



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:24 AM UTC

PDB ID : 4TWF / pdb_00004twf
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

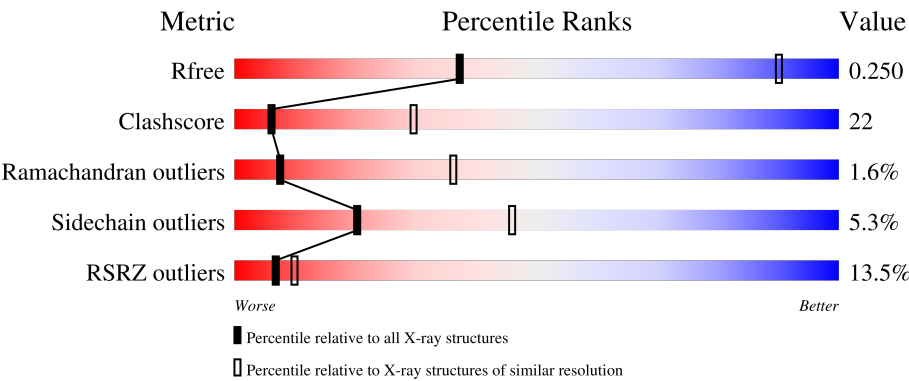
1 Overall quality at a glance i

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}	180053	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	307	7% 57% 35% 7%
1	B	307	19% 57% 37%
1	C	307	10% 57% 37% 5%
1	D	307	13% 66% 28% 5%

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Mol	Chain	Length	Quality of chain
1	E	307	14% 56% 37% 6%
1	F	307	12% 57% 36% 5%
1	G	307	19% 55% 39% 5%
1	H	307	13% 53% 39% 6%
1	I	307	13% 55% 40%
1	J	307	13% 60% 33% 6%

2 Entry composition

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:

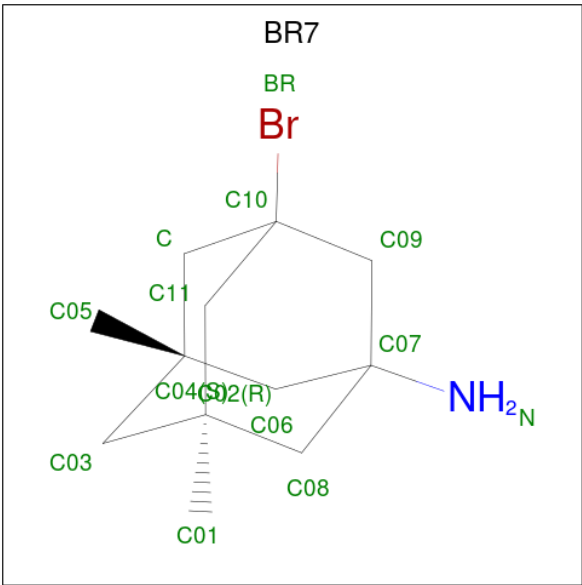
Chain	Residue	Modelled	Actual	Comment	Reference
A	152	ALA	ILE	conflict	UNP P0C7B7
A	164	GLY	-	insertion	UNP P0C7B7
A	247	SER	PHE	engineered mutation	UNP P0C7B7
A	289	ASN	MET	conflict	UNP P0C7B7
B	152	ALA	ILE	conflict	UNP P0C7B7
B	164	GLY	-	insertion	UNP P0C7B7
B	247	SER	PHE	engineered mutation	UNP P0C7B7
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 (CCD ID: BR7) (formula: C₁₂H₂₀BrN).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	Br	C	N	0	0
			14	1	12	1		
2	A	1	Total	Br	C	N	0	0
			14	1	12	1		
2	B	1	Total	Br	C	N	0	0
			14	1	12	1		
2	C	1	Total	Br	C	N	0	0
			14	1	12	1		
2	D	1	Total	Br	C	N	0	0
			14	1	12	1		
2	E	1	Total	Br	C	N	0	0
			14	1	12	1		
2	F	1	Total	Br	C	N	0	0
			14	1	12	1		
2	F	1	Total	Br	C	N	0	0
			14	1	12	1		
2	G	1	Total	Br	C	N	0	0
			14	1	12	1		
2	H	1	Total	Br	C	N	0	0
			14	1	12	1		
2	I	1	Total	Br	C	N	0	0
			14	1	12	1		
2	J	1	Total	Br	C	N	0	0
			14	1	12	1		

