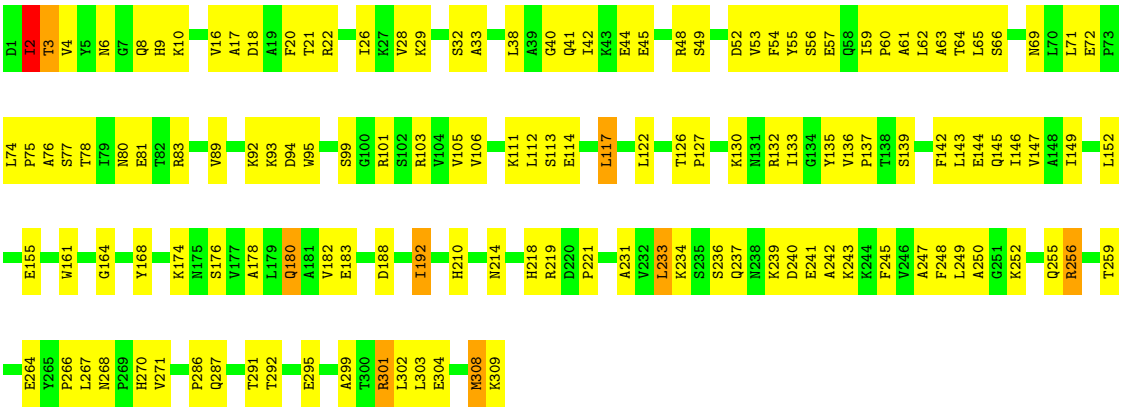
- Molecule 1: periplasmic iron-binding protein

Chain G:



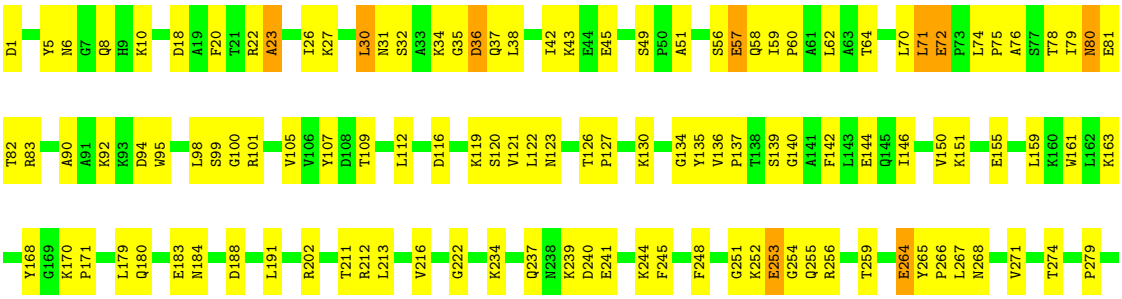
- Molecule 1: periplasmic iron-binding protein

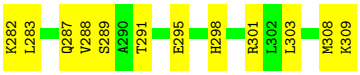
Chain H:



- Molecule 1: periplasmic iron-binding protein

Chain I:




K282
L283
Q287
V288
S289
A290
T291
E295
H298
R301
L302
L303
M308
K309

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	146.20Å 146.20Å 113.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 1.51	Depositor
% Data completeness (in resolution range)	97.3 (20.00-1.51)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.191 , 0.275	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22547	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

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: ZRC

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	0.39	0/2423	0.63	0/3280
1	B	0.36	0/2423	0.63	1/3280 (0.0%)
1	C	0.41	0/2423	0.65	2/3280 (0.1%)
1	D	0.37	0/2423	0.59	0/3280
1	E	0.38	0/2423	0.63	0/3280
1	F	0.37	0/2423	0.63	0/3280
1	G	0.34	0/2423	0.60	0/3280
1	H	0.35	0/2423	0.60	0/3280
1	I	0.36	0/2423	0.61	0/3280
All	All	0.37	0/21807	0.62	3/29520 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	195	TYR	CB-CG-CD1	5.81	124.49	121.00
1	B	205	GLY	N-CA-C	-5.34	99.75	113.10
1	C	196	TYR	CB-CG-CD2	5.22	124.13	121.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2378	0	2424	98	0
1	B	2378	0	2424	102	0
1	C	2378	0	2424	149	0
1	D	2378	0	2424	147	0
1	E	2378	0	2424	93	0
1	F	2378	0	2424	95	0
1	G	2378	0	2424	140	0
1	H	2378	0	2424	139	0
1	I	2378	0	2424	127	0
2	A	19	0	0	0	0
2	B	19	0	0	1	0
2	C	19	0	0	1	0
2	D	19	0	0	2	0
2	E	19	0	0	0	0
2	F	19	0	0	0	0
2	G	19	0	0	0	0
2	H	19	0	0	1	0
2	I	19	0	0	1	0
3	A	142	0	0	3	0
3	B	103	0	0	4	0
3	C	111	0	0	11	0
3	D	113	0	0	10	0
3	E	136	0	0	5	0
3	F	124	0	0	8	0
3	G	79	0	0	5	0
3	H	81	0	0	6	0
3	I	85	0	0	3	0
All	All	22547	0	21816	1086	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 25.

