Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 01:24 am GMT

PDB ID	:	4TWF
Title	:	X-ray structure of a pentameric ligand gated ion channel from Erwinia chrysanthemi (ELIC) in complex with bromomemantine
Authors	:	Ulens, C.; Spurny, R.; Thompson, A.J.; Alqazzaz, M.; Debaveye, S.; Lu, H.; Price, K.; Villalgordo, J.M.; Tresadern, G.; Lynch, J.W.; Lummis, S.C.R.
Deposited on	:	2014-06-30
Resolution	:	3.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

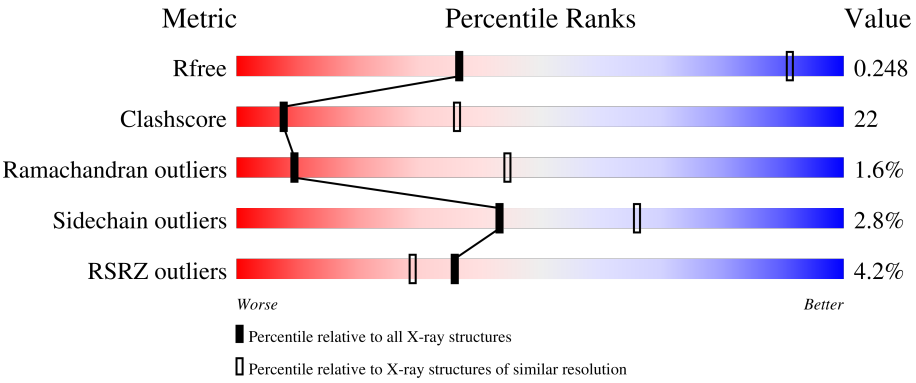
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.90 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	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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% 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	307	3% 59% 36%
1	B	307	4% 60% 38%
1	C	307	6% 60% 37%
1	D	307	4% 68% 29%

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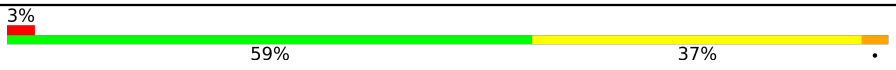
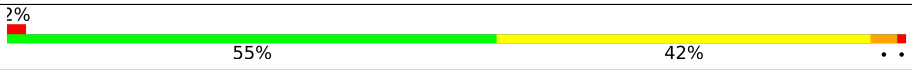
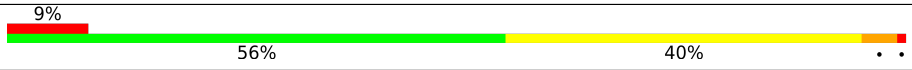
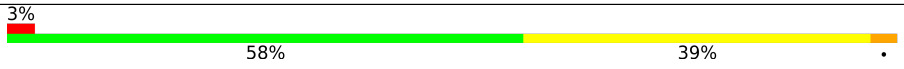
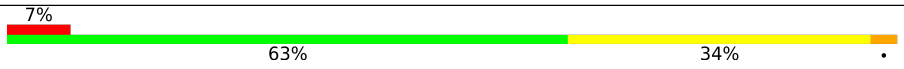
Mol	Chain	Length	Quality of chain
1	E	307	
1	F	307	
1	G	307	
1	H	307	
1	I	307	
1	J	307	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 25138 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 Cys-loop ligand-gated ion channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	B	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	C	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	D	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	E	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	F	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	G	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	H	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	I	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	J	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	ALA	ILE	conflict	UNP P0C7B7
A	164	GLY	-	insertion	UNP P0C7B7
A	247	SER	PHE	engineered mutation	UNP P0C7B7
A	289	ASN	MET	conflict	UNP P0C7B7
B	152	ALA	ILE	conflict	UNP P0C7B7
B	164	GLY	-	insertion	UNP P0C7B7
B	247	SER	PHE	engineered mutation	UNP P0C7B7
B	289	ASN	MET	conflict	UNP P0C7B7
C	152	ALA	ILE	conflict	UNP P0C7B7

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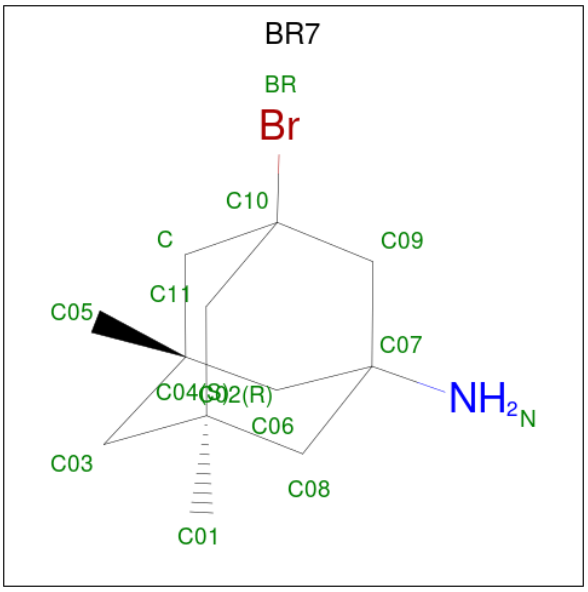
Chain	Residue	Modelled	Actual	Comment	Reference
C	164	GLY	-	insertion	UNP P0C7B7
C	247	SER	PHE	engineered mutation	UNP P0C7B7
C	289	ASN	MET	conflict	UNP P0C7B7
D	152	ALA	ILE	conflict	UNP P0C7B7
D	164	GLY	-	insertion	UNP P0C7B7
D	247	SER	PHE	engineered mutation	UNP P0C7B7
D	289	ASN	MET	conflict	UNP P0C7B7
E	152	ALA	ILE	conflict	UNP P0C7B7
E	164	GLY	-	insertion	UNP P0C7B7
E	247	SER	PHE	engineered mutation	UNP P0C7B7
E	289	ASN	MET	conflict	UNP P0C7B7
F	152	ALA	ILE	conflict	UNP P0C7B7
F	164	GLY	-	insertion	UNP P0C7B7
F	247	SER	PHE	engineered mutation	UNP P0C7B7
F	289	ASN	MET	conflict	UNP P0C7B7
G	152	ALA	ILE	conflict	UNP P0C7B7
G	164	GLY	-	insertion	UNP P0C7B7
G	247	SER	PHE	engineered mutation	UNP P0C7B7
G	289	ASN	MET	conflict	UNP P0C7B7
H	152	ALA	ILE	conflict	UNP P0C7B7
H	164	GLY	-	insertion	UNP P0C7B7
H	247	SER	PHE	engineered mutation	UNP P0C7B7
H	289	ASN	MET	conflict	UNP P0C7B7
I	152	ALA	ILE	conflict	UNP P0C7B7
I	164	GLY	-	insertion	UNP P0C7B7
I	247	SER	PHE	engineered mutation	UNP P0C7B7
I	289	ASN	MET	conflict	UNP P0C7B7
J	152	ALA	ILE	conflict	UNP P0C7B7
J	164	GLY	-	insertion	UNP P0C7B7
J	247	SER	PHE	engineered mutation	UNP P0C7B7
J	289	ASN	MET	conflict	UNP P0C7B7

- Molecule 2 is Bromomemantine (three-letter code: BR7) (formula: $C_{12}H_{20}BrN$).



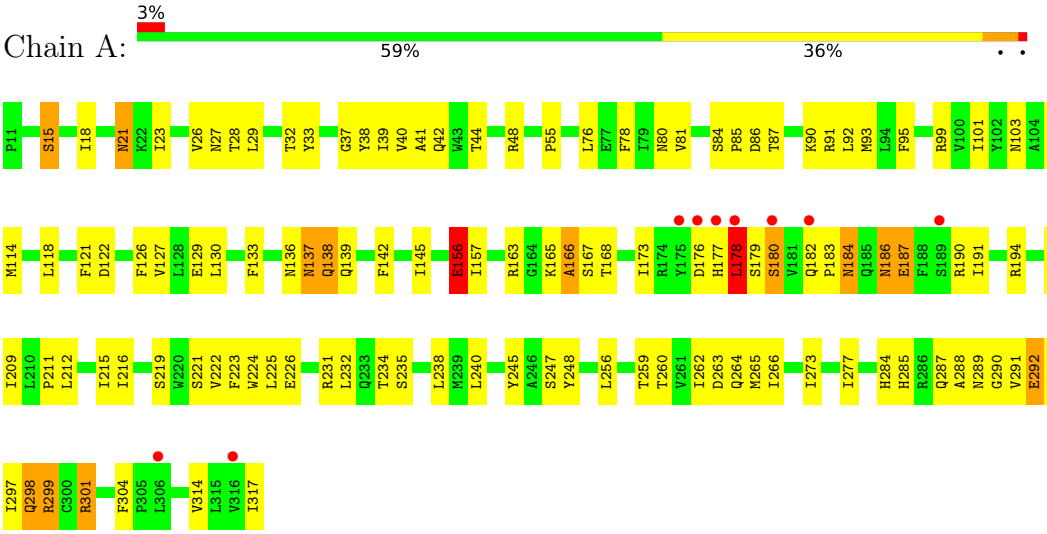
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Br	C	N		
2	A	1	14	1	12	1	0	0
			Total	Br	C	N		
2	A	1	14	1	12	1	0	0
			Total	Br	C	N		
2	B	1	14	1	12	1	0	0
			Total	Br	C	N		
2	C	1	14	1	12	1	0	0
			Total	Br	C	N		
2	D	1	14	1	12	1	0	0
			Total	Br	C	N		
2	E	1	14	1	12	1	0	0
			Total	Br	C	N		
2	F	1	14	1	12	1	0	0
			Total	Br	C	N		
2	F	1	14	1	12	1	0	0
			Total	Br	C	N		
2	G	1	14	1	12	1	0	0
			Total	Br	C	N		
2	H	1	14	1	12	1	0	0
			Total	Br	C	N		
2	I	1	14	1	12	1	0	0
			Total	Br	C	N		
2	J	1	14	1	12	1	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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

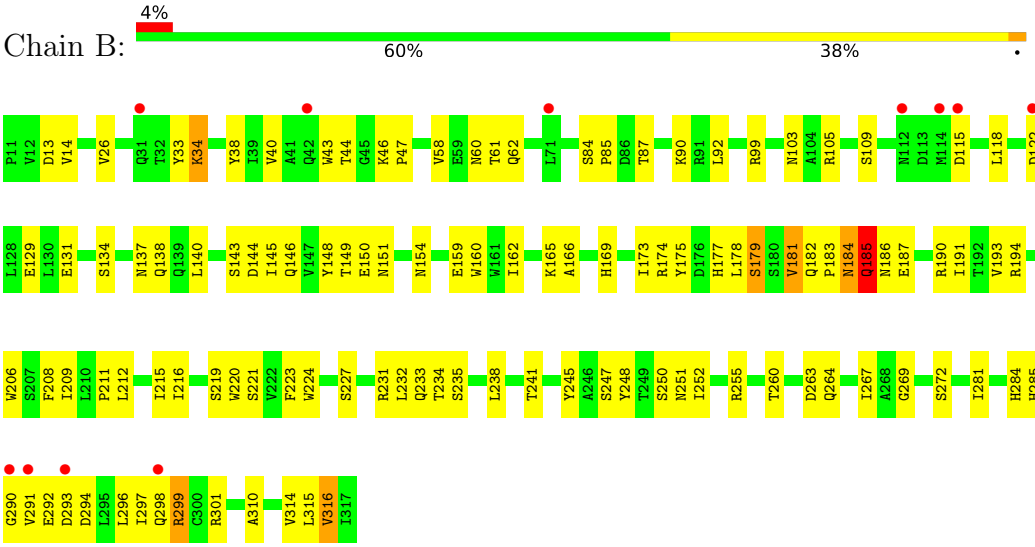
• Molecule 1: Cys-loop ligand-gated ion channel

Chain A:



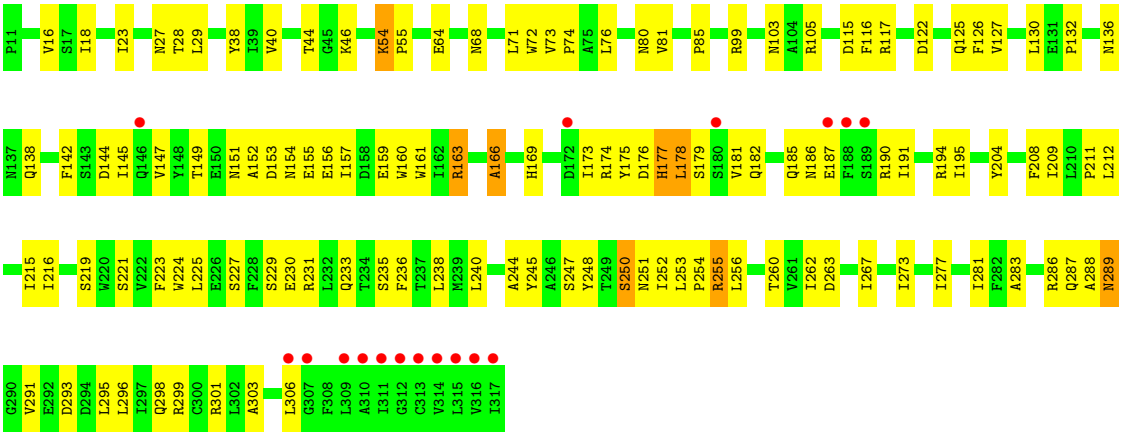
• Molecule 1: Cys-loop ligand-gated ion channel

Chain B:



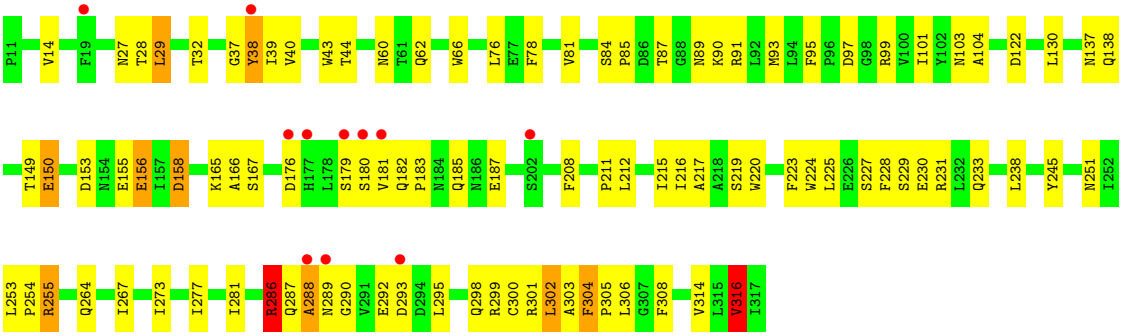
• Molecule 1: Cys-loop ligand-gated ion channel

Chain C:



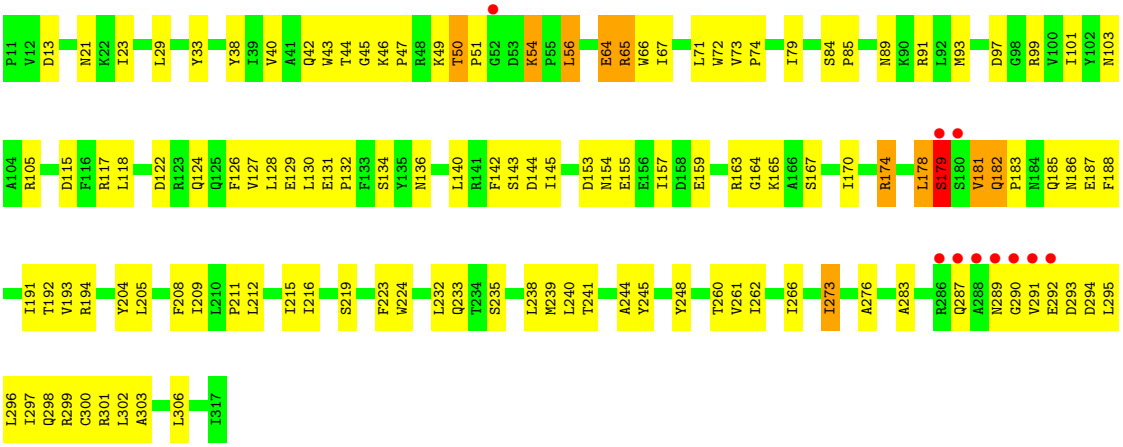
• Molecule 1: Cys-loop ligand-gated ion channel

Chain D:



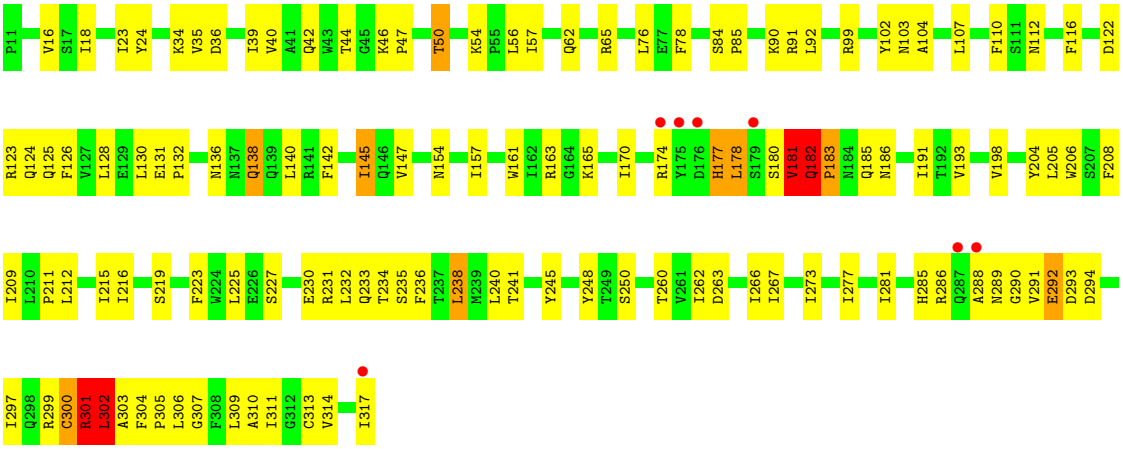
• Molecule 1: Cys-loop ligand-gated ion channel

Chain E:



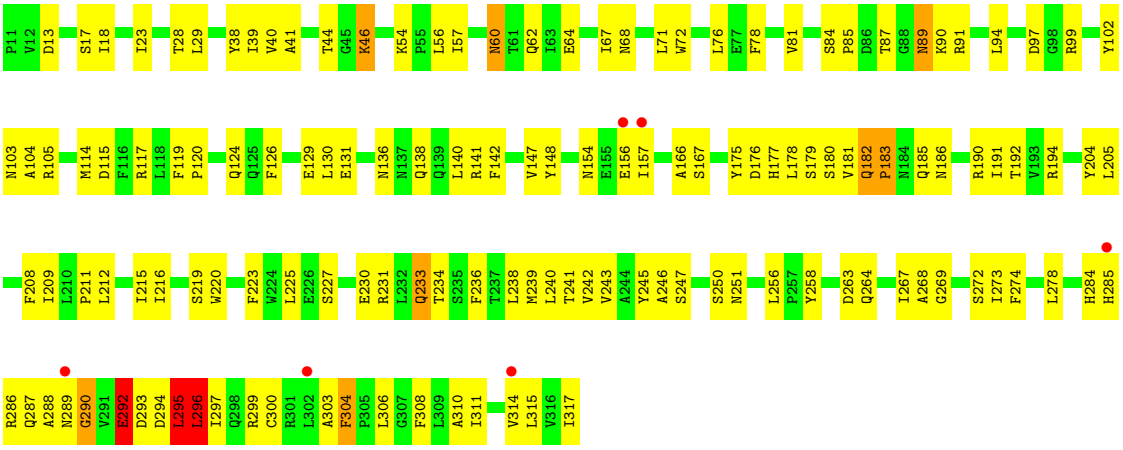
• Molecule 1: Cys-loop ligand-gated ion channel

Chain F:



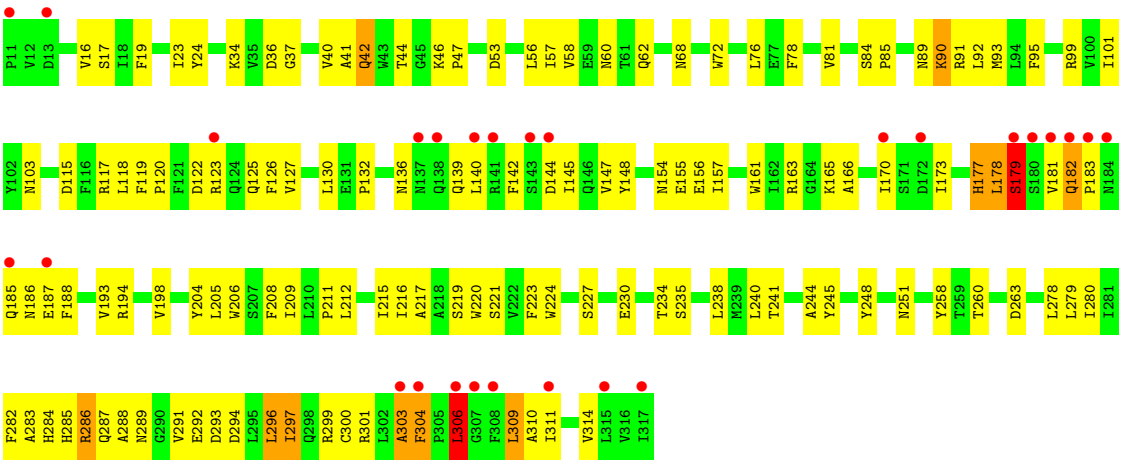
• Molecule 1: Cys-loop ligand-gated ion channel

Chain G:



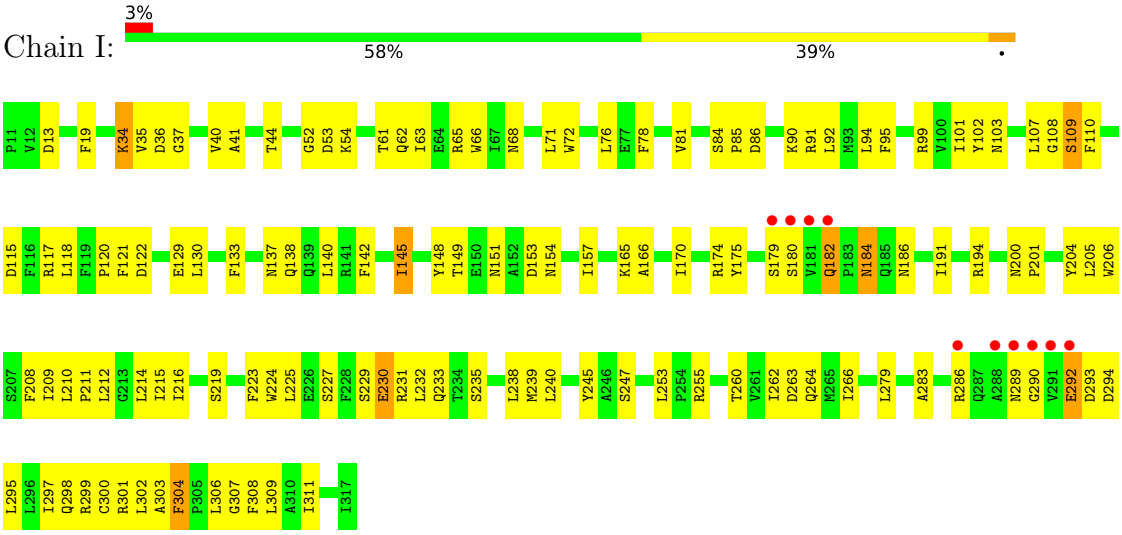
• Molecule 1: Cys-loop ligand-gated ion channel

Chain H:



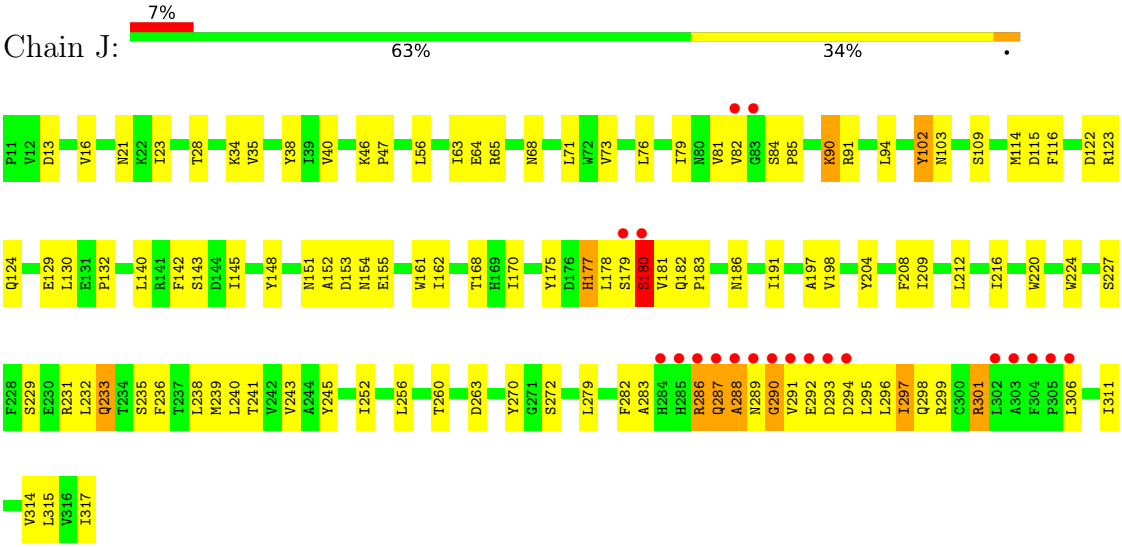
• Molecule 1: Cys-loop ligand-gated ion channel

Chain I:



• Molecule 1: Cys-loop ligand-gated ion channel

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	106.50Å 266.09Å 112.17Å 90.00° 107.70° 90.00°	Depositor
Resolution (Å)	49.83 – 3.90 49.83 – 3.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.83-3.90) 91.1 (49.83-3.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.95 (at 3.88Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.202 , 0.250 0.205 , 0.248	Depositor DCC
R_{free} test set	2719 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	106.1	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.22 , 77.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	25138	wwPDB-VP
Average B, all atoms (Å^2)	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BR7

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	0.42	0/2564	0.77	3/3495 (0.1%)
1	B	0.43	0/2564	0.75	2/3495 (0.1%)
1	C	0.42	0/2564	0.75	1/3495 (0.0%)
1	D	0.39	0/2564	0.72	0/3495
1	E	0.49	2/2564 (0.1%)	0.82	4/3495 (0.1%)
1	F	0.43	0/2564	0.78	3/3495 (0.1%)
1	G	0.41	0/2564	0.75	4/3495 (0.1%)
1	H	0.45	0/2564	0.80	3/3495 (0.1%)
1	I	0.41	0/2564	0.74	1/3495 (0.0%)
1	J	0.45	0/2564	0.76	3/3495 (0.1%)
All	All	0.43	2/25640 (0.0%)	0.77	24/34950 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	7
1	C	0	3
1	D	0	2
1	E	0	3
1	F	0	5
1	G	0	2
1	H	0	3
1	I	0	2
1	J	0	2
All	All	0	31

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	273	ILE	CA-CB	-7.06	1.38	1.54
1	E	54	LYS	CE-NZ	5.27	1.62	1.49

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	56	LEU	CB-CG-CD1	-13.99	87.22	111.00
1	A	301	ARG	NE-CZ-NH2	-11.40	114.60	120.30
1	H	296	LEU	CA-CB-CG	10.74	140.00	115.30
1	H	306	LEU	CA-CB-CG	8.49	134.84	115.30
1	F	178	LEU	CA-CB-CG	7.92	133.51	115.30
1	G	315	LEU	CA-CB-CG	7.64	132.88	115.30
1	G	238	LEU	CA-CB-CG	7.13	131.71	115.30
1	B	34	LYS	CD-CE-NZ	6.49	126.62	111.70
1	C	178	LEU	CA-CB-CG	6.47	130.18	115.30
1	I	182	GLN	CA-CB-CG	6.46	127.60	113.40
1	A	301	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	E	45	GLY	N-CA-C	-6.36	97.20	113.10
1	G	296	LEU	CA-CB-CG	5.79	128.63	115.30
1	J	288	ALA	N-CA-C	5.69	126.37	111.00
1	H	286	ARG	CB-CG-CD	5.64	126.26	111.60
1	F	182	GLN	CA-CB-CG	5.41	125.30	113.40
1	E	56	LEU	CB-CA-C	-5.34	100.06	110.20
1	E	181	VAL	N-CA-C	-5.31	96.67	111.00
1	F	238	LEU	CA-CB-CG	5.29	127.46	115.30
1	A	299	ARG	CA-CB-CG	5.23	124.90	113.40
1	B	181	VAL	N-CA-C	-5.20	96.95	111.00
1	J	178	LEU	CB-CG-CD2	-5.08	102.36	111.00
1	J	178	LEU	CA-CB-CG	5.05	126.93	115.30
1	G	182	GLN	C-N-CD	-5.04	109.51	120.60

There are no chirality outliers.

All (31) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	177	HIS	Peptide
1	A	178	LEU	Peptide
1	B	177	HIS	Peptide
1	B	178	LEU	Peptide
1	B	179	SER	Peptide
1	B	184	ASN	Peptide
1	B	185	GLN	Peptide

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Mol	Chain	Res	Type	Group
1	B	286	ARG	Peptide
1	B	316	VAL	Peptide
1	C	177	HIS	Sidechain
1	C	286	ARG	Peptide
1	C	288	ALA	Peptide
1	D	158	ASP	Peptide
1	D	286	ARG	Peptide
1	E	178	LEU	Peptide
1	E	179	SER	Peptide
1	E	46	LYS	Peptide
1	F	177	HIS	Peptide
1	F	180	SER	Peptide
1	F	181	VAL	Peptide
1	F	300	CYS	Peptide
1	F	301	ARG	Peptide
1	G	294	ASP	Peptide
1	G	295	LEU	Peptide
1	H	178	LEU	Peptide
1	H	179	SER	Peptide
1	H	293	ASP	Peptide
1	I	292	GLU	Peptide
1	I	34	LYS	Peptide
1	J	177	HIS	Peptide
1	J	180	SER	Peptide

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	2497	0	2468	117	0
1	B	2497	0	2468	115	0
1	C	2497	0	2468	118	0
1	D	2497	0	2468	79	0
1	E	2497	0	2468	118	0
1	F	2497	0	2468	126	0
1	G	2497	0	2468	124	0
1	H	2497	0	2468	130	0
1	I	2497	0	2468	134	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	2497	0	2468	116	0
2	A	28	0	40	2	0
2	B	14	0	20	4	0
2	C	14	0	20	5	0
2	D	14	0	20	0	0
2	E	14	0	20	2	0
2	F	28	0	40	1	0
2	G	14	0	20	3	0
2	H	14	0	20	0	0
2	I	14	0	20	1	0
2	J	14	0	20	2	0
All	All	25138	0	24920	1091	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 22.