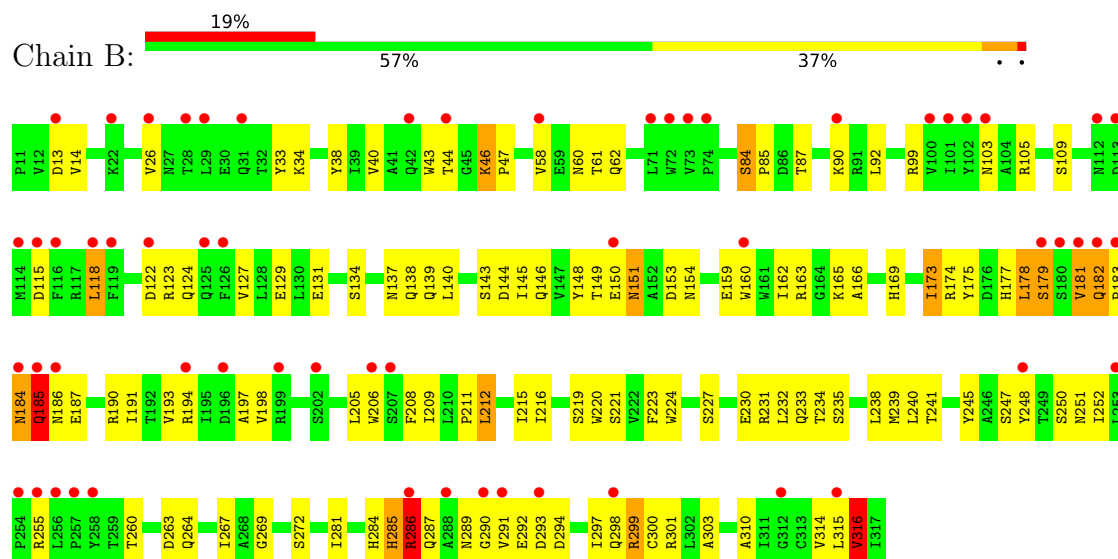
3 Residue-property plots

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.

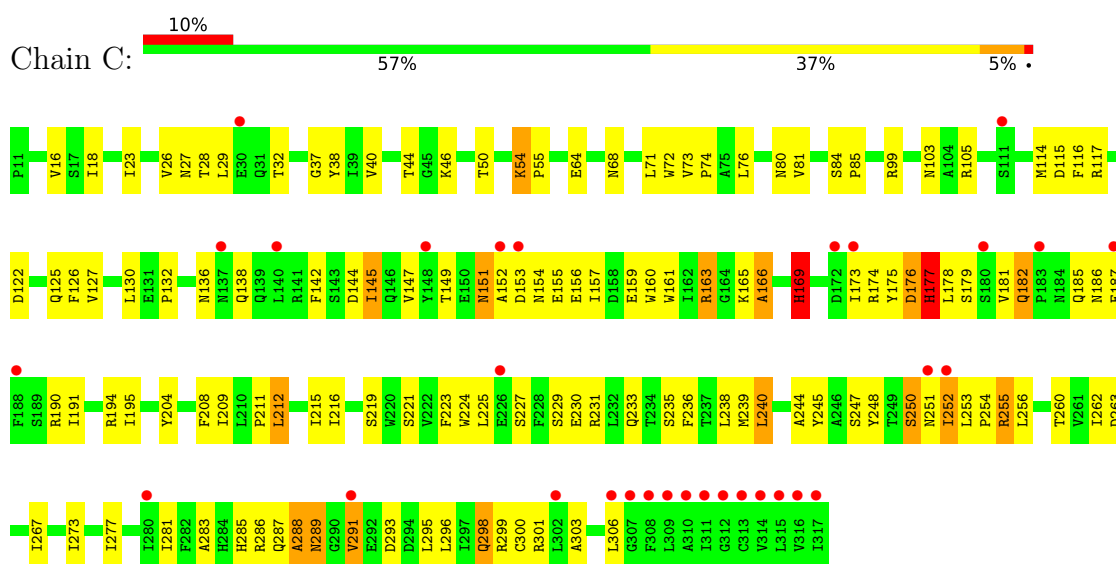
• Molecule 1: Cys-loop ligand-gated ion channel