All (1086) 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:259:THR:HG21	1:A:266:PRO:HG3	1.24	1.17
1:F:259:THR:HG21	1:F:266:PRO:HG3	1.14	1.11
1:H:80:ASN:HA	1:H:83:ARG:HG2	1.27	1.10
1:H:259:THR:HG21	1:H:266:PRO:HG3	1.35	1.07
1:G:259:THR:HG21	1:G:266:PRO:HG3	1.35	1.06
1:C:202:ARG:HH22	1:C:274:THR:HG23	1.07	1.06
1:E:202:ARG:HH22	1:E:274:THR:HG22	1.19	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:202:ARG:NH2	1:E:274:THR:HG22	1.72	1.05
1:C:162:LEU:HB3	1:C:308:MET:HE2	1.44	0.98
1:G:119:LYS:HA	1:G:119:LYS:HE2	1.40	0.98
1:I:259:THR:HG21	1:I:266:PRO:HG3	1.42	0.97
1:I:56:SER:HB3	1:I:62:LEU:HD11	1.45	0.97
1:B:93:LYS:HE2	1:B:93:LYS:H	1.30	0.96
1:I:80:ASN:HA	1:I:83:ARG:HG2	1.45	0.94
1:I:43:LYS:HD2	1:I:70:LEU:HD11	1.47	0.93
1:B:170:LYS:HD2	1:B:187:ILE:HD12	1.51	0.92
1:C:202:ARG:NH2	1:C:274:THR:HG23	1.84	0.91
1:C:202:ARG:HH22	1:C:274:THR:CG2	1.84	0.91
1:F:176:SER:O	1:F:180:GLN:HG2	1.72	0.90
1:I:71:LEU:HB3	1:I:94:ASP:HB2	1.55	0.89
1:D:256:ARG:HG3	1:D:256:ARG:HH11	1.37	0.88
1:C:162:LEU:HD22	1:C:308:MET:HE1	1.56	0.88
1:C:262:ARG:HG2	1:C:264:GLU:HG3	1.53	0.88
1:B:255:GLN:HB2	1:B:271:VAL:HG21	1.57	0.87
1:C:256:ARG:NH1	1:C:272:VAL:H	1.72	0.86
1:I:202:ARG:NH2	1:I:274:THR:HG22	1.90	0.86
1:A:159:LEU:HD13	1:A:302:LEU:HD22	1.56	0.86
1:H:259:THR:CG2	1:H:266:PRO:HG3	2.06	0.86
1:C:256:ARG:HD3	1:C:271:VAL:HG13	1.58	0.85
1:E:72:GLU:HG2	1:E:234:LYS:HG2	1.59	0.84
1:H:268:ASN:HD22	1:H:271:VAL:HG23	1.42	0.84
1:D:174:LYS:HE3	1:D:177:VAL:HG23	1.59	0.84
1:D:101:ARG:CZ	1:D:264:GLU:HG2	2.08	0.84
1:A:288:VAL:HB	3:A:471:HOH:O	1.77	0.83
1:E:85:LYS:HD2	1:E:85:LYS:N	1.94	0.83
1:H:17:ALA:HB1	1:H:28:VAL:HG21	1.58	0.83
1:A:304:GLU:HG2	1:A:309:LYS:HG2	1.58	0.83
1:B:93:LYS:HE2	1:B:93:LYS:N	1.94	0.83
1:B:2:ILE:HG23	1:B:241:GLU:OE2	1.79	0.82
1:E:85:LYS:HD2	1:E:85:LYS:H	1.44	0.82
1:C:120:SER:HB3	1:C:123:ASN:ND2	1.95	0.82
1:I:18:ASP:HB3	1:I:22:ARG:HH12	1.45	0.81
1:C:121:VAL:HB	3:C:460:HOH:O	1.78	0.81
1:A:278:GLU:HB2	1:A:282:LYS:NZ	1.96	0.81
1:E:202:ARG:HH22	1:E:274:THR:CG2	1.93	0.80
1:H:2:ILE:HD11	1:H:53:VAL:HG23	1.65	0.79
1:D:132:ARG:HH11	1:D:132:ARG:HB3	1.47	0.79
1:C:252:LYS:O	1:C:256:ARG:HG2	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:239:LYS:O	1:G:243:LYS:HG3	1.84	0.78
1:I:202:ARG:HH22	1:I:274:THR:HG22	1.46	0.78
1:G:202:ARG:NH2	1:G:274:THR:HG22	1.99	0.78
1:C:259:THR:HG23	1:C:273:SER:HA	1.66	0.78
1:I:279:PRO:HD2	1:I:282:LYS:HD2	1.64	0.77
1:G:72:GLU:HG3	1:G:73:PRO:HD2	1.66	0.77
1:F:280:ILE:O	1:F:280:ILE:HD13	1.85	0.77
1:H:255:GLN:HB3	1:H:271:VAL:HG21	1.66	0.77
1:G:90:ALA:HB3	1:G:93:LYS:HA	1.66	0.77
1:H:4:VAL:HG22	1:H:53:VAL:HB	1.65	0.77
1:C:52:ASP:HA	1:C:236:SER:HB2	1.66	0.77
1:I:240:ASP:O	1:I:244:LYS:HG2	1.85	0.76
1:F:11:GLU:HG2	1:F:12:ALA:N	2.00	0.76
1:G:234:LYS:HB3	1:G:234:LYS:NZ	2.01	0.76
1:I:309:LYS:NZ	1:I:309:LYS:HB3	2.00	0.76
1:D:42:ILE:HD13	1:D:233:LEU:HD21	1.68	0.76
1:G:292:THR:OG1	1:G:295:GLU:HG3	1.86	0.76
1:F:147:VAL:HG13	1:F:295:GLU:HG2	1.68	0.76
1:H:255:GLN:CB	1:H:271:VAL:HG21	2.16	0.75
1:C:48:ARG:HE	1:C:237:GLN:NE2	1.84	0.75
1:C:79:ILE:HD12	1:C:93:LYS:HG3	1.68	0.75
1:A:101:ARG:HH22	1:A:228:SER:HB3	1.51	0.74
1:C:195:TYR:CE2	1:C:196:TYR:CE1	2.74	0.74
1:D:132:ARG:HB3	1:D:132:ARG:NH1	2.00	0.74
1:E:262:ARG:HG2	1:E:264:GLU:HG3	1.69	0.74
1:I:130:LYS:HG2	1:I:168:TYR:HD2	1.52	0.74
1:A:130:LYS:HE3	1:A:131:ASN:HD22	1.52	0.74
1:B:60:PRO:O	1:B:64:THR:HG23	1.88	0.74
1:A:125:ALA:HB1	1:A:164:GLY:HA3	1.70	0.73
1:B:197:TRP:HE1	1:B:211:THR:HG22	1.53	0.73
1:I:80:ASN:HB3	1:I:83:ARG:NH2	2.03	0.73
1:F:9:HIS:CD2	1:F:11:GLU:HB3	2.23	0.73
1:H:99:SER:HA	1:H:267:LEU:HG	1.69	0.73
1:F:192:ILE:HG22	1:F:193:ASN:N	2.03	0.73
1:B:5:TYR:CE1	1:B:51:ALA:HB2	2.24	0.73
1:D:61:ALA:O	1:D:65:LEU:HD23	1.88	0.73
1:E:158:ALA:O	1:E:162:LEU:HD13	1.89	0.73
1:G:259:THR:CG2	1:G:266:PRO:HG3	2.15	0.72
1:F:259:THR:CG2	1:F:266:PRO:HG3	2.06	0.72
1:C:130:LYS:HD3	1:C:131:ASN:N	2.05	0.72
1:D:256:ARG:HG3	1:D:256:ARG:NH1	1.99	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:130:LYS:CD	1:G:168:TYR:HB3	2.19	0.72
1:A:47:SER:HA	1:A:235:SER:HB3	1.72	0.72
1:F:85:LYS:NZ	1:F:219:ARG:HH12	1.87	0.72
1:A:72:GLU:OE1	1:A:73:PRO:HD2	1.89	0.71
1:D:39:ALA:HB1	1:D:65:LEU:HD21	1.72	0.71
1:G:302:LEU:HD23	1:G:305:GLN:NE2	2.05	0.71
1:B:41:GLN:O	1:B:45:GLU:HG2	1.88	0.71
1:B:209:VAL:HG12	1:B:211:THR:H	1.53	0.71
1:E:3:THR:HG22	1:E:29:LYS:HD3	1.71	0.71
1:F:85:LYS:HZ1	1:F:284:GLU:HA	1.55	0.71
1:D:174:LYS:HE3	1:D:177:VAL:CG2	2.19	0.71
1:G:236:SER:HB3	1:G:239:LYS:HG2	1.73	0.71
1:B:197:TRP:NE1	1:B:211:THR:HG22	2.05	0.71
1:H:3:THR:HB	1:H:29:LYS:HE2	1.73	0.71
1:H:268:ASN:ND2	1:H:271:VAL:HG23	2.04	0.71
1:B:252:LYS:HE2	1:B:256:ARG:NH2	2.06	0.70
1:H:71:LEU:O	1:H:234:LYS:HE3	1.90	0.70
1:H:80:ASN:HA	1:H:83:ARG:CG	2.15	0.70
1:C:303:LEU:HG	1:C:309:LYS:HA	1.73	0.70
1:B:45:GLU:HB3	1:B:49:SER:HB3	1.73	0.70
1:C:104:VAL:HG23	3:C:511:HOH:O	1.90	0.70
1:B:45:GLU:CB	1:B:49:SER:HB3	2.21	0.70
1:C:259:THR:O	1:C:274:THR:HG22	1.92	0.70
1:H:8:GLN:HG3	1:H:9:HIS:H	1.54	0.70
1:H:259:THR:HG21	1:H:266:PRO:CG	2.20	0.70
1:D:265:TYR:HB3	1:D:280:ILE:HG23	1.74	0.70
1:D:259:THR:HG23	3:D:411:HOH:O	1.92	0.69
1:G:4:VAL:HB	1:G:30:LEU:HD23	1.73	0.69
1:A:143:LEU:O	1:A:146:ILE:HG23	1.93	0.69
1:C:255:GLN:HE21	1:C:268:ASN:H	1.39	0.69
1:A:89:VAL:HG12	3:A:465:HOH:O	1.92	0.69
1:I:259:THR:CG2	1:I:266:PRO:HG3	2.20	0.69
1:E:252:LYS:O	1:E:256:ARG:HG3	1.93	0.69
1:I:30:LEU:C	1:I:31:ASN:HD22	1.96	0.69
1:I:81:GLU:OE1	1:I:251:GLY:HA2	1.93	0.69
1:H:112:LEU:HD11	1:H:188:ASP:HB3	1.75	0.69
1:A:60:PRO:O	1:A:64:THR:HG23	1.93	0.68
1:I:126:THR:HB	1:I:127:PRO:HD2	1.75	0.68
1:I:43:LYS:HD2	1:I:70:LEU:CD1	2.22	0.68
1:A:112:LEU:HD11	1:A:188:ASP:HB3	1.75	0.68
1:G:300:THR:O	1:G:304:GLU:HG3	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:174:LYS:NZ	2:H:400:ZRC:O23	2.25	0.68
1:H:192:ILE:N	1:H:192:ILE:HD13	2.09	0.68
1:A:279:PRO:HD2	1:A:282:LYS:NZ	2.09	0.68
1:E:170:LYS:HD2	1:E:187:ILE:HD12	1.76	0.68
1:H:81:GLU:HB2	1:H:250:ALA:HB1	1.75	0.68
1:D:77:SER:HA	1:D:80:ASN:HD22	1.56	0.67
1:G:130:LYS:HD2	1:G:168:TYR:HB3	1.75	0.67
1:B:125:ALA:HB1	1:B:164:GLY:HA3	1.75	0.67
1:I:56:SER:HB3	1:I:62:LEU:CD1	2.21	0.67
1:I:60:PRO:O	1:I:64:THR:HG23	1.93	0.67
1:I:127:PRO:O	1:I:130:LYS:HG3	1.94	0.67
1:C:151:LYS:HD2	1:C:288:VAL:HG23	1.77	0.67
1:D:8:GLN:HE22	1:D:101:ARG:HH22	1.41	0.67
1:F:5:TYR:CE1	1:F:51:ALA:HB2	2.30	0.67
1:A:278:GLU:HB2	1:A:282:LYS:HZ2	1.59	0.67
1:D:255:GLN:O	1:D:259:THR:HG22	1.95	0.67
1:G:125:ALA:HB1	1:G:164:GLY:HA3	1.77	0.67
1:G:5:TYR:CE1	1:G:51:ALA:HB2	2.30	0.66
1:F:125:ALA:HB1	1:F:164:GLY:HA3	1.76	0.66
1:B:255:GLN:CB	1:B:271:VAL:HG21	2.26	0.66
1:C:197:TRP:HE1	1:C:211:THR:HG23	1.59	0.66
1:B:8:GLN:HA	1:B:57:GLU:HG3	1.77	0.66
1:A:252:LYS:HE3	1:A:256:ARG:NH2	2.10	0.66
1:B:106:VAL:HG22	1:B:211:THR:HG23	1.77	0.66
1:C:259:THR:CG2	1:C:273:SER:HA	2.24	0.66
1:D:80:ASN:O	1:D:83:ARG:HG2	1.95	0.66
1:I:59:ILE:N	1:I:60:PRO:HD2	2.11	0.66
1:C:236:SER:H	1:C:239:LYS:HE2	1.59	0.66
1:F:259:THR:HG21	1:F:266:PRO:CG	2.09	0.66
1:D:236:SER:HB3	1:D:239:LYS:HG2	1.78	0.65
1:I:266:PRO:HD2	3:I:417:HOH:O	1.96	0.65
1:D:240:ASP:HB2	3:D:508:HOH:O	1.95	0.65
1:G:8:GLN:HG3	1:G:9:HIS:H	1.61	0.65
1:G:33:ALA:HB3	1:G:38:LEU:CD2	2.26	0.65
1:I:119:LYS:O	1:I:216:VAL:HG23	1.97	0.65
1:A:279:PRO:HG2	1:A:282:LYS:HG3	1.79	0.65
1:F:192:ILE:HG22	1:F:193:ASN:H	1.61	0.65
1:C:121:VAL:HG21	1:C:222:GLY:HA3	1.79	0.65
1:A:133:ILE:HD11	1:A:191:LEU:HD13	1.77	0.65
1:D:201:ALA:HB3	3:D:512:HOH:O	1.97	0.65
1:D:15:ALA:CB	1:D:261:VAL:HG21	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:GLN:NE2	1:C:268:ASN:H	1.95	0.65
1:C:48:ARG:HH21	1:C:237:GLN:HG3	1.61	0.64
1:G:202:ARG:HH22	1:G:274:THR:HG22	1.59	0.64
1:A:110:ARG:HH21	1:A:210:HIS:CD2	2.15	0.64
1:A:82:THR:HB	1:A:267:LEU:HB3	1.79	0.64
1:H:78:THR:HG23	1:H:247:ALA:HA	1.77	0.64
1:D:155:GLU:OE2	1:D:298:HIS:HE1	1.81	0.64
1:H:292:THR:OG1	1:H:295:GLU:HG3	1.97	0.64
1:A:174:LYS:HB2	1:A:177:VAL:HG23	1.79	0.64
1:I:72:GLU:HG3	1:I:239:LYS:HD2	1.78	0.64
1:B:38:LEU:O	1:B:42:ILE:HG13	1.97	0.64
1:D:267:LEU:HD23	1:D:280:ILE:HD13	1.78	0.64
1:D:45:GLU:HB2	1:D:49:SER:HB2	1.79	0.64
1:C:119:LYS:O	1:C:216:VAL:HG13	1.97	0.64
1:F:245:PHE:O	1:F:249:LEU:HG	1.98	0.64
1:H:38:LEU:O	1:H:42:ILE:HG13	1.97	0.63
1:A:9:HIS:HB3	1:A:12:ALA:CB	2.28	0.63
1:G:162:LEU:HD22	1:G:308:MET:HE1	1.80	0.63
1:H:126:THR:HB	1:H:127:PRO:HD2	1.81	0.63
1:B:292:THR:OG1	1:B:295:GLU:HG3	1.98	0.63
1:H:8:GLN:HG3	1:H:9:HIS:N	2.13	0.63
1:B:5:TYR:CD1	1:B:51:ALA:HB2	2.33	0.63
1:B:101:ARG:NH2	1:B:226:THR:HG22	2.13	0.63
1:G:140:GLY:O	1:G:144:GLU:HG2	1.98	0.63
1:C:113:SER:C	1:C:115:LYS:H	2.02	0.63
1:H:18:ASP:O	1:H:22:ARG:HG3	1.98	0.63
1:H:57:GLU:HB2	1:H:101:ARG:NH2	2.14	0.63
1:F:192:ILE:CG2	1:F:193:ASN:H	2.12	0.63
1:G:9:HIS:HB3	1:G:12:ALA:HB3	1.80	0.63
1:B:252:LYS:HE3	1:B:270:HIS:O	1.99	0.63
1:C:2:ILE:HG13	1:C:28:VAL:HG13	1.81	0.62
1:E:287:GLN:HB3	3:E:498:HOH:O	1.99	0.62
1:I:202:ARG:HH22	1:I:274:THR:CG2	2.12	0.62
1:C:28:VAL:HG11	3:C:462:HOH:O	1.99	0.62
1:G:130:LYS:HA	1:G:168:TYR:HB2	1.79	0.62
1:C:107:TYR:CD1	1:C:117:LEU:HD11	2.34	0.62
1:C:162:LEU:HB3	1:C:308:MET:CE	2.25	0.62
1:H:33:ALA:HB3	1:H:38:LEU:HG	1.80	0.62
1:E:268:ASN:C	1:E:268:ASN:HD22	2.03	0.62
1:I:240:ASP:HB3	1:I:241:GLU:OE2	1.99	0.62
1:C:114:GLU:OE2	1:C:214:ASN:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:34:LYS:O	1:G:38:LEU:HD23	2.00	0.62
1:H:41:GLN:O	1:H:45:GLU:HG3	2.00	0.62
1:D:72:GLU:HG2	1:D:234:LYS:HA	1.82	0.62
1:I:101:ARG:NH1	2:I:400:ZRC:O1A	2.33	0.62
1:G:5:TYR:HB3	1:G:38:LEU:HD12	1.82	0.61
1:F:115:LYS:O	1:F:116:ASP:CG	2.39	0.61
1:F:85:LYS:HD2	1:F:281:ALA:HA	1.82	0.61
1:G:300:THR:O	1:G:303:LEU:HB3	1.99	0.61
1:H:54:PHE:CE2	1:H:56:SER:HB2	2.35	0.61
1:E:72:GLU:HG2	1:E:234:LYS:HA	1.83	0.61
1:F:122:LEU:HA	1:F:161:TRP:CD1	2.35	0.61
1:C:105:VAL:HG22	1:C:191:LEU:HD23	1.82	0.61
1:C:268:ASN:C	1:C:268:ASN:HD22	2.04	0.61
1:E:38:LEU:O	1:E:42:ILE:HG13	2.01	0.61
1:G:303:LEU:HD22	1:G:308:MET:CE	2.30	0.61
1:H:16:VAL:HG11	1:H:249:LEU:CD2	2.30	0.61
1:A:236:SER:HB3	1:A:239:LYS:HG2	1.83	0.61
1:G:162:LEU:HD22	1:G:308:MET:CE	2.31	0.61
1:C:120:SER:HB3	1:C:123:ASN:HD21	1.66	0.60
1:H:136:VAL:O	1:H:139:SER:HB3	2.01	0.60
1:B:237:GLN:H	1:B:237:GLN:NE2	1.99	0.60
1:C:5:TYR:CD1	1:C:51:ALA:HB2	2.36	0.60
1:C:17:ALA:O	1:C:20:PHE:HB3	2.00	0.60
1:F:38:LEU:HD13	3:F:494:HOH:O	2.01	0.60
1:G:2:ILE:HD11	1:G:28:VAL:HG22	1.81	0.60
1:G:104:VAL:HG12	1:G:105:VAL:N	2.16	0.60
1:G:202:ARG:HH22	1:G:274:THR:CG2	2.14	0.60
1:A:304:GLU:HA	1:A:309:LYS:HB3	1.84	0.60
1:C:162:LEU:HD22	1:C:308:MET:CE	2.30	0.60
1:H:3:THR:HB	1:H:29:LYS:HB3	1.82	0.60
1:H:95:TRP:HB3	1:H:231:ALA:HB2	1.82	0.60
1:I:252:LYS:NZ	1:I:256:ARG:HD2	2.17	0.60
1:E:125:ALA:HB1	1:E:164:GLY:HA3	1.83	0.60
1:F:280:ILE:HD13	1:F:280:ILE:C	2.22	0.60
1:G:1:ASP:OD1	1:G:27:LYS:HD3	2.01	0.60
1:G:2:ILE:HB	3:G:443:HOH:O	2.01	0.60
1:G:162:LEU:HB3	1:G:308:MET:HE2	1.83	0.60
1:A:45:GLU:HB3	1:A:49:SER:HB3	1.82	0.60
1:H:59:ILE:N	1:H:60:PRO:HD2	2.16	0.60
1:F:85:LYS:NZ	1:F:284:GLU:HA	2.17	0.60
1:A:203:GLU:OE1	1:A:204:LYS:HE2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:LYS:NZ	1:D:27:LYS:HB3	2.16	0.60
1:G:279:PRO:HD2	1:G:282:LYS:HG3	1.82	0.60
1:H:75:PRO:HB2	1:H:77:SER:OG	2.00	0.60
1:I:10:LYS:HE2	1:I:32:SER:HB2	1.84	0.60
1:C:121:VAL:CG2	1:C:222:GLY:HA3	2.32	0.60
1:G:53:VAL:HG22	1:G:232:VAL:HG22	1.83	0.60
1:B:59:ILE:HD11	1:B:227:TYR:HB2	1.82	0.59
1:D:279:PRO:HB2	1:D:282:LYS:HE2	1.84	0.59
1:G:70:LEU:HD22	3:G:470:HOH:O	2.02	0.59
1:A:108:ASP:OD2	1:A:110:ARG:HD2	2.02	0.59
1:F:77:SER:O	1:F:81:GLU:HG3	2.01	0.59
1:F:101:ARG:NH1	1:F:101:ARG:HB2	2.18	0.59
1:H:69:ASN:HB3	1:H:92:LYS:NZ	2.16	0.59
1:G:260:ALA:HA	1:G:274:THR:OG1	2.02	0.59
1:G:302:LEU:HD23	1:G:305:GLN:HE22	1.68	0.59
1:I:82:THR:HB	1:I:267:LEU:HB3	1.83	0.59
1:I:109:THR:HG22	1:I:109:THR:O	2.03	0.59
1:A:146:ILE:CD1	1:A:158:ALA:HB1	2.32	0.59
1:E:78:THR:HG22	1:E:96:VAL:HG21	1.84	0.59
1:F:192:ILE:CG2	1:F:193:ASN:N	2.64	0.59
1:G:130:LYS:HD3	1:G:168:TYR:HB3	1.84	0.59
1:E:148:ALA:O	1:E:152:LEU:HD23	2.03	0.59
1:G:3:THR:CG2	1:G:31:ASN:HD21	2.15	0.59
1:I:80:ASN:N	1:I:80:ASN:HD22	2.01	0.59
1:I:130:LYS:HG2	1:I:168:TYR:CD2	2.37	0.59
1:D:4:VAL:HB	1:D:30:LEU:HD23	1.85	0.59
1:F:99:SER:HA	1:F:267:LEU:HG	1.84	0.59
1:G:5:TYR:CD1	1:G:51:ALA:HB2	2.38	0.59
1:I:5:TYR:CE1	1:I:51:ALA:HB2	2.38	0.59
1:I:309:LYS:HB3	1:I:309:LYS:HZ3	1.68	0.59
1:B:245:PHE:O	1:B:248:PHE:HB3	2.02	0.58
1:C:266:PRO:HD2	3:C:457:HOH:O	2.03	0.58
1:D:79:ILE:HG12	1:D:96:VAL:HG22	1.85	0.58
1:C:106:VAL:HB	3:C:511:HOH:O	2.02	0.58
1:D:16:VAL:HG11	1:D:249:LEU:HD22	1.83	0.58
1:B:133:ILE:HD11	1:B:191:LEU:CD1	2.32	0.58
1:E:255:GLN:HE22	1:E:267:LEU:H	1.51	0.58
1:C:130:LYS:HD2	1:C:131:ASN:ND2	2.19	0.58
1:E:252:LYS:HE2	1:E:252:LYS:H	1.69	0.58
1:H:146:ILE:HD11	1:H:303:LEU:HD21	1.86	0.58
1:F:135:TYR:CD2	1:F:137:PRO:HD3	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:233:LEU:N	1:F:233:LEU:HD12	2.18	0.58
1:C:252:LYS:HG2	1:C:268:ASN:OD1	2.03	0.58
1:D:34:LYS:HB3	1:D:37:GLN:CD	2.24	0.58
1:D:96:VAL:HG13	3:D:513:HOH:O	2.03	0.58
1:E:180:GLN:NE2	1:E:184:ASN:HD21	2.01	0.58
1:I:22:ARG:HG3	3:I:426:HOH:O	2.02	0.58
1:D:4:VAL:HG13	1:D:53:VAL:HG22	1.85	0.58
1:H:17:ALA:HB1	1:H:28:VAL:CG2	2.33	0.58
1:B:8:GLN:HA	1:B:57:GLU:CG	2.34	0.58
1:C:106:VAL:CG2	1:C:211:THR:OG1	2.52	0.58
1:G:234:LYS:HB3	1:G:234:LYS:HZ2	1.68	0.58
1:B:59:ILE:N	1:B:60:PRO:HD2	2.18	0.57
1:H:80:ASN:CA	1:H:83:ARG:HG2	2.18	0.57
1:C:104:VAL:HG21	1:C:213:LEU:HD22	1.84	0.57
1:E:268:ASN:HD22	1:E:270:HIS:H	1.52	0.57
1:B:197:TRP:CD1	1:B:211:THR:HG22	2.39	0.57
1:I:31:ASN:HD22	1:I:31:ASN:N	2.00	0.57
1:F:178:ALA:HB3	1:F:192:ILE:HD11	1.86	0.57
1:G:255:GLN:O	1:G:259:THR:HG23	2.04	0.57
1:A:106:VAL:HG13	1:A:213:LEU:HD23	1.85	0.57
1:D:184:ASN:HB2	1:D:186:GLU:HG3	1.87	0.57
1:D:51:ALA:HB3	1:D:233:LEU:HD22	1.86	0.57
1:F:85:LYS:HB2	3:F:514:HOH:O	2.05	0.57
1:H:152:LEU:HD12	3:H:481:HOH:O	2.05	0.57
1:I:34:LYS:HE3	1:I:36:ASP:OD2	2.05	0.57
1:E:255:GLN:NE2	1:E:268:ASN:H	2.02	0.57
1:E:268:ASN:ND2	1:E:270:HIS:H	2.02	0.57
1:G:43:LYS:HZ3	1:G:65:LEU:HD23	1.69	0.57
1:G:90:ALA:CB	1:G:93:LYS:HA	2.34	0.57
1:H:83:ARG:HA	1:H:83:ARG:NE	2.19	0.57
1:I:179:LEU:O	1:I:183:GLU:HB2	2.05	0.57
1:C:268:ASN:HD22	1:C:269:PRO:N	2.03	0.56
1:B:83:ARG:HH11	1:B:83:ARG:HB3	1.71	0.56
1:D:47:SER:HA	1:D:235:SER:HB3	1.86	0.56
1:D:101:ARG:HH21	1:D:262:ARG:HE	1.53	0.56
2:D:400:ZRC:O1B	3:D:407:HOH:O	2.18	0.56
1:F:147:VAL:HG22	1:F:295:GLU:HG3	1.86	0.56
1:B:136:VAL:HG21	1:B:175:ASN:HD22	1.71	0.56
1:B:141:ALA:CB	1:B:193:ASN:HD21	2.18	0.56
1:C:22:ARG:HD3	1:D:184:ASN:HB3	1.87	0.56
1:C:197:TRP:HB3	1:C:213:LEU:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:SER:HA	1:D:80:ASN:ND2	2.20	0.56
1:D:255:GLN:CB	1:D:271:VAL:HG21	2.35	0.56
1:F:85:LYS:NZ	1:F:219:ARG:NH1	2.53	0.56
1:G:9:HIS:CE1	1:G:11:GLU:HB3	2.40	0.56
1:G:20:PHE:C	1:G:22:ARG:H	2.09	0.56
1:G:47:SER:HA	1:G:235:SER:HB3	1.86	0.56
1:B:8:GLN:NE2	1:B:57:GLU:HG2	2.21	0.56
1:D:41:GLN:O	1:D:45:GLU:HG3	2.04	0.56
1:D:252:LYS:HG3	1:D:253:GLU:H	1.70	0.56
1:H:92:LYS:HB2	1:H:94:ASP:OD1	2.06	0.56
1:D:57:GLU:OE2	1:D:57:GLU:N	2.36	0.56
1:F:256:ARG:HG2	1:F:271:VAL:HG13	1.86	0.56
1:A:16:VAL:HG11	1:A:249:LEU:CD2	2.36	0.56
1:B:43:LYS:NZ	1:B:64:THR:HB	2.19	0.56
1:D:11:GLU:CD	1:D:11:GLU:H	2.09	0.56
1:H:117:LEU:HD23	1:H:214:ASN:ND2	2.20	0.56
1:B:18:ASP:O	1:B:22:ARG:HB2	2.06	0.56
1:I:155:GLU:OE1	1:I:298:HIS:HE1	1.89	0.56
1:D:107:TYR:HB2	1:D:112:LEU:HD12	1.88	0.56
1:G:303:LEU:HD12	1:G:309:LYS:HB2	1.88	0.56
1:F:177:VAL:HA	1:F:180:GLN:CG	2.36	0.56
1:G:79:ILE:HD11	1:G:93:LYS:HB2	1.87	0.56
1:I:288:VAL:HG12	1:I:289:SER:O	2.05	0.56
1:D:137:PRO:HB3	1:D:308:MET:HE3	1.87	0.56
1:I:253:GLU:OE1	1:I:254:GLY:N	2.38	0.56
1:B:159:LEU:O	1:B:163:LYS:HG3	2.06	0.55
1:H:164:GLY:O	1:H:168:TYR:HD1	1.89	0.55
1:G:41:GLN:O	1:G:45:GLU:HG3	2.05	0.55