All (1091) 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:221:SER:HA	1:A:301:ARG:HH22	1.15	1.07
1:E:239:MET:HE3	1:E:273:ILE:HG21	1.37	1.06
1:I:63:ILE:HD13	1:I:90:LYS:HE3	1.40	1.04
1:I:299:ARG:HH12	1:I:302:LEU:HD23	1.21	1.01
1:C:298:GLN:O	1:C:301:ARG:NH1	1.98	0.97
1:H:286:ARG:HH12	1:H:297:ILE:HG21	1.29	0.94
1:H:287:GLN:OE1	1:H:292:GLU:N	2.03	0.92
1:F:145:ILE:HD12	1:F:191:ILE:HG21	1.50	0.92
1:J:115:ASP:H	1:J:124:GLN:HE22	0.99	0.91
1:E:223:PHE:HB3	1:E:301:ARG:NH1	1.86	0.90
1:F:301:ARG:HB3	1:F:303:ALA:H	1.32	0.89
1:H:296:LEU:HA	1:H:299:ARG:HB2	1.55	0.88
1:E:235:SER:HA	1:E:238:LEU:HD12	1.56	0.88
1:F:90:LYS:HE2	1:F:104:ALA:HB2	1.53	0.88
1:G:287:GLN:HB2	1:G:292:GLU:HB2	1.53	0.88
1:C:251:ASN:HD21	1:D:251:ASN:HD22	1.18	0.87
1:A:221:SER:HA	1:A:301:ARG:NH2	1.90	0.87
1:F:219:SER:HA	1:F:238:LEU:HD11	1.57	0.87
1:J:220:TRP:HE1	1:J:272:SER:HG	1.18	0.86
1:I:34:LYS:NZ	1:I:35:VAL:O	2.08	0.85
1:C:287:GLN:HG2	1:C:289:ASN:H	1.40	0.85
1:F:182:GLN:HB2	1:F:183:PRO:HD3	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:THR:OG1	1:E:56:LEU:HD11	1.76	0.85
1:G:156:GLU:OE1	1:H:117:ARG:NH1	2.08	0.85
1:E:182:GLN:H	1:E:183:PRO:HD2	1.42	0.85
1:J:115:ASP:N	1:J:124:GLN:HE22	1.74	0.84
1:J:123:ARG:HD3	1:J:198:VAL:HG22	1.59	0.84
1:E:50:THR:OG1	1:E:54:LYS:NZ	2.09	0.84
1:H:230:GLU:OE2	1:I:229:SER:OG	1.94	0.84
1:C:176:ASP:HB2	1:C:177:HIS:CD2	2.13	0.83
1:H:234:THR:OG1	1:I:233:GLN:NE2	2.11	0.83
1:I:255:ARG:HG2	1:I:255:ARG:HH11	1.43	0.83
1:I:76:LEU:HB3	1:I:130:LEU:HD11	1.60	0.82
1:B:38:TYR:HE1	1:B:105:ARG:HD2	1.44	0.82
1:H:93:MET:HB3	1:H:101:ILE:HB	1.61	0.82
1:D:81:VAL:HG21	1:D:85:PRO:HG3	1.61	0.82
1:I:90:LYS:HD2	1:I:91:ARG:N	1.94	0.82
1:H:156:GLU:HG3	1:H:157:ILE:HG13	1.62	0.81
1:F:50:THR:HG21	1:F:54:LYS:O	1.81	0.81
1:I:223:PHE:HE1	1:I:304:PHE:HE2	1.29	0.80
1:J:181:VAL:HG12	1:J:183:PRO:HD2	1.63	0.80
1:J:235:SER:HA	1:J:238:LEU:HD13	1.64	0.80
1:I:34:LYS:CG	1:I:109:SER:HA	2.12	0.80
1:C:153:ASP:OD1	1:C:154:ASN:N	2.15	0.79
1:H:42:GLN:HG2	1:H:101:ILE:HG12	1.63	0.79
2:A:402:BR7:BR	1:C:244:ALA:HA	2.38	0.79
1:H:286:ARG:NH1	1:H:297:ILE:HG21	1.98	0.79
1:C:251:ASN:ND2	1:D:251:ASN:HD22	1.82	0.78
1:D:62:GLN:HE22	1:E:67:ILE:HG22	1.47	0.78
1:I:219:SER:HA	1:I:238:LEU:HD23	1.63	0.78
1:F:174:ARG:NH1	1:F:186:ASN:HB2	1.98	0.78
1:D:97:ASP:OD1	1:D:99:ARG:NH1	2.16	0.77
1:G:287:GLN:HG2	1:G:289:ASN:H	1.49	0.77
1:D:289:ASN:OD1	1:D:290:GLY:N	2.17	0.77
1:E:239:MET:CE	1:E:273:ILE:HG21	2.12	0.77
1:C:229:SER:O	1:C:233:GLN:HG2	1.85	0.77
1:E:145:ILE:HD11	1:E:191:ILE:HG12	1.66	0.77
1:B:34:LYS:HD2	1:B:109:SER:HA	1.64	0.77
1:I:205:LEU:HD23	1:I:209:ILE:HG13	1.64	0.77
1:E:298:GLN:O	1:E:301:ARG:NH1	2.18	0.76
1:C:16:VAL:HB	1:C:145:ILE:HD11	1.66	0.76
1:J:282:PHE:HE2	1:J:297:ILE:HG12	1.50	0.76
1:C:301:ARG:HG3	1:C:301:ARG:HH11	1.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:34:LYS:HG2	1:I:109:SER:HA	1.68	0.75
1:C:40:VAL:HG13	1:C:103:ASN:HD21	1.52	0.74
1:C:298:GLN:C	1:C:301:ARG:HH12	1.90	0.74
1:H:224:TRP:CD1	1:H:301:ARG:HD3	2.23	0.74
1:J:23:ILE:HG12	1:J:35:VAL:HG22	1.68	0.74
1:B:219:SER:HA	1:B:238:LEU:CD2	2.18	0.74
1:G:311:ILE:O	1:G:314:VAL:HG22	1.87	0.74
1:E:239:MET:CE	1:E:273:ILE:HD13	2.18	0.74
1:D:302:LEU:HD23	1:D:305:PRO:HB2	1.70	0.73
1:H:219:SER:HA	1:H:238:LEU:HD22	1.70	0.73
1:G:287:GLN:HB2	1:G:292:GLU:CB	2.19	0.72
1:F:234:THR:OG1	1:G:233:GLN:OE1	2.07	0.72
1:E:219:SER:HA	1:E:238:LEU:HD22	1.72	0.72
1:G:99:ARG:HG2	1:G:99:ARG:HH11	1.54	0.72
1:F:90:LYS:CE	1:F:104:ALA:HB2	2.20	0.72
1:D:233:GLN:OE1	1:E:233:GLN:NE2	2.23	0.71
1:G:62:GLN:NE2	1:H:68:ASN:OD1	2.22	0.71
1:E:239:MET:HE3	1:E:273:ILE:CG2	2.17	0.71
1:C:176:ASP:HB2	1:C:177:HIS:HD2	1.55	0.71
1:A:163:ARG:HG2	1:A:163:ARG:HH11	1.55	0.71
1:H:40:VAL:HG13	1:H:103:ASN:HD21	1.55	0.71
1:I:44:THR:HA	1:I:99:ARG:HA	1.71	0.71
1:A:287:GLN:HG3	1:A:290:GLY:N	2.06	0.70
1:F:181:VAL:HG22	1:F:182:GLN:HA	1.73	0.70
1:F:289:ASN:OD1	1:F:290:GLY:N	2.24	0.70
1:B:224:TRP:CE2	1:B:301:ARG:HG2	2.26	0.70
1:B:252:ILE:HD11	1:C:250:SER:OG	1.92	0.70
1:H:283:ALA:HA	1:H:286:ARG:CZ	2.21	0.70
1:H:286:ARG:HH21	1:H:294:ASP:H	1.38	0.70
1:I:34:LYS:HE2	1:I:108:GLY:N	2.07	0.70
1:J:90:LYS:NZ	1:J:102:TYR:CD2	2.58	0.70
1:B:223:PHE:HB2	1:B:301:ARG:HD3	1.73	0.70
1:D:229:SER:O	1:D:233:GLN:HG2	1.92	0.70
1:F:116:PHE:CE2	1:F:124:GLN:NE2	2.60	0.70
1:E:51:PRO:HB2	1:E:54:LYS:HE3	1.73	0.70
1:F:178:LEU:HG	1:F:181:VAL:HB	1.73	0.70
1:J:162:ILE:HD13	1:J:197:ALA:HB2	1.74	0.69
1:G:46:LYS:N	1:G:46:LYS:HD3	2.07	0.69
1:B:87:THR:HG21	1:B:90:LYS:NZ	2.06	0.69
1:H:145:ILE:HD12	1:H:170:ILE:HD11	1.73	0.69
1:I:34:LYS:HZ3	1:I:108:GLY:H	1.38	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:13:ASP:HB3	1:E:143:SER:HB3	1.74	0.69
1:F:177:HIS:CD2	1:J:148:TYR:HH	2.10	0.69
1:J:286:ARG:NH1	1:J:287:GLN:HA	2.07	0.69
1:A:38:TYR:CD2	2:B:401:BR7:H20	2.28	0.69
1:E:239:MET:HE1	1:E:273:ILE:HD13	1.75	0.69
1:H:179:SER:HB2	1:H:181:VAL:H	1.57	0.69
1:A:42:GLN:HB2	1:A:101:ILE:HG12	1.75	0.69
1:A:205:LEU:HD23	1:A:209:ILE:HG13	1.74	0.68
1:J:81:VAL:HG21	1:J:85:PRO:HG3	1.75	0.68
1:G:167:SER:HB3	1:G:194:ARG:HB2	1.76	0.68
1:B:255:ARG:HG2	1:B:255:ARG:HH11	1.58	0.68
1:E:153:ASP:OD1	1:E:154:ASN:N	2.24	0.68
1:B:38:TYR:CE2	2:C:401:BR7:H20	2.29	0.68
1:I:165:LYS:HG3	1:I:166:ALA:H	1.60	0.67
1:J:287:GLN:HE21	1:J:289:ASN:H	1.40	0.67
1:A:314:VAL:O	1:A:317:ILE:HG22	1.93	0.67
1:F:76:LEU:HB3	1:F:130:LEU:HD11	1.76	0.67
1:H:42:GLN:HG2	1:H:101:ILE:HA	1.77	0.67
1:I:63:ILE:HD13	1:I:90:LYS:CE	2.22	0.67
1:G:178:LEU:HD22	2:G:401:BR7:H2	1.77	0.67
1:I:34:LYS:CE	1:I:108:GLY:H	2.08	0.67
1:A:157:ILE:HD11	1:B:115:ASP:HA	1.76	0.67
2:F:402:BR7:BR	1:H:244:ALA:HA	2.50	0.67
1:F:211:PRO:O	1:F:215:ILE:HG12	1.95	0.67
1:C:208:PHE:O	1:C:245:TYR:OH	2.12	0.66
1:E:145:ILE:HD13	1:E:191:ILE:HG23	1.77	0.66
1:I:34:LYS:HE3	1:I:35:VAL:H	1.60	0.66
1:C:235:SER:HA	1:C:238:LEU:HD13	1.76	0.66
1:A:219:SER:HA	1:A:238:LEU:HD23	1.77	0.66
1:A:224:TRP:CE3	1:B:281:ILE:HG21	2.31	0.66
1:I:53:ASP:H	1:I:54:LYS:HD2	1.60	0.66
1:J:220:TRP:NE1	1:J:272:SER:OG	2.20	0.66
1:F:145:ILE:HD11	1:F:191:ILE:HD13	1.78	0.66
1:A:221:SER:CA	1:A:301:ARG:HH22	2.01	0.66
1:H:241:THR:HA	1:I:240:LEU:HD23	1.78	0.66
1:A:287:GLN:HG2	1:A:289:ASN:H	1.61	0.66
1:E:129:GLU:HG2	1:E:192:THR:HG23	1.77	0.66
1:A:38:TYR:HE1	1:A:105:ARG:HD2	1.60	0.65
1:D:299:ARG:HG2	1:D:299:ARG:HH11	1.62	0.65
1:H:204:TYR:O	1:H:208:PHE:HB2	1.96	0.65
1:C:299:ARG:HA	1:C:301:ARG:NH1	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:34:LYS:HE2	1:I:108:GLY:H	1.58	0.65
1:J:287:GLN:HG2	1:J:288:ALA:N	2.10	0.65
1:B:143:SER:OG	1:B:144:ASP:OD1	2.14	0.65
1:F:303:ALA:O	1:F:307:GLY:N	2.28	0.65
1:F:301:ARG:HB3	1:F:303:ALA:N	2.10	0.64
1:I:34:LYS:NZ	1:I:108:GLY:H	1.95	0.64
1:J:293:ASP:N	1:J:293:ASP:OD1	2.30	0.64
1:A:15:SER:HB3	1:A:42:GLN:HG2	1.78	0.64
1:A:287:GLN:HA	1:A:292:GLU:OE2	1.97	0.64
1:A:173:ILE:HD13	1:A:190:ARG:HB3	1.79	0.64
1:B:62:GLN:NE2	1:C:68:ASN:OD1	2.30	0.64
1:B:40:VAL:HG13	1:B:103:ASN:HD21	1.61	0.64
1:I:230:GLU:HB3	1:J:233:GLN:HE22	1.61	0.64
1:F:294:ASP:HB2	1:F:297:ILE:HB	1.80	0.64
1:J:297:ILE:HG13	1:J:298:GLN:N	2.11	0.64
1:G:178:LEU:HG	1:G:179:SER:H	1.63	0.64
1:H:62:GLN:NE2	1:I:68:ASN:OD1	2.31	0.64
1:I:85:PRO:HA	1:I:108:GLY:HA3	1.80	0.63
1:C:27:ASN:OD1	1:C:255:ARG:NH1	2.31	0.63
1:C:301:ARG:NH1	1:C:301:ARG:HG3	2.12	0.63
1:E:208:PHE:O	1:E:245:TYR:OH	2.16	0.63
1:J:180:SER:OG	1:J:180:SER:O	2.08	0.63
1:H:309:LEU:HG	1:H:310:ALA:N	2.13	0.63
1:F:110:PHE:HE2	1:F:128:LEU:HG	1.64	0.63
1:C:149:THR:HG23	1:C:151:ASN:HD22	1.63	0.63
1:C:296:LEU:HA	1:C:299:ARG:HB2	1.79	0.63
1:I:227:SER:O	1:I:231:ARG:HG3	1.98	0.63
1:I:230:GLU:OE1	1:J:233:GLN:NE2	2.30	0.63
1:D:76:LEU:HB3	1:D:130:LEU:HD11	1.80	0.63
1:I:294:ASP:HB2	1:I:297:ILE:HG12	1.80	0.63
1:I:91:ARG:NH2	1:I:103:ASN:OD1	2.32	0.62
1:E:298:GLN:O	1:E:301:ARG:CZ	2.47	0.62
1:J:114:MET:HA	1:J:124:GLN:NE2	2.15	0.62
1:H:115:ASP:OD2	1:H:117:ARG:NH2	2.29	0.62
1:D:299:ARG:HG2	1:D:299:ARG:NH1	2.14	0.62
1:G:251:ASN:ND2	1:H:251:ASN:ND2	2.47	0.62
1:H:235:SER:HA	1:H:238:LEU:HD12	1.82	0.62
1:E:182:GLN:H	1:E:183:PRO:CD	2.11	0.62
1:I:61:THR:HG21	1:J:64:GLU:HG2	1.80	0.62
1:A:232:LEU:O	1:A:235:SER:OG	2.18	0.62
1:E:93:MET:HB3	1:E:101:ILE:HB	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:76:LEU:HB3	1:G:130:LEU:HD11	1.82	0.62
1:J:63:ILE:HD13	1:J:90:LYS:HE2	1.81	0.62
2:A:402:BR7:H3	1:E:244:ALA:HA	1.81	0.62
1:C:256:LEU:HD12	1:C:260:THR:HG22	1.82	0.62
1:I:54:LYS:HD2	1:I:54:LYS:H	1.64	0.62
1:H:227:SER:HB3	1:H:230:GLU:HG3	1.81	0.61
1:J:286:ARG:HD2	1:J:287:GLN:N	2.15	0.61
1:F:178:LEU:HD21	1:F:181:VAL:HG21	1.81	0.61
1:C:175:TYR:CE1	2:C:401:BR7:H4	2.36	0.61
1:G:216:ILE:HD12	1:G:269:GLY:HA2	1.82	0.61
1:J:123:ARG:NH1	1:J:197:ALA:O	2.33	0.61
1:B:87:THR:HG21	1:B:90:LYS:HZ2	1.66	0.61
1:C:130:LEU:HB3	1:C:191:ILE:HD12	1.82	0.61
1:G:97:ASP:OD1	1:G:99:ARG:NH1	2.33	0.61
1:J:286:ARG:O	1:J:287:GLN:HB3	2.00	0.61
1:C:253:LEU:HD21	1:C:262:ILE:HD12	1.81	0.61
1:H:81:VAL:HG21	1:H:85:PRO:HG3	1.82	0.61
1:I:63:ILE:HD12	1:I:90:LYS:HG3	1.83	0.61
1:J:282:PHE:CE2	1:J:297:ILE:HG12	2.34	0.61
1:B:146:GLN:HB3	1:B:148:TYR:CE1	2.35	0.61
1:B:212:LEU:O	1:B:216:ILE:HG12	2.00	0.61
1:H:44:THR:HA	1:H:99:ARG:HA	1.82	0.61
1:I:295:LEU:HA	1:I:298:GLN:HG2	1.83	0.61
1:J:91:ARG:NH2	1:J:103:ASN:OD1	2.34	0.61
1:G:208:PHE:O	1:G:245:TYR:OH	2.19	0.60
1:G:212:LEU:O	1:G:216:ILE:HG12	2.01	0.60
1:A:178:LEU:HD13	1:A:180:SER:HA	1.82	0.60
1:E:66:TRP:HB3	1:E:71:LEU:HD12	1.82	0.60
1:F:248:TYR:HB2	1:G:247:SER:HB3	1.82	0.60
1:G:38:TYR:CE1	1:G:105:ARG:HD2	2.35	0.60
1:I:299:ARG:HH12	1:I:302:LEU:CD2	2.05	0.60
1:G:38:TYR:HE1	1:G:105:ARG:HD2	1.66	0.60
1:G:300:CYS:HB2	1:G:303:ALA:HB3	1.83	0.60
1:A:28:THR:HB	1:A:256:LEU:HD21	1.83	0.60
1:F:136:ASN:ND2	1:F:185:GLN:HA	2.16	0.60
1:F:241:THR:HA	1:G:240:LEU:HD23	1.83	0.60
1:J:34:LYS:HZ3	1:J:109:SER:HG	1.50	0.60
1:C:155:GLU:HB3	1:C:161:TRP:CD1	2.36	0.60
1:F:90:LYS:HE3	1:F:102:TYR:OH	2.02	0.60
1:G:295:LEU:HD13	1:G:296:LEU:HB3	1.83	0.60
1:F:301:ARG:HG2	1:F:302:LEU:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:223:PHE:CE1	1:G:304:PHE:HE2	2.20	0.60
1:B:131:GLU:OE1	1:B:190:ARG:NH2	2.35	0.60
1:B:149:THR:O	1:B:151:ASN:N	2.34	0.60
1:C:54:LYS:HB3	1:C:55:PRO:HD2	1.83	0.60
1:C:219:SER:HA	1:C:238:LEU:HD23	1.83	0.60
1:H:221:SER:HA	1:H:224:TRP:CE3	2.37	0.60
1:I:255:ARG:HH11	1:I:255:ARG:CG	2.15	0.60
1:G:97:ASP:OD2	1:G:99:ARG:NH1	2.35	0.59
1:I:300:CYS:HB2	1:I:303:ALA:HB3	1.84	0.59
1:B:123:ARG:HD3	1:B:198:VAL:HG22	1.83	0.59
1:D:219:SER:HA	1:D:238:LEU:HD11	1.84	0.59
1:F:91:ARG:NH2	1:F:103:ASN:OD1	2.34	0.59
1:B:162:ILE:HD13	1:B:197:ALA:HB2	1.84	0.59
1:B:175:TYR:CE1	2:B:401:BR7:H4	2.37	0.59
1:G:251:ASN:HD21	1:H:251:ASN:ND2	2.00	0.59
1:A:208:PHE:O	1:A:245:TYR:OH	2.19	0.59
1:A:248:TYR:HB2	1:B:247:SER:HB3	1.85	0.59
1:B:219:SER:HA	1:B:238:LEU:HD22	1.84	0.59
1:E:299:ARG:HA	1:E:301:ARG:HG2	1.84	0.59
1:D:211:PRO:O	1:D:215:ILE:HG12	2.02	0.59
1:G:81:VAL:HG21	1:G:85:PRO:HG3	1.84	0.59
1:G:182:GLN:N	1:G:183:PRO:HD3	2.16	0.58
1:H:283:ALA:HA	1:H:286:ARG:NH2	2.19	0.58
1:H:287:GLN:HB3	1:H:289:ASN:H	1.66	0.58
1:J:34:LYS:HG2	1:J:109:SER:HA	1.85	0.58
1:B:138:GLN:HE22	1:B:184:ASN:ND2	2.00	0.58
1:E:223:PHE:HB3	1:E:301:ARG:CZ	2.33	0.58
1:G:180:SER:HA	1:G:182:GLN:HE22	1.66	0.58
1:I:41:ALA:HB3	1:I:102:TYR:HB3	1.85	0.58
1:F:306:LEU:O	1:F:310:ALA:N	2.35	0.58
1:G:289:ASN:OD1	1:G:290:GLY:N	2.33	0.58
1:A:136:ASN:HB2	1:A:187:GLU:HG3	1.85	0.58
1:A:212:LEU:O	1:A:216:ILE:HG12	2.02	0.58
1:H:42:GLN:HE21	1:H:101:ILE:HG23	1.68	0.58
1:H:76:LEU:HB3	1:H:130:LEU:HD11	1.85	0.58
1:D:219:SER:HA	1:D:238:LEU:HD21	1.86	0.58
1:F:206:TRP:HZ3	1:G:264:GLN:HE21	1.50	0.58
1:G:54:LYS:HD2	1:G:54:LYS:N	2.18	0.58
1:I:223:PHE:CE1	1:I:304:PHE:HE2	2.17	0.58
1:B:251:ASN:ND2	1:C:251:ASN:OD1	2.36	0.58
1:D:288:ALA:N	1:D:292:GLU:HG3	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:262:ILE:O	1:F:266:ILE:HG12	2.04	0.58
1:F:90:LYS:NZ	1:F:102:TYR:CZ	2.70	0.58
1:G:233:GLN:HA	1:G:236:PHE:HD1	1.68	0.58
1:A:93:MET:HE3	1:A:101:ILE:HB	1.85	0.57
1:I:81:VAL:HG21	1:I:85:PRO:HG3	1.86	0.57
1:I:175:TYR:CD1	2:I:401:BR7:H3	2.39	0.57
1:D:149:THR:HG23	1:D:165:LYS:HE2	1.86	0.57
1:H:17:SER:HB2	1:H:40:VAL:HB	1.86	0.57
1:I:90:LYS:HD2	1:I:91:ARG:H	1.69	0.57
1:I:219:SER:HA	1:I:238:LEU:CD2	2.33	0.57
1:I:148:TYR:OH	1:J:177:HIS:HD2	1.88	0.57
1:A:87:THR:HG21	1:A:90:LYS:NZ	2.19	0.57
1:A:91:ARG:HH11	1:B:134:SER:HA	1.70	0.57
1:E:145:ILE:CD1	1:E:191:ILE:HG12	2.34	0.57
1:E:239:MET:HE2	1:E:239:MET:N	2.19	0.57
1:I:299:ARG:HA	1:I:301:ARG:HG3	1.86	0.57
1:B:205:LEU:HD23	1:B:209:ILE:HG13	1.85	0.57
1:G:28:THR:HB	1:G:256:LEU:HD21	1.87	0.57
1:G:205:LEU:HD23	1:G:209:ILE:HG13	1.86	0.57
1:G:284:HIS:HB3	1:G:285:HIS:HD2	1.70	0.57
1:I:289:ASN:HD21	1:I:292:GLU:HG2	1.69	0.57
1:A:289:ASN:OD1	1:A:290:GLY:N	2.27	0.57
1:E:289:ASN:OD1	1:E:290:GLY:N	2.35	0.57
1:B:260:THR:O	1:B:264:GLN:HG3	2.05	0.57
1:H:208:PHE:O	1:H:245:TYR:OH	2.21	0.57
1:J:295:LEU:HA	1:J:298:GLN:HG2	1.86	0.57
1:H:300:CYS:HG	1:H:304:PHE:HE2	1.52	0.57
1:I:137:ASN:HA	1:I:140:LEU:O	2.04	0.57
1:A:44:THR:HA	1:A:99:ARG:HA	1.87	0.56
1:B:208:PHE:O	1:B:245:TYR:OH	2.22	0.56
1:D:208:PHE:O	1:D:245:TYR:OH	2.21	0.56
1:E:211:PRO:O	1:E:215:ILE:HG12	2.04	0.56
1:G:90:LYS:HD3	1:G:102:TYR:OH	2.05	0.56
1:I:115:ASP:OD2	1:I:117:ARG:NH2	2.38	0.56
1:E:179:SER:HB2	1:E:181:VAL:H	1.69	0.56
1:G:136:ASN:HD21	1:G:138:GLN:HB2	1.70	0.56
1:G:263:ASP:O	1:G:267:ILE:HG13	2.05	0.56
1:H:221:SER:HA	1:H:224:TRP:HE3	1.70	0.56
1:E:40:VAL:HG13	1:E:103:ASN:HD21	1.70	0.56
1:F:16:VAL:HA	1:F:40:VAL:O	2.05	0.56
1:H:248:TYR:HB2	1:I:247:SER:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:286:ARG:HH11	1:J:287:GLN:HA	1.71	0.56
1:B:159:GLU:OE2	1:C:29:LEU:HD21	2.05	0.56
1:D:212:LEU:O	1:D:216:ILE:HG12	2.04	0.56
1:F:145:ILE:CD1	1:F:191:ILE:HD13	2.34	0.56
1:F:227:SER:HB3	1:F:230:GLU:OE2	2.04	0.56
1:H:211:PRO:O	1:H:215:ILE:HG12	2.06	0.56
1:I:211:PRO:O	1:I:215:ILE:HG12	2.06	0.56
1:C:224:TRP:CD1	1:C:301:ARG:HD3	2.40	0.56
1:J:282:PHE:CE2	1:J:297:ILE:HG21	2.40	0.56
1:A:184:ASN:O	1:A:187:GLU:HG2	2.05	0.56
1:A:263:ASP:OD1	1:A:264:GLN:N	2.38	0.56
1:I:165:LYS:HG3	1:I:166:ALA:N	2.20	0.56
1:I:34:LYS:CE	1:I:35:VAL:H	2.19	0.56
1:A:295:LEU:HA	1:A:298:GLN:HE22	1.71	0.56
1:D:38:TYR:CD2	2:E:401:BR7:H20	2.41	0.56
1:C:177:HIS:CD2	1:C:177:HIS:N	2.74	0.55
1:E:49:LYS:HD2	1:E:50:THR:H	1.71	0.55
1:D:149:THR:HG21	1:D:165:LYS:O	2.05	0.55
1:H:23:ILE:HG21	1:H:126:PHE:CD1	2.40	0.55
1:A:211:PRO:O	1:A:215:ILE:HG12	2.06	0.55
1:E:91:ARG:NH2	1:E:103:ASN:OD1	2.40	0.55
1:G:176:ASP:OD1	1:G:177:HIS:N	2.37	0.55
1:B:232:LEU:O	1:B:235:SER:OG	2.23	0.55
1:E:115:ASP:O	1:E:124:GLN:NE2	2.39	0.55
1:J:102:TYR:HD2	1:J:103:ASN:N	2.05	0.55
1:J:123:ARG:CD	1:J:198:VAL:HG22	2.33	0.55
1:J:142:PHE:CD2	1:J:191:ILE:HG13	2.42	0.55
1:F:110:PHE:CE2	1:F:128:LEU:HG	2.41	0.55
1:F:281:ILE:HG21	1:J:224:TRP:CZ3	2.41	0.55
1:F:289:ASN:OD1	1:F:291:VAL:N	2.38	0.55
1:C:212:LEU:O	1:C:216:ILE:HG12	2.05	0.55
1:H:118:LEU:HD11	1:H:122:ASP:HA	1.87	0.55
1:B:224:TRP:CD1	1:B:301:ARG:NE	2.74	0.55
1:E:44:THR:HA	1:E:99:ARG:HA	1.89	0.55
1:E:67:ILE:HG23	1:E:71:LEU:O	2.06	0.55
1:A:186:ASN:N	1:A:186:ASN:OD1	2.39	0.55
1:D:38:TYR:CE2	2:E:401:BR7:H20	2.41	0.55
1:D:137:ASN:ND2	1:D:187:GLU:OE1	2.37	0.55
1:H:284:HIS:CD2	1:H:291:VAL:HG13	2.41	0.55
1:J:123:ARG:HD2	1:J:197:ALA:O	2.06	0.55
1:A:292:GLU:HG2	1:A:292:GLU:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:ASN:HD21	1:D:251:ASN:ND2	1.96	0.55
1:E:165:LYS:HD2	1:E:165:LYS:N	2.22	0.55
1:G:284:HIS:HB3	1:G:285:HIS:CD2	2.42	0.55
1:G:99:ARG:HG2	1:G:99:ARG:NH1	2.21	0.55
1:I:54:LYS:HD2	1:I:54:LYS:N	2.20	0.55
1:B:44:THR:HA	1:B:99:ARG:HA	1.89	0.54
1:F:181:VAL:O	1:F:182:GLN:NE2	2.40	0.54
1:G:44:THR:HA	1:G:99:ARG:HA	1.89	0.54
1:I:304:PHE:HA	1:I:307:GLY:H	1.71	0.54
1:B:173:ILE:O	1:B:187:GLU:HA	2.07	0.54
1:D:91:ARG:HH11	1:E:134:SER:HA	1.72	0.54
1:E:299:ARG:C	1:E:301:ARG:H	2.10	0.54
1:F:90:LYS:HE3	1:F:102:TYR:CZ	2.42	0.54
1:A:165:LYS:O	1:A:165:LYS:HG2	2.06	0.54
1:B:223:PHE:HB2	1:B:301:ARG:CD	2.36	0.54
1:E:174:ARG:HB2	1:E:187:GLU:HG2	1.87	0.54