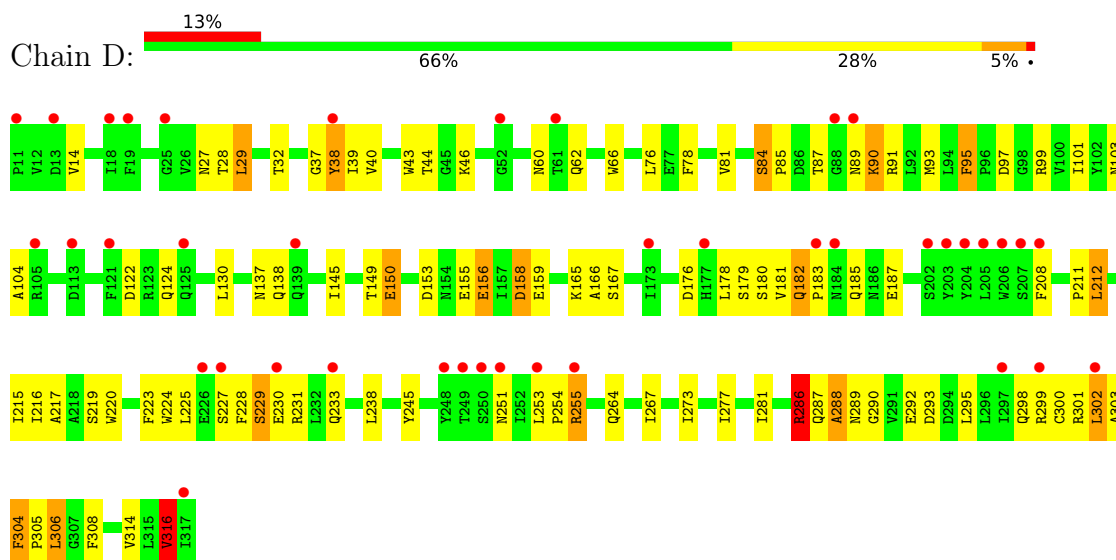
• Molecule 1: Cys-loop ligand-gated ion channel



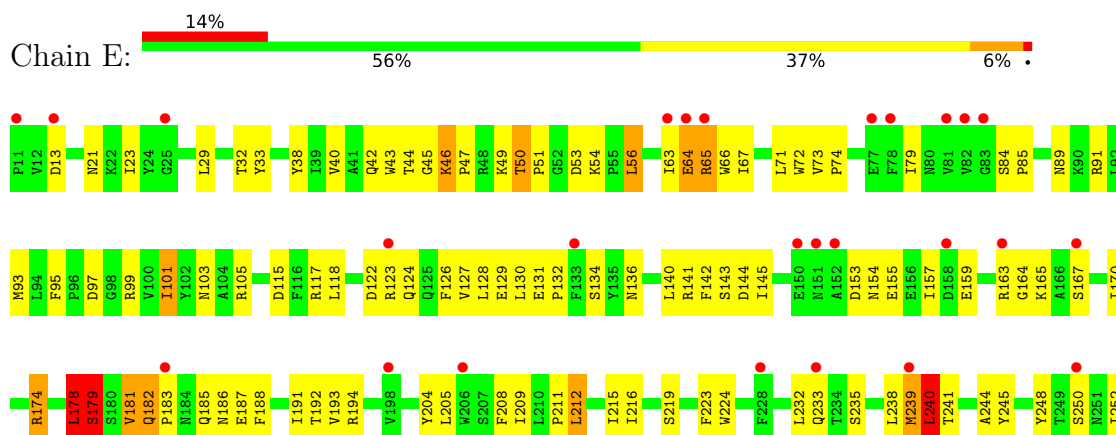
• Molecule 1: Cys-loop ligand-gated ion channel