1:F:203:GLU:HG3	1:F:204:LYS:N	2.20	0.55
1:H:236:SER:HB2	1:H:239:LYS:HG2	1.86	0.55
1:B:239:LYS:O	1:B:243:LYS:HG3	2.06	0.55
1:E:182:VAL:HG22	1:E:187:ILE:HG23	1.88	0.55
1:A:47:SER:HA	1:A:235:SER:CB	2.34	0.55
1:D:144:GLU:HG3	1:D:224:LEU:HD21	1.89	0.55
1:H:26:ILE:HD13	1:H:241:GLU:HG3	1.89	0.55
1:H:57:GLU:OE2	1:H:57:GLU:N	2.25	0.55
1:A:1:ASP:HB2	1:A:26:ILE:HG23	1.87	0.55
1:D:255:GLN:HB3	1:D:271:VAL:HG21	1.88	0.55
1:G:233:LEU:HD12	1:G:233:LEU:N	2.22	0.55
1:A:9:HIS:HB3	1:A:12:ALA:HB2	1.87	0.55
1:A:170:LYS:HG3	3:A:450:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:LEU:CD1	1:B:233:LEU:N	2.70	0.55
1:C:7:GLY:HA2	1:C:33:ALA:O	2.07	0.55
1:G:71:LEU:O	1:G:234:LYS:HD3	2.07	0.55
1:G:33:ALA:HB3	1:G:38:LEU:HD21	1.88	0.55
1:H:89:VAL:HG12	3:H:456:HOH:O	2.07	0.55
1:I:58:GLN:O	1:I:62:LEU:HD13	2.07	0.55
1:D:10:LYS:O	1:D:14:GLN:HG3	2.07	0.55
1:H:61:ALA:O	1:H:64:THR:HG22	2.07	0.55
1:I:255:GLN:CB	1:I:271:VAL:HG21	2.36	0.55
1:H:21:THR:HA	1:H:26:ILE:O	2.07	0.55
1:H:72:GLU:OE2	1:H:239:LYS:HD3	2.07	0.55
1:I:98:LEU:O	1:I:267:LEU:HB2	2.07	0.55
1:B:141:ALA:HB1	1:B:193:ASN:HD21	1.72	0.54
1:E:130:LYS:HD3	1:E:168:TYR:HD2	1.72	0.54
1:F:85:LYS:HZ3	1:F:219:ARG:HH12	1.54	0.54
1:A:9:HIS:ND1	1:A:262:ARG:HD3	2.22	0.54
1:H:40:GLY:O	1:H:44:GLU:HG3	2.06	0.54
1:I:27:LYS:HD3	1:I:27:LYS:C	2.27	0.54
1:B:91:ALA:O	1:B:93:LYS:HE3	2.07	0.54
1:G:71:LEU:CB	1:G:94:ASP:HB2	2.37	0.54
1:G:72:GLU:OE1	1:G:239:LYS:HD3	2.07	0.54
1:G:92:LYS:C	1:G:93:LYS:HG2	2.28	0.54
1:G:256:ARG:HG2	1:G:271:VAL:HG13	1.88	0.54
1:H:192:ILE:HD13	1:H:192:ILE:H	1.70	0.54
1:D:39:ALA:O	1:D:43:LYS:HG2	2.08	0.54
1:C:143:LEU:HA	1:C:146:ILE:HD12	1.89	0.54
1:H:245:PHE:O	1:H:248:PHE:HB3	2.07	0.54
1:C:262:ARG:CG	1:C:264:GLU:HG3	2.30	0.54
1:G:146:ILE:HD13	1:G:162:LEU:HD11	1.89	0.54
1:G:303:LEU:HD22	1:G:308:MET:HE1	1.89	0.54
1:I:151:LYS:HD2	1:I:288:VAL:HG13	1.88	0.54
1:C:51:ALA:HB3	1:C:233:LEU:CD2	2.38	0.54
1:I:34:LYS:HE2	1:I:37:GLN:HG3	1.89	0.54
1:I:183:GLU:OE1	1:I:211:THR:HG23	2.08	0.54
1:A:252:LYS:NZ	1:H:237:GLN:HB3	2.23	0.54
1:C:236:SER:O	1:C:237:GLN:HB2	2.08	0.54
1:D:34:LYS:HE3	1:D:36:ASP:H	1.73	0.54
1:F:147:VAL:HG13	1:F:295:GLU:CG	2.37	0.54
1:G:183:GLU:HA	1:G:211:THR:HG23	1.90	0.54
1:I:146:ILE:O	1:I:150:VAL:HG23	2.08	0.54
1:C:303:LEU:CG	1:C:309:LYS:HA	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:202:ARG:NH2	1:E:274:THR:CG2	2.57	0.54
1:H:255:GLN:HB2	1:H:271:VAL:HG21	1.88	0.54
1:C:130:LYS:HD3	1:C:130:LYS:C	2.29	0.53
1:I:57:GLU:HG2	1:I:58:GLN:HG3	1.89	0.53
1:I:137:PRO:HA	1:I:142:PHE:CD2	2.43	0.53
1:C:51:ALA:HB3	1:C:233:LEU:HD21	1.90	0.53
1:E:216:VAL:HG13	3:E:436:HOH:O	2.08	0.53
1:F:173:ALA:HB3	1:F:174:LYS:CE	2.38	0.53
1:C:166:LYS:HD2	3:C:417:HOH:O	2.07	0.53
1:G:303:LEU:CD1	1:G:309:LYS:HB2	2.38	0.53
1:A:75:PRO:HD3	1:A:243:LYS:HZ2	1.73	0.53
1:C:125:ALA:HB1	1:C:164:GLY:HA3	1.90	0.53
1:G:242:ALA:O	1:G:246:VAL:HG23	2.09	0.53
1:G:255:GLN:HB2	1:G:271:VAL:HG21	1.89	0.53
1:D:262:ARG:HG2	1:D:264:GLU:HG3	1.90	0.53
1:G:104:VAL:HG12	1:G:105:VAL:H	1.72	0.53
1:E:196:TYR:O	1:E:200:PHE:CD1	2.62	0.53
1:E:268:ASN:HD22	1:E:269:PRO:N	2.06	0.53
1:F:41:GLN:O	1:F:45:GLU:HG3	2.09	0.53
1:B:9:HIS:NE2	1:B:11:GLU:HG2	2.23	0.53
1:C:51:ALA:O	1:C:233:LEU:HD22	2.09	0.53
1:E:43:LYS:HA	3:E:527:HOH:O	2.08	0.53
1:F:8:GLN:OE1	1:F:12:ALA:HB3	2.08	0.53
1:I:252:LYS:CD	1:I:256:ARG:HD2	2.39	0.53
1:B:22:ARG:O	1:F:110:ARG:NH1	2.39	0.53
1:G:255:GLN:CB	1:G:271:VAL:HG21	2.39	0.53
1:B:233:LEU:N	1:B:233:LEU:HD12	2.24	0.53
1:G:67:ALA:HA	1:G:92:LYS:NZ	2.24	0.53
1:H:114:GLU:HA	1:H:117:LEU:HD22	1.90	0.53
1:E:252:LYS:H	1:E:252:LYS:CD	2.22	0.53
1:F:255:GLN:HB2	1:F:271:VAL:HG21	1.90	0.53
1:G:33:ALA:HB3	1:G:38:LEU:HD22	1.89	0.53
1:G:256:ARG:HB3	1:G:256:ARG:NH1	2.23	0.53
1:A:297:GLU:HA	1:A:297:GLU:OE2	2.09	0.52
1:G:21:THR:HG22	1:G:21:THR:O	2.09	0.52
1:E:79:ILE:HG12	1:E:96:VAL:HG22	1.90	0.52
1:B:22:ARG:HG2	1:F:184:ASN:O	2.09	0.52
1:B:291:THR:CG2	1:B:296:LYS:HE2	2.39	0.52
1:D:145:GLN:O	1:D:149:ILE:HG13	2.10	0.52
1:D:233:LEU:HD12	1:D:233:LEU:N	2.24	0.52
1:G:121:VAL:CG1	1:G:222:GLY:HA3	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:THR:OG1	1:C:266:PRO:HG3	2.09	0.52
1:I:253:GLU:CD	1:I:254:GLY:H	2.12	0.52
1:B:36:ASP:HB2	3:B:489:HOH:O	2.09	0.52
1:C:48:ARG:HE	1:C:237:GLN:HE21	1.54	0.52
1:E:252:LYS:H	1:E:252:LYS:CE	2.23	0.52
1:I:122:LEU:HA	1:I:161:TRP:CD1	2.44	0.52
1:E:161:TRP:CE3	1:E:162:LEU:HD12	2.45	0.52
1:H:16:VAL:HG11	1:H:249:LEU:HD23	1.91	0.52
1:H:105:VAL:HG23	3:H:480:HOH:O	2.09	0.52
1:C:33:ALA:HB3	1:C:38:LEU:HD21	1.92	0.52
1:D:6:ASN:OD1	1:D:55:TYR:HD2	1.93	0.52
1:H:268:ASN:HD22	1:H:271:VAL:CG2	2.18	0.52
1:B:216:VAL:HG23	3:B:437:HOH:O	2.10	0.52
1:G:59:ILE:N	1:G:60:PRO:CD	2.73	0.52
1:H:66:SER:O	1:H:92:LYS:HE2	2.10	0.52
1:H:240:ASP:HA	1:H:243:LYS:HD2	1.91	0.52
1:H:304:GLU:HA	1:H:309:LYS:O	2.09	0.52
1:I:34:LYS:HE2	1:I:37:GLN:CG	2.40	0.52
1:I:34:LYS:HG2	1:I:37:GLN:CD	2.30	0.52
1:I:59:ILE:N	1:I:60:PRO:CD	2.73	0.52
1:D:33:ALA:HB1	1:D:37:GLN:OE1	2.10	0.52
1:G:80:ASN:OD1	1:G:83:ARG:NH2	2.41	0.52
1:A:8:GLN:CG	1:A:9:HIS:H	2.23	0.51
1:C:4:VAL:HG22	1:C:53:VAL:HB	1.92	0.51
1:C:121:VAL:HG23	1:C:216:VAL:HG21	1.92	0.51
1:C:300:THR:O	1:C:304:GLU:HG3	2.10	0.51
1:C:304:GLU:HG2	1:C:309:LYS:HG3	1.91	0.51
1:D:103:ARG:HD2	1:D:145:GLN:HB2	1.92	0.51
1:F:5:TYR:CD1	1:F:51:ALA:HB2	2.44	0.51
1:H:152:LEU:HD11	1:H:286:PRO:HB2	1.92	0.51
1:I:245:PHE:O	1:I:248:PHE:HB3	2.09	0.51
1:F:262:ARG:HH11	1:F:264:GLU:HG3	1.74	0.51
1:G:2:ILE:HG13	1:G:2:ILE:O	2.09	0.51
1:I:140:GLY:O	1:I:144:GLU:HG2	2.10	0.51
1:D:26:ILE:HD13	1:D:241:GLU:HB3	1.91	0.51
1:G:104:VAL:HG11	1:G:213:LEU:HB3	1.93	0.51
1:H:6:ASN:OD1	1:H:8:GLN:HB3	2.11	0.51
1:I:34:LYS:HG2	1:I:37:GLN:OE1	2.09	0.51
1:I:259:THR:HG21	1:I:266:PRO:CG	2.29	0.51
1:B:202:ARG:NH2	1:B:274:THR:O	2.43	0.51
1:G:252:LYS:O	1:G:256:ARG:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ARG:NH2	1:A:183:GLU:O	2.32	0.51
1:I:20:PHE:CZ	1:I:26:ILE:HD12	2.45	0.51
1:A:9:HIS:HB3	1:A:12:ALA:HB3	1.92	0.51
1:C:1:ASP:OD1	1:C:27:LYS:HG2	2.11	0.51
1:D:10:LYS:HD2	1:D:14:GLN:NE2	2.25	0.51
1:F:114:GLU:O	1:F:117:LEU:HB2	2.10	0.51
1:I:18:ASP:HB3	1:I:22:ARG:NH1	2.21	0.51
1:E:45:GLU:HG3	1:E:49:SER:HB2	1.91	0.51
1:F:137:PRO:HA	1:F:142:PHE:CD2	2.46	0.51
1:I:121:VAL:HB	1:I:222:GLY:HA3	1.92	0.51
1:A:245:PHE:O	1:A:249:LEU:HG	2.10	0.51
1:C:174:LYS:HG3	1:C:177:VAL:HG23	1.93	0.51
1:D:106:VAL:HG22	1:D:211:THR:OG1	2.11	0.51
1:E:146:ILE:HG12	1:E:162:LEU:HD11	1.93	0.51
1:G:136:VAL:HG21	1:G:175:ASN:HD22	1.76	0.51
1:I:234:LYS:O	1:I:239:LYS:NZ	2.44	0.51
1:I:252:LYS:HZ3	1:I:256:ARG:HD2	1.76	0.51
1:C:43:LYS:HE3	1:C:64:THR:HG22	1.93	0.51
1:C:109:THR:HG21	1:C:212:ARG:NE	2.26	0.51
1:F:191:LEU:O	1:F:192:ILE:HG13	2.11	0.51
1:H:239:LYS:O	1:H:243:LYS:HG3	2.11	0.51
1:I:34:LYS:CE	1:I:37:GLN:HG3	2.40	0.51
1:C:255:GLN:CB	1:C:271:VAL:HG21	2.41	0.51
1:E:255:GLN:O	1:E:259:THR:HB	2.11	0.51
1:F:51:ALA:O	1:F:233:LEU:HD22	2.11	0.51
1:G:137:PRO:HA	1:G:142:PHE:CD2	2.46	0.51
1:I:1:ASP:OD1	1:I:27:LYS:HB3	2.12	0.51
1:D:236:SER:O	1:D:239:LYS:HG3	2.11	0.50
1:E:256:ARG:HD3	3:E:504:HOH:O	2.11	0.50
1:F:54:PHE:CE2	1:F:56:SER:HB2	2.46	0.50
1:I:79:ILE:HG22	1:I:83:ARG:NH1	2.26	0.50
1:B:174:LYS:NZ	2:B:400:ZRC:O23	2.45	0.50
1:C:15:ALA:HB2	1:C:261:VAL:HG11	1.93	0.50
1:C:109:THR:HG21	1:C:212:ARG:CD	2.41	0.50
1:D:76:ALA:O	1:D:80:ASN:ND2	2.44	0.50
1:E:77:SER:O	1:E:81:GLU:HG3	2.11	0.50
1:H:234:LYS:HE2	3:H:450:HOH:O	2.11	0.50
1:H:252:LYS:HE2	1:H:270:HIS:CB	2.41	0.50
1:I:248:PHE:CD1	1:I:253:GLU:OE1	2.63	0.50
1:F:58:GLN:HG3	1:F:61:ALA:H	1.76	0.50
1:H:38:LEU:HB3	1:H:54:PHE:HE1	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:80:ASN:HA	1:I:83:ARG:CG	2.30	0.50
1:D:34:LYS:HD2	1:D:35:GLY:N	2.26	0.50
1:E:255:GLN:CB	1:E:271:VAL:HG21	2.41	0.50
1:G:51:ALA:O	1:G:233:LEU:HD22	2.11	0.50
1:G:258:LEU:HD11	1:G:264:GLU:OE1	2.11	0.50
1:C:130:LYS:HE2	1:C:168:TYR:HA	1.94	0.50
1:E:74:LEU:CD1	1:E:96:VAL:HG23	2.42	0.50
1:B:111:LYS:HE2	1:B:111:LYS:HA	1.94	0.50
1:C:52:ASP:HA	1:C:236:SER:CB	2.37	0.50
1:C:252:LYS:HE2	1:C:270:HIS:CD2	2.46	0.50
1:D:34:LYS:O	1:D:37:GLN:HG2	2.11	0.50
1:F:133:ILE:HD11	1:F:191:LEU:HD13	1.93	0.50
1:D:217:ARG:NH1	1:D:278:GLU:OE2	2.45	0.50
1:G:3:THR:HG23	1:G:31:ASN:HD21	1.77	0.50
1:C:195:TYR:HE2	1:C:196:TYR:CE1	2.29	0.50
1:E:6:ASN:HD21	1:E:8:GLN:HB2	1.75	0.50
1:H:236:SER:HB2	1:H:239:LYS:CG	2.42	0.50
1:E:252:LYS:HE2	1:E:252:LYS:N	2.27	0.49
1:G:12:ALA:O	1:G:16:VAL:HG22	2.12	0.49
1:A:269:PRO:HG3	1:H:48:ARG:CZ	2.41	0.49
1:E:8:GLN:NE2	1:E:55:TYR:CE1	2.79	0.49
1:E:304:GLU:HG3	1:E:309:LYS:HD3	1.92	0.49
1:H:53:VAL:CG2	1:H:242:ALA:HB1	2.42	0.49
1:A:37:GLN:O	1:A:41:GLN:HB2	2.12	0.49
1:D:42:ILE:CD1	1:D:233:LEU:HD21	2.39	0.49
1:D:287:GLN:OE1	1:D:288:VAL:N	2.46	0.49
1:I:80:ASN:HB3	1:I:83:ARG:CZ	2.42	0.49
1:A:51:ALA:O	1:A:233:LEU:HD22	2.13	0.49
1:A:146:ILE:HD11	1:A:302:LEU:CD1	2.42	0.49
1:B:89:VAL:HG22	3:B:408:HOH:O	2.11	0.49
1:D:71:LEU:HD13	1:D:231:ALA:CB	2.43	0.49
1:E:297:GLU:O	1:E:301:ARG:HG2	2.12	0.49
1:H:122:LEU:HD21	1:H:149:ILE:HD13	1.94	0.49
1:D:4:VAL:HG13	1:D:53:VAL:CG2	2.42	0.49
1:D:217:ARG:HA	1:D:283:LEU:O	2.12	0.49
1:G:121:VAL:HG11	1:G:222:GLY:HA3	1.93	0.49
1:A:4:VAL:HB	1:A:30:LEU:HD23	1.93	0.49
1:A:142:PHE:O	1:A:146:ILE:HG22	2.13	0.49
1:C:90:ALA:HB2	1:C:95:TRP:CE2	2.46	0.49
1:D:117:LEU:N	1:D:117:LEU:HD12	2.27	0.49
1:D:268:ASN:HD22	1:D:268:ASN:C	2.15	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:148:ALA:O	1:E:152:LEU:CD2	2.61	0.49
1:G:66:SER:OG	1:G:92:LYS:HE3	2.13	0.49
1:I:38:LEU:O	1:I:42:ILE:HG13	2.13	0.49
1:C:301:ARG:HA	1:C:304:GLU:OE1	2.13	0.49
1:E:41:GLN:O	1:E:45:GLU:HG2	2.11	0.49
1:H:54:PHE:HD2	1:H:62:LEU:HD23	1.78	0.49
1:H:106:VAL:HB	1:H:192:ILE:HD11	1.94	0.49
1:A:248:PHE:O	1:A:254:GLY:HA3	2.13	0.49
1:C:40:GLY:O	1:C:44:GLU:HG3	2.12	0.49
1:E:191:LEU:N	1:E:191:LEU:HD22	2.27	0.49
1:G:234:LYS:HB3	1:G:234:LYS:HZ3	1.78	0.49
1:A:110:ARG:HE	1:A:210:HIS:CG	2.31	0.49
1:C:48:ARG:NH2	1:C:237:GLN:HG3	2.26	0.49
1:D:101:ARG:NH2	1:D:262:ARG:HE	2.11	0.49
1:F:155:GLU:OE2	1:F:298:HIS:HE1	1.96	0.49
1:H:2:ILE:HG23	1:H:2:ILE:O	2.13	0.49
1:I:268:ASN:HB3	1:I:271:VAL:HG23	1.95	0.49
1:C:122:LEU:HA	1:C:161:TRP:CD1	2.48	0.49
1:D:37:GLN:HG3	3:D:494:HOH:O	2.13	0.49
1:D:256:ARG:NH2	1:D:274:THR:HG22	2.27	0.49
1:F:140:GLY:O	1:F:144:GLU:HG2	2.13	0.49
1:H:81:GLU:HB3	1:H:250:ALA:O	2.13	0.49
1:D:8:GLN:NE2	1:D:101:ARG:HH22	2.11	0.48
1:D:232:VAL:HG23	1:D:246:VAL:HG21	1.95	0.48
1:I:105:VAL:HG22	1:I:191:LEU:HD23	1.94	0.48
1:D:101:ARG:NH1	1:D:264:GLU:HG2	2.28	0.48
1:E:255:GLN:HB2	1:E:271:VAL:HG21	1.95	0.48
1:A:304:GLU:HG2	1:A:309:LYS:CG	2.39	0.48
1:D:17:ALA:O	1:D:20:PHE:HB3	2.13	0.48
1:F:111:LYS:HD2	1:F:111:LYS:N	2.28	0.48
1:F:237:GLN:O	1:F:238:ASN:ND2	2.46	0.48
1:H:2:ILE:HD13	1:H:2:ILE:C	2.34	0.48
1:H:99:SER:OG	1:H:264:GLU:HG2	2.13	0.48
1:I:76:ALA:O	1:I:80:ASN:ND2	2.46	0.48
1:B:256:ARG:HA	1:B:259:THR:HG22	1.94	0.48
1:C:53:VAL:HG23	1:C:242:ALA:HB1	1.96	0.48
1:C:255:GLN:HB2	1:C:271:VAL:HG21	1.95	0.48
1:E:256:ARG:O	1:E:259:THR:HG22	2.13	0.48
1:F:191:LEU:C	1:F:192:ILE:HG13	2.34	0.48
1:G:245:PHE:O	1:G:249:LEU:HG	2.13	0.48
1:I:100:GLY:O	1:I:264:GLU:HG3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:107:TYR:O	1:I:211:THR:HA	2.14	0.48
1:I:309:LYS:HB3	1:I:309:LYS:HZ2	1.78	0.48
1:B:8:GLN:HG3	1:B:9:HIS:N	2.28	0.48
1:C:46:GLY:O	1:C:47:SER:C	2.51	0.48
1:C:72:GLU:OE1	1:C:73:PRO:HD2	2.13	0.48
1:D:74:LEU:HD12	1:D:96:VAL:HG23	1.95	0.48
1:D:197:TRP:CD1	1:D:211:THR:HG23	2.47	0.48
1:E:200:PHE:CD1	1:E:200:PHE:N	2.81	0.48
1:E:200:PHE:N	1:E:200:PHE:HD1	2.11	0.48
1:G:303:LEU:HD13	1:G:303:LEU:O	2.13	0.48
1:D:90:ALA:HB2	1:D:95:TRP:CD2	2.49	0.48
1:F:72:GLU:OE2	1:F:239:LYS:HD3	2.14	0.48
1:A:111:LYS:HE2	1:A:111:LYS:HB3	1.74	0.48
1:C:22:ARG:HG2	3:C:433:HOH:O	2.13	0.48
1:G:47:SER:HA	1:G:235:SER:CB	2.43	0.48
1:G:220:ASP:OD1	1:G:221:PRO:HD2	2.14	0.48
1:I:119:LYS:O	1:I:216:VAL:CG2	2.60	0.48
1:B:255:GLN:O	1:B:259:THR:HG22	2.14	0.48
1:C:59:ILE:N	1:C:60:PRO:HD2	2.29	0.48
1:D:43:LYS:HZ3	1:D:68:ALA:CB	2.26	0.48
1:F:58:GLN:HB2	3:F:508:HOH:O	2.13	0.48
1:G:71:LEU:HB3	1:G:94:ASP:HB2	1.96	0.48
1:H:256:ARG:CB	1:H:256:ARG:HH11	2.26	0.48
1:B:117:LEU:HD22	1:B:214:ASN:HB2	1.95	0.47
1:C:183:GLU:HG2	1:C:211:THR:CG2	2.44	0.47
1:F:240:ASP:OD1	1:F:241:GLU:HG3	2.14	0.47
1:G:256:ARG:CB	1:G:256:ARG:HH11	2.27	0.47
1:G:282:LYS:HA	1:G:282:LYS:HE2	1.95	0.47
1:H:76:ALA:O	1:H:80:ASN:ND2	2.46	0.47
1:H:143:LEU:O	1:H:147:VAL:HG23	2.13	0.47
1:B:9:HIS:CE1	1:B:11:GLU:HG2	2.49	0.47
1:D:180:GLN:NE2	1:D:184:ASN:OD1	2.46	0.47
1:E:41:GLN:O	1:E:42:ILE:C	2.51	0.47
1:G:2:ILE:HG21	1:G:241:GLU:O	2.14	0.47
1:G:5:TYR:CB	1:G:38:LEU:HD12	2.44	0.47
1:I:80:ASN:N	1:I:80:ASN:ND2	2.61	0.47
1:C:113:SER:C	1:C:115:LYS:N	2.67	0.47
1:D:34:LYS:HD2	1:D:35:GLY:H	1.79	0.47
1:D:197:TRP:NE1	1:D:211:THR:HG23	2.30	0.47
1:G:237:GLN:HA	1:G:237:GLN:NE2	2.29	0.47
1:B:117:LEU:N	1:B:117:LEU:HD12	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:59:ILE:N	1:E:60:PRO:CD	2.78	0.47
1:G:233:LEU:HD12	1:G:233:LEU:H	1.80	0.47
1:I:134:GLY:HA2	1:I:170:LYS:O	2.15	0.47
1:I:252:LYS:HD2	1:I:256:ARG:HD2	1.96	0.47
1:C:170:LYS:HE3	1:C:170:LYS:HB2	1.67	0.47
1:D:267:LEU:CD2	1:D:280:ILE:HD13	2.44	0.47
1:D:279:PRO:HD2	1:D:282:LYS:HG3	1.96	0.47
1:E:151:LYS:HE3	1:E:295:GLU:OE1	2.13	0.47
1:I:72:GLU:HG2	1:I:234:LYS:HA	1.97	0.47
1:I:252:LYS:O	1:I:256:ARG:HG3	2.15	0.47
1:A:279:PRO:CG	1:A:282:LYS:HE3	2.44	0.47
1:C:239:LYS:O	1:C:243:LYS:HG3	2.15	0.47
1:D:43:LYS:HZ1	1:D:64:THR:C	2.18	0.47
1:F:101:ARG:HB2	1:F:101:ARG:HH11	1.79	0.47
1:H:133:ILE:O	1:H:133:ILE:HG23	2.14	0.47
1:I:98:LEU:C	1:I:267:LEU:HD22	2.34	0.47
1:I:135:TYR:O	1:I:171:PRO:HA	2.15	0.47
1:D:142:PHE:HE2	1:D:308:MET:HE1	1.80	0.47
1:E:74:LEU:HD13	1:E:96:VAL:HG23	1.97	0.47
1:F:138:THR:HG23	3:F:441:HOH:O	2.13	0.47
1:G:21:THR:O	1:G:25:GLY:HA2	2.15	0.47
1:I:127:PRO:HA	1:I:168:TYR:CD2	2.50	0.47
1:F:59:ILE:N	1:F:60:PRO:CD	2.77	0.47
1:H:59:ILE:N	1:H:60:PRO:CD	2.77	0.47
1:A:57:GLU:HG2	1:A:101:ARG:NH1	2.29	0.47
1:A:217:ARG:HH11	1:A:217:ARG:HG2	1.80	0.47
1:C:147:VAL:O	1:C:151:LYS:HG3	2.14	0.47
1:D:197:TRP:HE1	1:D:211:THR:HG23	1.80	0.47
1:D:240:ASP:O	1:D:244:LYS:HG3	2.15	0.47
1:F:262:ARG:HH11	1:F:262:ARG:HG2	1.79	0.47
1:G:303:LEU:HD22	1:G:308:MET:HE3	1.97	0.47
1:A:10:LYS:HE2	1:I:81:GLU:OE2	2.15	0.46
1:A:135:TYR:CD2	1:A:137:PRO:HD3	2.50	0.46
1:B:6:ASN:HD22	1:B:32:SER:HB3	1.79	0.46
1:E:122:LEU:HA	1:E:161:TRP:CD1	2.49	0.46
1:G:71:LEU:HB2	1:G:94:ASP:HB2	1.96	0.46
1:H:55:TYR:CE1	1:H:249:LEU:HD13	2.51	0.46
1:H:71:LEU:HD23	1:H:233:LEU:HD12	1.97	0.46
1:D:256:ARG:NH2	1:D:274:THR:CG2	2.78	0.46
1:F:103:ARG:NH1	3:F:411:HOH:O	2.48	0.46
1:H:99:SER:HB2	1:H:264:GLU:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:146:ILE:CD1	1:H:303:LEU:HD21	2.44	0.46
1:H:183:GLU:OE2	1:H:210:HIS:HB2	2.14	0.46
1:H:252:LYS:HE2	1:H:270:HIS:HB3	1.97	0.46
1:A:106:VAL:HG13	1:A:213:LEU:CD2	2.45	0.46
1:D:33:ALA:HB3	1:D:38:LEU:HG	1.97	0.46
1:D:65:LEU:N	1:D:65:LEU:HD22	2.30	0.46
1:F:228:SER:HB3	3:F:500:HOH:O	2.15	0.46
1:D:43:LYS:NZ	1:D:68:ALA:HB2	2.30	0.46
1:E:109:THR:HG21	1:E:212:ARG:HG2	1.96	0.46
1:E:112:LEU:HD22	1:E:112:LEU:N	2.31	0.46
1:G:3:THR:CG2	1:G:31:ASN:ND2	2.79	0.46
1:G:112:LEU:HD21	1:G:132:ARG:HH12	1.79	0.46
1:G:301:ARG:O	1:G:305:GLN:HG3	2.15	0.46
1:H:69:ASN:HB3	1:H:92:LYS:HZ2	1.80	0.46
1:H:122:LEU:HA	1:H:161:TRP:CD1	2.51	0.46
1:I:18:ASP:O	1:I:22:ARG:NH1	2.49	0.46
1:B:258:LEU:C	1:B:260:ALA:H	2.19	0.46
1:H:99:SER:CB	1:H:264:GLU:HG2	2.46	0.46
1:H:135:TYR:CE2	1:H:308:MET:HE3	2.50	0.46
1:I:101:ARG:HG2	1:I:264:GLU:CD	2.36	0.46
1:A:146:ILE:HD11	1:A:302:LEU:HD12	1.97	0.46
1:A:279:PRO:HD2	1:A:282:LYS:HZ2	1.79	0.46
1:B:7:GLY:HA2	1:B:33:ALA:O	2.16	0.46
1:B:41:GLN:O	1:B:45:GLU:CG	2.61	0.46
1:B:117:LEU:HD22	1:B:214:ASN:CB	2.45	0.46
1:B:117:LEU:HD12	1:B:117:LEU:H	1.79	0.46