1:G:154:ASN:O	1:G:157:ILE:HG22	2.08	0.54
1:F:132:PRO:HD3	1:F:142:PHE:CE2	2.42	0.54
1:I:101:ILE:HD13	1:J:179:SER:HB2	1.88	0.54
1:C:211:PRO:HG2	1:C:245:TYR:OH	2.08	0.54
1:E:287:GLN:HA	1:E:292:GLU:HB3	1.90	0.54
1:G:225:LEU:HB2	1:G:231:ARG:HG3	1.89	0.54
1:A:81:VAL:O	1:E:105:ARG:NH2	2.41	0.54
1:A:224:TRP:N	1:A:301:ARG:HH11	2.04	0.54
1:F:212:LEU:O	1:F:216:ILE:HG12	2.07	0.54
1:F:223:PHE:HE2	1:F:300:CYS:HG	1.54	0.54
1:H:279:LEU:O	1:H:283:ALA:N	2.28	0.54
1:A:260:THR:N	1:A:263:ASP:OD2	2.33	0.54
1:G:91:ARG:NH2	1:G:103:ASN:OD1	2.41	0.54
1:G:129:GLU:HG2	1:G:192:THR:HG23	1.89	0.54
1:I:299:ARG:C	1:I:301:ARG:H	2.11	0.54
1:J:155:GLU:O	1:J:161:TRP:NE1	2.40	0.54
1:A:15:SER:O	1:A:41:ALA:HA	2.07	0.54
1:B:314:VAL:C	1:B:316:VAL:H	2.11	0.54
1:C:299:ARG:HA	1:C:301:ARG:HH11	1.73	0.54
1:D:300:CYS:HG	1:D:304:PHE:HE2	1.55	0.54
1:F:136:ASN:ND2	1:F:138:GLN:HG3	2.22	0.54
1:G:216:ILE:O	1:G:219:SER:HB3	2.08	0.54
1:J:34:LYS:NZ	1:J:109:SER:OG	2.34	0.54
1:A:235:SER:HA	1:A:238:LEU:HD13	1.89	0.54
1:C:132:PRO:HD3	1:C:142:PHE:CE2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:TYR:HD2	2:B:401:BR7:H20	1.72	0.54
1:C:99:ARG:NH2	1:D:180:SER:OG	2.40	0.54
1:J:301:ARG:HD2	1:J:301:ARG:O	2.08	0.54
1:F:23:ILE:HG12	1:F:35:VAL:HG22	1.90	0.53
1:H:144:ASP:O	1:H:145:ILE:HG13	2.08	0.53
1:I:95:PHE:HE2	1:J:181:VAL:CG2	2.20	0.53
1:D:37:GLY:C	1:D:38:TYR:HD1	2.11	0.53
1:E:154:ASN:HB3	1:E:157:ILE:HD13	1.88	0.53
1:I:174:ARG:HA	1:I:186:ASN:O	2.08	0.53
1:J:286:ARG:HG3	1:J:294:ASP:OD2	2.09	0.53
1:B:263:ASP:O	1:B:267:ILE:HG13	2.08	0.53
1:G:296:LEU:HA	1:G:299:ARG:HB3	1.90	0.53
1:A:163:ARG:HG2	1:A:163:ARG:NH1	2.24	0.53
1:B:224:TRP:CD2	1:B:301:ARG:HG2	2.42	0.53
1:B:289:ASN:OD1	1:B:290:GLY:N	2.35	0.53
1:F:182:GLN:HB2	1:F:183:PRO:CD	2.35	0.53
1:J:283:ALA:HB2	1:J:297:ILE:HD11	1.91	0.53
1:C:251:ASN:HB3	1:C:252:ILE:HD13	1.91	0.53
1:E:50:THR:HG1	1:E:56:LEU:HD11	1.70	0.53
1:A:294:ASP:OD2	1:A:297:ILE:HB	2.08	0.53
1:F:46:LYS:HD2	1:F:47:PRO:N	2.23	0.53
1:F:154:ASN:O	1:F:157:ILE:HG22	2.09	0.53
1:F:236:PHE:CE2	1:J:238:LEU:HD11	2.43	0.53
1:G:97:ASP:CG	1:G:99:ARG:NH1	2.62	0.53
1:G:223:PHE:HE1	1:G:304:PHE:HE2	1.55	0.53
1:I:232:LEU:O	1:I:235:SER:OG	2.21	0.53
1:I:34:LYS:HE3	1:I:107:LEU:HD12	1.90	0.53
1:J:279:LEU:O	1:J:282:PHE:HB3	2.08	0.53
1:C:221:SER:HA	1:C:224:TRP:HE3	1.73	0.53
1:E:205:LEU:HD23	1:E:209:ILE:HG13	1.90	0.53
1:E:295:LEU:HA	1:E:298:GLN:HG2	1.91	0.53
1:H:16:VAL:HB	1:H:145:ILE:HG12	1.91	0.53
1:H:286:ARG:NH2	1:H:294:ASP:HB3	2.24	0.53
1:H:303:ALA:O	1:H:306:LEU:HG	2.09	0.53
1:J:227:SER:O	1:J:231:ARG:NH1	2.42	0.53
1:A:180:SER:O	1:A:180:SER:OG	2.20	0.53
1:C:46:LYS:HD3	1:C:46:LYS:N	2.24	0.53
1:D:122:ASP:OD1	1:D:122:ASP:N	2.42	0.53
1:D:176:ASP:OD1	1:D:176:ASP:N	2.39	0.53
1:E:299:ARG:HG3	1:E:299:ARG:HH11	1.74	0.53
1:F:174:ARG:CZ	1:F:186:ASN:HB2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:225:LEU:HB2	1:F:231:ARG:HG3	1.91	0.53
1:G:23:ILE:HG21	1:G:126:PHE:CD1	2.44	0.53
1:I:54:LYS:H	1:I:54:LYS:CD	2.22	0.53
1:J:132:PRO:HG3	1:J:140:LEU:HD22	1.90	0.52
1:A:226:GLU:OE2	1:B:285:HIS:CE1	2.62	0.52
1:D:299:ARG:HA	1:D:301:ARG:HG3	1.91	0.52
1:H:294:ASP:HB3	1:H:297:ILE:HB	1.90	0.52
1:B:26:VAL:HG21	1:B:160:TRP:CZ2	2.44	0.52
1:C:219:SER:HA	1:C:238:LEU:CD2	2.39	0.52
1:G:181:VAL:C	1:G:183:PRO:HD3	2.30	0.52
1:G:233:GLN:O	1:G:236:PHE:HB2	2.09	0.52
1:E:33:TYR:OH	1:E:127:VAL:N	2.37	0.52
1:I:212:LEU:O	1:I:216:ILE:HG12	2.10	0.52
1:A:224:TRP:CG	1:A:301:ARG:HD3	2.45	0.52
1:B:238:LEU:HD21	1:C:236:PHE:CE2	2.44	0.52
1:G:157:ILE:HD12	1:H:258:TYR:CE2	2.45	0.52
1:A:91:ARG:HB3	1:A:103:ASN:HB2	1.91	0.52
1:B:40:VAL:HG13	1:B:103:ASN:ND2	2.23	0.52
1:C:159:GLU:HG2	1:C:160:TRP:CD1	2.45	0.52
1:C:295:LEU:O	1:C:299:ARG:HG3	2.09	0.52
1:D:93:MET:HB3	1:D:101:ILE:HB	1.92	0.52
1:E:79:ILE:HD11	1:E:131:GLU:HB3	1.92	0.52
1:F:260:THR:HG23	1:F:263:ASP:OD2	2.10	0.52
1:B:14:VAL:HG22	1:B:43:TRP:HB3	1.91	0.52
1:F:90:LYS:HE2	1:F:104:ALA:CB	2.32	0.52
1:F:112:ASN:ND2	1:F:125:GLN:O	2.43	0.52
1:B:118:LEU:CD1	1:B:122:ASP:HA	2.40	0.52
1:A:221:SER:C	1:A:301:ARG:HH12	2.13	0.52
1:B:38:TYR:HE2	2:C:401:BR7:H6	1.74	0.52
1:I:92:LEU:HD13	1:I:94:LEU:HD21	1.92	0.52
1:G:105:ARG:NH2	1:H:81:VAL:O	2.43	0.52
1:A:136:ASN:N	1:A:139:GLN:OE1	2.43	0.51
1:H:224:TRP:CE2	1:H:301:ARG:HB3	2.45	0.51
1:J:151:ASN:OD1	1:J:152:ALA:N	2.43	0.51
1:D:97:ASP:CG	1:D:99:ARG:NH1	2.64	0.51
1:I:65:ARG:NH2	1:J:68:ASN:HD22	2.07	0.51
1:D:40:VAL:HG13	1:D:103:ASN:ND2	2.25	0.51
1:F:157:ILE:HD13	1:G:115:ASP:HA	1.91	0.51
1:B:87:THR:CG2	1:B:90:LYS:HZ2	2.22	0.51
1:D:14:VAL:HG22	1:D:43:TRP:HB3	1.92	0.51
1:E:21:ASN:HD21	1:E:38:TYR:HE1	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:240:LEU:HD23	1:J:241:THR:HA	1.91	0.51
1:J:208:PHE:O	1:J:245:TYR:OH	2.29	0.51
1:B:216:ILE:O	1:B:219:SER:HB3	2.10	0.51
1:B:224:TRP:CD1	1:C:281:ILE:HG21	2.46	0.51
1:C:223:PHE:HB3	1:C:301:ARG:HG2	1.92	0.51
1:F:227:SER:HB3	1:F:230:GLU:HG3	1.93	0.51
1:A:27:ASN:HB3	1:A:32:THR:HB	1.93	0.51
1:B:33:TYR:C	1:B:34:LYS:HD3	2.30	0.51
1:B:38:TYR:CE1	1:B:105:ARG:HD2	2.35	0.51
1:C:44:THR:HA	1:C:99:ARG:HA	1.93	0.51
1:F:157:ILE:HD11	1:G:114:MET:O	2.10	0.51
1:J:28:THR:HB	1:J:256:LEU:HD21	1.92	0.51
1:C:156:GLU:H	1:C:156:GLU:CD	2.14	0.51
1:G:242:VAL:HG21	1:G:273:ILE:HD11	1.93	0.51
1:G:211:PRO:O	1:G:215:ILE:HG12	2.11	0.51
1:G:274:PHE:O	1:G:278:LEU:HG	2.10	0.51
1:C:176:ASP:CB	1:C:177:HIS:HD2	2.22	0.51
1:I:260:THR:HG23	1:I:263:ASP:OD2	2.10	0.51
1:D:220:TRP:CE3	1:D:305:PRO:HB3	2.45	0.51
1:D:303:ALA:O	1:D:306:LEU:HG	2.11	0.51
1:E:72:TRP:CH2	1:E:140:LEU:HD12	2.46	0.51
1:I:34:LYS:CE	1:I:107:LEU:HD12	2.40	0.51
1:A:38:TYR:CE1	1:A:105:ARG:HD2	2.43	0.50
1:D:298:GLN:HG3	1:D:298:GLN:O	2.11	0.50
1:E:72:TRP:CZ2	1:E:74:PRO:HB3	2.46	0.50
1:F:23:ILE:HG21	1:F:126:PHE:CD1	2.46	0.50
1:H:283:ALA:HA	1:H:286:ARG:NH1	2.26	0.50
1:H:306:LEU:O	1:H:309:LEU:HB3	2.10	0.50
1:F:136:ASN:HD21	1:F:138:GLN:HG3	1.76	0.50
1:G:90:LYS:HE3	1:G:104:ALA:HB1	1.92	0.50
1:H:289:ASN:CG	1:H:292:GLU:HB3	2.31	0.50
1:B:248:TYR:HB2	1:C:247:SER:HB3	1.92	0.50
1:C:295:LEU:HA	1:C:298:GLN:HG2	1.94	0.50
1:G:131:GLU:OE1	1:G:190:ARG:NH2	2.38	0.50
1:I:52:GLY:HA3	1:I:54:LYS:HD3	1.94	0.50
1:A:87:THR:HG21	1:A:90:LYS:HZ2	1.76	0.50
1:D:29:LEU:CD1	1:D:255:ARG:NH1	2.74	0.50
1:H:125:GLN:HE22	1:H:194:ARG:HH11	1.58	0.50
1:A:224:TRP:H	1:A:301:ARG:HH11	1.59	0.50
1:A:287:GLN:CG	1:A:289:ASN:H	2.24	0.50
1:C:211:PRO:O	1:C:215:ILE:HG12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:167:SER:HB3	1:E:194:ARG:HB2	1.94	0.50
1:J:71:LEU:HD22	1:J:73:VAL:CG2	2.42	0.50
1:J:115:ASP:H	1:J:124:GLN:NE2	1.84	0.50
1:J:153:ASP:CG	1:J:154:ASN:H	2.15	0.50
1:C:221:SER:HA	1:C:224:TRP:CE3	2.46	0.50
1:H:205:LEU:HD23	1:H:209:ILE:HG13	1.94	0.50
1:A:55:PRO:HG3	1:A:95:PHE:CE2	2.47	0.50
1:C:29:LEU:HB2	1:C:255:ARG:HD2	1.94	0.50
1:G:91:ARG:HB3	1:G:103:ASN:HB2	1.93	0.50
1:G:178:LEU:CD2	2:G:401:BR7:H2	2.41	0.50
1:I:90:LYS:NZ	1:I:102:TYR:CD1	2.80	0.50
1:I:95:PHE:HB2	1:I:99:ARG:O	2.12	0.50
1:D:27:ASN:HB3	1:D:32:THR:HB	1.93	0.50
1:E:91:ARG:HB3	1:E:103:ASN:HB2	1.94	0.50
1:F:223:PHE:HE2	1:F:300:CYS:SG	2.35	0.50
1:I:138:GLN:NE2	1:I:184:ASN:HB3	2.27	0.50
1:J:186:ASN:OD1	1:J:186:ASN:N	2.45	0.50
1:F:185:GLN:HG3	1:F:185:GLN:O	2.11	0.49
1:G:64:GLU:HA	1:G:67:ILE:HD12	1.94	0.49
1:G:239:MET:HA	1:G:273:ILE:HD13	1.93	0.49
1:C:81:VAL:HG21	1:C:85:PRO:HG3	1.93	0.49
1:E:299:ARG:HG3	1:E:299:ARG:NH1	2.27	0.49
1:C:16:VAL:HB	1:C:145:ILE:CD1	2.39	0.49
1:D:91:ARG:HB3	1:D:103:ASN:HB2	1.94	0.49
1:F:36:ASP:HB2	1:F:107:LEU:HD13	1.93	0.49
1:G:293:ASP:OD1	1:G:293:ASP:N	2.44	0.49
1:H:155:GLU:HB3	1:H:161:TRP:CD1	2.47	0.49
1:H:282:PHE:CD2	1:H:286:ARG:HD3	2.47	0.49
1:F:116:PHE:CD2	1:F:124:GLN:NE2	2.80	0.49
1:I:142:PHE:CD2	1:I:191:ILE:HG13	2.47	0.49
1:A:122:ASP:OD1	1:A:122:ASP:N	2.44	0.49
1:B:87:THR:HG21	1:B:90:LYS:HZ1	1.77	0.49
1:C:132:PRO:HD3	1:C:142:PHE:HE2	1.77	0.49
1:I:279:LEU:O	1:I:283:ALA:N	2.36	0.49
1:F:142:PHE:HB3	1:F:170:ILE:HD13	1.94	0.49
1:H:36:ASP:OD2	1:H:37:GLY:N	2.45	0.49
1:I:306:LEU:HA	1:I:309:LEU:HB2	1.95	0.49
1:A:93:MET:HB3	1:A:101:ILE:HB	1.94	0.49
1:C:38:TYR:CE2	1:C:105:ARG:HD2	2.48	0.49
1:E:296:LEU:HA	1:E:299:ARG:HB3	1.95	0.49
1:F:250:SER:HB3	1:J:252:ILE:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:260:THR:N	1:I:263:ASP:OD2	2.34	0.49
1:J:229:SER:O	1:J:233:GLN:HG3	2.11	0.49
1:A:219:SER:HA	1:A:238:LEU:CD2	2.40	0.49
1:C:18:ILE:HB	1:C:147:VAL:HG22	1.93	0.49
1:G:114:MET:HB3	1:G:124:GLN:NE2	2.27	0.49
1:G:233:GLN:HA	1:G:236:PHE:CD1	2.48	0.49
1:H:16:VAL:HA	1:H:40:VAL:O	2.13	0.49
1:I:95:PHE:HE2	1:J:181:VAL:HG21	1.77	0.49
1:I:204:TYR:O	1:I:208:PHE:HB2	2.13	0.49
1:D:217:ALA:HA	1:D:220:TRP:CE3	2.47	0.49
1:E:295:LEU:HA	1:E:298:GLN:OE1	2.12	0.49
1:C:125:GLN:OE1	1:C:194:ARG:HD3	2.13	0.48
1:E:23:ILE:HG21	1:E:126:PHE:CD1	2.48	0.48
1:E:295:LEU:HA	1:E:298:GLN:CD	2.34	0.48
1:G:223:PHE:HE1	1:G:304:PHE:CE2	2.31	0.48
1:I:295:LEU:O	1:I:299:ARG:HB2	2.13	0.48
1:B:211:PRO:O	1:B:215:ILE:HG12	2.12	0.48
1:F:181:VAL:HG22	1:F:182:GLN:CA	2.43	0.48
1:I:40:VAL:HG22	1:I:103:ASN:ND2	2.28	0.48
1:A:29:LEU:HD21	1:E:159:GLU:OE2	2.13	0.48
1:C:231:ARG:NH2	1:C:293:ASP:OD1	2.46	0.48
1:E:72:TRP:HH2	1:E:140:LEU:HD12	1.78	0.48
1:I:63:ILE:CD1	1:I:90:LYS:HG3	2.43	0.48
1:J:314:VAL:O	1:J:317:ILE:HG13	2.13	0.48
1:A:176:ASP:OD1	1:A:176:ASP:N	2.46	0.48
1:C:76:LEU:HB3	1:C:130:LEU:HD21	1.93	0.48
1:H:224:TRP:CZ2	1:H:301:ARG:HB3	2.49	0.48
1:I:255:ARG:CG	1:I:255:ARG:NH1	2.75	0.48
1:B:129:GLU:OE1	1:B:190:ARG:HD3	2.12	0.48
1:F:62:GLN:NE2	1:G:68:ASN:OD1	2.42	0.48
1:F:178:LEU:HD11	1:F:181:VAL:HG23	1.95	0.48
1:G:90:LYS:HZ2	1:G:104:ALA:HB1	1.77	0.48
1:A:78:PHE:O	1:A:81:VAL:HG12	2.14	0.48
1:C:260:THR:HG23	1:C:263:ASP:OD2	2.14	0.48
1:D:39:ILE:HD11	1:D:78:PHE:CE1	2.49	0.48
1:F:123:ARG:HD2	1:F:198:VAL:HG22	1.96	0.48
1:H:127:VAL:HG22	1:H:194:ARG:HG2	1.95	0.48
1:H:182:GLN:H	1:H:183:PRO:CD	2.27	0.48
1:I:34:LYS:HG3	1:I:109:SER:HA	1.94	0.48
1:A:133:PHE:CE1	1:E:89:ASN:HB2	2.48	0.48
1:B:299:ARG:HG3	1:B:299:ARG:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:ASN:OD1	1:C:138:GLN:HB2	2.14	0.48
1:I:115:ASP:OD2	1:I:117:ARG:NE	2.47	0.48
1:I:145:ILE:HD12	1:I:191:ILE:HG21	1.96	0.48
1:I:293:ASP:OD1	1:I:293:ASP:N	2.45	0.48
1:A:284:HIS:HB3	1:A:285:HIS:CD2	2.49	0.48
1:E:40:VAL:HG22	1:E:103:ASN:ND2	2.29	0.48
1:E:212:LEU:O	1:E:216:ILE:HG12	2.14	0.48
1:G:56:LEU:HD12	1:G:57:ILE:H	1.79	0.48
1:H:78:PHE:O	1:H:81:VAL:HG12	2.14	0.48
1:J:287:GLN:HG3	1:J:292:GLU:H	1.78	0.48
1:A:18:ILE:HD13	1:A:39:ILE:HG23	1.96	0.48
1:B:221:SER:HA	1:B:301:ARG:NH2	2.28	0.48
1:B:287:GLN:HA	1:B:292:GLU:HB3	1.96	0.48
1:B:294:ASP:HB3	1:B:297:ILE:CG2	2.43	0.48
1:H:42:GLN:HG2	1:H:101:ILE:CG1	2.40	0.48
1:I:34:LYS:CD	1:I:35:VAL:H	2.27	0.48
1:A:26:VAL:HG13	1:A:114:MET:HE1	1.96	0.48
1:A:156:GLU:H	1:A:156:GLU:HG3	1.34	0.48
1:A:215:ILE:O	1:A:219:SER:N	2.46	0.48
1:D:84:SER:HA	1:D:85:PRO:HD3	1.57	0.48
1:D:264:GLN:HA	1:D:267:ILE:HD12	1.95	0.48
1:G:178:LEU:HG	1:G:179:SER:N	2.29	0.48
1:A:223:PHE:HB2	1:A:301:ARG:HD2	1.96	0.47
1:A:259:THR:HA	1:A:263:ASP:OD2	2.14	0.47
1:B:58:VAL:HB	1:B:92:LEU:HB2	1.95	0.47
1:C:144:ASP:O	1:C:145:ILE:HG13	2.14	0.47
1:G:17:SER:HB2	1:G:40:VAL:HB	1.96	0.47
1:H:215:ILE:O	1:H:219:SER:N	2.45	0.47
1:I:289:ASN:OD1	1:I:290:GLY:N	2.46	0.47
1:E:142:PHE:CD2	1:E:191:ILE:HG13	2.49	0.47
1:E:235:SER:O	1:E:239:MET:HE2	2.15	0.47
1:F:204:TYR:O	1:F:209:ILE:HG12	2.14	0.47
1:I:223:PHE:CZ	1:I:279:LEU:HD21	2.49	0.47
1:A:21:ASN:HD22	1:A:37:GLY:HA2	1.79	0.47
1:D:253:LEU:HG	1:D:254:PRO:HD2	1.95	0.47
1:E:294:ASP:HB3	1:E:297:ILE:HG22	1.96	0.47
1:F:122:ASP:OD1	1:F:122:ASP:N	2.42	0.47
1:A:226:GLU:OE2	1:B:285:HIS:NE2	2.47	0.47
1:C:40:VAL:HA	1:C:103:ASN:ND2	2.29	0.47
1:D:87:THR:HG21	1:D:90:LYS:HE3	1.96	0.47
1:E:51:PRO:HD2	1:E:54:LYS:NZ	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:287:GLN:CB	1:G:292:GLU:HB2	2.36	0.47
1:I:86:ASP:N	1:I:107:LEU:O	2.36	0.47
1:I:231:ARG:HG2	1:I:231:ARG:HH11	1.78	0.47
1:C:263:ASP:O	1:C:267:ILE:HG13	2.14	0.47
1:D:62:GLN:O	1:D:66:TRP:HD1	1.98	0.47
1:D:150:GLU:H	1:D:150:GLU:HG2	1.47	0.47
1:D:153:ASP:HA	1:D:155:GLU:OE2	2.15	0.47
1:G:46:LYS:HD3	1:G:46:LYS:H	1.78	0.47
1:E:118:LEU:CD1	1:E:122:ASP:HA	2.45	0.47
1:E:174:ARG:HA	1:E:186:ASN:O	2.14	0.47
1:F:263:ASP:O	1:F:267:ILE:HG13	2.15	0.47
1:H:154:ASN:HA	1:H:156:GLU:HG2	1.95	0.47
1:H:291:VAL:HG12	1:H:291:VAL:O	2.15	0.47
1:B:169:HIS:CE1	1:B:194:ARG:HH11	2.33	0.47
1:C:185:GLN:N	1:C:185:GLN:OE1	2.47	0.47
1:E:64:GLU:OE1	1:E:65:ARG:N	2.48	0.47
1:F:92:LEU:HD23	1:F:92:LEU:HA	1.73	0.47
1:F:123:ARG:CZ	1:F:198:VAL:HG13	2.45	0.47
1:H:224:TRP:NE1	1:H:301:ARG:HD3	2.30	0.47
1:J:63:ILE:HD13	1:J:90:LYS:CE	2.45	0.47
1:A:224:TRP:H	1:A:301:ARG:NH1	2.12	0.47
1:B:255:ARG:HH11	1:B:255:ARG:CG	2.28	0.47
1:C:178:LEU:CG	1:C:179:SER:H	2.28	0.47
1:D:185:GLN:OE1	1:D:185:GLN:N	2.48	0.47
1:A:287:GLN:HG2	1:A:288:ALA:N	2.29	0.47
1:B:294:ASP:HB3	1:B:297:ILE:HB	1.96	0.47
1:C:29:LEU:CB	1:C:255:ARG:HD2	2.45	0.47
1:E:122:ASP:HB2	1:E:124:GLN:HE21	1.79	0.47
1:G:241:THR:HA	1:H:240:LEU:HD23	1.95	0.47
1:H:178:LEU:HD21	1:H:186:ASN:HA	1.97	0.47
1:J:286:ARG:HD2	1:J:286:ARG:C	2.34	0.47
1:B:234:THR:O	1:B:238:LEU:HD12	2.15	0.46
1:D:273:ILE:O	1:D:277:ILE:HG12	2.15	0.46
1:E:122:ASP:OD1	1:E:122:ASP:N	2.48	0.46
1:G:87:THR:HG23	1:G:90:LYS:NZ	2.30	0.46
1:J:212:LEU:O	1:J:216:ILE:HG12	2.15	0.46
1:J:295:LEU:O	1:J:295:LEU:HD23	2.15	0.46
1:A:299:ARG:C	1:A:301:ARG:H	2.18	0.46
1:B:13:ASP:CG	1:B:143:SER:HB3	2.36	0.46
1:B:169:HIS:CE1	1:B:194:ARG:NH1	2.83	0.46
1:C:23:ILE:HG21	1:C:126:PHE:CD1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:LEU:HD21	1:C:181:VAL:HG13	1.96	0.46
1:E:163:ARG:HA	1:E:163:ARG:HD3	1.60	0.46
1:I:121:PHE:HZ	1:I:205:LEU:HD21	1.79	0.46
1:I:216:ILE:O	1:I:219:SER:HB3	2.15	0.46
1:J:84:SER:HA	1:J:85:PRO:HD3	1.75	0.46
1:C:155:GLU:O	1:C:161:TRP:NE1	2.48	0.46
1:E:40:VAL:HG13	1:E:103:ASN:ND2	2.29	0.46
1:E:128:LEU:HB2	1:E:193:VAL:HB	1.98	0.46
1:F:16:VAL:HB	1:F:145:ILE:HD11	1.97	0.46
1:F:236:PHE:CD2	1:J:238:LEU:HD11	2.50	0.46
1:H:136:ASN:HA	1:H:188:PHE:CD1	2.50	0.46
1:F:288:ALA:HB3	1:F:292:GLU:OE2	2.16	0.46
1:H:41:ALA:C	1:H:42:GLN:HG3	2.35	0.46
1:J:71:LEU:HD22	1:J:73:VAL:HG22	1.97	0.46
1:A:240:LEU:HD23	1:E:241:THR:HA	1.97	0.46
1:C:251:ASN:ND2	1:D:251:ASN:ND2	2.58	0.46
1:D:89:ASN:O	1:D:104:ALA:HA	2.16	0.46
1:D:228:PHE:HA	1:D:231:ARG:CZ	2.46	0.46
1:A:38:TYR:HE1	1:A:105:ARG:CD	2.26	0.46
1:G:90:LYS:HZ2	1:G:104:ALA:CA	2.29	0.46
1:H:90:LYS:HA	1:H:103:ASN:O	2.16	0.46
1:I:255:ARG:HG2	1:I:255:ARG:NH1	2.20	0.46
1:B:61:THR:HG21	1:C:64:GLU:HG3	1.97	0.46
1:C:221:SER:HB2	1:D:281:ILE:HD11	1.98	0.46
1:F:301:ARG:HD2	1:F:303:ALA:HB2	1.97	0.46
1:H:19:PHE:CE1	1:H:148:TYR:HD2	2.34	0.46
1:H:118:LEU:CD1	1:H:122:ASP:HA	2.45	0.46
1:I:307:GLY:O	1:I:311:ILE:HG13	2.15	0.46
1:A:80:ASN:ND2	1:A:127:VAL:O	2.45	0.46
1:A:95:PHE:CZ	1:B:181:VAL:HB	2.51	0.46
1:A:208:PHE:HE2	1:A:248:TYR:CZ	2.34	0.46
1:B:284:HIS:HA	1:B:293:ASP:OD1	2.16	0.46
1:C:71:LEU:HD22	1:C:73:VAL:HG22	1.98	0.46
1:C:248:TYR:O	1:C:252:ILE:HG12	2.16	0.46
1:J:233:GLN:HA	1:J:236:PHE:HD1	1.81	0.46
1:A:223:PHE:H	1:A:301:ARG:NH1	2.13	0.46
1:C:216:ILE:O	1:C:219:SER:HB3	2.16	0.46
1:F:128:LEU:HB2	1:F:193:VAL:HB	1.98	0.46
1:G:71:LEU:HD11	1:G:94:LEU:HD21	1.98	0.46
1:I:78:PHE:O	1:I:81:VAL:HG12	2.15	0.46
1:I:90:LYS:HD2	1:I:90:LYS:C	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:224:TRP:CD1	1:I:301:ARG:HD3	2.50	0.46
1:J:315:LEU:HA	1:J:315:LEU:HD12	1.55	0.46
1:B:174:ARG:NH2	1:I:13:ASP:OD1	2.48	0.46
1:D:225:LEU:HD21	1:E:232:LEU:HD22	1.99	0.46
1:G:216:ILE:HD12	1:G:269:GLY:CA	2.46	0.46
1:A:42:GLN:CB	1:A:101:ILE:HG12	2.46	0.45
1:A:234:THR:OG1	1:B:233:GLN:NE2	2.49	0.45
1:C:204:TYR:O	1:C:209:ILE:HG12	2.16	0.45
1:I:149:THR:O	1:I:151:ASN:N	2.45	0.45
1:J:123:ARG:NH1	1:J:197:ALA:H	2.14	0.45
1:J:175:TYR:CE1	2:J:401:BR7:H4	2.51	0.45
1:J:311:ILE:HA	1:J:314:VAL:HG23	1.97	0.45
1:A:23:ILE:HG21	1:A:126:PHE:CD1	2.51	0.45
1:A:92:LEU:HD23	1:A:92:LEU:HA	1.59	0.45
1:B:146:GLN:N	1:B:146:GLN:OE1	2.49	0.45
1:I:36:ASP:OD1	1:I:37:GLY:N	2.49	0.45