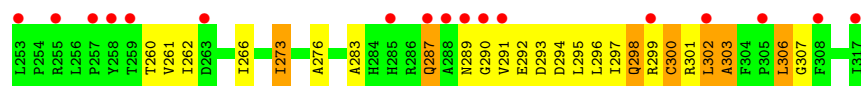


• Molecule 1: Cys-loop ligand-gated ion channel

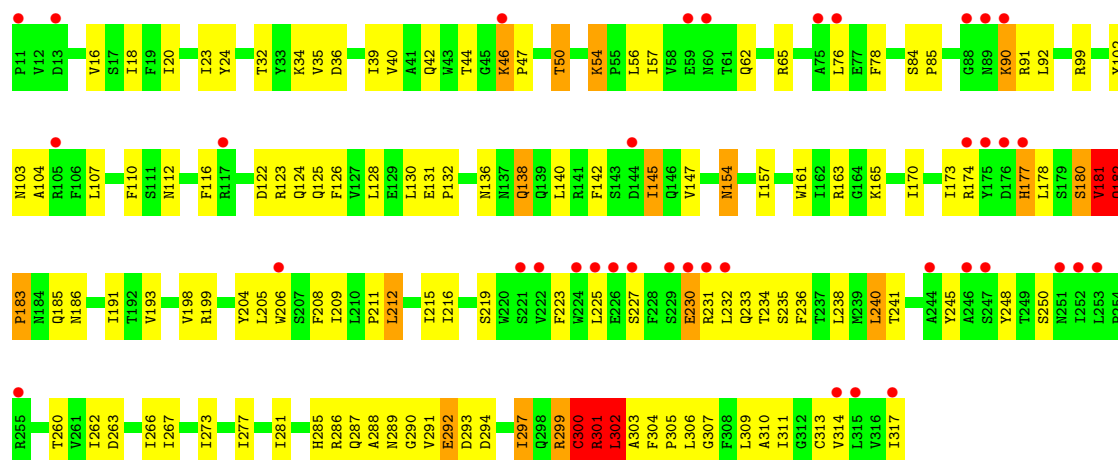


• Molecule 1: Cys-loop ligand-gated ion channel

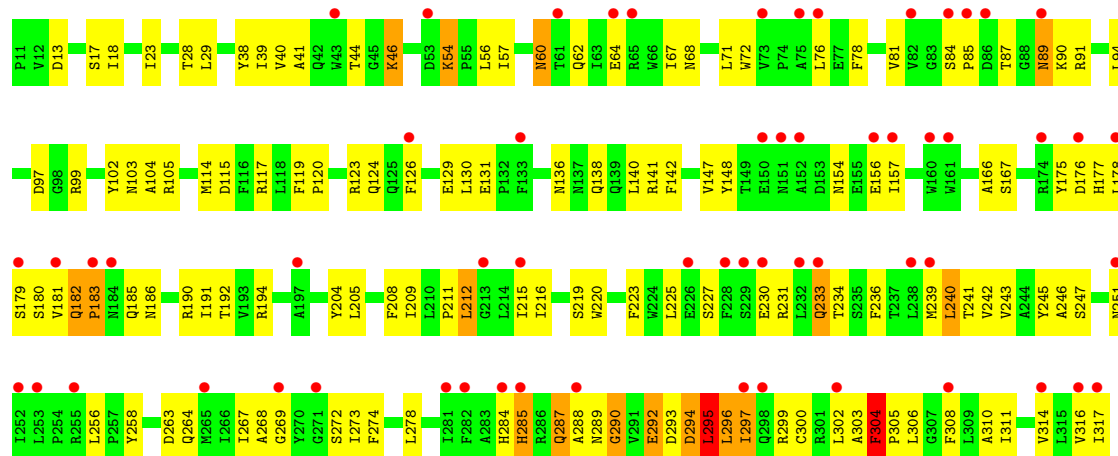




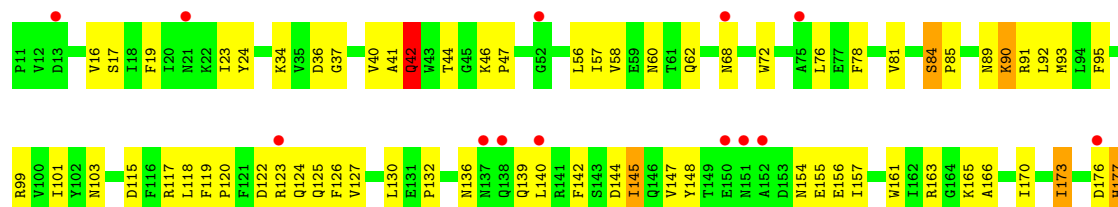
• Molecule 1: Cys-loop ligand-gated ion channel