1:A:159:LEU:HD12	1:A:159:LEU:HA	1.81	0.46
1:B:28:VAL:HG12	1:B:30:LEU:CD1	2.46	0.46
1:B:83:ARG:HB3	1:B:83:ARG:NH1	2.31	0.46
1:B:245:PHE:CE2	1:B:249:LEU:HD11	2.51	0.46
1:D:15:ALA:HB3	1:D:261:VAL:HG21	1.97	0.46
1:D:125:ALA:HB1	1:D:164:GLY:HA3	1.98	0.46
1:G:2:ILE:O	1:G:4:VAL:HG23	2.15	0.46
1:C:82:THR:HB	1:C:267:LEU:HB3	1.97	0.46
1:F:112:LEU:HD13	1:F:117:LEU:HD11	1.97	0.46
1:H:192:ILE:N	1:H:192:ILE:CD1	2.78	0.46
1:A:151:LYS:HD2	1:A:288:VAL:CG2	2.46	0.46
1:B:71:LEU:O	1:B:234:LYS:HE3	2.15	0.46
1:C:245:PHE:O	1:C:248:PHE:HB3	2.15	0.46
1:C:280:ILE:HG23	1:C:281:ALA:N	2.31	0.46
1:D:242:ALA:O	1:D:246:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:11:GLU:HG3	1:F:261:VAL:HG12	1.96	0.46
1:F:34:LYS:O	1:F:38:LEU:HD22	2.16	0.46
1:I:120:SER:HB3	1:I:123:ASN:ND2	2.30	0.46
1:A:137:PRO:HA	1:A:142:PHE:CD2	2.50	0.45
1:C:26:ILE:HD13	1:C:26:ILE:HA	1.85	0.45
1:C:92:LYS:O	1:C:93:LYS:HB3	2.15	0.45
1:D:279:PRO:O	1:D:282:LYS:HG2	2.16	0.45
1:H:219:ARG:O	1:H:286:PRO:HB3	2.17	0.45
1:I:112:LEU:HB2	1:I:116:ASP:HB2	1.98	0.45
1:I:159:LEU:O	1:I:163:LYS:HG3	2.16	0.45
1:B:106:VAL:HG22	1:B:211:THR:CG2	2.45	0.45
1:C:113:SER:O	1:C:115:LYS:N	2.44	0.45
1:C:255:GLN:O	1:C:259:THR:HB	2.16	0.45
1:F:174:LYS:HG3	1:F:176:SER:OG	2.16	0.45
1:A:130:LYS:HA	1:A:168:TYR:HB3	1.97	0.45
1:A:300:THR:O	1:A:304:GLU:HG3	2.16	0.45
1:B:119:LYS:O	1:B:216:VAL:HG13	2.17	0.45
1:C:268:ASN:C	1:C:268:ASN:ND2	2.68	0.45
1:I:31:ASN:N	1:I:31:ASN:ND2	2.65	0.45
1:C:219:ARG:O	1:C:286:PRO:HB3	2.16	0.45
1:D:74:LEU:CD1	1:D:96:VAL:HG23	2.47	0.45
1:E:72:GLU:CG	1:E:234:LYS:HA	2.45	0.45
1:G:10:LYS:HE2	1:G:32:SER:HB3	1.99	0.45
1:G:243:LYS:HG2	3:G:471:HOH:O	2.15	0.45
1:H:155:GLU:HG3	1:H:302:LEU:HD11	1.98	0.45
1:B:245:PHE:O	1:B:249:LEU:HG	2.16	0.45
1:F:85:LYS:CE	1:F:219:ARG:HH22	2.29	0.45
1:F:270:HIS:CG	1:I:237:GLN:HG3	2.51	0.45
1:H:52:ASP:HA	1:H:236:SER:OG	2.17	0.45
1:A:256:ARG:HG3	1:A:271:VAL:HG13	1.98	0.45
1:B:291:THR:HG21	1:B:296:LYS:HE2	1.99	0.45
1:C:106:VAL:HG23	1:C:211:THR:OG1	2.16	0.45
1:D:4:VAL:HG22	1:D:53:VAL:HG22	1.98	0.45
1:E:54:PHE:CD2	1:E:65:LEU:HD12	2.52	0.45
1:G:20:PHE:C	1:G:22:ARG:N	2.70	0.45
1:A:212:ARG:HH11	1:A:212:ARG:HG2	1.81	0.45
1:B:106:VAL:HB	1:B:192:ILE:HD11	1.97	0.45
1:D:117:LEU:HD22	1:D:214:ASN:HB2	1.99	0.45
1:D:137:PRO:HB3	1:D:308:MET:CE	2.47	0.45
1:A:57:GLU:CG	1:A:101:ARG:NH1	2.79	0.45
1:A:181:ALA:O	1:A:186:GLU:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:VAL:HB	1:B:214:ASN:HB3	1.98	0.45
1:D:245:PHE:CE1	1:D:249:LEU:HD21	2.52	0.45
1:E:192:ILE:HB	3:E:536:HOH:O	2.17	0.45
1:F:233:LEU:N	1:F:233:LEU:CD1	2.80	0.45
1:I:22:ARG:O	1:I:23:ALA:HB2	2.17	0.45
1:A:252:LYS:HE3	1:A:256:ARG:HH22	1.78	0.45
1:B:193:ASN:HB3	1:B:195:TYR:CE1	2.52	0.45
1:E:90:ALA:HB2	1:E:95:TRP:CE2	2.52	0.45
1:G:239:LYS:HB3	1:G:243:LYS:HE3	1.99	0.45
1:G:279:PRO:HB2	1:G:282:LYS:HG2	1.98	0.45
1:B:140:GLY:O	1:B:144:GLU:HG2	2.16	0.45
1:D:27:LYS:HB3	1:D:27:LYS:HZ3	1.81	0.45
1:F:31:ASN:HB2	3:G:476:HOH:O	2.17	0.45
1:F:93:LYS:HD3	3:F:511:HOH:O	2.17	0.45
1:H:76:ALA:HB1	1:H:80:ASN:HD21	1.81	0.45
1:B:151:LYS:HE2	1:B:295:GLU:OE2	2.17	0.44
1:D:43:LYS:HZ3	1:D:68:ALA:HB3	1.82	0.44
1:F:255:GLN:HE22	1:F:267:LEU:H	1.64	0.44
1:I:265:TYR:CE2	1:I:283:LEU:HD11	2.51	0.44
1:A:252:LYS:HE3	1:A:256:ARG:CZ	2.46	0.44
1:E:59:ILE:HB	1:E:60:PRO:HD3	1.98	0.44
1:G:80:ASN:HA	1:G:83:ARG:HB2	1.99	0.44
1:G:120:SER:HB3	1:G:123:ASN:ND2	2.33	0.44
1:H:62:LEU:HD13	1:H:95:TRP:HB2	1.98	0.44
1:A:159:LEU:HG	1:A:163:LYS:HE3	1.99	0.44
1:C:54:PHE:CE2	1:C:56:SER:HB3	2.52	0.44
1:C:218:HIS:HB3	3:C:500:HOH:O	2.18	0.44
1:E:262:ARG:CG	1:E:264:GLU:HG3	2.44	0.44
1:H:21:THR:O	1:H:21:THR:HG22	2.17	0.44
1:H:122:LEU:CD2	1:H:149:ILE:HD13	2.47	0.44
1:A:146:ILE:HD12	1:A:158:ALA:HB1	1.99	0.44
1:B:30:LEU:HD12	1:B:30:LEU:N	2.33	0.44
1:C:54:PHE:CZ	1:C:56:SER:HB3	2.52	0.44
1:D:94:ASP:OD1	1:D:94:ASP:N	2.49	0.44
1:E:41:GLN:O	1:E:44:GLU:N	2.49	0.44
1:H:57:GLU:HB2	1:H:101:ARG:HH22	1.80	0.44
1:I:256:ARG:HG2	1:I:271:VAL:HG13	1.99	0.44
1:B:51:ALA:HB3	1:B:233:LEU:CD2	2.47	0.44
1:F:85:LYS:CE	1:F:219:ARG:HH12	2.30	0.44
1:H:76:ALA:HB1	1:H:80:ASN:ND2	2.32	0.44
1:A:8:GLN:CG	1:A:9:HIS:N	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:VAL:HG23	1:B:285:ALA:HB2	2.00	0.44
1:D:256:ARG:HA	1:D:256:ARG:HD2	1.71	0.44
1:E:161:TRP:HE3	1:E:162:LEU:HD12	1.82	0.44
1:E:300:THR:HG23	1:E:309:LYS:HE2	2.00	0.44
1:H:142:PHE:O	1:H:145:GLN:HB3	2.17	0.44
1:A:162:LEU:HB3	1:A:306:ALA:CB	2.48	0.44
1:C:119:LYS:HE3	3:C:489:HOH:O	2.17	0.44
1:C:303:LEU:HG	1:C:309:LYS:CA	2.46	0.44
1:D:174:LYS:HE2	3:D:466:HOH:O	2.16	0.44
1:E:71:LEU:O	1:E:234:LYS:HE3	2.18	0.44
1:E:90:ALA:HB2	1:E:95:TRP:CD2	2.53	0.44
1:E:107:TYR:CD1	1:E:117:LEU:HD11	2.52	0.44
1:H:2:ILE:HD11	1:H:53:VAL:CG2	2.43	0.44
1:I:78:THR:O	1:I:81:GLU:HB2	2.18	0.44
1:B:90:ALA:O	1:B:93:LYS:HE2	2.18	0.44
1:F:279:PRO:O	1:F:282:LYS:HB2	2.17	0.44
1:G:5:TYR:CD2	1:G:38:LEU:HD12	2.53	0.44
1:H:266:PRO:HA	3:H:479:HOH:O	2.17	0.44
1:I:81:GLU:OE1	1:I:268:ASN:ND2	2.51	0.44
1:B:13:ALA:HA	1:B:16:VAL:HG12	2.00	0.44
1:E:151:LYS:NZ	1:E:295:GLU:OE1	2.47	0.44
1:E:174:LYS:HB2	1:E:177:VAL:HG23	1.99	0.44
1:G:205:GLY:O	1:G:207:GLN:N	2.51	0.44
1:G:223:ALA:HB3	1:G:286:PRO:HD3	2.00	0.44
1:H:2:ILE:HG13	1:H:242:ALA:HA	2.00	0.44
1:I:45:GLU:HB2	1:I:49:SER:HB2	1.99	0.43
1:A:9:HIS:NE2	1:A:11:GLU:HB3	2.33	0.43
1:C:140:GLY:O	1:C:144:GLU:HG2	2.19	0.43
1:D:117:LEU:HD22	1:D:214:ASN:CB	2.48	0.43
1:I:255:GLN:HB2	1:I:271:VAL:HG21	1.99	0.43
1:C:6:ASN:HB2	1:C:30:LEU:HD22	2.00	0.43
1:C:256:ARG:HH12	1:C:272:VAL:HB	1.82	0.43
1:D:72:GLU:OE2	1:D:234:LYS:HG2	2.18	0.43
1:G:9:HIS:HB3	1:G:12:ALA:CB	2.46	0.43
1:G:145:GLN:O	1:G:149:ILE:HG13	2.18	0.43
1:G:298:HIS:O	1:G:302:LEU:HG	2.18	0.43
1:H:252:LYS:O	1:H:256:ARG:HG3	2.18	0.43
1:C:5:TYR:CE1	1:C:51:ALA:HB2	2.53	0.43
1:C:155:GLU:OE2	1:C:298:HIS:HE1	2.00	0.43
1:D:217:ARG:HH11	1:D:217:ARG:HG2	1.84	0.43
1:E:130:LYS:O	1:E:132:ARG:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:LYS:HE3	1:D:131:ASN:ND2	2.34	0.43
1:E:255:GLN:HE22	1:E:267:LEU:N	2.14	0.43
1:A:101:ARG:O	1:A:101:ARG:HG2	2.19	0.43
1:B:101:ARG:HG3	1:B:264:GLU:HG2	2.01	0.43
1:B:292:THR:O	1:B:296:LYS:HG3	2.18	0.43
1:C:108:ASP:OD2	1:C:110:ARG:HB2	2.18	0.43
1:C:248:PHE:CE2	1:C:254:GLY:HA2	2.54	0.43
1:D:223:ALA:HB3	1:D:286:PRO:HD3	2.01	0.43
1:C:12:ALA:HB1	1:C:258:LEU:CD1	2.49	0.43
1:E:57:GLU:HG2	1:E:58:GLN:HG2	2.00	0.43
1:F:1:ASP:HA	1:F:26:ILE:HG23	2.00	0.43
1:D:183:GLU:OE1	1:D:211:THR:HG22	2.19	0.43
1:E:42:ILE:HD12	1:E:65:LEU:HD11	2.01	0.43
1:F:144:GLU:OE1	1:F:144:GLU:HA	2.19	0.43
1:F:232:VAL:HG13	1:F:242:ALA:HB1	2.01	0.43
1:G:130:LYS:HA	1:G:168:TYR:CB	2.46	0.43
1:H:9:HIS:CD2	1:H:10:LYS:N	2.87	0.43
1:I:6:ASN:ND2	1:I:8:GLN:H	2.17	0.43
1:I:255:GLN:HG3	1:I:268:ASN:HB2	2.01	0.43
1:A:106:VAL:CG2	1:A:192:ILE:HG12	2.48	0.43
1:D:265:TYR:CD1	1:D:265:TYR:N	2.86	0.43
1:E:45:GLU:HG2	1:E:45:GLU:H	1.66	0.43
1:H:20:PHE:CE2	1:H:26:ILE:HB	2.54	0.43
1:I:22:ARG:HG3	1:I:22:ARG:HH11	1.84	0.43
1:I:34:LYS:CG	1:I:37:GLN:HG3	2.48	0.43
1:A:182:VAL:HG12	1:A:211:THR:HG22	2.01	0.43
1:D:55:TYR:CE1	1:D:249:LEU:HD13	2.54	0.43
1:E:112:LEU:HD12	1:E:116:ASP:HB2	2.01	0.43
1:G:267:LEU:HD23	1:G:267:LEU:HA	1.86	0.43
1:I:20:PHE:CE2	1:I:26:ILE:HB	2.54	0.43
1:I:180:GLN:O	1:I:184:ASN:ND2	2.51	0.43
1:A:38:LEU:O	1:A:41:GLN:HB3	2.19	0.42
1:A:103:ARG:HD2	1:A:145:GLN:HB2	2.01	0.42
1:B:40:GLY:O	1:B:44:GLU:HG2	2.19	0.42
1:B:43:LYS:HZ1	1:B:64:THR:HB	1.84	0.42
1:D:80:ASN:HA	1:D:83:ARG:HD3	1.99	0.42
1:D:115:LYS:HD2	1:D:116:ASP:OD1	2.18	0.42
1:D:255:GLN:HB2	1:D:271:VAL:HG21	2.00	0.42
1:F:7:GLY:HA2	1:F:33:ALA:O	2.19	0.42
1:F:11:GLU:HG3	1:F:261:VAL:CG1	2.49	0.42
1:H:117:LEU:N	1:H:117:LEU:CD1	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:99:SER:HA	1:I:267:LEU:HD13	2.01	0.42
1:I:303:LEU:HD23	1:I:308:MET:SD	2.59	0.42
1:A:59:ILE:N	1:A:60:PRO:CD	2.82	0.42
1:A:217:ARG:NH1	1:A:278:GLU:OE1	2.52	0.42
1:C:26:ILE:HG13	1:C:241:GLU:OE1	2.19	0.42
1:F:16:VAL:HG11	1:F:249:LEU:CD2	2.49	0.42
1:H:113:SER:O	1:H:117:LEU:HD13	2.20	0.42
1:A:203:GLU:HG3	1:A:204:LYS:N	2.34	0.42
1:A:309:LYS:O	1:A:309:LYS:HG3	2.19	0.42
1:C:3:THR:O	1:C:51:ALA:HA	2.19	0.42
1:D:152:LEU:O	1:D:153:LYS:HD3	2.19	0.42
1:D:256:ARG:NE	3:D:411:HOH:O	2.51	0.42
1:I:234:LYS:HD2	1:I:234:LYS:C	2.39	0.42
1:C:27:LYS:HD3	1:C:27:LYS:N	2.35	0.42
1:C:228:SER:HB3	3:C:476:HOH:O	2.18	0.42
1:C:256:ARG:HH12	1:C:272:VAL:H	1.58	0.42
1:C:306:ALA:HB3	1:C:308:MET:HE3	2.01	0.42
1:F:104:VAL:HG12	1:F:215:PHE:CE2	2.55	0.42
1:G:67:ALA:HA	1:G:92:LYS:HZ2	1.84	0.42
1:B:90:ALA:HB2	1:B:95:TRP:CE2	2.55	0.42
1:D:58:GLN:HG3	1:D:60:PRO:HD2	2.00	0.42
1:D:193:ASN:HB3	1:D:195:TYR:CE1	2.54	0.42
1:D:252:LYS:HG3	1:D:253:GLU:N	2.34	0.42
1:D:303:LEU:CD2	1:D:308:MET:HE1	2.50	0.42
1:E:18:ASP:O	1:E:22:ARG:HG3	2.19	0.42
1:G:69:ASN:O	1:G:234:LYS:HG3	2.20	0.42
1:H:93:LYS:HE3	3:H:466:HOH:O	2.19	0.42
1:H:180:GLN:HA	1:H:183:GLU:HB3	2.00	0.42
1:A:267:LEU:HD23	1:A:267:LEU:HA	1.91	0.42
1:B:24:THR:HB	1:B:26:ILE:HG13	2.02	0.42
1:D:12:ALA:O	1:D:16:VAL:HG23	2.19	0.42
1:D:245:PHE:O	1:D:249:LEU:HG	2.20	0.42
1:E:6:ASN:ND2	1:E:8:GLN:H	2.17	0.42
1:F:83:ARG:HD3	3:F:457:HOH:O	2.20	0.42
1:F:84:GLY:O	1:F:85:LYS:C	2.57	0.42
1:G:2:ILE:CG1	1:G:28:VAL:HG22	2.50	0.42
1:G:146:ILE:O	1:G:150:VAL:HG23	2.20	0.42
1:H:45:GLU:HB2	1:H:49:SER:HB2	2.02	0.42
1:I:8:GLN:HE21	1:I:8:GLN:HB2	1.67	0.42
1:A:75:PRO:CD	1:A:243:LYS:HZ2	2.32	0.42
1:B:52:ASP:HA	1:B:236:SER:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:VAL:CG2	1:B:211:THR:HG23	2.45	0.42
1:D:86:GLY:HA2	1:D:287:GLN:HG2	2.00	0.42
1:D:144:GLU:CG	1:D:224:LEU:HD21	2.49	0.42
1:D:199:ALA:O	1:D:203:GLU:OE1	2.37	0.42
2:D:400:ZRC:O3A	2:D:400:ZRC:O31	2.38	0.42
1:E:57:GLU:O	1:E:101:ARG:NH2	2.52	0.42
1:H:174:LYS:HA	1:H:174:LYS:HD3	1.83	0.42
1:H:301:ARG:HA	1:H:304:GLU:OE1	2.19	0.42
1:I:291:THR:HA	1:I:295:GLU:OE1	2.20	0.42
1:B:17:ALA:O	1:B:20:PHE:HB3	2.20	0.42
1:E:112:LEU:HD12	1:E:116:ASP:CB	2.50	0.42
1:H:176:SER:O	1:H:180:GLN:NE2	2.53	0.42
1:C:198:HIS:HB3	1:C:275:PHE:CD2	2.54	0.41
1:D:265:TYR:CZ	1:D:283:LEU:HD11	2.56	0.41
1:H:42:ILE:HD12	1:H:65:LEU:HD11	2.02	0.41
1:H:130:LYS:O	1:H:132:ARG:HG3	2.20	0.41
1:A:76:ALA:O	1:A:80:ASN:HB2	2.20	0.41
1:A:206:VAL:HA	1:A:209:VAL:HG22	2.01	0.41
1:A:279:PRO:HD2	1:A:282:LYS:HZ1	1.83	0.41
1:E:71:LEU:C	1:E:234:LYS:HG3	2.40	0.41
1:F:173:ALA:HB3	1:F:174:LYS:HE3	2.01	0.41
1:G:143:LEU:O	1:G:147:VAL:HG23	2.19	0.41
1:H:117:LEU:HD23	1:H:214:ASN:HB2	2.02	0.41
1:B:106:VAL:CG2	1:B:211:THR:CG2	2.98	0.41
1:C:121:VAL:CG2	1:C:216:VAL:HG21	2.50	0.41
1:C:130:LYS:O	1:C:132:ARG:HG3	2.19	0.41
1:C:233:LEU:N	1:C:233:LEU:HD12	2.35	0.41
1:I:92:LYS:HB2	1:I:94:ASP:OD2	2.20	0.41
1:I:109:THR:O	1:I:109:THR:CG2	2.68	0.41
1:A:106:VAL:HG22	1:A:192:ILE:HG12	2.02	0.41
1:B:59:ILE:N	1:B:60:PRO:CD	2.84	0.41
1:D:59:ILE:N	1:D:60:PRO:CD	2.84	0.41
1:D:134:GLY:HA2	1:D:170:LYS:O	2.20	0.41
1:D:225:VAL:HG23	1:D:285:ALA:HB2	2.02	0.41
1:E:109:THR:HG21	1:E:212:ARG:CG	2.50	0.41
1:E:152:LEU:HD21	1:E:288:VAL:HG12	2.03	0.41
1:F:217:ARG:HG2	1:F:217:ARG:HH11	1.85	0.41
1:G:234:LYS:NZ	1:G:234:LYS:CB	2.79	0.41
1:B:131:ASN:CA	1:B:170:LYS:HE3	2.51	0.41
1:C:55:TYR:CD1	1:C:249:LEU:HD13	2.56	0.41
1:C:79:ILE:HD12	1:C:93:LYS:CG	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:ALA:HB2	1:C:95:TRP:CD2	2.55	0.41
1:C:149:ILE:O	1:C:153:LYS:N	2.47	0.41
1:F:178:ALA:CB	1:F:192:ILE:HD11	2.50	0.41
1:F:255:GLN:NE2	1:F:268:ASN:H	2.19	0.41
1:G:69:ASN:C	1:G:71:LEU:H	2.24	0.41
1:G:233:LEU:H	1:G:233:LEU:CD1	2.33	0.41
1:I:298:HIS:HD2	3:I:456:HOH:O	2.02	0.41
1:A:8:GLN:HG2	1:A:9:HIS:H	1.86	0.41
1:B:103:ARG:NH2	3:B:403:HOH:O	2.40	0.41
1:B:237:GLN:H	1:B:237:GLN:CD	2.22	0.41
1:C:48:ARG:HD2	3:C:472:HOH:O	2.21	0.41
1:C:236:SER:OG	1:C:239:LYS:HE2	2.21	0.41
1:D:18:ASP:O	1:D:22:ARG:HG3	2.20	0.41
1:D:107:TYR:CD1	1:D:117:LEU:HD21	2.55	0.41
1:E:83:ARG:HG3	1:E:83:ARG:HH11	1.84	0.41
1:E:252:LYS:HE2	1:E:268:ASN:OD1	2.20	0.41
1:F:38:LEU:O	1:F:42:ILE:HG13	2.20	0.41
1:H:2:ILE:O	1:H:28:VAL:HA	2.20	0.41
1:C:101:ARG:O	1:C:225:VAL:HA	2.21	0.41
1:C:225:VAL:HG23	1:C:285:ALA:HB2	2.02	0.41
1:C:268:ASN:HA	1:C:269:PRO:HD2	1.94	0.41
1:D:65:LEU:N	1:D:65:LEU:CD2	2.84	0.41
1:E:268:ASN:ND2	1:E:269:PRO:HD2	2.36	0.41
1:F:240:ASP:O	1:F:244:LYS:HG3	2.20	0.41
1:A:51:ALA:HB3	1:A:233:LEU:HD22	2.02	0.41
1:A:71:LEU:HB2	1:A:94:ASP:HB2	2.02	0.41
1:C:5:TYR:HE2	1:C:41:GLN:HG2	1.86	0.41
1:C:236:SER:OG	1:C:239:LYS:HG3	2.20	0.41
1:C:268:ASN:ND2	1:C:270:HIS:H	2.18	0.41
1:G:2:ILE:CD1	1:G:28:VAL:HG22	2.47	0.41
1:G:70:LEU:C	1:G:234:LYS:HG2	2.41	0.41
1:G:164:GLY:O	1:G:168:TYR:CE1	2.74	0.41
1:G:265:TYR:CE2	1:G:277:LEU:HB3	2.55	0.41
1:H:6:ASN:O	1:H:32:SER:HA	2.19	0.41
1:H:137:PRO:HA	1:H:142:PHE:CD2	2.56	0.41
1:B:147:VAL:HG11	1:B:291:THR:HG23	2.03	0.41
1:B:202:ARG:HH22	1:B:274:THR:C	2.25	0.41
1:C:92:LYS:O	1:C:93:LYS:CB	2.69	0.41
1:C:303:LEU:HG	1:C:309:LYS:H	1.86	0.41
1:D:51:ALA:HB3	1:D:233:LEU:CD2	2.51	0.41
1:D:103:ARG:HD3	3:D:431:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:TYR:HB2	3:D:501:HOH:O	2.21	0.41
1:D:175:ASN:HD22	1:D:192:ILE:HG22	1.86	0.41
1:D:184:ASN:HB2	1:D:186:GLU:CG	2.51	0.41
1:E:151:LYS:CE	1:E:295:GLU:OE1	2.68	0.41
1:F:46:GLY:O	1:F:48:ARG:N	2.54	0.41
1:F:85:LYS:HB3	1:F:86:GLY:H	1.55	0.41
1:G:104:VAL:CG1	1:G:105:VAL:N	2.83	0.41
1:H:60:PRO:HA	1:H:63:ALA:HB3	2.01	0.41
1:H:74:LEU:HA	1:H:75:PRO:HD3	1.91	0.41
1:H:111:LYS:HD2	1:H:188:ASP:OD1	2.21	0.41
1:H:144:GLU:OE2	1:H:291:THR:HG21	2.20	0.41
1:I:136:VAL:O	1:I:139:SER:HB3	2.20	0.41
1:I:255:GLN:HG3	1:I:268:ASN:CB	2.51	0.41
1:B:2:ILE:HG22	1:B:52:ASP:OD1	2.20	0.41
1:B:71:LEU:HD12	1:B:94:ASP:OD2	2.21	0.41
1:C:166:LYS:HD3	1:C:166:LYS:C	2.40	0.41
1:D:106:VAL:HG21	1:D:179:LEU:CD1	2.51	0.41
1:D:181:ALA:HA	1:D:186:GLU:OE1	2.20	0.41
1:E:262:ARG:HE	1:E:264:GLU:CD	2.24	0.41
1:G:3:THR:HB	1:G:50:PRO:O	2.20	0.41
1:H:143:LEU:HD11	1:H:299:ALA:HB3	2.03	0.41
1:H:218:HIS:O	1:H:219:ARG:HB2	2.21	0.41
1:A:57:GLU:HG2	1:A:101:ARG:HH12	1.86	0.40
1:C:304:GLU:CG	1:C:309:LYS:HG3	2.51	0.40
1:G:9:HIS:HB2	1:G:262:ARG:HD2	2.03	0.40
1:G:111:LYS:HD2	3:G:455:HOH:O	2.20	0.40
1:H:106:VAL:HG12	1:H:192:ILE:CD1	2.51	0.40
1:H:117:LEU:HD23	1:H:214:ASN:CG	2.42	0.40
1:H:178:ALA:O	1:H:182:VAL:HG23	2.21	0.40
1:I:90:ALA:HB2	1:I:95:TRP:CD2	2.55	0.40
1:A:217:ARG:HB3	1:A:284:GLU:OE2	2.20	0.40
1:C:52:ASP:HB3	1:C:242:ALA:HB2	2.03	0.40
1:G:182:VAL:HG12	1:G:211:THR:HG22	2.04	0.40
1:G:256:ARG:NH1	1:G:256:ARG:CB	2.85	0.40
1:I:20:PHE:HZ	1:I:26:ILE:HD12	1.86	0.40
1:A:206:VAL:O	1:A:209:VAL:HG22	2.21	0.40
1:C:10:LYS:O	1:C:14:GLN:HG2	2.21	0.40
2:C:400:ZRC:O23	2:C:400:ZRC:O2A	2.39	0.40
1:G:39:ALA:HA	1:G:65:LEU:HD11	2.03	0.40
1:H:59:ILE:H	1:H:60:PRO:HD2	1.85	0.40
1:H:149:ILE:HG12	1:H:221:PRO:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:74:LEU:HA	1:I:75:PRO:HD3	1.87	0.40
1:I:112:LEU:HD12	1:I:112:LEU:C	2.41	0.40
1:B:21:THR:O	1:B:25:GLY:N	2.46	0.40
1:B:297:GLU:O	1:B:301:ARG:HG2	2.21	0.40
1:C:52:ASP:CA	1:C:236:SER:HB2	2.45	0.40
1:D:127:PRO:HG3	1:D:168:TYR:CZ	2.55	0.40
1:G:202:ARG:NH2	1:G:274:THR:CG2	2.74	0.40
1:H:2:ILE:CG2	1:H:28:VAL:HG12	2.51	0.40
1:H:33:ALA:HB3	1:H:38:LEU:CG	2.49	0.40
1:I:35:GLY:HA3	1:I:57:GLU:OE2	2.21	0.40
1:C:251:GLY:O	1:C:255:GLN:HG2	2.22	0.40
1:D:180:GLN:HE21	1:D:184:ASN:CG	2.23	0.40
1:I:255:GLN:HB3	1:I:271:VAL:HG21	2.03	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	307/309 (99%)	288 (94%)	19 (6%)	0	100	100
1	B	307/309 (99%)	288 (94%)	17 (6%)	2 (1%)	22	5
1	C	307/309 (99%)	283 (92%)	20 (6%)	4 (1%)	12	1
1	D	307/309 (99%)	291 (95%)	14 (5%)	2 (1%)	22	5
1	E	307/309 (99%)	291 (95%)	12 (4%)	4 (1%)	12	1
1	F	307/309 (99%)	292 (95%)	13 (4%)	2 (1%)	22	5
1	G	307/309 (99%)	281 (92%)	23 (8%)	3 (1%)	15	3
1	H	307/309 (99%)	287 (94%)	18 (6%)	2 (1%)	22	5
1	I	307/309 (99%)	291 (95%)	15 (5%)	1 (0%)	41	18
All	All	2763/2781 (99%)	2592 (94%)	151 (6%)	20 (1%)	22	5