1:C:176:ASP:C	1:C:177:HIS:HD2	2.19	0.45
1:D:227:SER:HB3	1:D:230:GLU:CG	2.46	0.45
1:E:182:GLN:N	1:E:183:PRO:HD2	2.21	0.45
1:H:42:GLN:CG	1:H:101:ILE:HG12	2.42	0.45
1:H:119:PHE:CD1	1:H:120:PRO:HA	2.51	0.45
1:C:225:LEU:HB2	1:C:231:ARG:HG3	1.99	0.45
1:D:44:THR:HA	1:D:99:ARG:HA	1.98	0.45
1:E:84:SER:HA	1:E:85:PRO:HD3	1.85	0.45
1:E:118:LEU:HD11	1:E:122:ASP:HA	1.98	0.45
1:H:72:TRP:HH2	1:H:140:LEU:HD12	1.82	0.45
1:H:72:TRP:CH2	1:H:140:LEU:HD12	2.52	0.45
1:H:286:ARG:HH21	1:H:294:ASP:N	2.10	0.45
1:I:253:LEU:HD21	1:I:262:ILE:HD12	1.99	0.45
1:D:180:SER:OG	1:D:180:SER:O	2.27	0.45
1:D:181:VAL:HG11	1:D:185:GLN:HB2	1.98	0.45
1:E:178:LEU:HD21	1:E:185:GLN:O	2.17	0.45
1:G:239:MET:O	1:G:243:VAL:HG23	2.17	0.45
1:J:16:VAL:HA	1:J:40:VAL:O	2.17	0.45
1:B:38:TYR:CD2	2:C:401:BR7:H20	2.51	0.45
1:B:62:GLN:HE22	1:C:68:ASN:CG	2.18	0.45
1:G:287:GLN:HG2	1:G:288:ALA:N	2.31	0.45
1:J:46:LYS:HA	1:J:47:PRO:HD3	1.80	0.45
1:B:186:ASN:OD1	1:B:186:ASN:N	2.47	0.45
1:C:212:LEU:HD23	1:C:245:TYR:CD2	2.51	0.45
1:I:62:GLN:O	1:I:66:TRP:HD1	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:PHE:N	1:A:301:ARG:NH1	2.65	0.45
1:C:169:HIS:C	1:C:169:HIS:CD2	2.91	0.45
1:G:183:PRO:HG2	1:G:185:GLN:H	1.81	0.45
1:H:278:LEU:O	1:H:282:PHE:N	2.30	0.45
1:H:286:ARG:HH12	1:H:297:ILE:CG2	2.15	0.45
1:A:33:TYR:OH	1:A:127:VAL:N	2.41	0.44
1:A:222:VAL:HG13	1:A:223:PHE:CD2	2.51	0.44
1:B:137:ASN:ND2	1:B:187:GLU:OE2	2.47	0.44
1:B:299:ARG:C	1:B:301:ARG:H	2.18	0.44
1:C:16:VAL:HA	1:C:40:VAL:O	2.17	0.44
1:C:173:ILE:HD13	1:C:190:ARG:HB3	1.99	0.44
1:D:216:ILE:O	1:D:219:SER:HB2	2.17	0.44
1:F:208:PHE:O	1:F:245:TYR:OH	2.33	0.44
1:H:56:LEU:HD12	1:H:57:ILE:N	2.32	0.44
1:I:95:PHE:CE2	1:J:181:VAL:HG23	2.52	0.44
1:I:153:ASP:OD1	1:I:154:ASN:N	2.50	0.44
1:F:90:LYS:CE	1:F:102:TYR:CZ	3.01	0.44
1:F:216:ILE:O	1:F:219:SER:HB3	2.17	0.44
1:G:181:VAL:HG22	1:G:183:PRO:HD3	1.99	0.44
1:B:122:ASP:OD1	1:B:122:ASP:N	2.49	0.44
1:G:186:ASN:OD1	1:G:186:ASN:N	2.51	0.44
1:J:182:GLN:N	1:J:183:PRO:CD	2.80	0.44
1:A:194:ARG:HG3	1:A:194:ARG:HH11	1.83	0.44
1:B:137:ASN:HA	1:B:140:LEU:O	2.18	0.44
1:B:206:TRP:CD1	1:B:206:TRP:N	2.84	0.44
1:B:315:LEU:HD23	1:B:315:LEU:HA	1.82	0.44
1:F:178:LEU:CG	1:F:181:VAL:HB	2.45	0.44
1:H:285:HIS:O	1:H:285:HIS:CG	2.70	0.44
1:H:286:ARG:O	1:H:287:GLN:NE2	2.51	0.44
1:A:248:TYR:HE1	1:B:250:SER:OG	2.01	0.44
1:B:40:VAL:HG22	1:B:103:ASN:ND2	2.33	0.44
1:B:175:TYR:CD1	2:B:401:BR7:H4	2.52	0.44
1:E:132:PRO:HD3	1:E:142:PHE:CE2	2.52	0.44
1:F:39:ILE:HD11	1:F:78:PHE:CE1	2.52	0.44
1:G:136:ASN:ND2	1:G:138:GLN:H	2.15	0.44
1:G:175:TYR:CE1	2:G:401:BR7:H4	2.53	0.44
1:H:286:ARG:O	1:H:286:ARG:CG	2.65	0.44
1:I:294:ASP:HB2	1:I:297:ILE:CG1	2.48	0.44
1:A:216:ILE:O	1:A:219:SER:HB3	2.17	0.44
1:C:283:ALA:O	1:C:293:ASP:HA	2.17	0.44
1:E:232:LEU:O	1:E:235:SER:OG	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:132:PRO:HG3	1:F:140:LEU:HD22	2.00	0.44
1:F:313:CYS:O	1:F:317:ILE:HG12	2.18	0.44
1:H:84:SER:HA	1:H:85:PRO:HD3	1.72	0.44
1:I:34:LYS:HD3	1:I:108:GLY:O	2.17	0.44
1:I:186:ASN:N	1:I:186:ASN:OD1	2.50	0.44
1:B:174:ARG:HA	1:B:186:ASN:O	2.17	0.44
1:E:240:LEU:HD22	1:E:240:LEU:HA	1.64	0.44
1:H:223:PHE:CE1	1:H:304:PHE:HZ	2.36	0.44
1:J:175:TYR:CD1	2:J:401:BR7:H3	2.52	0.44
1:F:40:VAL:HG22	1:F:103:ASN:ND2	2.33	0.44
1:I:61:THR:HG21	1:J:64:GLU:CG	2.47	0.44
1:B:127:VAL:HA	1:B:193:VAL:O	2.18	0.44
1:B:286:ARG:HA	1:B:286:ARG:HD3	1.28	0.44
1:E:42:GLN:HG3	1:E:101:ILE:HA	1.99	0.44
1:F:40:VAL:HG13	1:F:103:ASN:HD21	1.83	0.44
1:G:90:LYS:NZ	1:G:104:ALA:HB1	2.32	0.44
1:H:136:ASN:ND2	1:H:139:GLN:HG3	2.33	0.44
1:H:287:GLN:OE1	1:H:292:GLU:HG2	2.18	0.44
1:I:52:GLY:HA3	1:I:54:LYS:NZ	2.33	0.44
1:I:145:ILE:HG22	1:I:170:ILE:HD11	2.00	0.44
1:I:308:PHE:HA	1:I:311:ILE:HD12	1.99	0.44
1:E:130:LEU:HB3	1:E:191:ILE:HB	2.00	0.43
1:E:212:LEU:HD23	1:E:245:TYR:CE2	2.53	0.43
1:E:224:TRP:CD1	1:E:224:TRP:N	2.85	0.43
1:G:269:GLY:O	1:G:273:ILE:HG13	2.17	0.43
1:J:132:PRO:CG	1:J:140:LEU:HD22	2.48	0.43
1:J:153:ASP:OD1	1:J:154:ASN:N	2.42	0.43
1:C:154:ASN:HB3	1:C:157:ILE:HG12	1.98	0.43
1:C:289:ASN:CG	1:C:291:VAL:H	2.21	0.43
1:F:123:ARG:C	1:F:124:GLN:HG2	2.39	0.43
1:F:260:THR:H	1:F:263:ASP:HB2	1.83	0.43
1:G:18:ILE:HB	1:G:147:VAL:HG22	2.01	0.43
1:G:18:ILE:HD13	1:G:39:ILE:HG12	1.99	0.43
1:G:230:GLU:O	1:G:234:THR:OG1	2.18	0.43
1:B:165:LYS:O	1:B:165:LYS:HG3	2.19	0.43
1:C:103:ASN:HD22	1:C:103:ASN:HA	1.60	0.43
1:E:47:PRO:HG3	1:E:97:ASP:O	2.18	0.43
1:E:145:ILE:HD13	1:E:191:ILE:CG2	2.45	0.43
1:F:177:HIS:CE1	1:J:148:TYR:HH	2.31	0.43
1:I:118:LEU:HD11	1:I:122:ASP:HA	1.99	0.43
1:J:301:ARG:HD2	1:J:301:ARG:C	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:VAL:O	1:A:293:ASP:N	2.51	0.43
1:C:303:ALA:HA	1:C:306:LEU:HD23	2.01	0.43
1:D:165:LYS:HA	1:D:165:LYS:HD2	1.83	0.43
1:E:219:SER:HA	1:E:238:LEU:CD2	2.46	0.43
1:F:62:GLN:OE1	1:F:65:ARG:HD3	2.18	0.43
1:F:65:ARG:HD2	1:G:68:ASN:ND2	2.33	0.43
1:G:314:VAL:O	1:G:317:ILE:HG12	2.19	0.43
1:H:173:ILE:O	1:H:187:GLU:HA	2.18	0.43
1:A:142:PHE:CD2	1:A:191:ILE:HG13	2.53	0.43
1:D:220:TRP:CZ2	1:D:308:PHE:HD2	2.35	0.43
1:E:155:GLU:OE1	1:E:163:ARG:NH1	2.49	0.43
1:I:299:ARG:HG2	1:I:301:ARG:CZ	2.49	0.43
1:A:137:ASN:N	1:A:187:GLU:OE1	2.51	0.43
1:C:255:ARG:O	1:C:255:ARG:HG2	2.11	0.43
1:D:289:ASN:OD1	1:D:292:GLU:HG2	2.17	0.43
1:E:145:ILE:HD12	1:E:170:ILE:HG12	2.00	0.43
1:E:273:ILE:O	1:E:276:ALA:N	2.51	0.43
1:E:300:CYS:HA	1:E:303:ALA:HB3	2.00	0.43
1:F:181:VAL:HG22	1:F:182:GLN:N	2.34	0.43
1:G:204:TYR:O	1:G:208:PHE:HB2	2.19	0.43
1:H:91:ARG:HB3	1:H:103:ASN:HB2	2.01	0.43
1:A:166:ALA:HA	1:A:194:ARG:O	2.18	0.43
1:B:84:SER:HA	1:B:85:PRO:HD3	1.79	0.43
1:C:145:ILE:HD12	1:C:191:ILE:HG12	2.00	0.43
1:D:28:THR:HG21	1:D:254:PRO:HB2	2.00	0.43
1:F:44:THR:HA	1:F:99:ARG:HA	2.00	0.43
1:F:165:LYS:HD2	1:F:165:LYS:HA	1.57	0.43
1:G:136:ASN:CG	1:G:185:GLN:HG3	2.39	0.43
1:H:286:ARG:NH1	1:H:297:ILE:HD13	2.34	0.43
1:I:34:LYS:HZ2	1:I:110:PHE:HE1	1.66	0.43
1:J:204:TYR:O	1:J:209:ILE:HG12	2.19	0.43
1:J:296:LEU:HD12	1:J:296:LEU:H	1.83	0.43
1:A:121:PHE:HZ	1:A:205:LEU:HD21	1.82	0.43
1:B:165:LYS:HA	1:B:165:LYS:HD2	1.89	0.43
1:G:117:ARG:HG2	1:G:258:TYR:CD1	2.53	0.43
1:H:89:ASN:HB2	1:I:133:PHE:CE1	2.54	0.43
1:H:125:GLN:HE22	1:H:194:ARG:HD3	1.84	0.43
1:J:13:ASP:HB3	1:J:143:SER:HB3	2.01	0.43
1:J:40:VAL:HG22	1:J:103:ASN:ND2	2.33	0.43
1:J:295:LEU:HA	1:J:298:GLN:CG	2.49	0.43
1:C:175:TYR:O	1:C:186:ASN:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:ARG:HA	1:D:286:ARG:HD3	1.59	0.43
1:F:42:GLN:OE1	1:G:179:SER:OG	2.36	0.43
1:H:300:CYS:SG	1:H:304:PHE:HE2	2.42	0.43
1:I:302:LEU:HD12	1:I:303:ALA:N	2.33	0.43
1:B:220:TRP:NE1	1:B:272:SER:OG	2.42	0.43
1:D:227:SER:HB3	1:D:230:GLU:HG3	2.01	0.43
1:E:56:LEU:O	1:E:93:MET:HA	2.19	0.43
1:F:301:ARG:HH11	1:F:303:ALA:HB2	1.84	0.43
1:I:40:VAL:HG13	1:I:103:ASN:ND2	2.34	0.43
1:C:174:ARG:HB3	1:C:187:GLU:HG2	1.99	0.42
1:D:286:ARG:NH1	1:D:287:GLN:NE2	2.67	0.42
1:G:90:LYS:CE	1:G:104:ALA:HB1	2.48	0.42
1:A:129:GLU:OE2	1:A:190:ARG:NH1	2.52	0.42
1:B:26:VAL:HG21	1:B:160:TRP:HZ2	1.83	0.42
1:B:118:LEU:HD12	1:B:122:ASP:HA	2.00	0.42
1:B:227:SER:O	1:B:231:ARG:NH1	2.52	0.42
1:D:29:LEU:HD23	1:D:29:LEU:HA	1.78	0.42
1:E:262:ILE:O	1:E:266:ILE:HG12	2.19	0.42
1:F:174:ARG:HH12	1:F:186:ASN:HD22	1.65	0.42
1:G:78:PHE:O	1:G:81:VAL:HG12	2.20	0.42
1:H:165:LYS:HG3	1:H:165:LYS:O	2.19	0.42
1:H:206:TRP:N	1:H:206:TRP:CD1	2.87	0.42
1:J:65:ARG:HA	1:J:68:ASN:OD1	2.19	0.42
1:A:76:LEU:HB3	1:A:130:LEU:HD11	2.00	0.42
1:A:204:TYR:O	1:A:208:PHE:HB2	2.19	0.42
1:B:92:LEU:HD23	1:B:92:LEU:HA	1.85	0.42
1:C:155:GLU:HB3	1:C:161:TRP:CG	2.54	0.42
1:D:95:PHE:HB2	1:D:99:ARG:O	2.18	0.42
1:F:123:ARG:CD	1:F:198:VAL:HG22	2.48	0.42
1:G:29:LEU:HD23	1:G:29:LEU:HA	1.79	0.42
1:G:84:SER:HA	1:G:85:PRO:HD3	1.79	0.42
1:H:260:THR:H	1:H:263:ASP:HB2	1.84	0.42
1:C:115:ASP:OD2	1:C:117:ARG:NE	2.50	0.42
1:E:118:LEU:HA	1:E:261:VAL:HG23	2.00	0.42
1:G:227:SER:HB3	1:G:230:GLU:CD	2.39	0.42
1:H:119:PHE:CG	1:H:120:PRO:HA	2.54	0.42
1:I:225:LEU:HD21	1:J:232:LEU:HD22	2.02	0.42
1:J:21:ASN:ND2	1:J:38:TYR:HE1	2.17	0.42
1:J:260:THR:H	1:J:263:ASP:HB2	1.84	0.42
1:A:137:ASN:OD1	1:A:138:GLN:HG2	2.18	0.42
1:C:16:VAL:HB	1:C:145:ILE:CG1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:TRP:CD1	1:D:301:ARG:HD3	2.55	0.42
1:E:136:ASN:HA	1:E:188:PHE:CD2	2.54	0.42
1:E:294:ASP:HB3	1:E:297:ILE:CG2	2.49	0.42
1:E:295:LEU:HA	1:E:298:GLN:CG	2.48	0.42
1:F:240:LEU:HD21	1:J:240:LEU:HD13	2.01	0.42
1:H:91:ARG:NH2	1:H:103:ASN:OD1	2.52	0.42
1:H:182:GLN:H	1:H:183:PRO:HD2	1.84	0.42
1:H:279:LEU:HD23	1:H:279:LEU:HA	1.90	0.42
1:H:288:ALA:C	1:H:289:ASN:HD22	2.22	0.42
1:E:283:ALA:O	1:E:293:ASP:HA	2.20	0.42
1:J:282:PHE:HD2	1:J:297:ILE:HD13	1.83	0.42
1:A:84:SER:HA	1:A:85:PRO:HD3	1.86	0.42
1:F:248:TYR:HE1	1:G:250:SER:HG	1.63	0.42
1:F:311:ILE:HA	1:F:314:VAL:HB	2.01	0.42
1:G:136:ASN:ND2	1:G:185:GLN:HG3	2.35	0.42
1:G:268:ALA:HB1	1:G:308:PHE:HE1	1.84	0.42
1:H:123:ARG:CD	1:H:198:VAL:HG22	2.50	0.42
1:J:287:GLN:NE2	1:J:290:GLY:N	2.68	0.42
1:B:291:VAL:O	1:B:291:VAL:HG22	2.20	0.42
1:C:178:LEU:HG	1:C:179:SER:H	1.84	0.42
1:F:24:TYR:CE2	1:F:34:LYS:HD2	2.55	0.42
1:F:248:TYR:CE1	1:G:246:ALA:HB1	2.54	0.42
1:J:233:GLN:HA	1:J:236:PHE:CD1	2.54	0.42
1:A:157:ILE:HD11	1:B:115:ASP:CA	2.47	0.42
1:A:262:ILE:O	1:A:266:ILE:HG12	2.20	0.42
1:C:227:SER:HB3	1:C:230:GLU:HG3	2.01	0.42
1:D:155:GLU:H	1:D:155:GLU:CD	2.23	0.42
1:I:118:LEU:CD1	1:I:122:ASP:HA	2.49	0.42
1:I:208:PHE:O	1:I:245:TYR:OH	2.38	0.42
1:I:286:ARG:HD3	1:I:286:ARG:HA	1.80	0.42
1:A:205:LEU:HD23	1:A:205:LEU:HA	1.82	0.42
1:E:117:ARG:O	1:E:260:THR:HA	2.20	0.42
1:F:273:ILE:O	1:F:277:ILE:HG12	2.20	0.42
1:G:13:ASP:OD1	1:G:141:ARG:NH1	2.48	0.42
1:I:95:PHE:CE2	1:J:181:VAL:CG2	3.02	0.42
1:J:82:VAL:HB	1:J:109:SER:CB	2.50	0.42
1:A:40:VAL:HG22	1:A:103:ASN:HD22	1.85	0.41
1:A:182:GLN:N	1:A:183:PRO:CD	2.83	0.41
1:B:145:ILE:HD12	1:B:191:ILE:HG21	2.02	0.41
1:C:72:TRP:CZ2	1:C:74:PRO:HB3	2.55	0.41
1:D:223:PHE:HB3	1:D:301:ARG:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:293:ASP:O	1:E:295:LEU:N	2.53	0.41
1:F:227:SER:HB3	1:F:230:GLU:CG	2.50	0.41
1:F:281:ILE:HD13	1:J:224:TRP:CZ3	2.55	0.41
1:I:283:ALA:HA	1:I:297:ILE:HD11	2.01	0.41
1:A:40:VAL:HG22	1:A:103:ASN:ND2	2.34	0.41
1:B:182:GLN:N	1:B:183:PRO:CD	2.83	0.41
1:B:221:SER:HA	1:B:301:ARG:CZ	2.50	0.41
1:B:314:VAL:O	1:B:316:VAL:N	2.51	0.41
1:C:166:ALA:HA	1:C:194:ARG:O	2.20	0.41
1:D:137:ASN:OD1	1:D:138:GLN:N	2.53	0.41
1:E:302:LEU:O	1:E:306:LEU:HG	2.19	0.41
1:F:18:ILE:HB	1:F:147:VAL:HG22	2.01	0.41
1:G:148:TYR:OH	1:H:177:HIS:CE1	2.74	0.41
1:G:306:LEU:O	1:G:310:ALA:N	2.50	0.41
1:H:95:PHE:HE1	1:H:101:ILE:HD12	1.85	0.41
1:I:223:PHE:HE1	1:I:304:PHE:CE2	2.20	0.41
1:J:56:LEU:HD23	1:J:94:LEU:HD12	2.03	0.41
1:A:273:ILE:O	1:A:277:ILE:HG12	2.21	0.41
1:B:46:LYS:HA	1:B:47:PRO:HD3	1.95	0.41
1:B:184:ASN:O	1:B:186:ASN:N	2.54	0.41
1:C:273:ILE:O	1:C:277:ILE:HG12	2.20	0.41
1:F:56:LEU:HD12	1:F:57:ILE:N	2.35	0.41
1:F:232:LEU:O	1:F:235:SER:OG	2.38	0.41
1:H:19:PHE:N	1:H:19:PHE:CD1	2.88	0.41
1:H:217:ALA:HA	1:H:220:TRP:CE3	2.55	0.41
1:I:19:PHE:O	1:I:37:GLY:HA3	2.20	0.41
1:J:76:LEU:HB3	1:J:130:LEU:HD11	2.02	0.41
1:A:145:ILE:HG23	1:A:168:THR:HG21	2.03	0.41
1:C:303:ALA:O	1:C:306:LEU:HG	2.20	0.41
1:D:91:ARG:NH2	1:D:103:ASN:OD1	2.53	0.41
1:F:123:ARG:NH1	1:F:198:VAL:HG13	2.35	0.41
1:H:132:PRO:HD3	1:H:142:PHE:CE2	2.56	0.41
1:I:71:LEU:HD12	1:I:72:TRP:N	2.36	0.41
1:J:145:ILE:HG23	1:J:168:THR:CG2	2.50	0.41
1:B:123:ARG:C	1:B:124:GLN:HG2	2.40	0.41
1:C:175:TYR:HE1	2:C:401:BR7:H15	1.85	0.41
1:F:285:HIS:O	1:F:285:HIS:CG	2.74	0.41
1:F:302:LEU:N	1:F:305:PRO:HD2	2.35	0.41
1:H:230:GLU:OE2	1:I:229:SER:CB	2.67	0.41
1:I:120:PRO:HG2	1:I:121:PHE:CE2	2.55	0.41
1:C:28:THR:HG22	1:C:116:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:182:GLN:N	1:E:183:PRO:CD	2.78	0.41
1:E:291:VAL:HG12	1:E:291:VAL:O	2.20	0.41
1:F:84:SER:HA	1:F:85:PRO:HD3	1.86	0.41
1:G:220:TRP:NE1	1:G:272:SER:OG	2.49	0.41
1:H:58:VAL:HB	1:H:92:LEU:HB2	2.02	0.41
1:H:286:ARG:O	1:H:286:ARG:HG3	2.20	0.41
1:I:206:TRP:CD1	1:I:210:LEU:HD12	2.54	0.41
1:I:262:ILE:O	1:I:266:ILE:HG12	2.21	0.41
1:J:79:ILE:HB	1:J:129:GLU:HB2	2.02	0.41
1:J:289:ASN:OD1	1:J:290:GLY:N	2.44	0.41
1:B:216:ILE:HD12	1:B:269:GLY:HA2	2.01	0.41
1:C:166:ALA:HB2	1:C:195:ILE:HG12	2.02	0.41
1:F:161:TRP:HE3	1:F:163:ARG:HH21	1.66	0.41
1:F:304:PHE:HB3	1:F:305:PRO:HD3	2.03	0.41
1:G:54:LYS:HD2	1:G:54:LYS:H	1.86	0.41
1:H:92:LEU:HD23	1:H:92:LEU:HA	1.85	0.41
1:I:214:LEU:HD12	1:J:270:TYR:HB3	2.02	0.41
1:A:247:SER:HB3	1:E:248:TYR:HB2	2.03	0.41
1:F:91:ARG:HB3	1:F:103:ASN:HB2	2.03	0.41
1:G:242:VAL:CG2	1:G:273:ILE:HD11	2.50	0.41
1:H:46:LYS:HA	1:H:47:PRO:HD3	1.95	0.41
1:I:121:PHE:CZ	1:I:205:LEU:HD21	2.55	0.41
1:J:90:LYS:HE3	1:J:91:ARG:N	2.36	0.41
1:A:133:PHE:CD1	1:E:89:ASN:HB2	2.55	0.41
1:C:122:ASP:OD1	1:C:122:ASP:N	2.49	0.41
1:C:163:ARG:HE	1:C:163:ARG:HB3	1.63	0.41
1:E:164:GLY:C	1:E:165:LYS:HD2	2.41	0.41
1:F:130:LEU:HD12	1:F:131:GLU:H	1.86	0.41
1:F:205:LEU:HD23	1:F:209:ILE:HG13	2.02	0.41
1:H:185:GLN:N	1:H:185:GLN:OE1	2.54	0.41
1:H:212:LEU:O	1:H:216:ILE:HG12	2.21	0.41
1:H:311:ILE:O	1:H:314:VAL:HB	2.20	0.41
1:A:225:LEU:HB2	1:A:231:ARG:HG3	2.03	0.41
1:B:289:ASN:OD1	1:B:292:GLU:N	2.54	0.41
1:C:125:GLN:HE22	1:C:194:ARG:HE	1.69	0.41
1:D:302:LEU:HA	1:D:305:PRO:HG2	2.03	0.41
1:E:296:LEU:HA	1:E:296:LEU:HD12	1.91	0.41
1:F:181:VAL:CG2	1:F:182:GLN:N	2.84	0.41
1:F:306:LEU:HA	1:F:309:LEU:HB2	2.03	0.41
1:H:147:VAL:HG21	1:H:193:VAL:HG11	2.03	0.41
1:H:208:PHE:HE2	1:H:248:TYR:CZ	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:280:ILE:O	1:H:283:ALA:HB3	2.21	0.41
1:B:310:ALA:O	1:B:314:VAL:HG23	2.21	0.40
1:C:208:PHE:HE2	1:C:248:TYR:CZ	2.40	0.40
1:G:157:ILE:HD13	1:H:115:ASP:HA	2.03	0.40
1:A:178:LEU:HB2	1:A:179:SER:O	2.21	0.40
1:A:212:LEU:HD11	1:A:265:MET:HB3	2.03	0.40
1:A:287:GLN:HG2	1:A:289:ASN:N	2.32	0.40
1:B:241:THR:HA	1:C:240:LEU:HD23	2.02	0.40
1:G:72:TRP:HH2	1:G:140:LEU:HD12	1.87	0.40
1:G:142:PHE:CD2	1:G:191:ILE:HG13	2.56	0.40
1:H:24:TYR:CE2	1:H:34:LYS:HD2	2.56	0.40
1:H:145:ILE:HD12	1:H:170:ILE:CD1	2.47	0.40
1:H:163:ARG:HG3	1:H:198:VAL:HG23	2.02	0.40
1:J:145:ILE:HG22	1:J:170:ILE:HD11	2.02	0.40
1:J:239:MET:O	1:J:243:VAL:HG23	2.21	0.40
1:A:222:VAL:O	1:A:225:LEU:HB2	2.22	0.40
1:B:181:VAL:O	1:B:185:GLN:HB2	2.21	0.40
1:C:174:ARG:HA	1:C:186:ASN:O	2.21	0.40
1:D:314:VAL:C	1:D:316:VAL:N	2.75	0.40
1:F:286:ARG:NE	1:F:294:ASP:OD2	2.55	0.40
1:F:299:ARG:C	1:F:301:ARG:N	2.74	0.40
1:I:84:SER:HA	1:I:85:PRO:HD3	1.71	0.40
1:J:40:VAL:HG13	1:J:103:ASN:HD21	1.86	0.40
1:J:116:PHE:HD2	1:J:122:ASP:OD2	2.05	0.40
1:B:118:LEU:H	1:B:118:LEU:HG	1.76	0.40
1:B:127:VAL:HG22	1:B:194:ARG:HG2	2.03	0.40
1:B:208:PHE:HE1	1:B:248:TYR:CZ	2.40	0.40
1:D:293:ASP:O	1:D:295:LEU:HD23	2.22	0.40
1:F:181:VAL:HG13	1:F:182:GLN:NE2	2.35	0.40
1:G:41:ALA:HB3	1:G:102:TYR:HB3	2.04	0.40
1:G:60:ASN:OD1	1:G:89:ASN:HB3	2.21	0.40
1:G:119:PHE:CD1	1:G:120:PRO:HA	2.56	0.40
1:H:40:VAL:HG12	1:H:42:GLN:NE2	2.37	0.40
1:I:200:ASN:HA	1:I:201:PRO:HD3	1.97	0.40
1:A:86:ASP:HB3	1:A:107:LEU:HB3	2.04	0.40
1:B:34:LYS:HE2	1:B:109:SER:OG	2.21	0.40
1:C:80:ASN:ND2	1:C:127:VAL:O	2.40	0.40
1:C:253:LEU:HG	1:C:254:PRO:HD2	2.03	0.40
1:E:43:TRP:HH2	1:E:73:VAL:HG13	1.86	0.40
1:E:144:ASP:C	1:E:145:ILE:HG13	2.42	0.40
1:E:204:TYR:HA	1:E:208:PHE:HD1	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:39:ILE:HD13	1:G:39:ILE:HG21	1.86	0.40
1:J:123:ARG:NH1	1:J:124:GLN:O	2.54	0.40
1:J:153:ASP:CG	1:J:154:ASN:N	2.74	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	305/307 (99%)	278 (91%)	23 (8%)	4 (1%)	12 48
1	B	305/307 (99%)	280 (92%)	19 (6%)	6 (2%)	7 40
1	C	305/307 (99%)	281 (92%)	20 (7%)	4 (1%)	12 48
1	D	305/307 (99%)	273 (90%)	23 (8%)	9 (3%)	4 33
1	E	305/307 (99%)	277 (91%)	26 (8%)	2 (1%)	22 60
1	F	305/307 (99%)	280 (92%)	20 (7%)	5 (2%)	9 44
1	G	305/307 (99%)	280 (92%)	18 (6%)	7 (2%)	6 38
1	H	305/307 (99%)	280 (92%)	19 (6%)	6 (2%)	7 40
1	I	305/307 (99%)	276 (90%)	25 (8%)	4 (1%)	12 48
1	J	305/307 (99%)	279 (92%)	24 (8%)	2 (1%)	22 60
All	All	3050/3070 (99%)	2784 (91%)	217 (7%)	49 (2%)	9 44