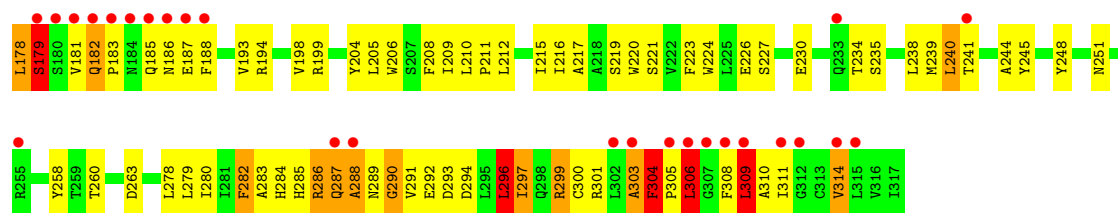


• Molecule 1: Cys-loop ligand-gated ion channel

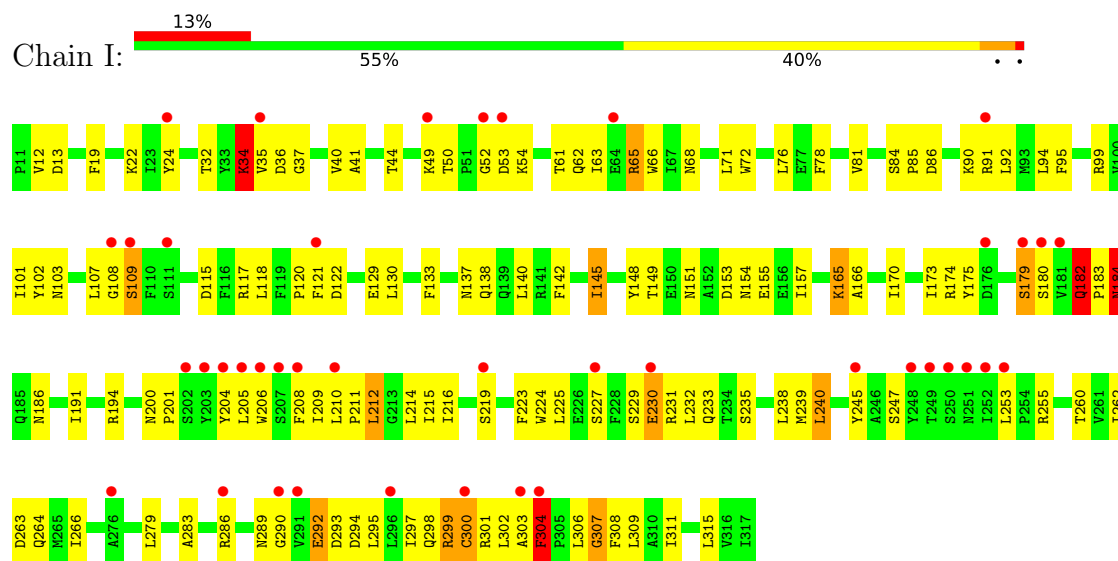


• Molecule 1: Cys-loop ligand-gated ion channel

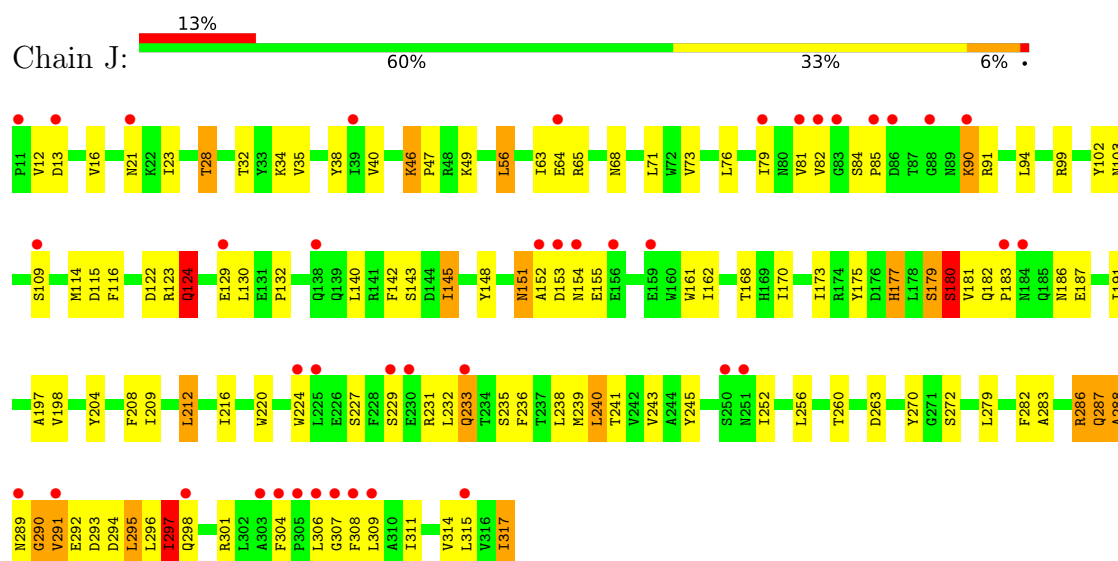




• Molecule 1: Cys-loop ligand-gated ion channel



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



4 Data and refinement statistics

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) 91.0 (49.83-3.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.95 (at 3.88Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.202 , 0.250 0.207 , 0.250	Depositor DCC
R_{free} test set	2719 reflections (5.03%)	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)	0.20 , 74.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