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	195	TYR
1	F	85	LYS
1	C	46	GLY
1	D	252	LYS
1	F	47	SER
1	G	8	GLN
1	G	206	VAL
1	H	308	MET
1	I	23	ALA
1	E	114	GLU
1	B	93	LYS
1	C	47	SER
1	C	114	GLU
1	E	217	ARG
1	B	217	ARG
1	E	35	GLY
1	H	2	ILE
1	E	42	ILE
1	G	2	ILE
1	D	192	ILE

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	245/245 (100%)	233 (95%)	12 (5%)	25 3
1	B	245/245 (100%)	233 (95%)	12 (5%)	25 3
1	C	245/245 (100%)	234 (96%)	11 (4%)	27 5
1	D	245/245 (100%)	233 (95%)	12 (5%)	25 3
1	E	245/245 (100%)	236 (96%)	9 (4%)	34 8
1	F	245/245 (100%)	235 (96%)	10 (4%)	30 6
1	G	245/245 (100%)	238 (97%)	7 (3%)	42 13
1	H	245/245 (100%)	235 (96%)	10 (4%)	30 6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	I	245/245 (100%)	232 (95%)	13 (5%)	22 3
All	All	2205/2205 (100%)	2109 (96%)	96 (4%)	28 5

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	GLU
1	A	60	PRO
1	A	80	ASN
1	A	101	ARG
1	A	103	ARG
1	A	106	VAL
1	A	115	LYS
1	A	146	ILE
1	A	187	ILE
1	A	191	LEU
1	A	216	VAL
1	A	301	ARG
1	B	1	ASP
1	B	14	GLN
1	B	93	LYS
1	B	103	ARG
1	B	175	ASN
1	B	183	GLU
1	B	188	ASP
1	B	211	THR
1	B	237	GLN
1	B	239	LYS
1	B	253	GLU
1	B	278	GLU
1	C	8	GLN
1	C	18	ASP
1	C	103	ARG
1	C	174	LYS
1	C	188	ASP
1	C	207	GLN
1	C	211	THR
1	C	239	LYS
1	C	253	GLU
1	C	259	THR
1	C	268	ASN
1	D	53	VAL