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	150	GLU
1	B	154	ASN
1	B	179	SER
1	B	185	GLN

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Mol	Chain	Res	Type
1	C	152	ALA
1	D	156	GLU
1	D	179	SER
1	D	288	ALA
1	E	179	SER
1	F	181	VAL
1	F	182	GLN
1	F	302	LEU
1	G	295	LEU
1	H	179	SER
1	H	303	ALA
1	I	179	SER
1	A	156	GLU
1	A	180	SER
1	E	182	GLN
1	F	301	ARG
1	G	183	PRO
1	H	304	PHE
1	I	184	ASN
1	J	287	GLN
1	A	166	ALA
1	C	289	ASN
1	D	60	ASN
1	H	166	ALA
1	B	166	ALA
1	C	166	ALA
1	C	182	GLN
1	D	166	ALA
1	F	183	PRO
1	G	292	GLU
1	I	109	SER
1	J	290	GLY
1	B	60	ASN
1	D	182	GLN
1	G	166	ALA
1	H	60	ASN
1	G	60	ASN
1	H	182	GLN
1	I	304	PHE
1	A	304	PHE
1	G	304	PHE
1	G	290	GLY

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Mol	Chain	Res	Type
1	D	183	PRO
1	D	304	PHE
1	D	316	VAL

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	274/274 (100%)	260 (95%)	14 (5%)	24	53
1	B	274/274 (100%)	271 (99%)	3 (1%)	73	84
1	C	274/274 (100%)	270 (98%)	4 (2%)	65	80
1	D	274/274 (100%)	264 (96%)	10 (4%)	35	61
1	E	274/274 (100%)	268 (98%)	6 (2%)	52	71
1	F	274/274 (100%)	267 (97%)	7 (3%)	46	68
1	G	274/274 (100%)	266 (97%)	8 (3%)	42	65
1	H	274/274 (100%)	267 (97%)	7 (3%)	46	68
1	I	274/274 (100%)	265 (97%)	9 (3%)	38	63
1	J	274/274 (100%)	264 (96%)	10 (4%)	35	61
All	All	2740/2740 (100%)	2662 (97%)	78 (3%)	43	66

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	SER
1	A	21	ASN
1	A	48	ARG
1	A	118	LEU
1	A	137	ASN
1	A	138	GLN
1	A	156	GLU
1	A	167	SER
1	A	178	LEU
1	A	184	ASN

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Mol	Chain	Res	Type
1	A	186	ASN
1	A	187	GLU
1	A	292	GLU
1	A	298	GLN
1	B	296	LEU
1	B	298	GLN
1	B	299	ARG
1	C	54	LYS
1	C	163	ARG
1	C	250	SER
1	C	255	ARG
1	D	29	LEU
1	D	38	TYR
1	D	150	GLU
1	D	156	GLU
1	D	158	ASP
1	D	167	SER
1	D	255	ARG
1	D	286	ARG
1	D	302	LEU
1	D	316	VAL
1	E	29	LEU
1	E	50	THR
1	E	64	GLU
1	E	65	ARG
1	E	174	ARG
1	E	179	SER
1	F	50	THR
1	F	138	GLN
1	F	145	ILE
1	F	233	GLN
1	F	292	GLU
1	F	293	ASP
1	F	302	LEU
1	G	46	LYS
1	G	89	ASN
1	G	233	GLN
1	G	286	ARG
1	G	292	GLU
1	G	295	LEU
1	G	296	LEU
1	G	297	ILE

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Mol	Chain	Res	Type
1	H	42	GLN
1	H	53	ASP
1	H	90	LYS
1	H	177	HIS
1	H	297	ILE
1	H	306	LEU
1	H	309	LEU
1	I	129	GLU
1	I	145	ILE
1	I	157	ILE
1	I	180	SER
1	I	182	GLN
1	I	194	ARG
1	I	230	GLU
1	I	239	MET
1	I	264	GLN
1	J	90	LYS
1	J	102	TYR
1	J	180	SER
1	J	233	GLN
1	J	286	ARG
1	J	291	VAL
1	J	297	ILE
1	J	299	ARG
1	J	301	ARG
1	J	306	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	285	HIS
1	B	62	GLN
1	B	103	ASN
1	B	169	HIS
1	B	184	ASN
1	B	185	GLN
1	B	233	GLN
1	C	103	ASN
1	C	151	ASN
1	C	169	HIS
1	C	177	HIS

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Mol	Chain	Res	Type
1	C	285	HIS
1	C	287	GLN
1	D	62	GLN
1	D	182	GLN
1	D	251	ASN
1	D	287	GLN
1	E	139	GLN
1	E	186	ASN
1	F	151	ASN
1	F	182	GLN
1	F	185	GLN
1	F	186	ASN
1	G	124	GLN
1	G	136	ASN
1	G	182	GLN
1	G	251	ASN
1	G	285	HIS
1	H	42	GLN
1	H	125	GLN
1	H	251	ASN
1	H	289	ASN
1	I	184	ASN
1	I	233	GLN
1	I	264	GLN
1	J	124	GLN
1	J	177	HIS
1	J	185	GLN
1	J	233	GLN
1	J	287	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

12 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	BR7	E	401	-	13,16,16	4.33	11 (84%)	24,30,30	3.98	10 (41%)
2	BR7	A	402	-	13,16,16	4.66	11 (84%)	24,30,30	3.54	11 (45%)
2	BR7	B	401	-	13,16,16	4.50	11 (84%)	24,30,30	4.06	10 (41%)
2	BR7	G	401	-	13,16,16	4.45	10 (76%)	24,30,30	3.29	13 (54%)
2	BR7	F	401	-	13,16,16	4.28	9 (69%)	24,30,30	3.45	11 (45%)
2	BR7	J	401	-	13,16,16	4.25	9 (69%)	24,30,30	3.20	11 (45%)
2	BR7	D	401	-	13,16,16	4.46	10 (76%)	24,30,30	3.84	10 (41%)
2	BR7	F	402	-	13,16,16	4.52	10 (76%)	24,30,30	3.48	12 (50%)
2	BR7	A	401	-	13,16,16	4.24	10 (76%)	24,30,30	3.28	12 (50%)
2	BR7	I	401	-	13,16,16	4.45	9 (69%)	24,30,30	3.11	8 (33%)
2	BR7	C	401	-	13,16,16	4.56	11 (84%)	24,30,30	3.76	11 (45%)
2	BR7	H	401	-	13,16,16	4.34	9 (69%)	24,30,30	3.43	11 (45%)

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	BR7	E	401	-	-	-	0/4/3/3
2	BR7	A	402	-	-	-	0/4/3/3
2	BR7	B	401	-	-	-	0/4/3/3
2	BR7	G	401	-	-	-	0/4/3/3
2	BR7	F	401	-	-	-	0/4/3/3
2	BR7	J	401	-	-	-	0/4/3/3
2	BR7	D	401	-	-	-	0/4/3/3
2	BR7	F	402	-	-	-	0/4/3/3
2	BR7	A	401	-	-	-	0/4/3/3
2	BR7	I	401	-	-	-	0/4/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BR7	C	401	-	-	-	0/4/3/3
2	BR7	H	401	-	-	-	0/4/3/3

All (120) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	402	BR7	C09-C10	-12.75	1.37	1.53
2	C	401	BR7	C09-C10	-12.59	1.38	1.53
2	F	402	BR7	C09-C10	-12.56	1.38	1.53
2	I	401	BR7	C09-C10	-12.53	1.38	1.53
2	D	401	BR7	C09-C10	-12.52	1.38	1.53
2	H	401	BR7	C09-C10	-12.46	1.38	1.53
2	G	401	BR7	C09-C10	-12.34	1.38	1.53
2	B	401	BR7	C09-C10	-12.23	1.38	1.53
2	F	401	BR7	C09-C10	-12.15	1.38	1.53
2	A	401	BR7	C09-C10	-11.85	1.38	1.53
2	J	401	BR7	C09-C10	-11.82	1.38	1.53
2	E	401	BR7	C09-C10	-11.66	1.39	1.53
2	J	401	BR7	C11-C02	-5.10	1.47	1.53
2	E	401	BR7	C11-C02	-5.06	1.47	1.53
2	B	401	BR7	C11-C02	-5.04	1.47	1.53
2	D	401	BR7	C03-C02	-4.99	1.47	1.53
2	B	401	BR7	C03-C02	-4.84	1.47	1.53
2	I	401	BR7	C11-C02	-4.81	1.47	1.53
2	G	401	BR7	C11-C02	-4.77	1.48	1.53
2	I	401	BR7	C03-C02	-4.74	1.48	1.53
2	H	401	BR7	C03-C02	-4.65	1.48	1.53
2	C	401	BR7	C03-C02	-4.59	1.48	1.53
2	G	401	BR7	C03-C02	-4.58	1.48	1.53
2	A	401	BR7	C11-C02	-4.57	1.48	1.53
2	C	401	BR7	C11-C02	-4.56	1.48	1.53
2	D	401	BR7	C11-C02	-4.55	1.48	1.53
2	F	401	BR7	C11-C02	-4.54	1.48	1.53
2	A	402	BR7	C11-C02	-4.46	1.48	1.53
2	A	401	BR7	C03-C02	-4.37	1.48	1.53
2	F	402	BR7	C11-C02	-4.35	1.48	1.53
2	E	401	BR7	C03-C02	-4.32	1.48	1.53
2	J	401	BR7	C03-C02	-4.30	1.48	1.53
2	F	402	BR7	C03-C02	-4.29	1.48	1.53
2	F	401	BR7	C03-C02	-4.28	1.48	1.53
2	H	401	BR7	C11-C02	-4.26	1.48	1.53
2	A	402	BR7	C03-C02	-4.03	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	402	BR7	C08-C02	-3.95	1.49	1.53
2	C	401	BR7	C08-C02	-3.87	1.49	1.53
2	A	402	BR7	C-C04	-3.78	1.49	1.53
2	F	402	BR7	C08-C02	-3.57	1.49	1.53
2	J	401	BR7	C08-C02	-3.49	1.49	1.53
2	F	401	BR7	C08-C02	-3.48	1.49	1.53
2	G	401	BR7	C08-C02	-3.44	1.49	1.53
2	B	401	BR7	C03-C04	-3.40	1.49	1.53
2	F	402	BR7	C-C04	-3.40	1.49	1.53
2	C	401	BR7	C03-C04	-3.37	1.49	1.53
2	A	402	BR7	C-C10	-3.31	1.49	1.53
2	A	402	BR7	C06-C04	-3.29	1.49	1.53
2	D	401	BR7	C08-C02	-3.28	1.49	1.53
2	I	401	BR7	C08-C02	-3.28	1.49	1.53
2	E	401	BR7	C-C04	-3.27	1.49	1.53
2	A	401	BR7	C08-C02	-3.26	1.49	1.53
2	H	401	BR7	C08-C02	-3.21	1.49	1.53
2	D	401	BR7	C03-C04	-3.20	1.49	1.53
2	G	401	BR7	C-C04	-3.17	1.49	1.53
2	G	401	BR7	C03-C04	-3.14	1.50	1.53
2	B	401	BR7	C-C04	-3.13	1.50	1.53
2	E	401	BR7	C08-C02	-3.11	1.50	1.53
2	C	401	BR7	C06-C04	-3.09	1.50	1.53
2	F	402	BR7	C05-C04	-3.08	1.47	1.54
2	J	401	BR7	C06-C04	-3.04	1.50	1.53
2	B	401	BR7	C08-C02	-3.00	1.50	1.53
2	A	402	BR7	C05-C04	-2.97	1.48	1.54
2	A	401	BR7	C-C04	-2.96	1.50	1.53
2	F	402	BR7	C06-C04	-2.95	1.50	1.53
2	F	402	BR7	C03-C04	-2.94	1.50	1.53
2	E	401	BR7	C03-C04	-2.91	1.50	1.53
2	F	401	BR7	C03-C04	-2.90	1.50	1.53
2	I	401	BR7	C06-C04	-2.89	1.50	1.53
2	B	401	BR7	C-C10	-2.81	1.49	1.53
2	E	401	BR7	C06-C04	-2.76	1.50	1.53
2	A	401	BR7	C06-C04	-2.75	1.50	1.53
2	F	401	BR7	C-C04	-2.74	1.50	1.53
2	E	401	BR7	C05-C04	-2.73	1.48	1.54
2	A	402	BR7	C03-C04	-2.65	1.50	1.53
2	H	401	BR7	C-C04	-2.63	1.50	1.53
2	I	401	BR7	C-C04	-2.63	1.50	1.53
2	F	402	BR7	C-C10	-2.61	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	401	BR7	C05-C04	-2.60	1.48	1.54
2	A	401	BR7	C-C10	-2.60	1.50	1.53
2	C	401	BR7	C-C10	-2.59	1.50	1.53
2	D	401	BR7	C01-C02	-2.57	1.48	1.54
2	F	402	BR7	C01-C02	-2.56	1.49	1.54
2	H	401	BR7	C03-C04	-2.54	1.50	1.53
2	D	401	BR7	C05-C04	-2.54	1.49	1.54
2	J	401	BR7	C05-C04	-2.54	1.49	1.54
2	H	401	BR7	C06-C04	-2.53	1.50	1.53
2	G	401	BR7	C01-C02	-2.52	1.49	1.54
2	C	401	BR7	C05-C04	-2.52	1.49	1.54
2	I	401	BR7	C03-C04	-2.50	1.50	1.53
2	B	401	BR7	C06-C04	-2.50	1.50	1.53
2	I	401	BR7	C01-C02	-2.49	1.49	1.54
2	B	401	BR7	C01-C02	-2.49	1.49	1.54
2	G	401	BR7	C-C10	-2.48	1.50	1.53
2	H	401	BR7	C05-C04	-2.47	1.49	1.54
2	A	402	BR7	C01-C02	-2.46	1.49	1.54
2	C	401	BR7	C-C04	-2.46	1.50	1.53
2	E	401	BR7	C-C10	-2.43	1.50	1.53
2	D	401	BR7	C-C04	-2.42	1.50	1.53
2	A	401	BR7	C05-C04	-2.41	1.49	1.54
2	J	401	BR7	C-C04	-2.39	1.50	1.53
2	G	401	BR7	C05-C04	-2.38	1.49	1.54
2	B	401	BR7	C11-C10	-2.37	1.50	1.53
2	D	401	BR7	C06-C04	-2.31	1.51	1.53
2	B	401	BR7	C05-C04	-2.31	1.49	1.54
2	E	401	BR7	C11-C10	-2.31	1.50	1.53
2	C	401	BR7	C01-C02	-2.30	1.49	1.54
2	F	401	BR7	C01-C02	-2.28	1.49	1.54
2	F	401	BR7	C05-C04	-2.24	1.49	1.54
2	C	401	BR7	C11-C10	-2.24	1.50	1.53
2	H	401	BR7	C01-C02	-2.23	1.49	1.54
2	E	401	BR7	C01-C02	-2.23	1.49	1.54
2	A	402	BR7	C11-C10	-2.20	1.50	1.53
2	A	401	BR7	C01-C02	-2.17	1.49	1.54
2	G	401	BR7	C06-C04	-2.16	1.51	1.53
2	J	401	BR7	C01-C02	-2.15	1.49	1.54
2	A	401	BR7	C03-C04	-2.07	1.51	1.53
2	D	401	BR7	C11-C10	-2.04	1.50	1.53
2	F	401	BR7	C06-C04	-2.00	1.51	1.53
2	J	401	BR7	C03-C04	-2.00	1.51	1.53

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	BR7	C-C10-C11	-14.02	102.70	110.55
2	E	401	BR7	C-C10-C11	-13.47	103.01	110.55
2	B	401	BR7	C-C10-C11	-13.33	103.09	110.55
2	C	401	BR7	C-C10-C11	-12.71	103.44	110.55
2	H	401	BR7	C-C10-C11	-11.91	103.88	110.55
2	F	401	BR7	C-C10-C11	-10.92	104.44	110.55
2	F	402	BR7	C-C10-C11	-10.50	104.67	110.55
2	I	401	BR7	C-C10-C11	-10.44	104.70	110.55
2	A	401	BR7	C-C10-C11	-10.18	104.85	110.55
2	J	401	BR7	C-C10-C11	-9.83	105.04	110.55
2	G	401	BR7	C-C10-C11	-9.21	105.39	110.55
2	A	402	BR7	C-C10-C11	-7.85	106.15	110.55
2	A	402	BR7	BR-C10-C	-7.50	101.75	108.48
2	B	401	BR7	C-C04-C03	-7.35	100.99	108.69
2	D	401	BR7	C-C10-C09	7.30	114.63	110.55
2	E	401	BR7	C-C10-C09	7.05	114.50	110.55
2	A	402	BR7	BR-C10-C09	6.88	114.65	108.48
2	A	402	BR7	C-C10-C09	6.82	114.36	110.55
2	B	401	BR7	C-C10-C09	6.66	114.28	110.55
2	F	401	BR7	C-C10-C09	6.48	114.18	110.55
2	C	401	BR7	C-C04-C03	-6.31	102.07	108.69
2	B	401	BR7	C06-C04-C03	6.27	115.25	108.69
2	E	401	BR7	C-C04-C03	-6.25	102.13	108.69
2	E	401	BR7	BR-C10-C09	5.96	113.83	108.48
2	J	401	BR7	BR-C10-C09	5.88	113.76	108.48
2	H	401	BR7	C-C10-C09	5.71	113.75	110.55
2	B	401	BR7	BR-C10-C09	5.70	113.59	108.48
2	F	402	BR7	C-C10-C09	5.69	113.73	110.55
2	C	401	BR7	C-C10-C09	5.67	113.72	110.55
2	A	401	BR7	BR-C10-C09	5.64	113.54	108.48
2	C	401	BR7	C06-C04-C03	5.63	114.59	108.69
2	G	401	BR7	C-C10-C09	5.53	113.64	110.55
2	G	401	BR7	BR-C10-C09	5.48	113.40	108.48
2	G	401	BR7	C08-C02-C03	5.22	114.16	108.69
2	J	401	BR7	C06-C04-C03	5.22	114.15	108.69
2	E	401	BR7	C06-C04-C03	5.06	113.99	108.69
2	I	401	BR7	C06-C04-C03	5.04	113.97	108.69
2	C	401	BR7	BR-C10-C09	5.01	112.97	108.48
2	F	402	BR7	C06-C04-C03	4.85	113.78	108.69
2	F	402	BR7	BR-C10-C09	4.85	112.83	108.48
2	A	401	BR7	C-C10-C09	4.83	113.25	110.55
2	D	401	BR7	C06-C04-C03	4.75	113.66	108.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	401	BR7	C06-C04-C03	4.73	113.65	108.69
2	A	402	BR7	C06-C04-C03	4.59	113.50	108.69
2	D	401	BR7	C08-C02-C03	4.53	113.44	108.69
2	A	402	BR7	C-C04-C03	-4.50	103.97	108.69
2	F	402	BR7	C08-C02-C03	4.41	113.31	108.69
2	A	401	BR7	C06-C04-C03	4.39	113.29	108.69
2	F	401	BR7	C08-C02-C03	4.35	113.25	108.69
2	F	402	BR7	BR-C10-C	-4.21	104.70	108.48
2	I	401	BR7	C-C10-C09	4.19	112.89	110.55
2	F	401	BR7	BR-C10-C09	4.18	112.23	108.48
2	J	401	BR7	C-C04-C03	-4.12	104.37	108.69
2	F	401	BR7	C11-C10-C09	-4.08	108.27	110.55
2	I	401	BR7	C-C04-C03	-4.07	104.42	108.69
2	F	401	BR7	C-C04-C03	-3.99	104.50	108.69
2	A	401	BR7	C-C04-C03	-3.97	104.52	108.69
2	C	401	BR7	C08-C02-C03	3.97	112.85	108.69
2	I	401	BR7	BR-C10-C09	3.93	112.01	108.48
2	G	401	BR7	C-C04-C03	-3.91	104.58	108.69
2	H	401	BR7	C08-C02-C03	3.83	112.70	108.69
2	F	402	BR7	C-C04-C03	-3.79	104.71	108.69
2	H	401	BR7	C-C04-C03	-3.79	104.72	108.69
2	G	401	BR7	C06-C04-C03	3.76	112.63	108.69
2	D	401	BR7	C-C04-C03	-3.70	104.81	108.69
2	I	401	BR7	C08-C02-C03	3.68	112.55	108.69
2	F	401	BR7	C06-C04-C03	3.60	112.47	108.69
2	H	401	BR7	BR-C10-C11	3.57	111.68	108.48
2	F	402	BR7	BR-C10-C11	3.55	111.66	108.48
2	J	401	BR7	C08-C02-C03	3.54	112.39	108.69
2	H	401	BR7	C-C04-C06	-3.52	104.99	108.69
2	E	401	BR7	C08-C02-C03	3.52	112.38	108.69
2	B	401	BR7	C08-C02-C03	3.49	112.35	108.69
2	E	401	BR7	C11-C10-C09	-3.45	108.62	110.55
2	A	401	BR7	BR-C10-C	-3.45	105.39	108.48
2	J	401	BR7	C11-C02-C03	-3.42	105.11	108.69
2	A	401	BR7	C08-C02-C03	3.37	112.22	108.69
2	F	401	BR7	C07-C06-C04	3.12	112.71	110.81
2	I	401	BR7	C-C04-C06	-3.11	105.42	108.69
2	F	401	BR7	C-C04-C06	-3.08	105.46	108.69
2	G	401	BR7	C-C04-C06	-3.07	105.47	108.69
2	A	402	BR7	C11-C10-C09	-3.05	108.84	110.55
2	J	401	BR7	C11-C10-C09	-3.02	108.86	110.55
2	D	401	BR7	C-C04-C06	-2.99	105.55	108.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	401	BR7	C-C04-C06	-2.95	105.59	108.69
2	A	401	BR7	C11-C10-C09	-2.90	108.92	110.55
2	F	402	BR7	C-C04-C06	-2.89	105.65	108.69
2	F	402	BR7	C11-C10-C09	-2.87	108.94	110.55
2	A	402	BR7	C08-C02-C03	2.87	111.69	108.69
2	A	401	BR7	C11-C02-C03	-2.79	105.76	108.69
2	G	401	BR7	C07-C08-C02	-2.75	109.13	110.81
2	J	401	BR7	C-C10-C09	2.74	112.08	110.55
2	I	401	BR7	C11-C02-C08	-2.73	105.83	108.69
2	G	401	BR7	C11-C02-C08	-2.71	105.84	108.69
2	G	401	BR7	C11-C10-C09	-2.70	109.04	110.55
2	A	401	BR7	C-C04-C06	-2.62	105.94	108.69
2	D	401	BR7	BR-C10-C09	2.56	110.77	108.48
2	G	401	BR7	C05-C04-C06	2.55	114.22	110.56
2	G	401	BR7	C11-C02-C03	-2.53	106.04	108.69
2	F	402	BR7	C07-C08-C02	-2.49	109.29	110.81
2	H	401	BR7	C11-C10-C09	-2.49	109.16	110.55
2	B	401	BR7	C-C04-C06	-2.48	106.09	108.69
2	D	401	BR7	C07-C08-C02	-2.46	109.31	110.81
2	D	401	BR7	C11-C10-C09	-2.46	109.17	110.55
2	G	401	BR7	C07-C06-C04	2.46	112.31	110.81
2	C	401	BR7	C07-C08-C02	-2.45	109.31	110.81
2	F	402	BR7	C11-C02-C08	-2.44	106.13	108.69
2	C	401	BR7	C-C04-C06	-2.43	106.14	108.69
2	A	402	BR7	BR-C10-C11	2.41	110.64	108.48
2	A	402	BR7	C11-C02-C08	-2.39	106.18	108.69
2	E	401	BR7	C07-C08-C02	-2.34	109.38	110.81
2	A	401	BR7	BR-C10-C11	2.28	110.52	108.48
2	E	401	BR7	C01-C02-C11	-2.27	107.30	110.56
2	H	401	BR7	BR-C10-C09	2.24	110.49	108.48
2	F	401	BR7	C11-C02-C03	-2.23	106.35	108.69
2	H	401	BR7	C11-C02-C03	-2.23	106.35	108.69
2	A	402	BR7	C07-C08-C02	-2.20	109.47	110.81
2	H	401	BR7	C11-C02-C08	-2.19	106.39	108.69
2	F	401	BR7	C11-C02-C08	-2.18	106.40	108.69
2	J	401	BR7	C11-C02-C08	-2.18	106.40	108.69
2	E	401	BR7	C11-C02-C08	-2.16	106.42	108.69
2	C	401	BR7	C05-C04-C	2.16	113.67	110.56
2	A	401	BR7	C11-C02-C08	-2.13	106.46	108.69
2	C	401	BR7	C11-C02-C03	-2.10	106.48	108.69
2	C	401	BR7	C11-C10-C09	-2.10	109.38	110.55
2	B	401	BR7	C01-C02-C11	-2.04	107.62	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	401	BR7	C01-C02-C03	2.04	113.49	110.56
2	B	401	BR7	C11-C10-C09	-2.02	109.42	110.55
2	D	401	BR7	C11-C02-C03	-2.01	106.58	108.69
2	B	401	BR7	BR-C10-C	-2.00	106.68	108.48

There are no chirality outliers.

There are no torsion outliers.

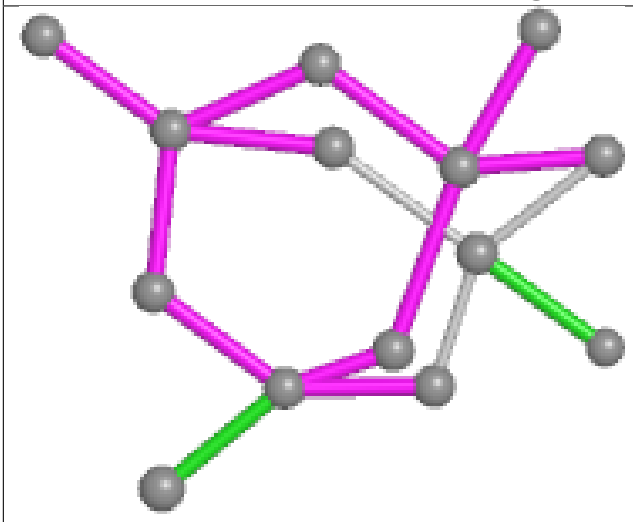
There are no ring outliers.

8 monomers are involved in 20 short contacts:

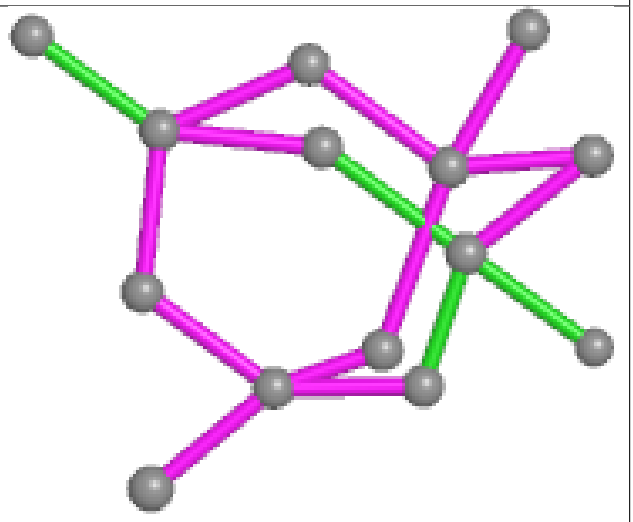
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	401	BR7	2	0
2	A	402	BR7	2	0
2	B	401	BR7	4	0
2	G	401	BR7	3	0
2	J	401	BR7	2	0
2	F	402	BR7	1	0
2	I	401	BR7	1	0
2	C	401	BR7	5	0

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.

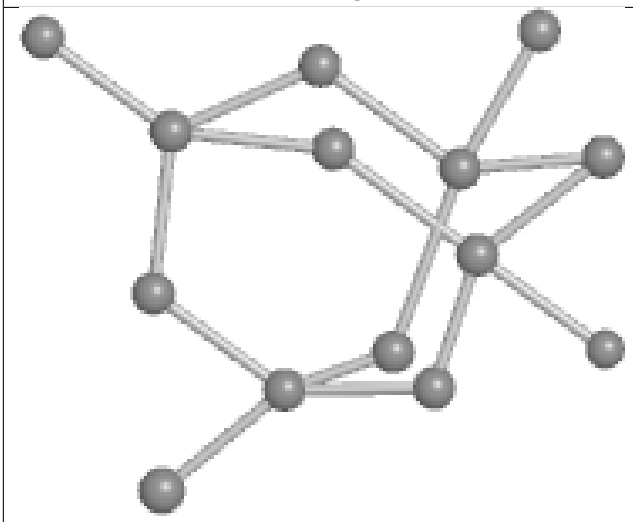
Ligand BR7 E 401



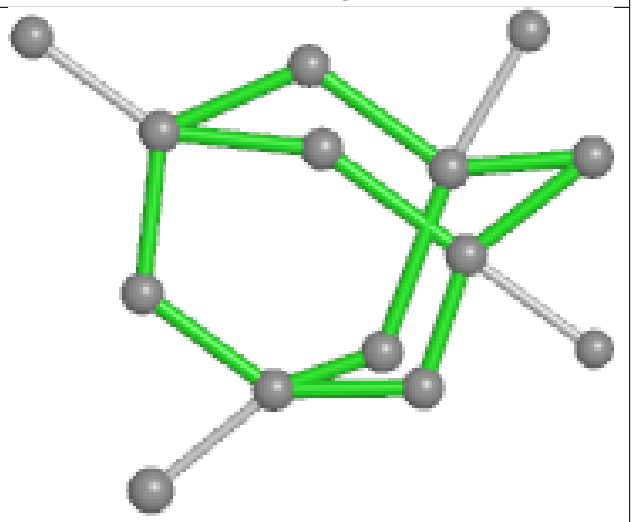
Bond lengths



Bond angles

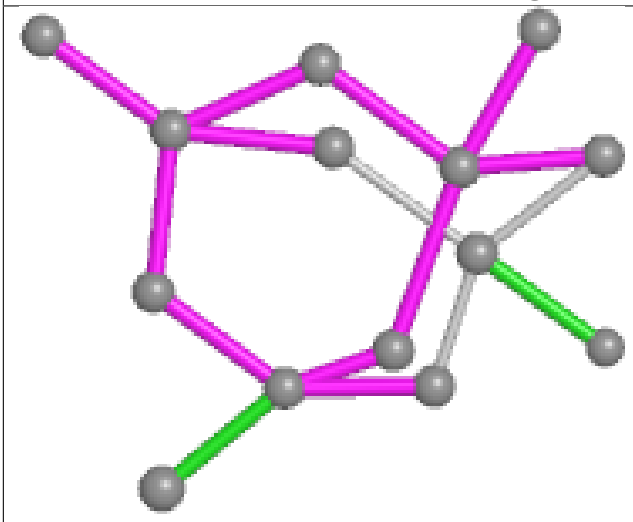


Torsions

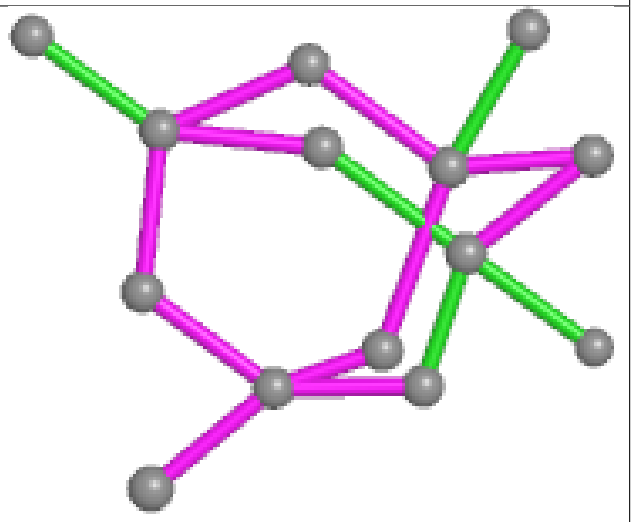


Rings

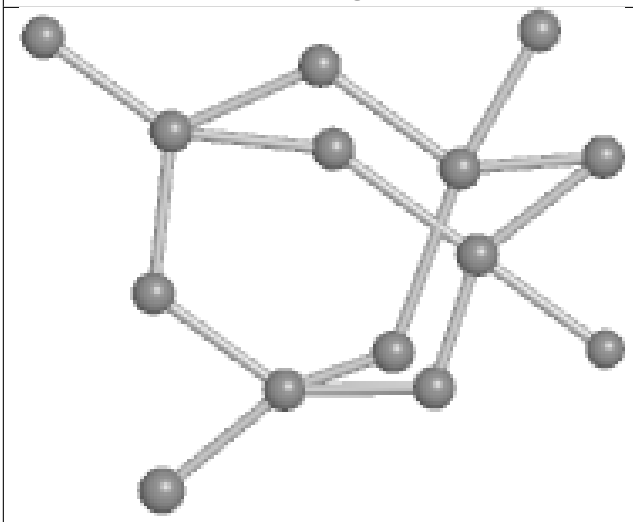
Ligand BR7 A 402



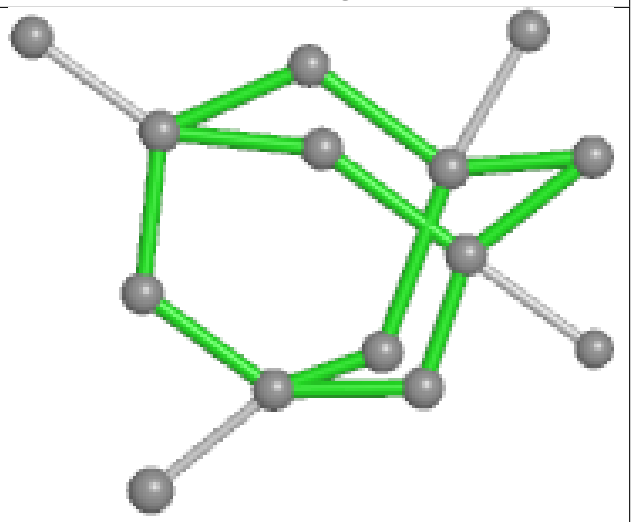
Bond lengths



Bond angles

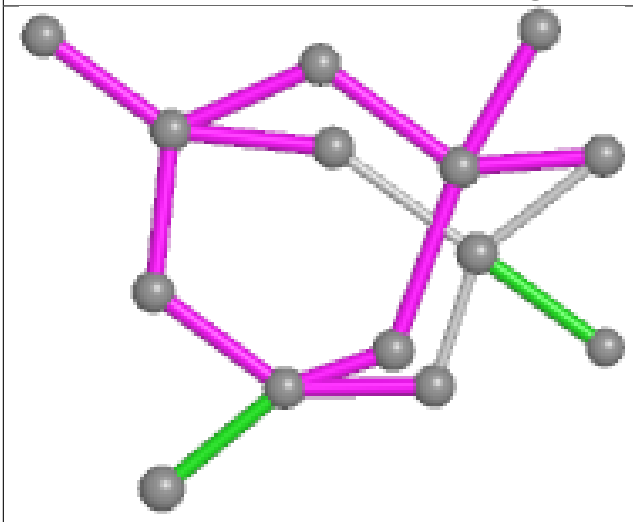


Torsions

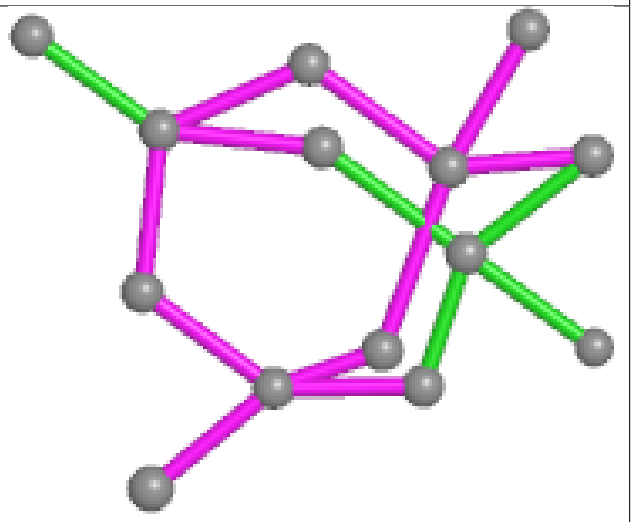


Rings

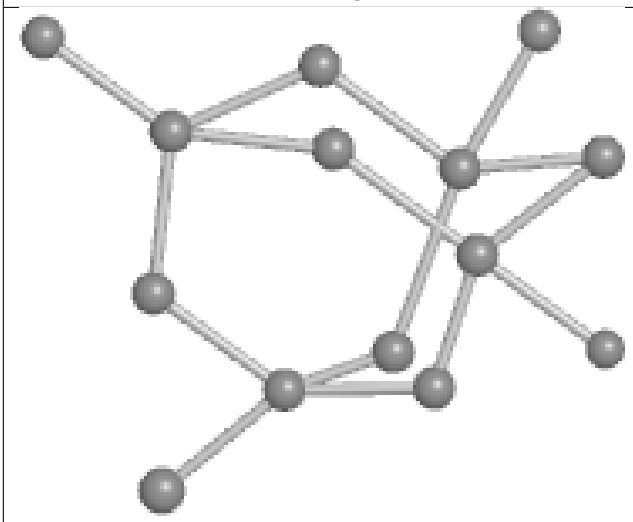
Ligand BR7 B 401



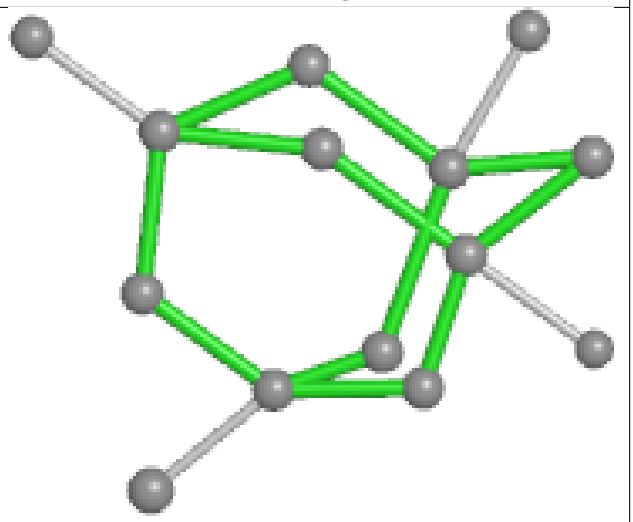
Bond lengths



Bond angles

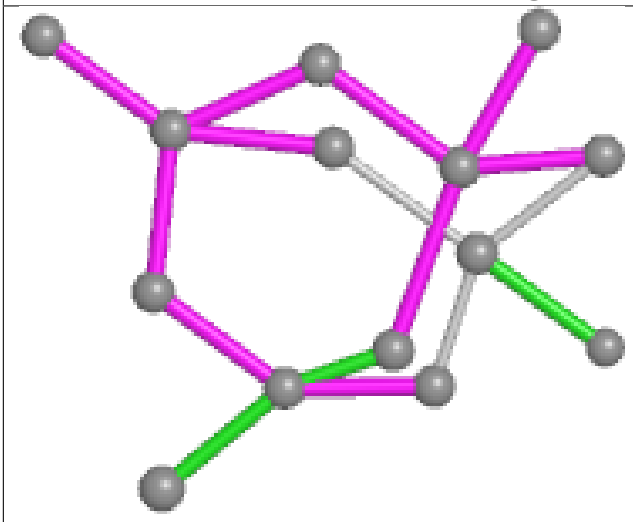


Torsions

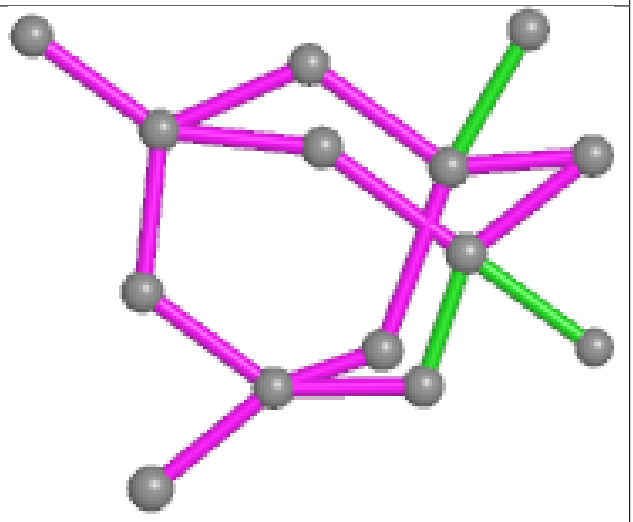


Rings

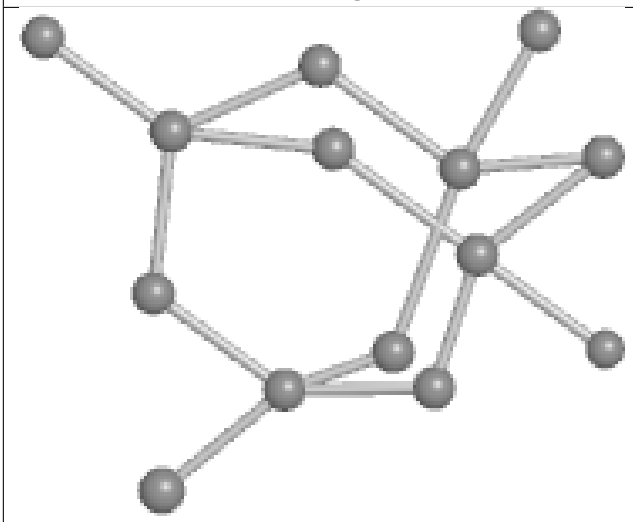
Ligand BR7 G 401



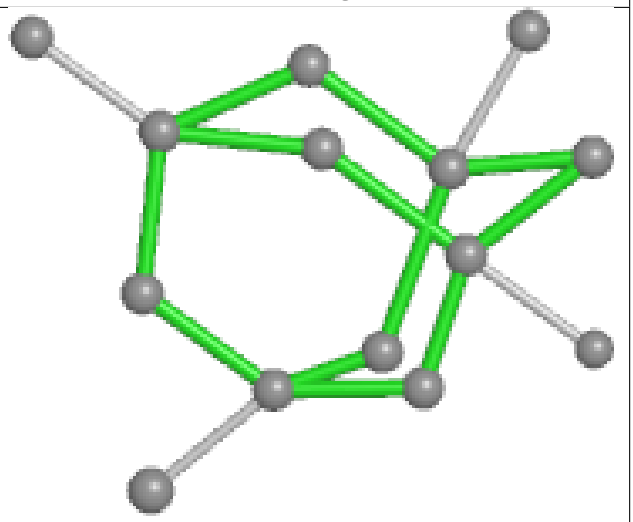
Bond lengths



Bond angles

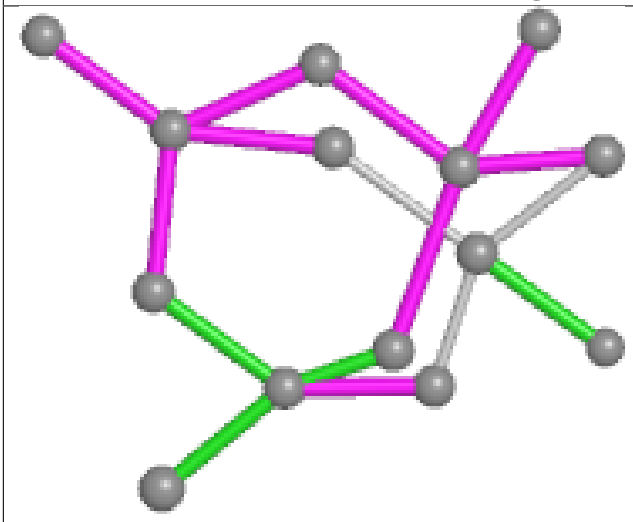


Torsions

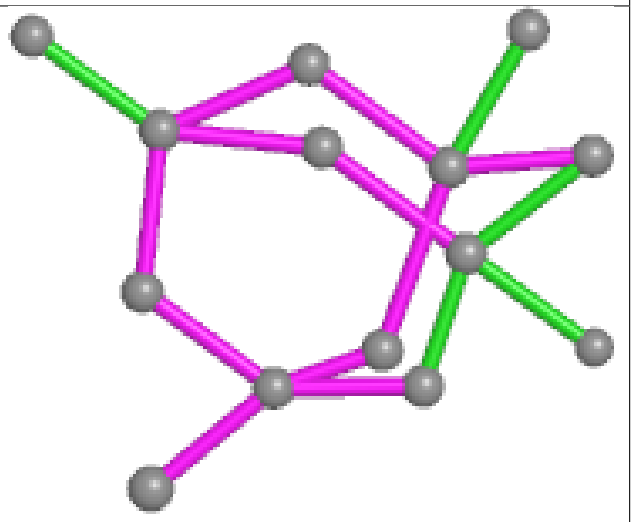


Rings

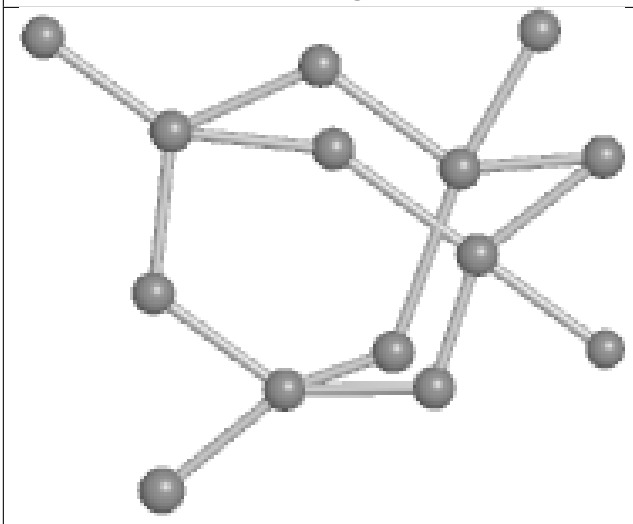
Ligand BR7 F 401



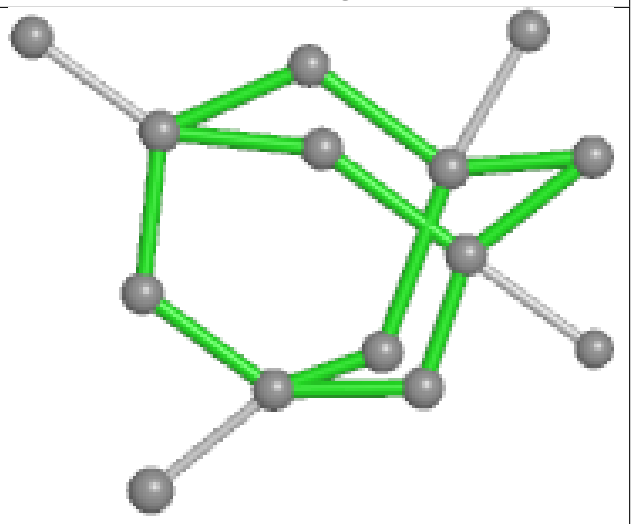
Bond lengths



Bond angles

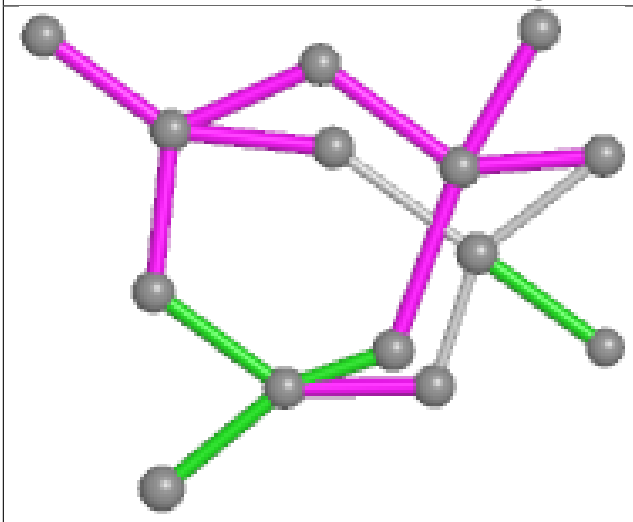


Torsions

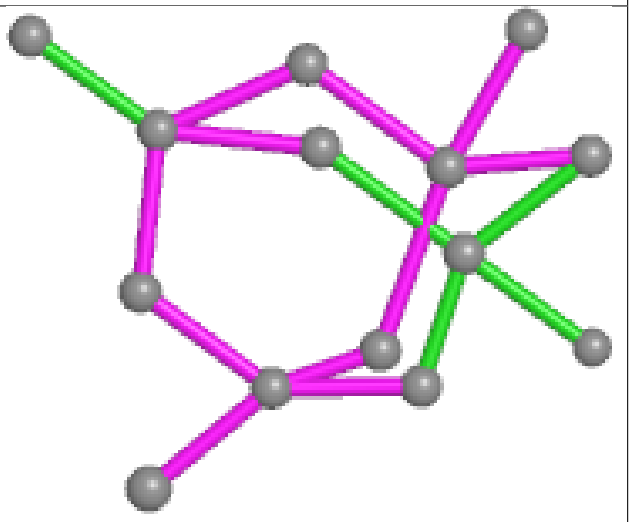


Rings

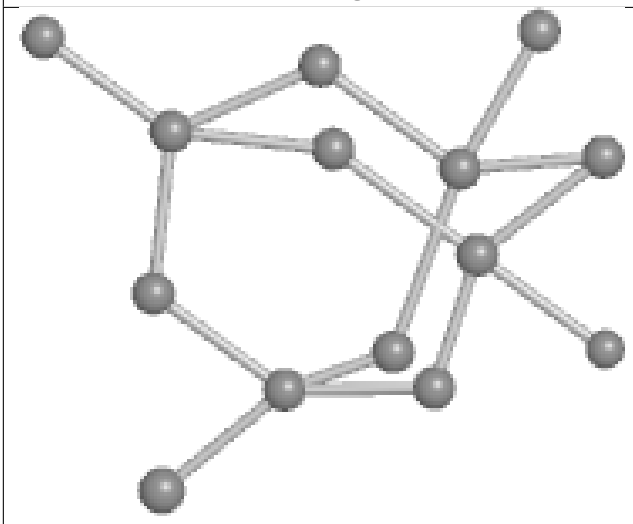
Ligand BR7 J 401



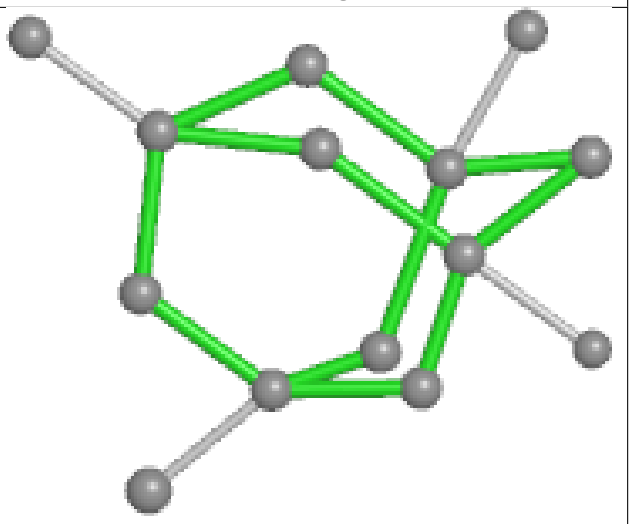
Bond lengths



Bond angles

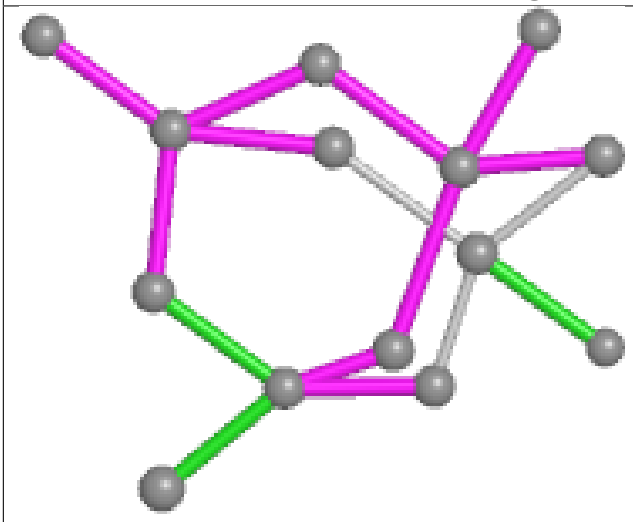


Torsions

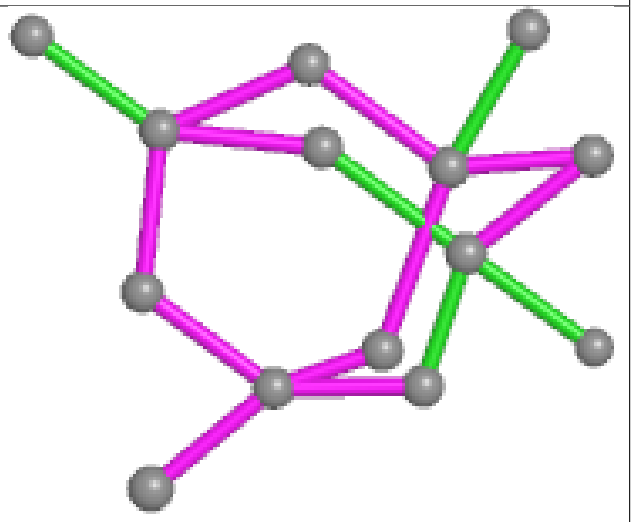


Rings

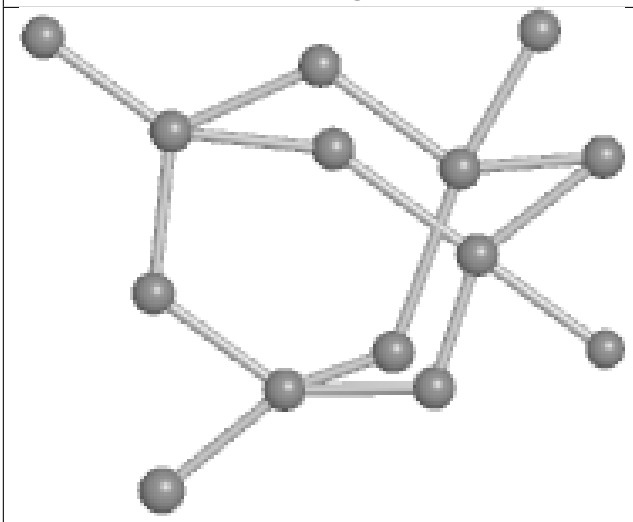
Ligand BR7 D 401



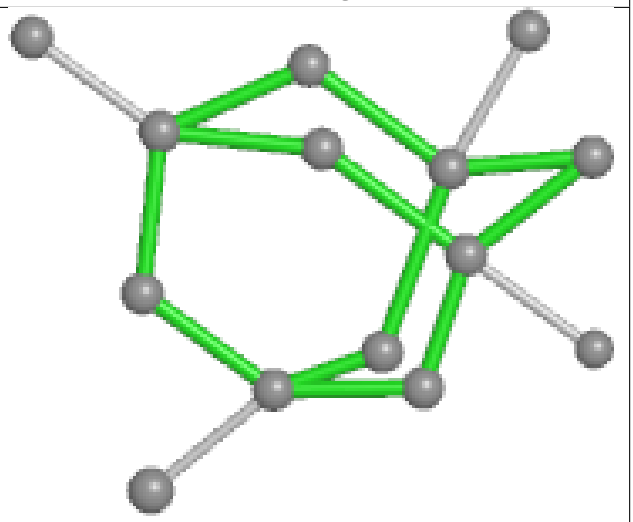
Bond lengths



Bond angles

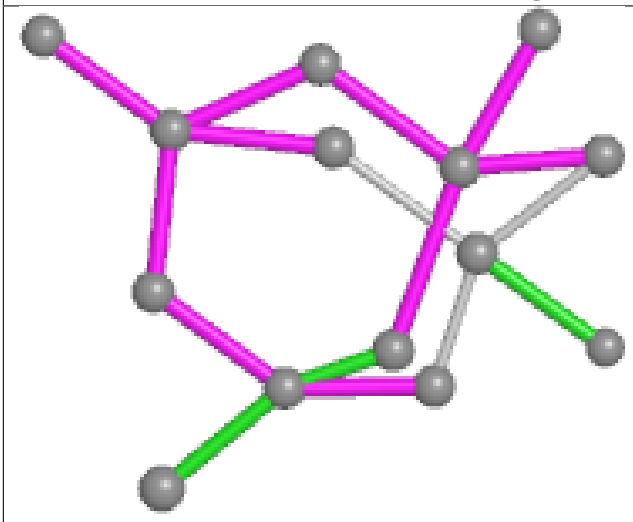


Torsions

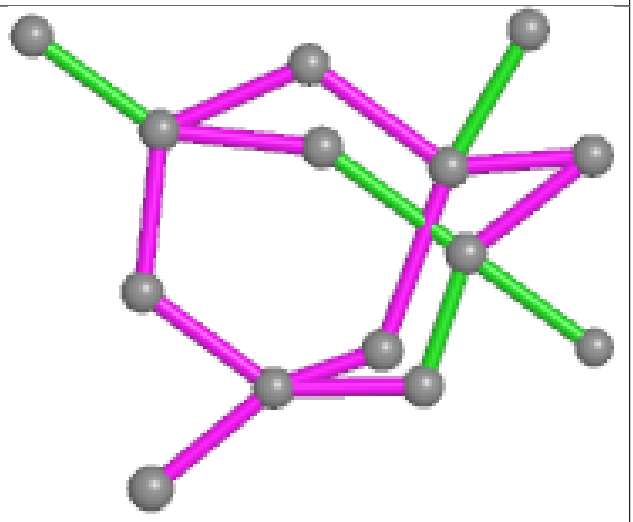


Rings

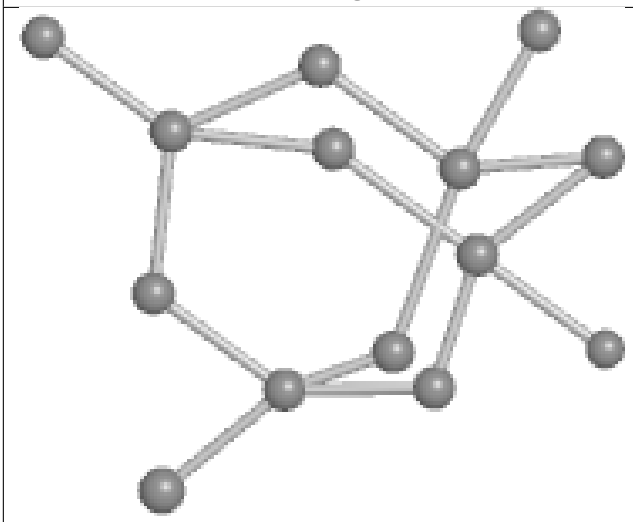
Ligand BR7 F 402



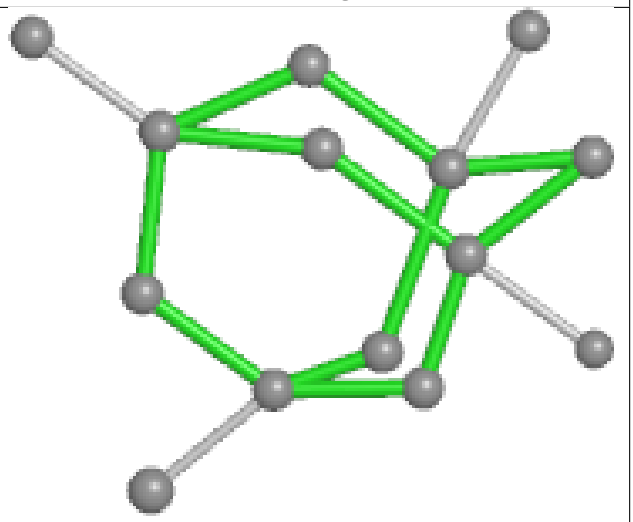
Bond lengths



Bond angles

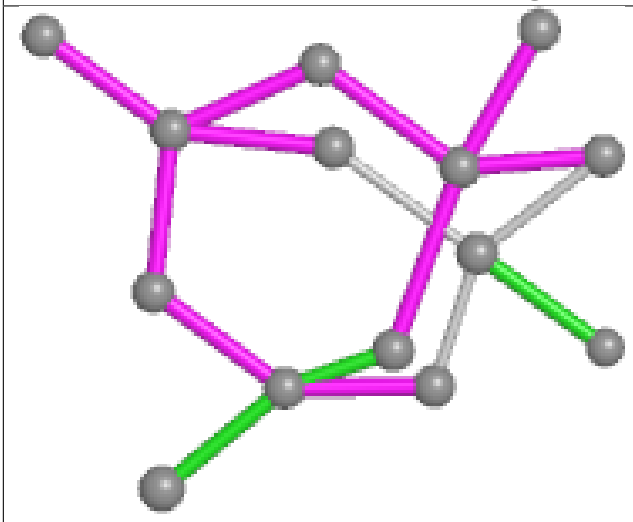


Torsions

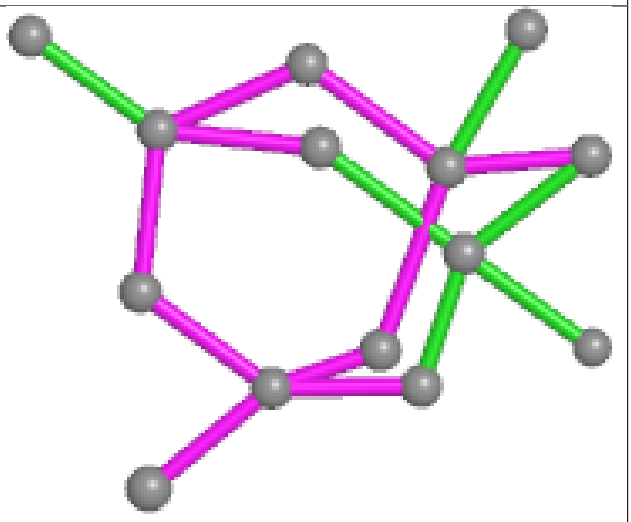


Rings

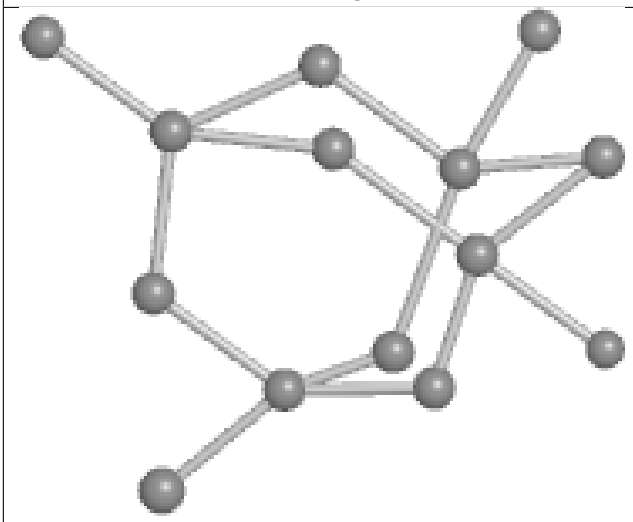
Ligand BR7 A 401



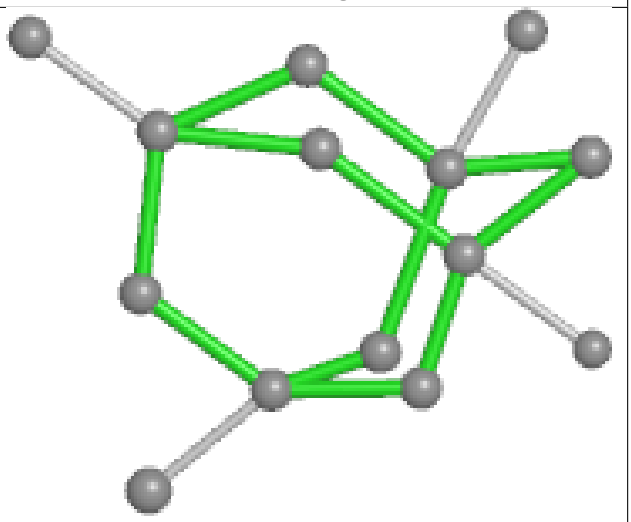
Bond lengths



Bond angles

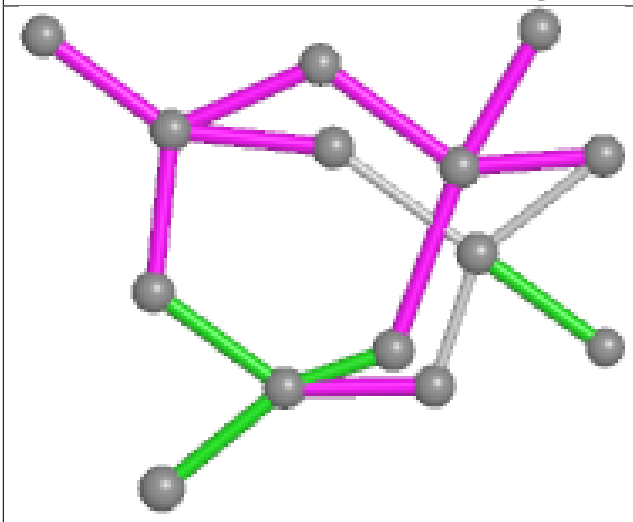


Torsions

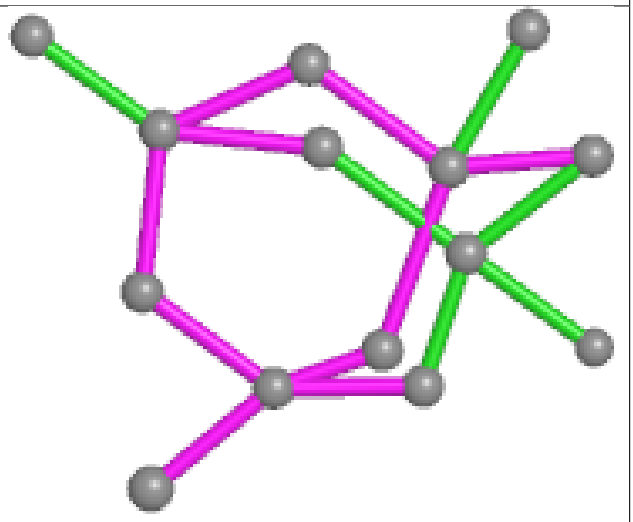


Rings

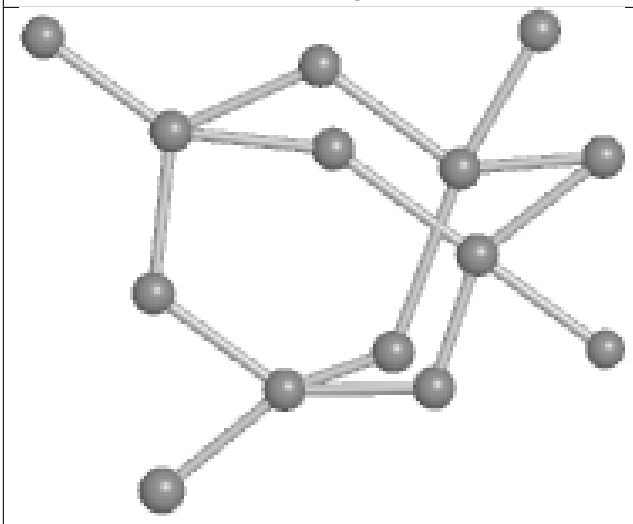
Ligand BR7 I 401



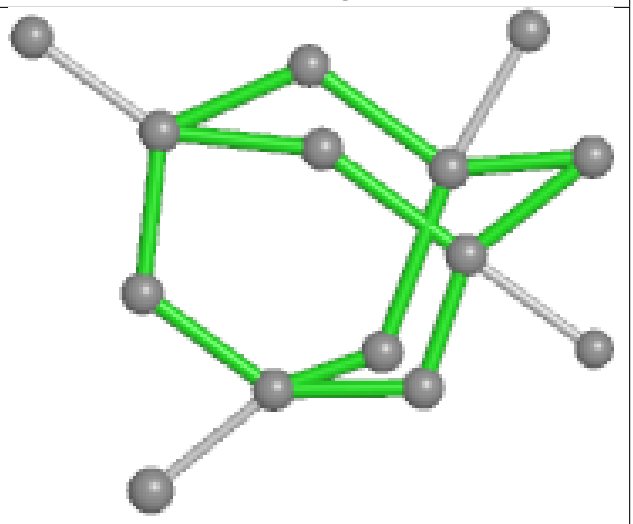
Bond lengths



Bond angles

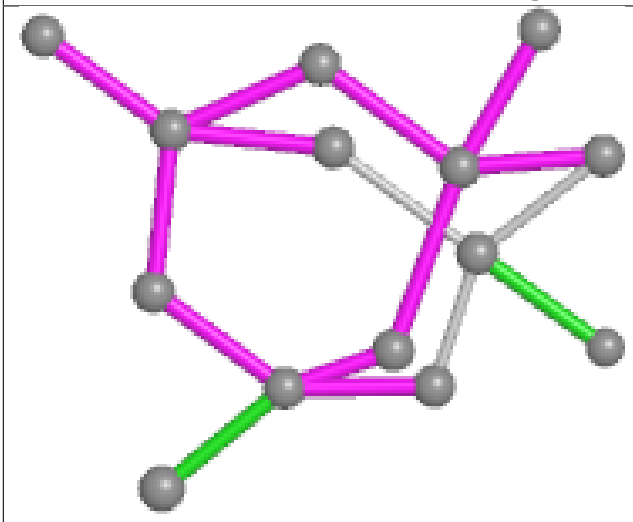


Torsions

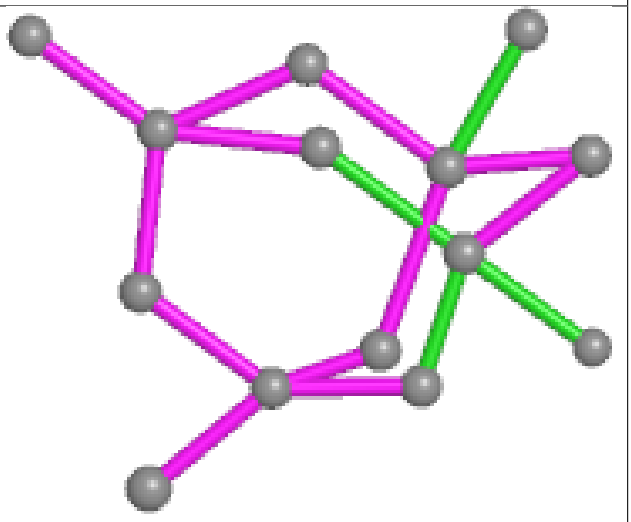


Rings

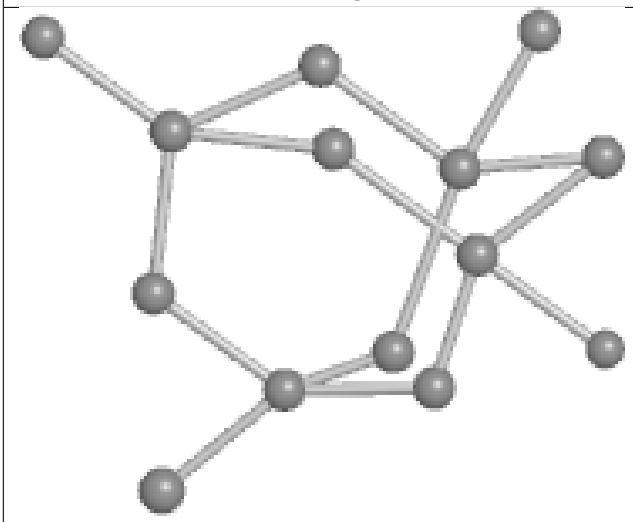
Ligand BR7 C 401



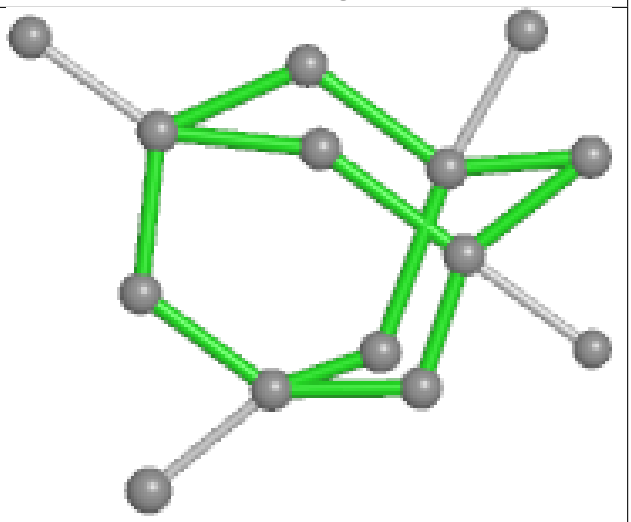
Bond lengths



Bond angles

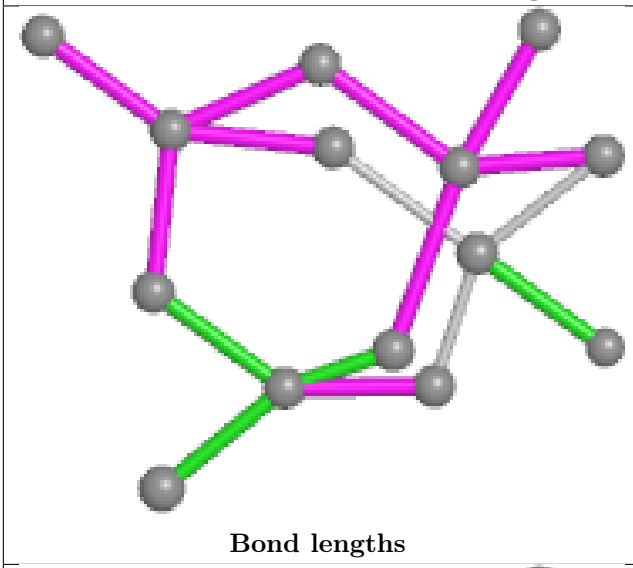


Torsions

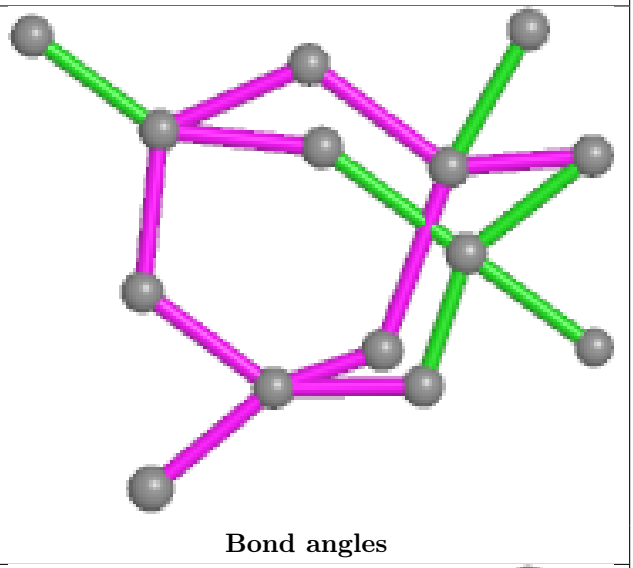


Rings

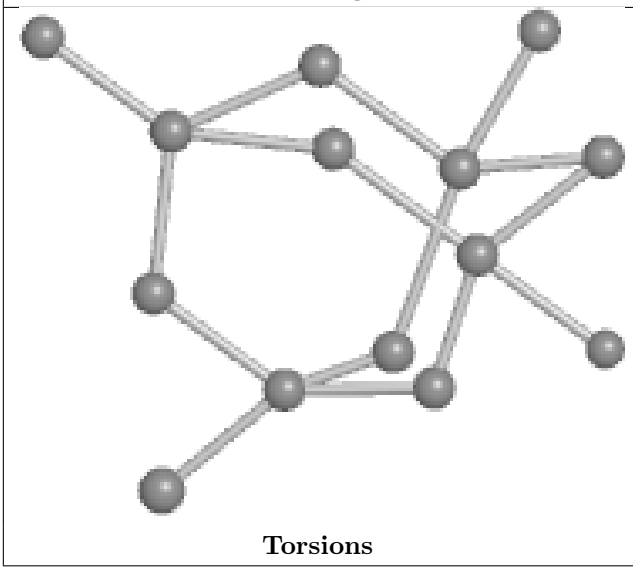
Ligand BR7 H 401



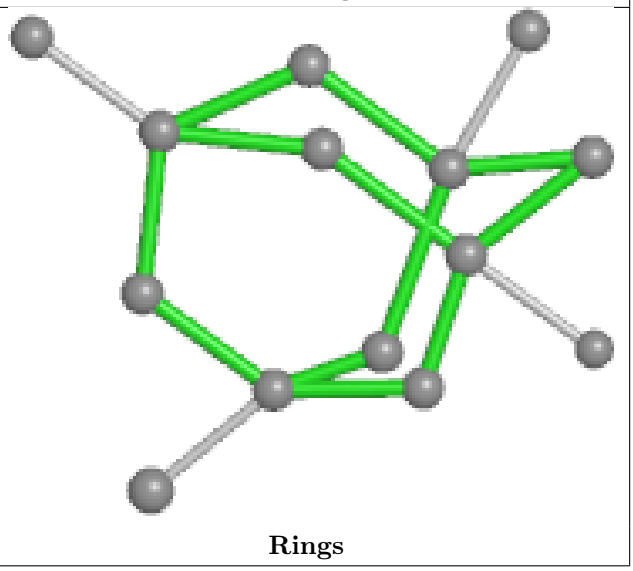
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	307/307 (100%)	-0.20	9 (2%) 51 40	89, 136, 232, 324	0
1	B	307/307 (100%)	-0.12	12 (3%) 39 30	78, 123, 237, 352	0
1	C	307/307 (100%)	-0.26	17 (5%) 25 20	71, 119, 234, 291	0
1	D	307/307 (100%)	-0.13	11 (3%) 42 33	73, 121, 228, 325	0
1	E	307/307 (100%)	-0.26	10 (3%) 46 36	83, 129, 235, 381	0
1	F	307/307 (100%)	-0.21	7 (2%) 60 50	84, 138, 250, 372	0
1	G	307/307 (100%)	-0.18	6 (1%) 65 55	78, 122, 221, 324	0
1	H	307/307 (100%)	-0.11	27 (8%) 10 7	79, 133, 250, 378	0
1	I	307/307 (100%)	-0.26	10 (3%) 46 36	76, 131, 234, 327	0
1	J	307/307 (100%)	-0.21	20 (6%) 18 13	91, 139, 272, 347	0
All	All	3070/3070 (100%)	-0.19	129 (4%) 36 29	71, 129, 243, 381	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	290	GLY	10.3