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Mol	Chain	Res	Type
1	D	103	ARG
1	D	115	LYS
1	D	132	ARG
1	D	167	GLU
1	D	214	ASN
1	D	216	VAL
1	D	240	ASP
1	D	256	ARG
1	D	264	GLU
1	D	268	ASN
1	D	287	GLN
1	E	103	ARG
1	E	139	SER
1	E	188	ASP
1	E	200	PHE
1	E	219	ARG
1	E	252	LYS
1	E	259	THR
1	E	268	ASN
1	E	280	ILE
1	F	8	GLN
1	F	11	GLU
1	F	111	LYS
1	F	114	GLU
1	F	115	LYS
1	F	174	LYS
1	F	191	LEU
1	F	240	ASP
1	F	280	ILE
1	F	287	GLN
1	G	55	TYR
1	G	94	ASP
1	G	103	ARG
1	G	168	TYR
1	G	278	GLU
1	G	288	VAL
1	G	294	SER
1	H	2	ILE
1	H	3	THR
1	H	103	ARG
1	H	117	LEU
1	H	180	GLN

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Mol	Chain	Res	Type
1	H	192	ILE
1	H	233	LEU
1	H	256	ARG
1	H	287	GLN
1	H	301	ARG
1	I	30	LEU
1	I	36	ASP
1	I	57	GLU
1	I	71	LEU
1	I	72	GLU
1	I	80	ASN
1	I	188	ASP
1	I	212	ARG
1	I	213	LEU
1	I	253	GLU
1	I	264	GLU
1	I	287	GLN
1	I	301	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	14	GLN
1	A	58	GLN
1	A	131	ASN
1	A	208	ASN
1	A	210	HIS
1	A	238	ASN
1	A	298	HIS
1	B	123	ASN
1	B	175	ASN
1	B	193	ASN
1	B	214	ASN
1	B	237	GLN
1	B	270	HIS
1	B	298	HIS
1	C	8	GLN
1	C	9	HIS
1	C	123	ASN
1	C	131	ASN
1	C	175	ASN

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Mol	Chain	Res	Type
1	C	180	GLN
1	C	237	GLN
1	C	255	GLN
1	C	268	ASN
1	C	270	HIS
1	C	298	HIS
1	D	14	GLN
1	D	80	ASN
1	D	123	ASN
1	D	175	ASN
1	D	180	GLN
1	D	193	ASN
1	D	218	HIS
1	D	268	ASN
1	D	298	HIS
1	E	6	ASN
1	E	180	GLN
1	E	238	ASN
1	E	255	GLN
1	E	270	HIS
1	E	298	HIS
1	F	37	GLN
1	F	123	ASN
1	F	184	ASN
1	F	218	HIS
1	F	238	ASN
1	F	255	GLN
1	F	270	HIS
1	F	298	HIS
1	G	31	ASN
1	G	58	GLN
1	G	69	ASN
1	G	123	ASN
1	G	175	ASN
1	G	184	ASN
1	G	208	ASN
1	G	237	GLN
1	G	255	GLN
1	G	298	HIS
1	G	305	GLN
1	H	9	HIS
1	H	14	GLN

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Mol	Chain	Res	Type
1	H	37	GLN
1	H	41	GLN
1	H	80	ASN
1	H	175	ASN
1	H	180	GLN
1	H	208	ASN
1	H	214	ASN
1	H	255	GLN
1	H	268	ASN
1	H	270	HIS
1	H	287	GLN
1	H	298	HIS
1	I	6	ASN
1	I	8	GLN
1	I	31	ASN
1	I	69	ASN
1	I	80	ASN
1	I	175	ASN
1	I	184	ASN
1	I	193	ASN
1	I	207	GLN
1	I	238	ASN
1	I	298	HIS
1	I	305	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

9 ligands are 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	ZRC	D	400	1	6,23,25	3.37	5 (83%)	3,66,78	0.27	0
2	ZRC	B	400	1	6,23,25	2.96	5 (83%)	3,66,78	0.23	0
2	ZRC	E	400	1	6,23,25	3.69	5 (83%)	3,66,78	0.31	0
2	ZRC	F	400	1	6,23,25	4.87	5 (83%)	3,66,78	0.29	0
2	ZRC	A	400	1	6,23,25	2.87	5 (83%)	3,66,78	0.25	0
2	ZRC	H	400	1	6,23,25	3.13	5 (83%)	3,66,78	0.21	0
2	ZRC	I	400	1	6,23,25	3.05	5 (83%)	3,66,78	0.19	0
2	ZRC	C	400	1	6,23,25	3.03	5 (83%)	3,66,78	0.23	0
2	ZRC	G	400	1	6,23,25	3.33	5 (83%)	3,66,78	0.23	0

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	400	ZRC	ZR2-OP2	7.74	2.43	2.11
2	F	400	ZRC	ZR2-O00	7.19	2.28	2.10
2	E	400	ZRC	ZR2-OP2	5.81	2.35	2.11
2	D	400	ZRC	ZR2-OP2	5.29	2.33	2.11
2	G	400	ZRC	ZR2-OP2	4.78	2.31	2.11
2	H	400	ZRC	ZR2-O00	4.57	2.21	2.10
2	C	400	ZRC	ZR2-OP2	4.49	2.30	2.11
2	A	400	ZRC	ZR2-OP2	3.93	2.27	2.11
2	I	400	ZRC	ZR2-OP2	3.89	2.27	2.11
2	B	400	ZRC	ZR2-O00	3.88	2.20	2.10
2	E	400	ZRC	P-OP1	-3.87	1.48	1.54
2	G	400	ZRC	P-OP3	-3.65	1.48	1.54
2	D	400	ZRC	P-OP1	-3.58	1.48	1.54
2	I	400	ZRC	P-OP3	-3.56	1.48	1.54
2	E	400	ZRC	P-OP3	-3.48	1.48	1.54
2	G	400	ZRC	P-OP1	-3.47	1.48	1.54
2	H	400	ZRC	P-OP3	-3.44	1.49	1.54
2	F	400	ZRC	P-OP3	-3.43	1.49	1.54
2	E	400	ZRC	ZR2-O00	3.40	2.19	2.10
2	G	400	ZRC	P-OP2	-3.34	1.49	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	ZRC	P-OP1	-3.30	1.49	1.54
2	B	400	ZRC	P-OP3	-3.30	1.49	1.54
2	I	400	ZRC	P-OP2	-3.26	1.49	1.54
2	H	400	ZRC	P-OP2	-3.26	1.49	1.54
2	D	400	ZRC	ZR2-O00	3.24	2.18	2.10
2	F	400	ZRC	P-OP1	-3.17	1.49	1.54
2	B	400	ZRC	P-OP2	-3.12	1.49	1.54
2	A	400	ZRC	P-OP2	-3.09	1.49	1.54
2	D	400	ZRC	P-OP3	-3.08	1.49	1.54
2	H	400	ZRC	P-OP1	-3.07	1.49	1.54
2	C	400	ZRC	P-OP2	-3.05	1.49	1.54
2	E	400	ZRC	P-OP2	-3.02	1.49	1.54
2	F	400	ZRC	P-OP2	-3.01	1.49	1.54
2	C	400	ZRC	P-OP1	-3.00	1.49	1.54
2	I	400	ZRC	ZR2-O00	2.96	2.18	2.10
2	I	400	ZRC	P-OP1	-2.95	1.49	1.54
2	C	400	ZRC	P-OP3	-2.93	1.49	1.54
2	A	400	ZRC	P-OP1	-2.89	1.49	1.54
2	A	400	ZRC	P-OP3	-2.86	1.49	1.54
2	C	400	ZRC	ZR2-O00	2.83	2.17	2.10
2	A	400	ZRC	ZR2-O00	2.81	2.17	2.10
2	D	400	ZRC	P-OP2	-2.72	1.50	1.54
2	G	400	ZRC	ZR2-O00	2.68	2.17	2.10
2	B	400	ZRC	ZR2-OP2	2.46	2.21	2.11
2	H	400	ZRC	ZR2-OP2	2.42	2.21	2.11