1	A	176	ASP	10.0
1	I	179	SER	8.7
1	I	180	SER	8.5
1	A	177	HIS	8.0
1	J	290	GLY	6.9
1	C	313	CYS	5.9
1	C	180	SER	5.6
1	H	180	SER	5.6
1	J	306	LEU	5.4
1	J	305	PRO	5.3
1	D	177	HIS	4.9
1	J	291	VAL	4.9

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Mol	Chain	Res	Type	RSRZ
1	J	289	ASN	4.7
1	F	287	GLN	4.6
1	E	291	VAL	4.4
1	J	286	ARG	4.4
1	E	287	GLN	4.2
1	F	288	ALA	4.2
1	E	288	ALA	4.1
1	F	317	ILE	4.0
1	E	289	ASN	4.0
1	F	176	ASP	4.0
1	A	178	LEU	3.9
1	H	306	LEU	3.9
1	F	174	ARG	3.8
1	C	314	VAL	3.8
1	H	137	ASN	3.8
1	I	291	VAL	3.8
1	F	179	SER	3.8
1	G	285	HIS	3.7
1	J	287	GLN	3.7
1	J	180	SER	3.7
1	J	304	PHE	3.7
1	C	317	ILE	3.7
1	I	289	ASN	3.7
1	G	156	GLU	3.6
1	D	179	SER	3.5
1	I	181	VAL	3.5
1	C	146	GLN	3.5
1	E	180	SER	3.4
1	C	306	LEU	3.4
1	A	175	TYR	3.4
1	F	175	TYR	3.4
1	C	187	GLU	3.3
1	A	182	GLN	3.3
1	H	123	ARG	3.3
1	B	291	VAL	3.3
1	I	288	ALA	3.3
1	J	303	ALA	3.3
1	D	180	SER	3.3
1	J	285	HIS	3.2
1	H	181	VAL	3.2
1	B	31	GLN	3.1
1	B	293	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	172	ASP	3.1
1	J	284	HIS	3.1
1	H	308	PHE	3.1
1	C	311	ILE	3.0
1	C	315	LEU	3.0
1	C	316	VAL	3.0
1	H	179	SER	2.9
1	H	303	ALA	2.9
1	B	290	GLY	2.9
1	D	202	SER	2.9
1	H	184	ASN	2.9
1	B	289	ASN	2.8
1	B	122	ASP	2.8
1	H	11	PRO	2.8
1	I	290	GLY	2.8
1	D	176	ASP	2.8
1	B	112	ASN	2.8
1	H	182	GLN	2.8
1	J	179	SER	2.7
1	I	286	ARG	2.6
1	H	317	ILE	2.6
1	B	298	GLN	2.6
1	H	140	LEU	2.6
1	C	312	GLY	2.6
1	J	302	LEU	2.6
1	B	114	MET	2.6
1	E	52	GLY	2.6
1	H	141	ARG	2.5
1	J	288	ALA	2.5
1	D	288	ALA	2.5
1	A	306	LEU	2.5
1	H	307	GLY	2.5
1	G	314	VAL	2.5
1	B	115	ASP	2.5
1	H	185	GLN	2.5
1	C	309	LEU	2.5
1	J	82	VAL	2.4
1	H	187	GLU	2.4
1	B	71	LEU	2.4
1	G	302	LEU	2.4
1	J	294	ASP	2.4
1	J	83	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	189	SER	2.4
1	C	310	ALA	2.3
1	E	292	GLU	2.3
1	G	157	ILE	2.3
1	D	19	PHE	2.3
1	G	289	ASN	2.3
1	H	183	PRO	2.3
1	C	307	GLY	2.3
1	J	293	ASP	2.2
1	H	138	GLN	2.2
1	D	293	ASP	2.2
1	H	304	PHE	2.2
1	H	172	ASP	2.2
1	C	188	PHE	2.2
1	A	316	VAL	2.2
1	E	179	SER	2.2
1	J	292	GLU	2.2
1	D	38	TYR	2.2
1	H	143	SER	2.1
1	H	315	LEU	2.1
1	H	13	ASP	2.1
1	H	170	ILE	2.1
1	E	286	ARG	2.1
1	D	289	ASN	2.1
1	I	182	GLN	2.1
1	H	311	ILE	2.1
1	I	292	GLU	2.1
1	H	144	ASP	2.1
1	C	189	SER	2.0
1	A	180	SER	2.0
1	D	181	VAL	2.0
1	B	42	GLN	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 monosaccharides in this entry.

6.4 Ligands (i)

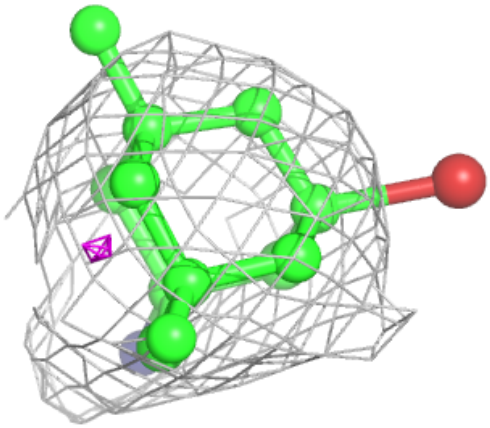
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

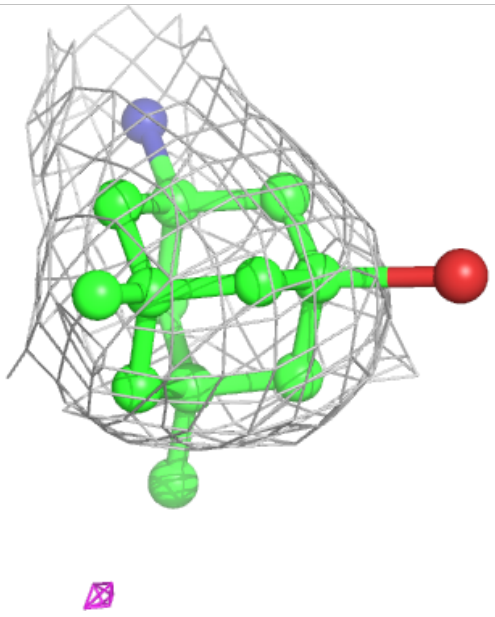
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BR7	A	401	14/14	0.94	0.43	112,142,147,354	0
2	BR7	F	401	14/14	0.94	0.42	99,129,135,272	0
2	BR7	F	402	14/14	0.94	0.24	110,131,138,389	0
2	BR7	C	401	14/14	0.95	0.46	111,127,145,217	0
2	BR7	B	401	14/14	0.96	0.17	104,108,119,265	0
2	BR7	E	401	14/14	0.96	0.61	84,110,120,309	0
2	BR7	H	401	14/14	0.96	0.41	129,141,153,250	0
2	BR7	J	401	14/14	0.96	0.48	98,112,125,194	0
2	BR7	I	401	14/14	0.97	0.15	86,100,119,321	0
2	BR7	A	402	14/14	0.97	0.27	98,109,129,224	0
2	BR7	G	401	14/14	0.98	0.41	77,115,131,268	0
2	BR7	D	401	14/14	0.98	0.38	98,111,119,277	0

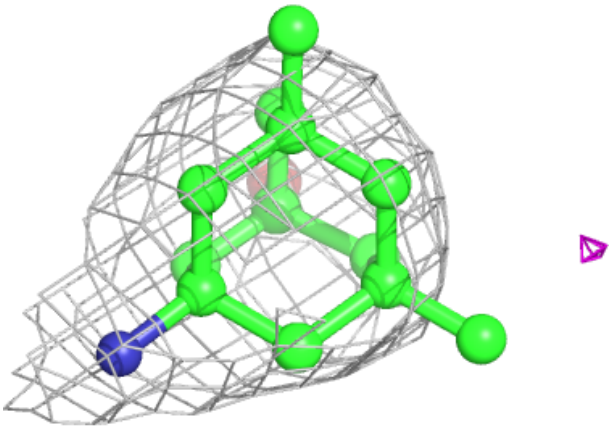
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BR7 A 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

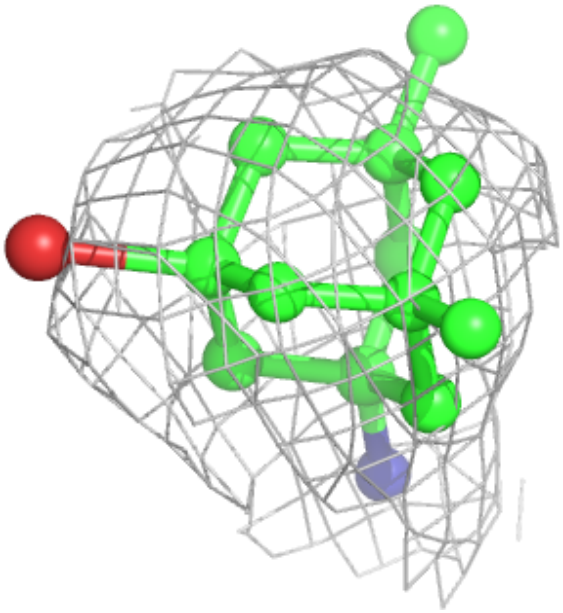


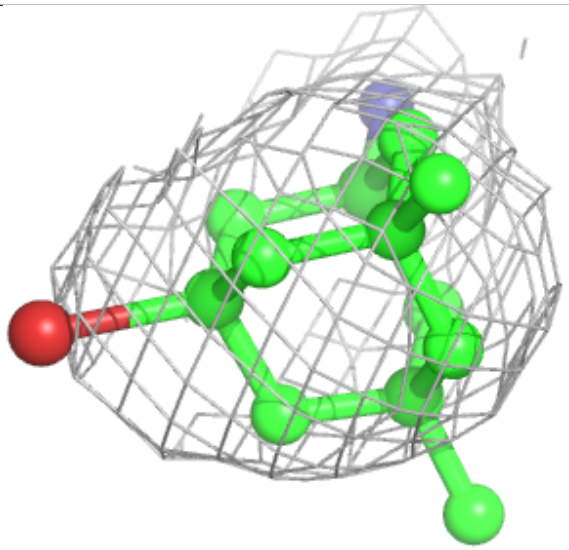


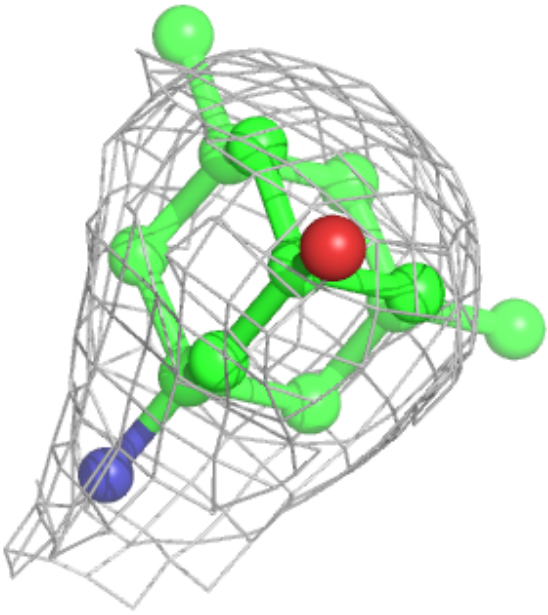


Electron density around BR7 F 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

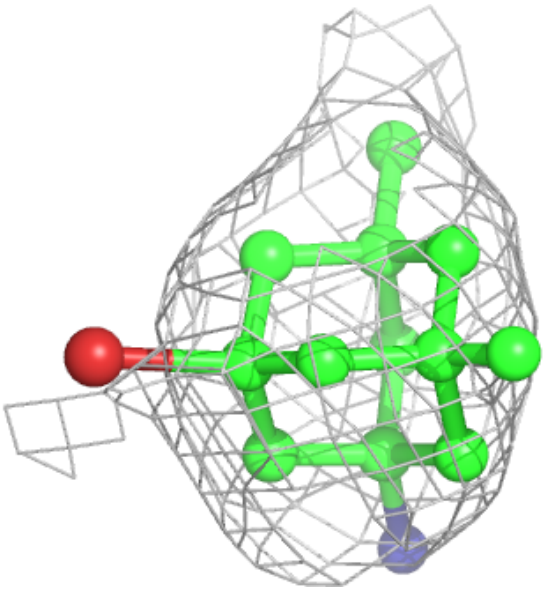


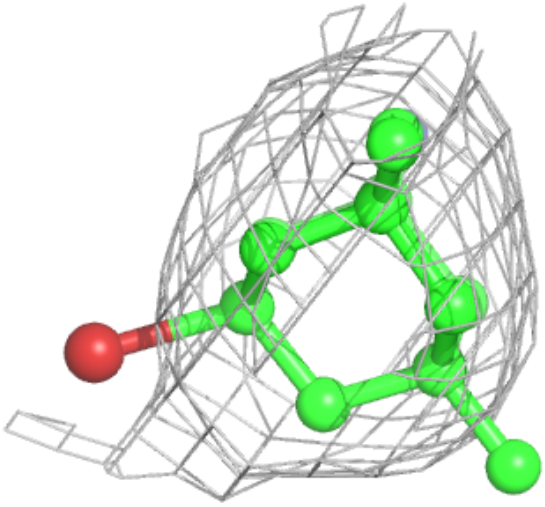


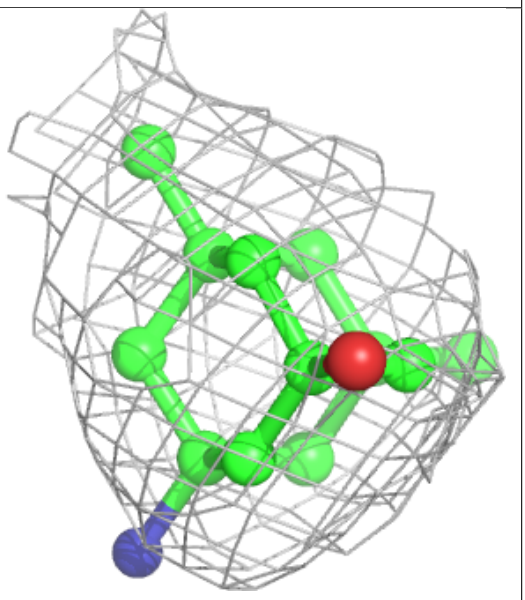


Electron density around BR7 F 402:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

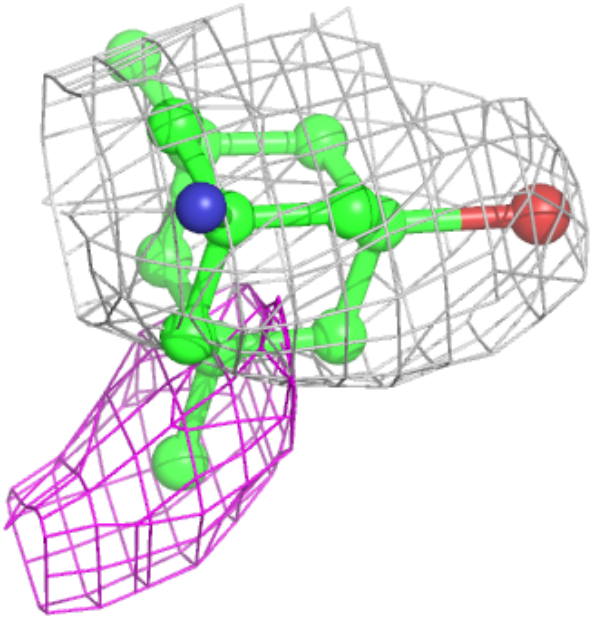


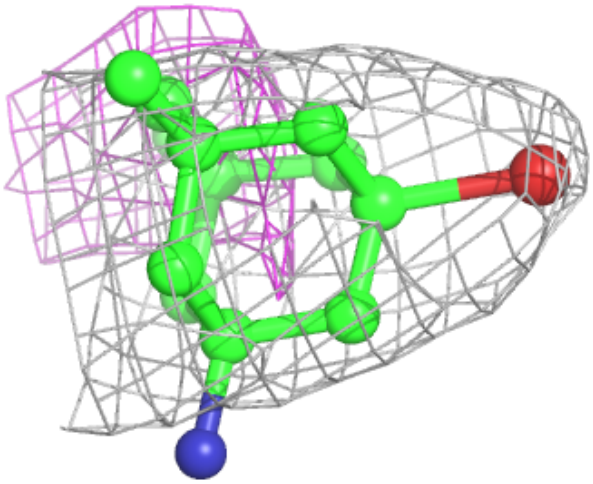


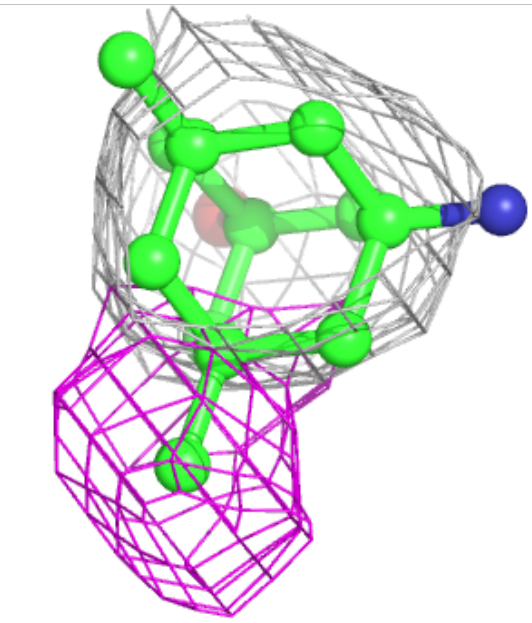


Electron density around BR7 C 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

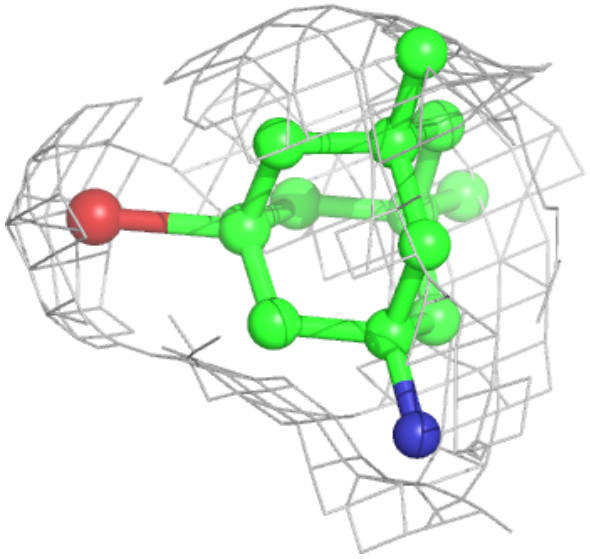


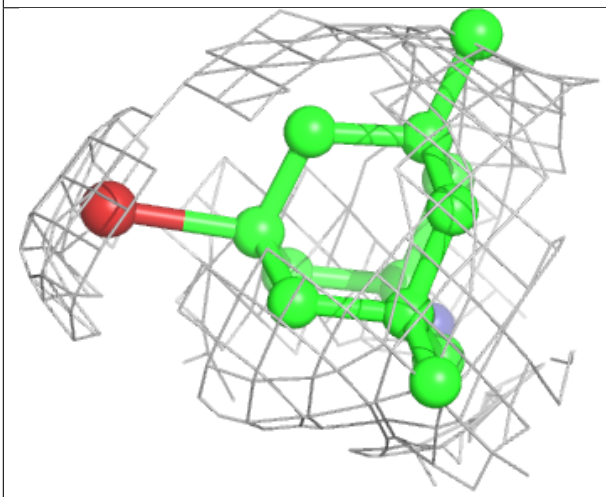


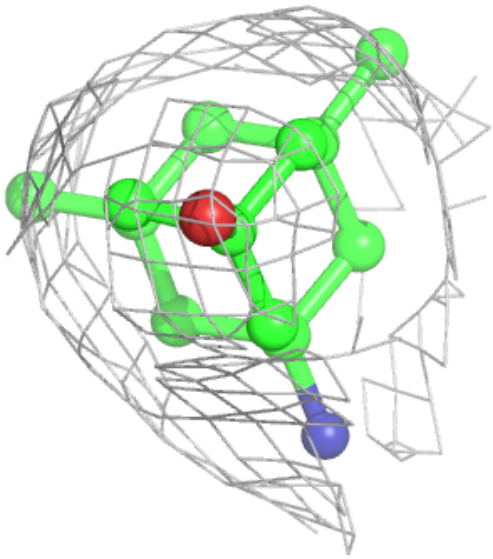


Electron density around BR7 B 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

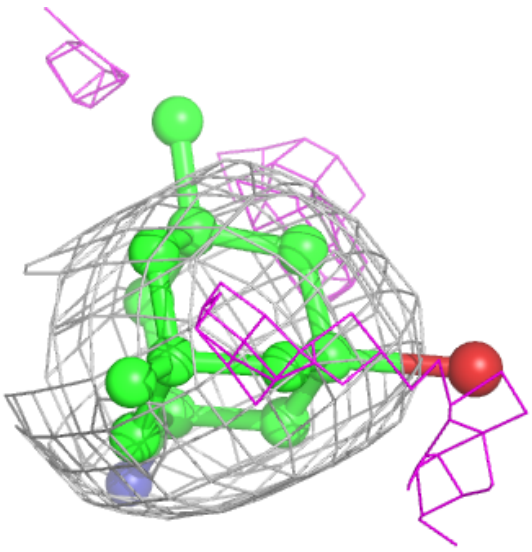


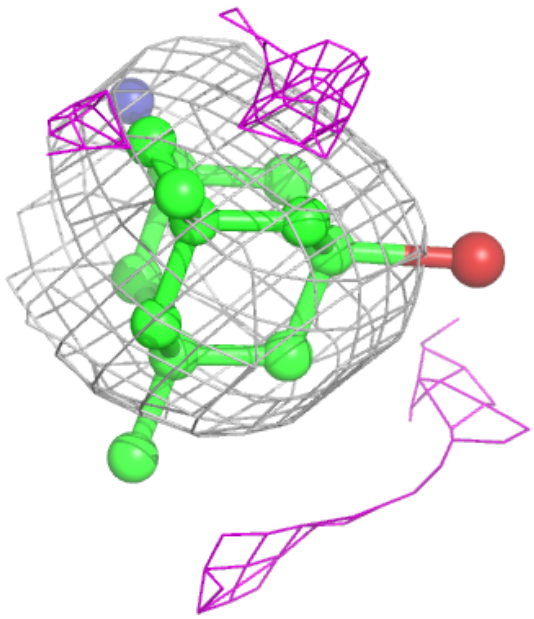


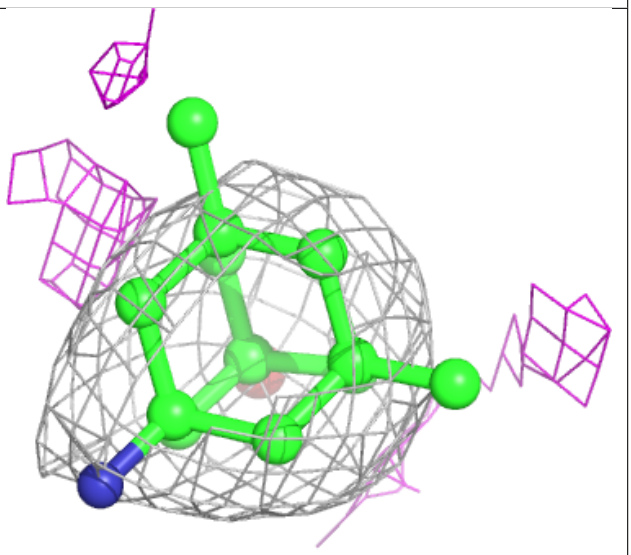


Electron density around BR7 E 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

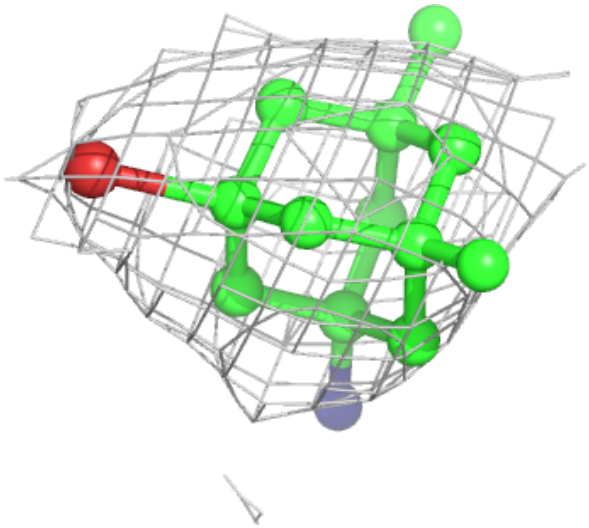


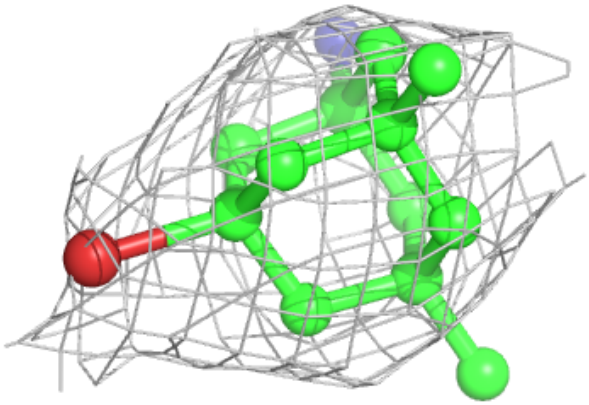


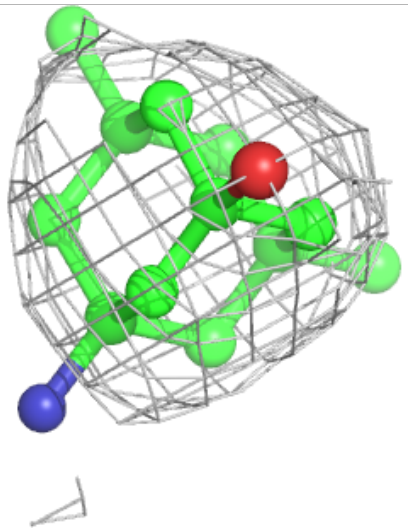


Electron density around BR7 H 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

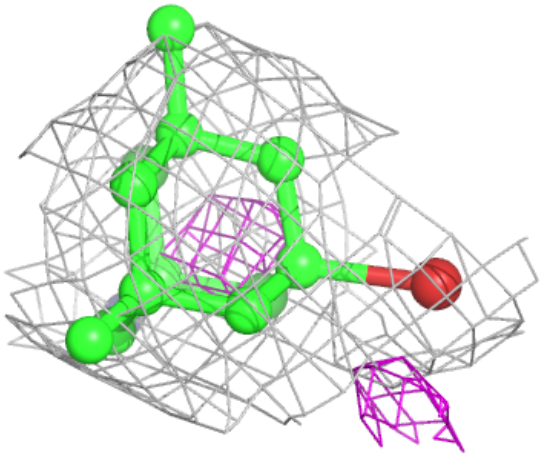


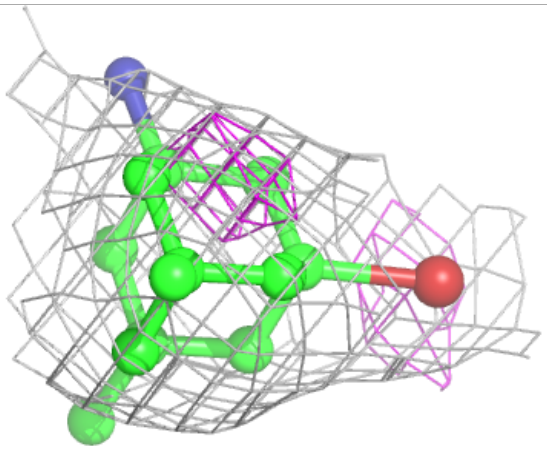


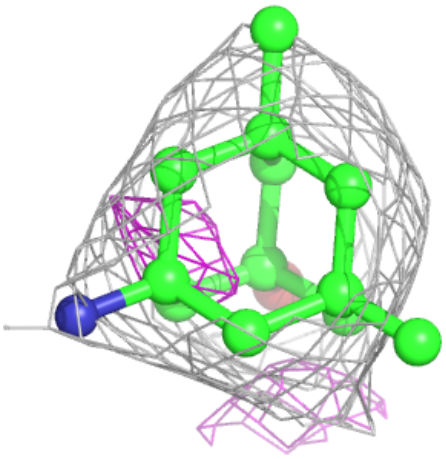


Electron density around BR7 J 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

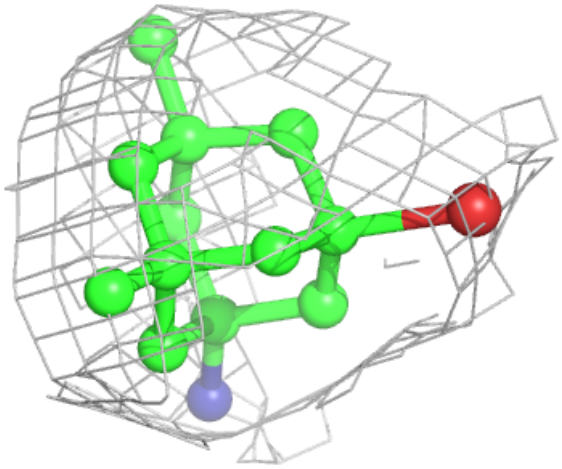


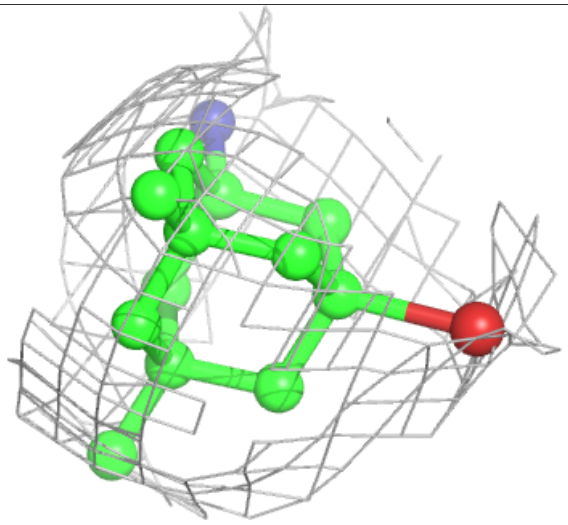


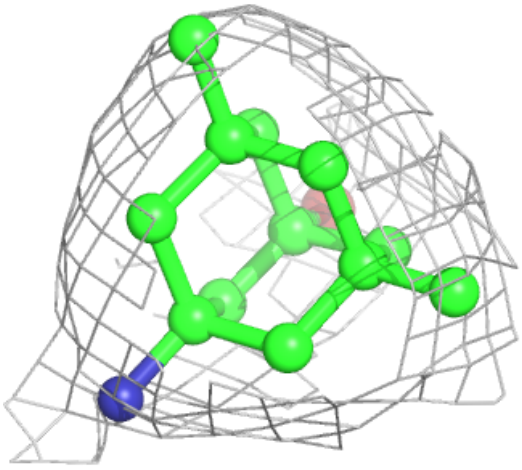


Electron density around BR7 I 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

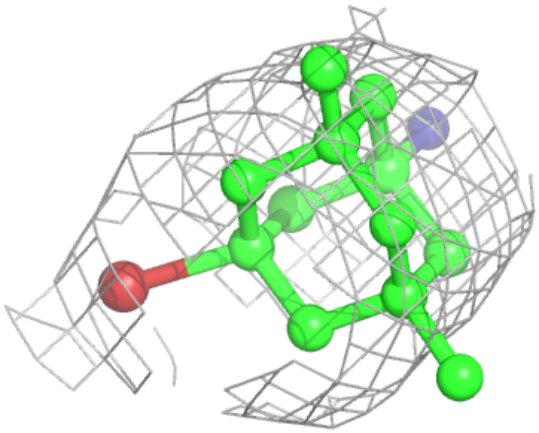


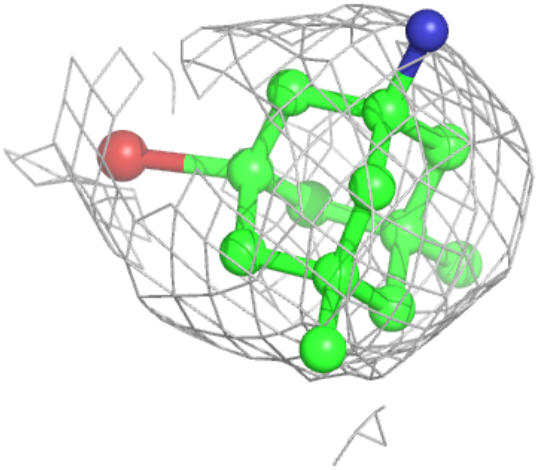


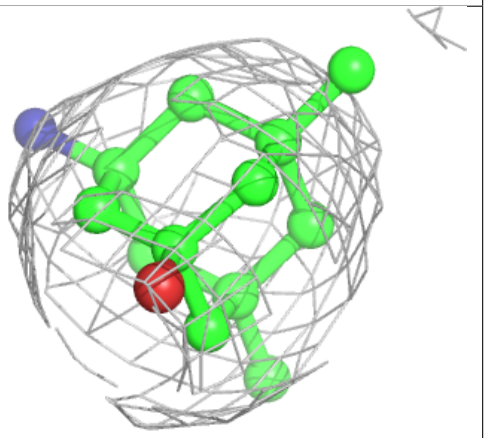


Electron density around BR7 A 402:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

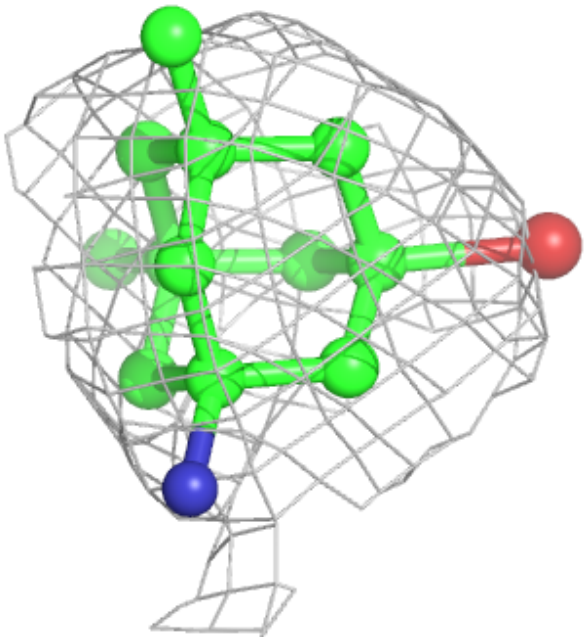


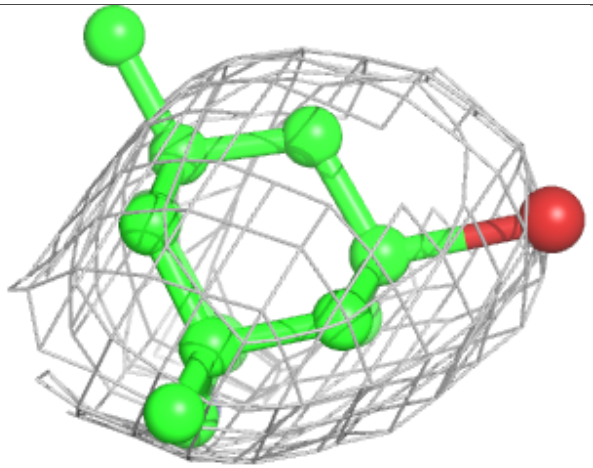


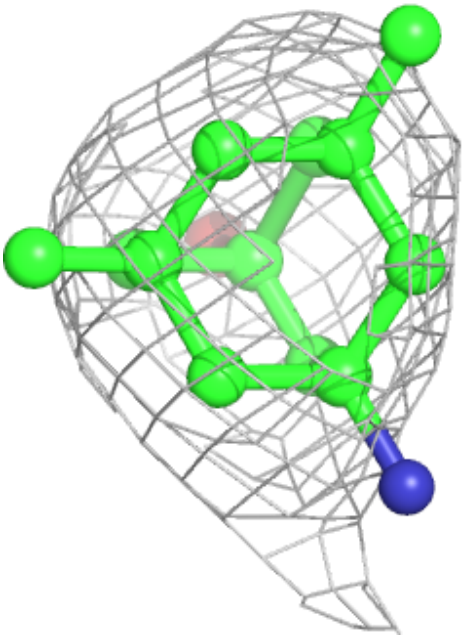


Electron density around BR7 G 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

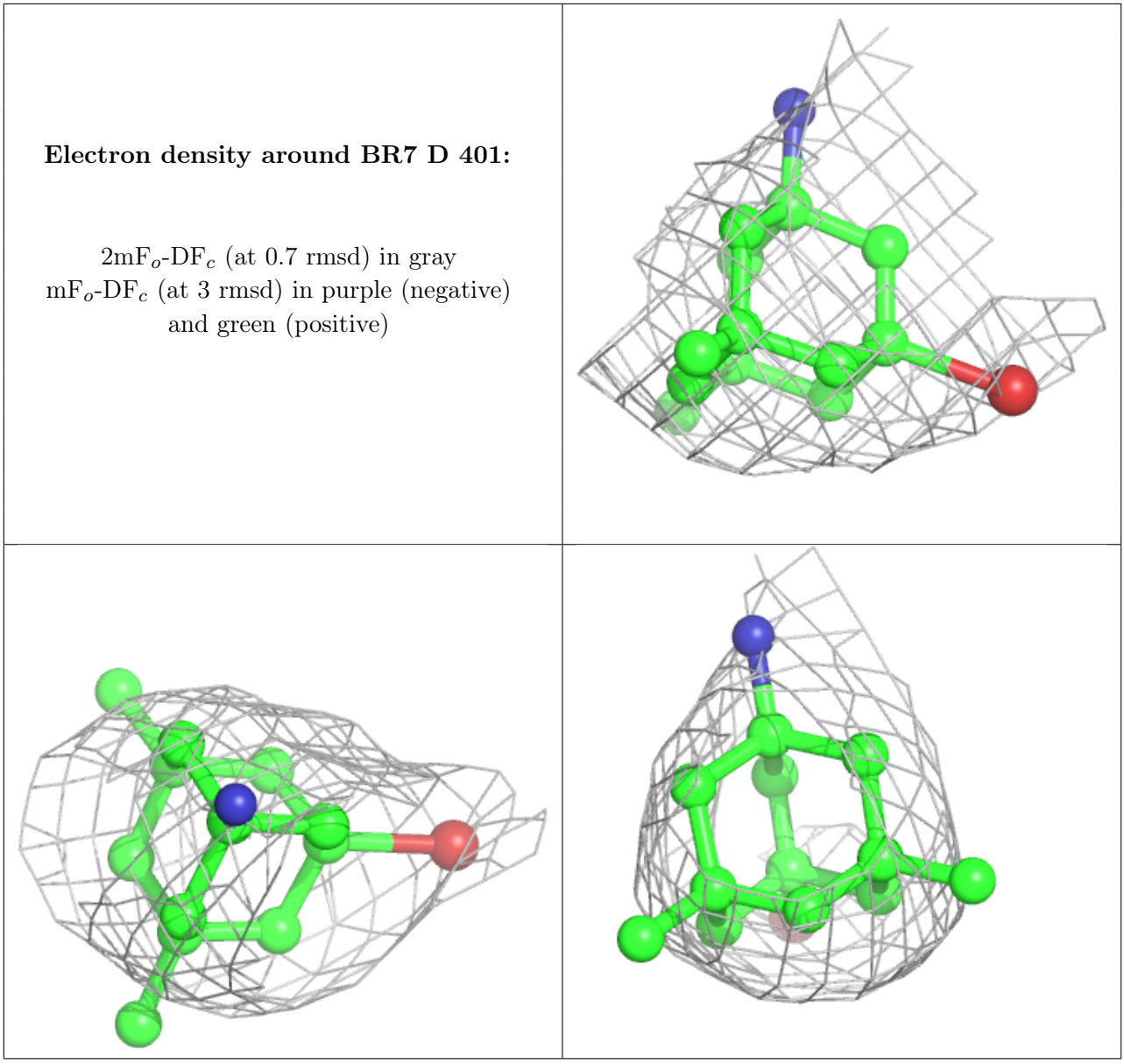






Electron density around BR7 D 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.