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

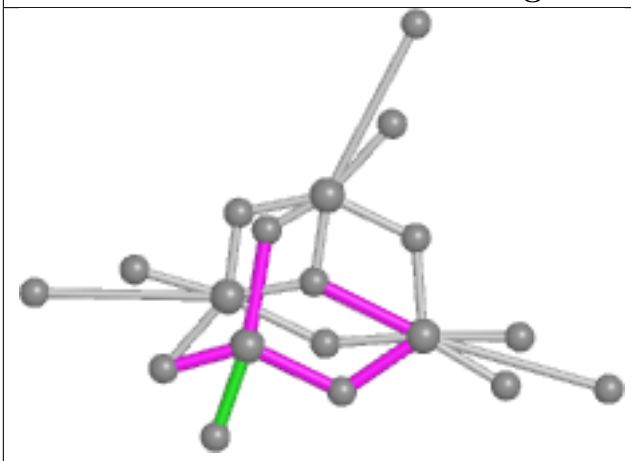
5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	400	ZRC	2	0
2	B	400	ZRC	1	0
2	H	400	ZRC	1	0
2	I	400	ZRC	1	0
2	C	400	ZRC	1	0

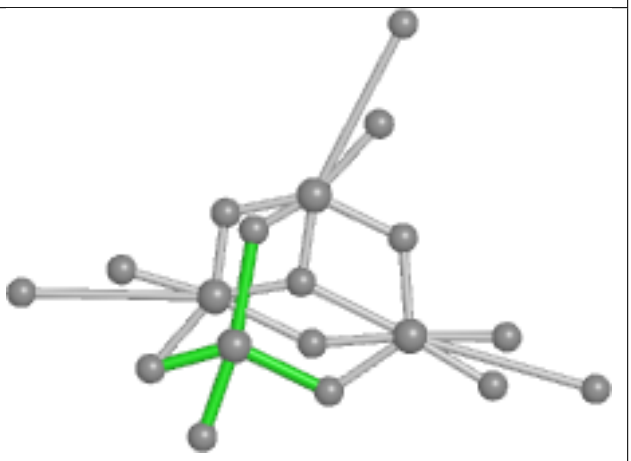
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

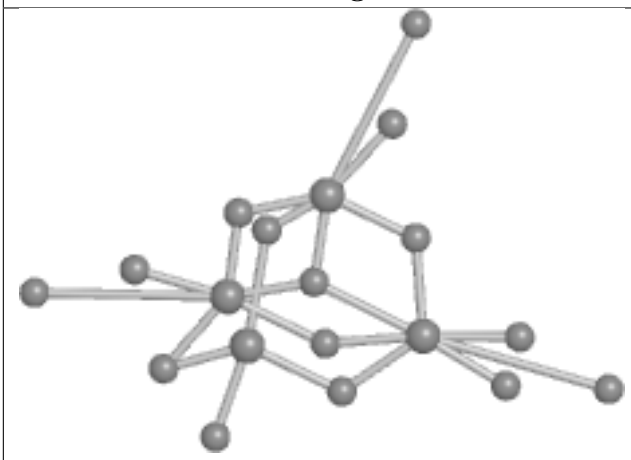
Ligand ZRC D 400



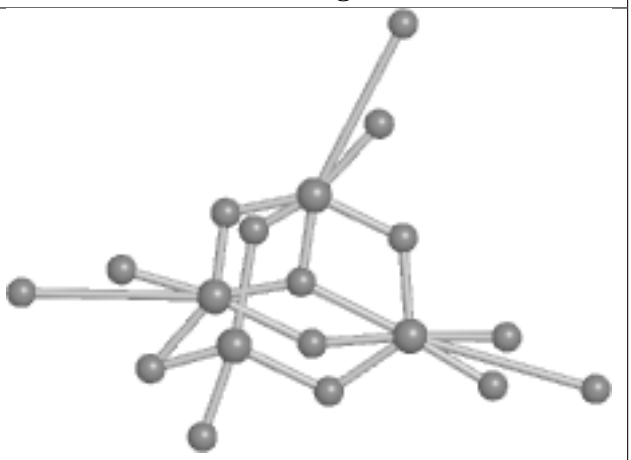
Bond lengths



Bond angles

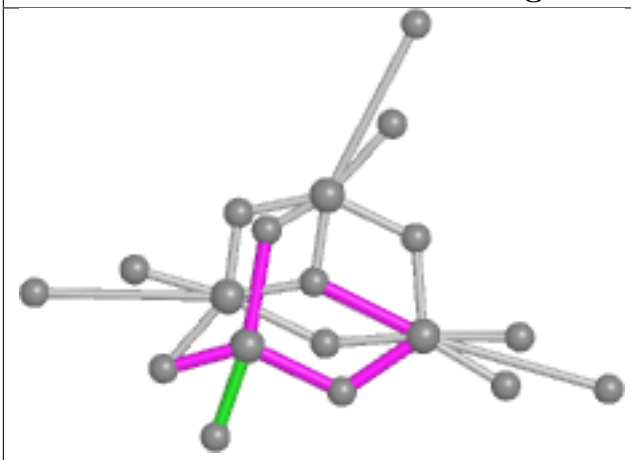


Torsions

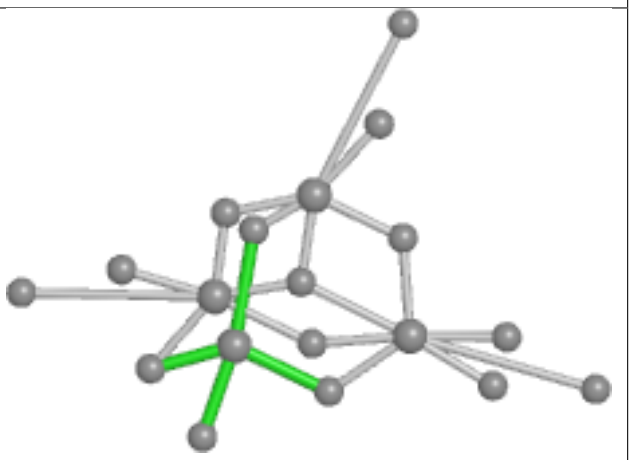


Rings

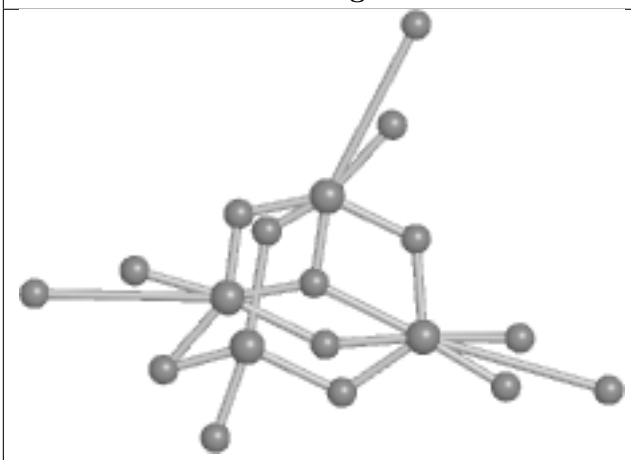
Ligand ZRC B 400



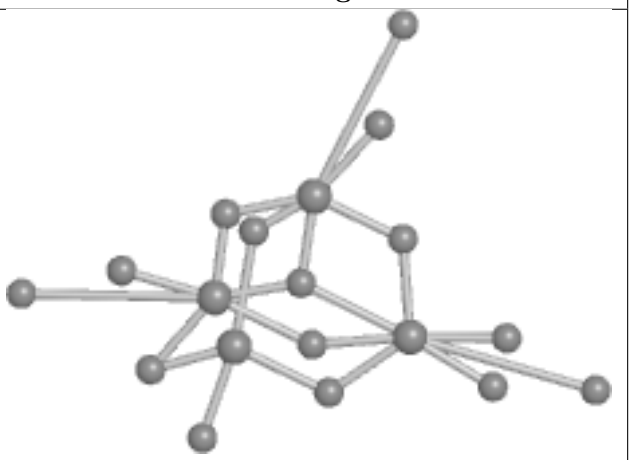
Bond lengths



Bond angles

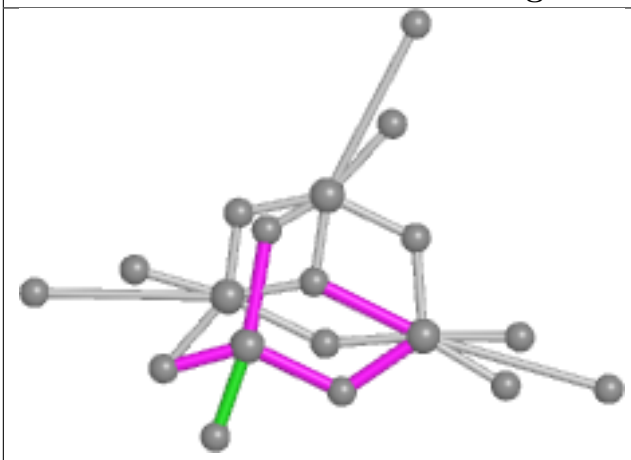


Torsions

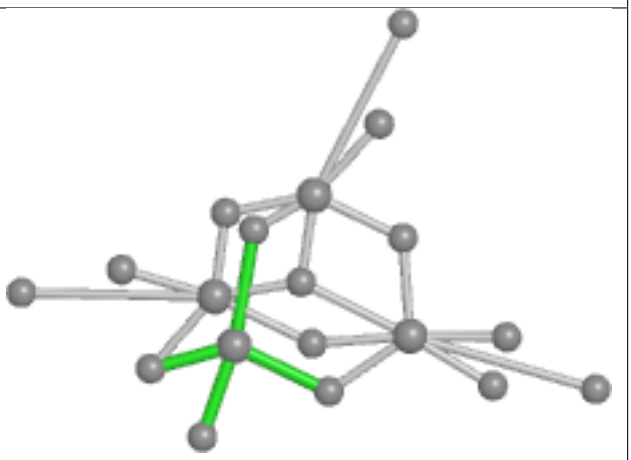


Rings

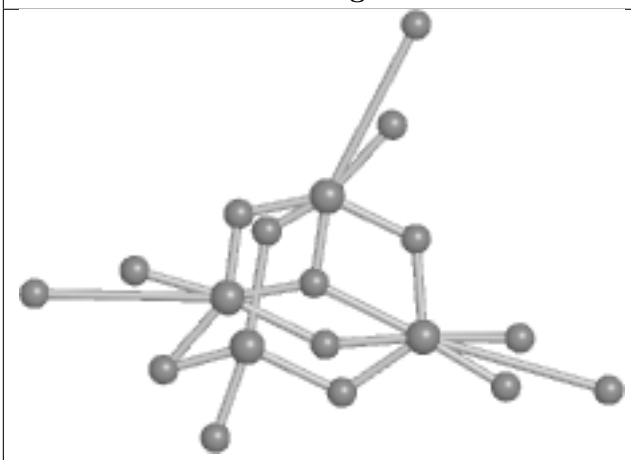
Ligand ZRC E 400



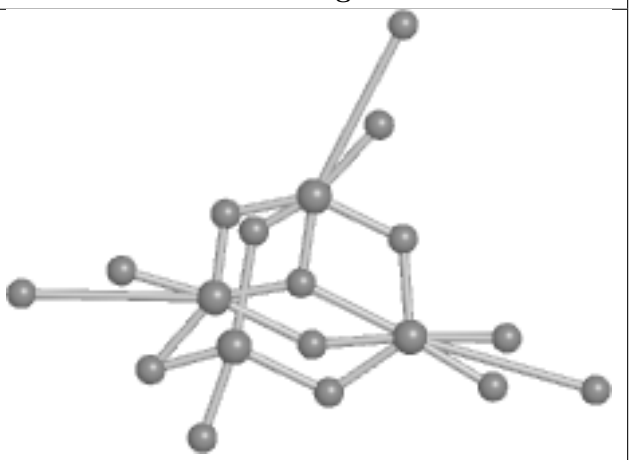
Bond lengths



Bond angles

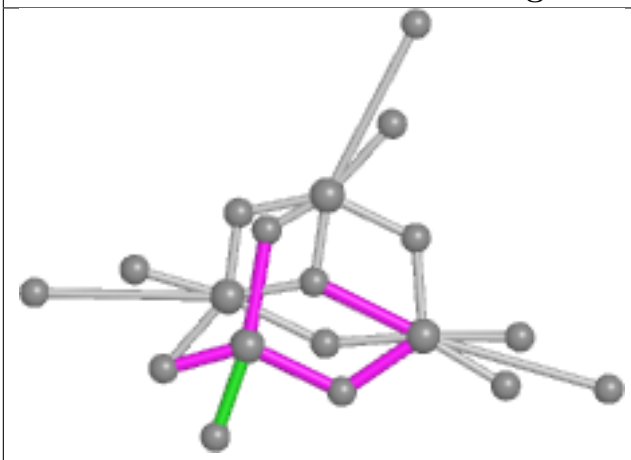


Torsions

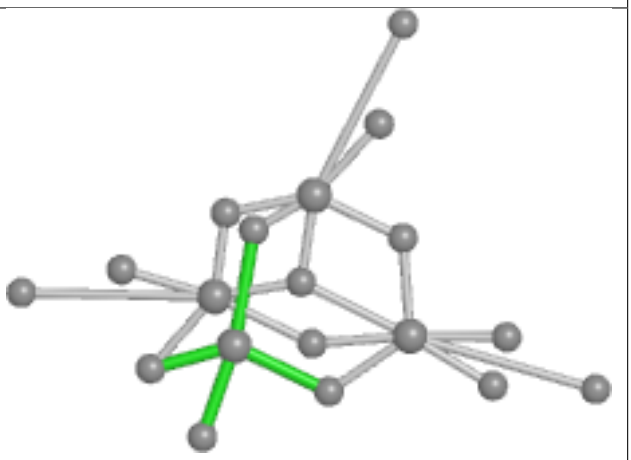


Rings

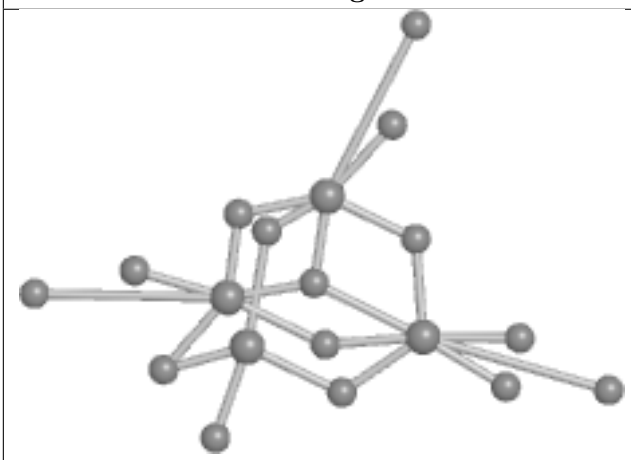
Ligand ZRC F 400



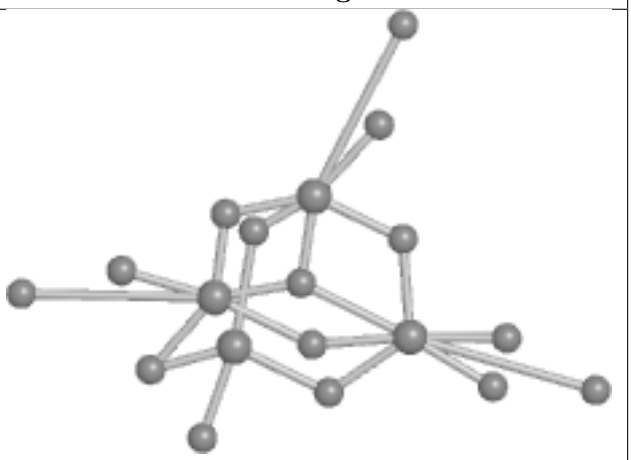
Bond lengths



Bond angles

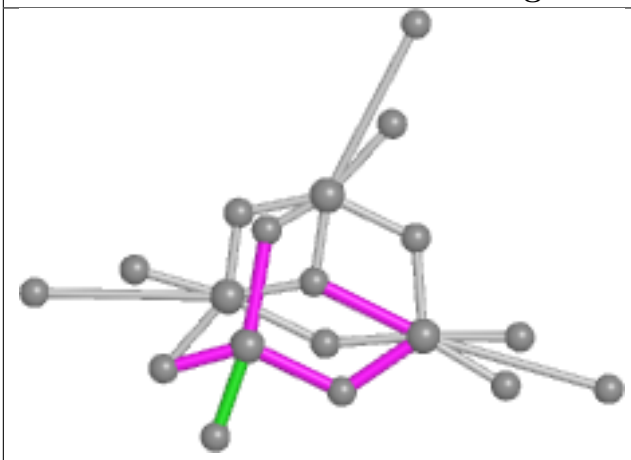


Torsions

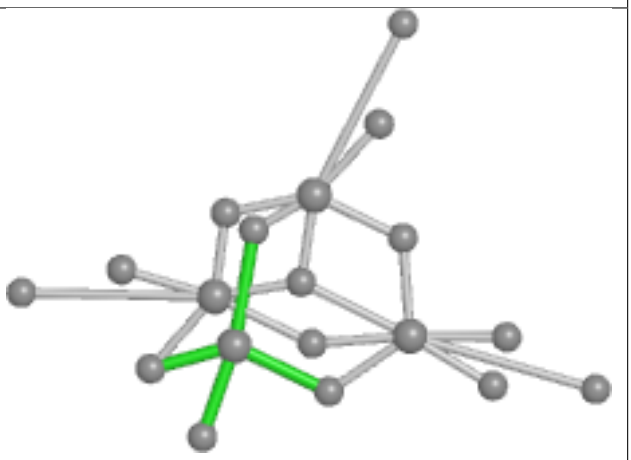


Rings

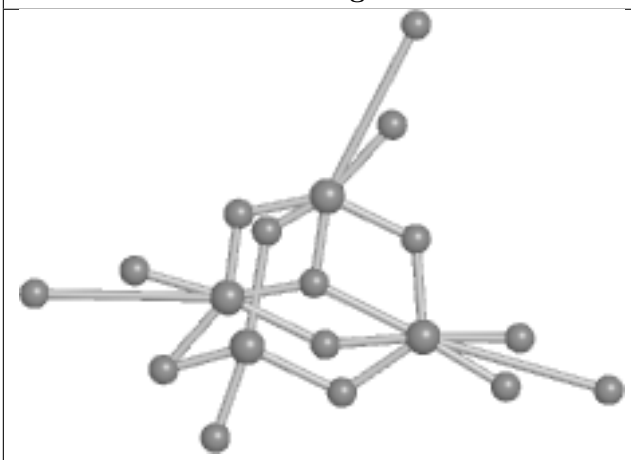
Ligand ZRC A 400



Bond lengths



Bond angles



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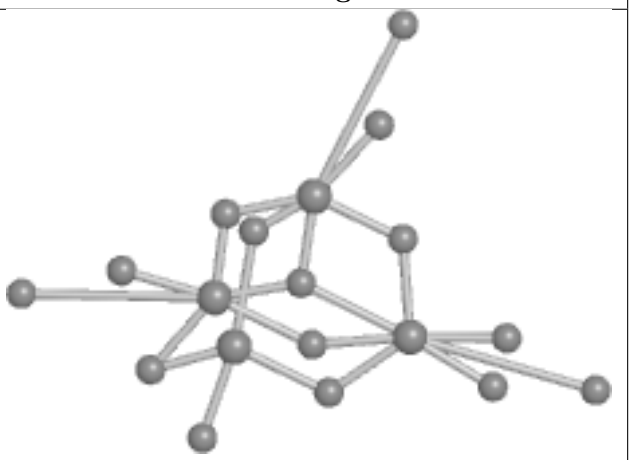
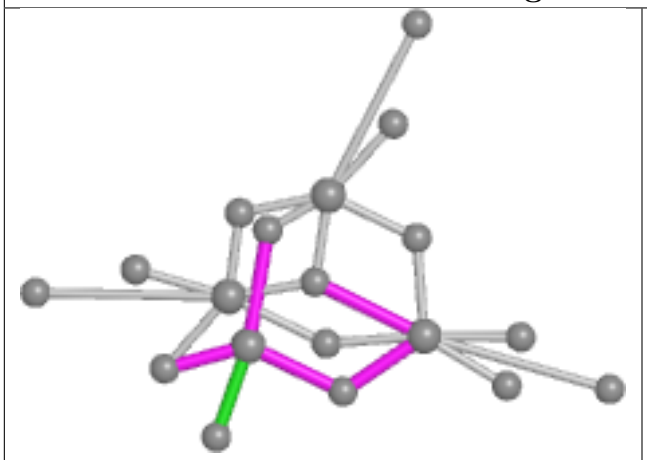


Rings

Ligand ZRC H 400



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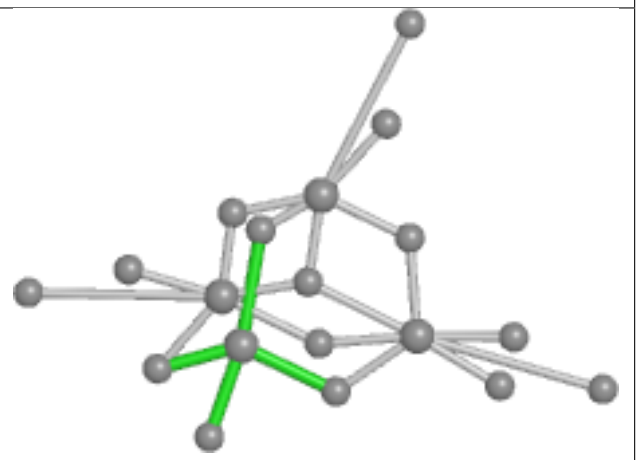
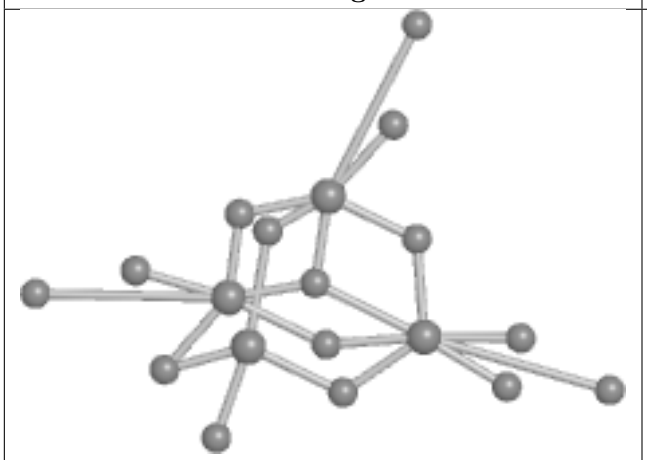


Bond angles



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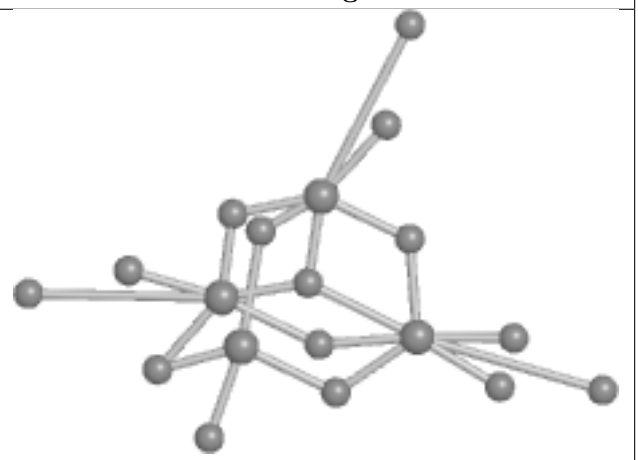
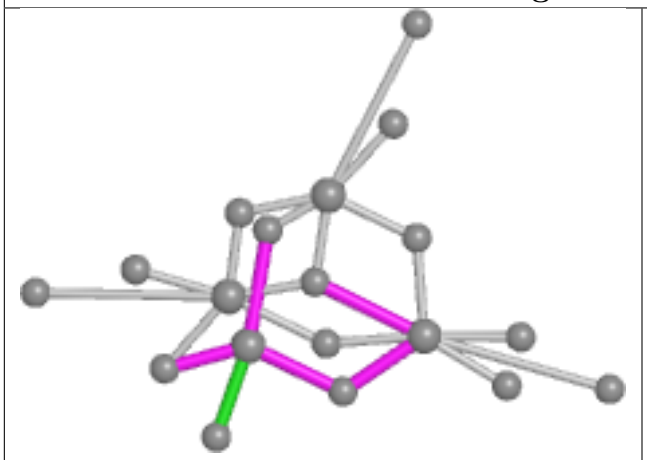


Rings

Ligand ZRC I 400



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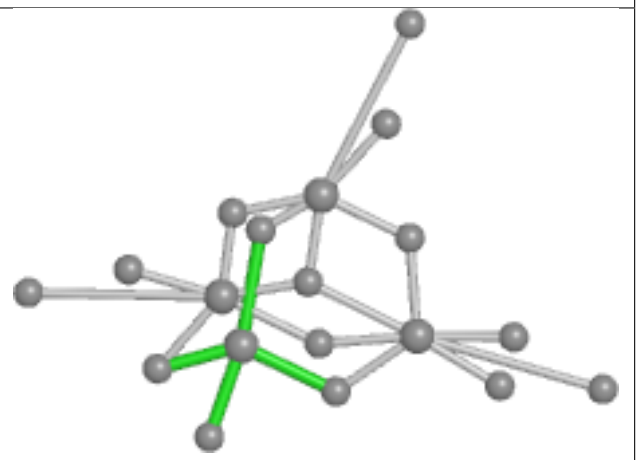
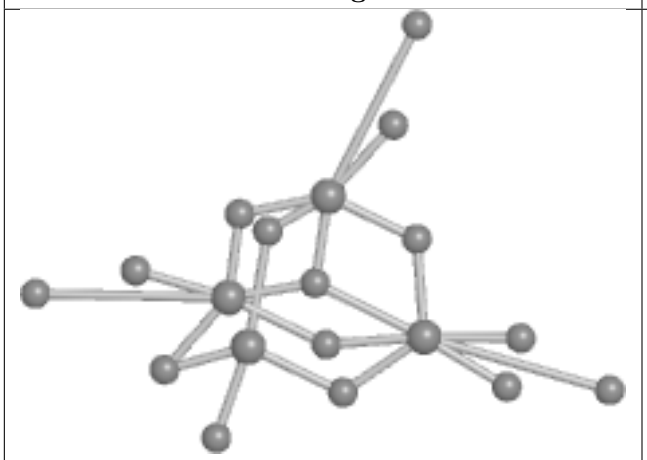


Bond angles



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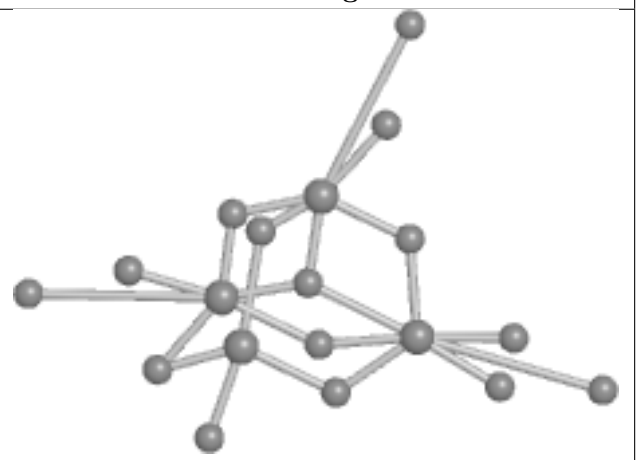
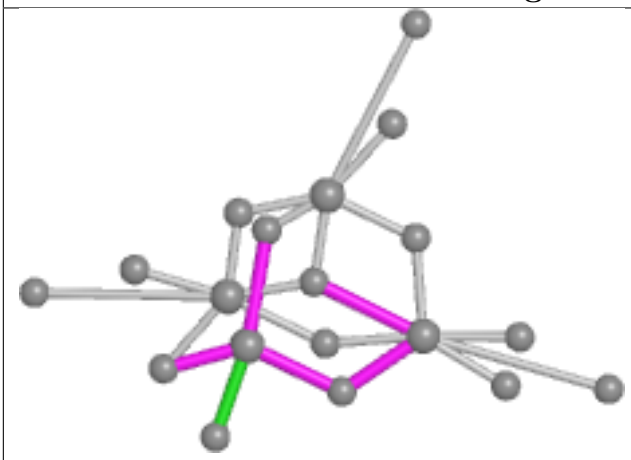


Rings

Ligand ZRC C 400



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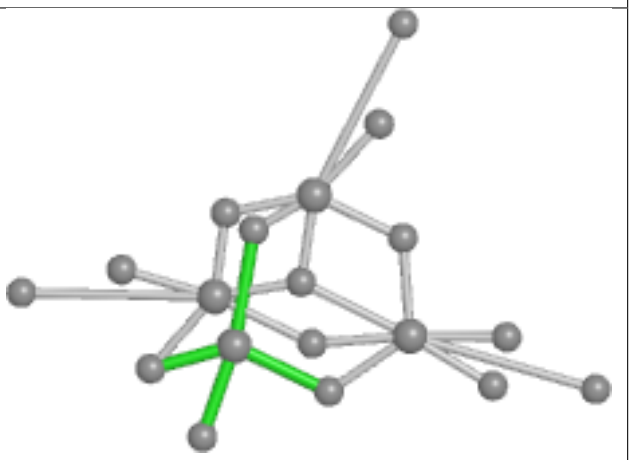
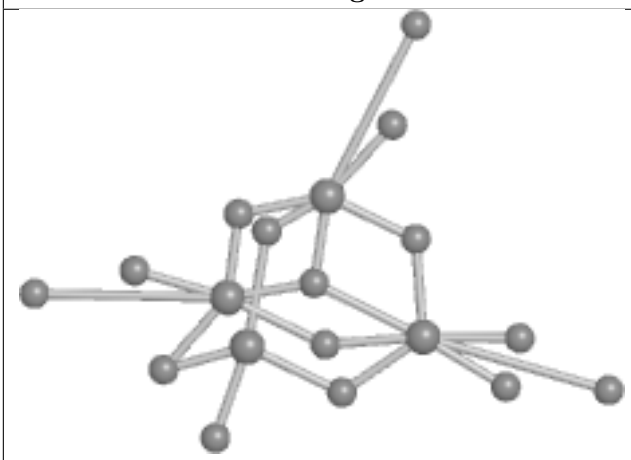
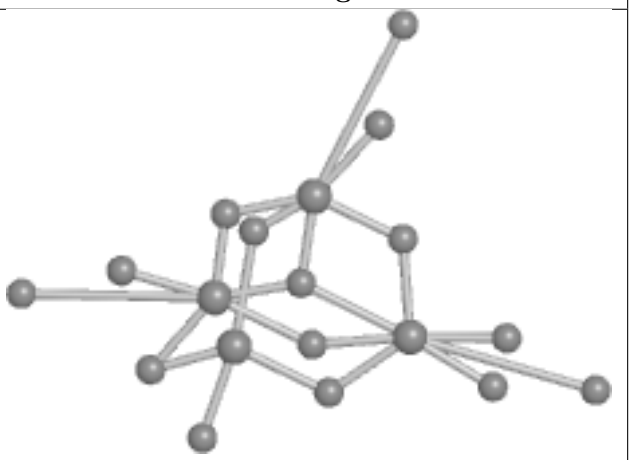


Bond angles

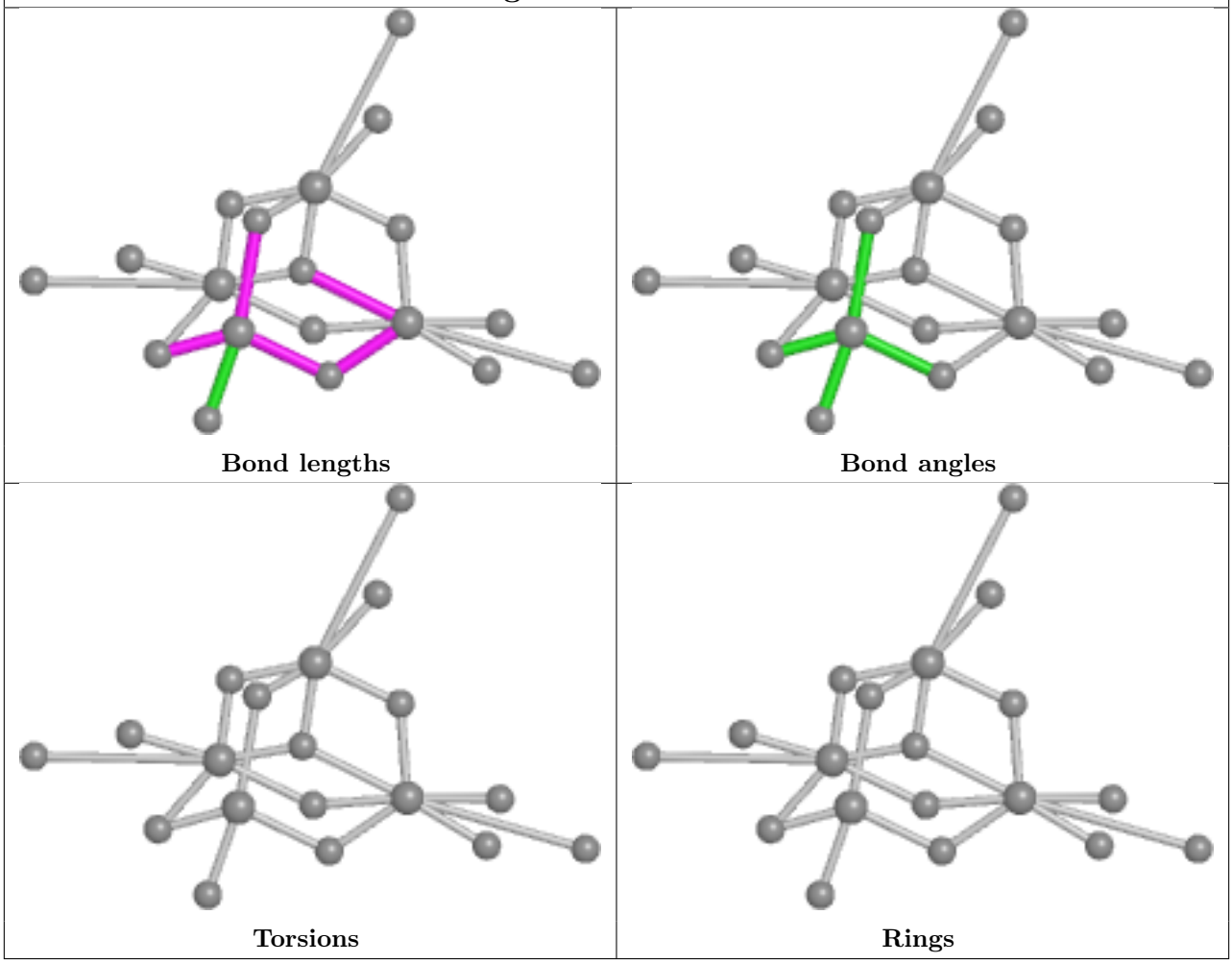


Torsions



Rings

Ligand ZRC G 400



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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.