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	0.55	0/2564	1.07	16/3495 (0.5%)
1	B	0.54	0/2564	1.10	16/3495 (0.5%)
1	C	0.55	0/2564	1.09	16/3495 (0.5%)
1	D	0.50	0/2564	1.08	13/3495 (0.4%)
1	E	0.68	4/2564 (0.2%)	1.19	21/3495 (0.6%)
1	F	0.57	0/2564	1.14	12/3495 (0.3%)
1	G	0.52	0/2564	1.08	8/3495 (0.2%)
1	H	0.56	0/2564	1.17	21/3495 (0.6%)
1	I	0.52	0/2564	1.11	12/3495 (0.3%)
1	J	0.57	0/2564	1.10	13/3495 (0.4%)
All	All	0.56	4/25640 (0.0%)	1.11	148/34950 (0.4%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	273	ILE	CA-CB	-11.76	1.38	1.54
1	E	239	MET	SD-CE	6.97	1.97	1.79
1	E	240	LEU	N-CA	-6.42	1.38	1.46
1	E	239	MET	CA-C	-5.05	1.46	1.52

All (148) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	54	LYS	CA-C-N	-10.96	108.78	119.85
1	F	54	LYS	C-N-CA	-10.96	108.78	119.85
1	E	45	GLY	N-CA-C	-10.77	97.20	112.60
1	G	182	GLN	CA-C-N	10.16	132.54	119.84
1	G	182	GLN	C-N-CA	10.16	132.54	119.84
1	D	84	SER	CA-C-N	9.45	130.16	120.14
1	D	84	SER	C-N-CA	9.45	130.16	120.14
1	I	304	PHE	CA-C-N	-9.43	108.58	118.85
1	I	304	PHE	C-N-CA	-9.43	108.58	118.85
1	H	308	PHE	N-CA-C	-9.24	102.01	113.20
1	F	180	SER	N-CA-C	-9.17	102.21	112.57
1	E	298	GLN	N-CA-C	-9.12	101.58	112.89
1	I	34	LYS	N-CA-C	9.09	122.96	109.24
1	H	304	PHE	CA-C-N	-8.95	109.44	119.28
1	H	304	PHE	C-N-CA	-8.95	109.44	119.28
1	E	46	LYS	CA-C-N	8.39	128.44	119.89
1	E	46	LYS	C-N-CA	8.39	128.44	119.89
1	J	307	GLY	N-CA-C	8.23	124.87	114.66
1	H	84	SER	CA-C-N	8.22	128.85	120.14
1	H	84	SER	C-N-CA	8.22	128.85	120.14
1	F	300	CYS	N-CA-C	-8.20	104.28	112.97
1	E	181	VAL	N-CA-C	-8.17	96.67	108.11
1	A	287	GLN	N-CA-C	8.17	119.40	108.38
1	H	287	GLN	N-CA-C	8.02	120.91	108.96
1	J	46	LYS	CA-C-N	7.92	127.97	119.90
1	J	46	LYS	C-N-CA	7.92	127.97	119.90
1	E	56	LEU	CB-CG-CD1	-7.83	87.22	110.70
1	H	282	PHE	N-CA-C	-7.81	102.72	111.07
1	E	240	LEU	N-CA-C	-7.80	102.78	111.28
1	F	46	LYS	CA-C-N	7.75	127.81	119.90
1	F	46	LYS	C-N-CA	7.75	127.81	119.90
1	D	229	SER	N-CA-C	-7.70	102.83	111.07
1	E	300	CYS	N-CA-C	-7.66	104.85	112.97
1	I	300	CYS	N-CA-C	-7.65	104.36	112.93
1	I	155	GLU	N-CA-C	7.50	119.35	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	316	VAL	CB-CA-C	-7.49	102.22	112.04
1	B	181	VAL	N-CA-C	-7.48	96.95	107.80
1	J	291	VAL	N-CA-C	7.40	120.36	112.96
1	A	298	GLN	N-CA-C	-7.34	104.30	113.18
1	J	288	ALA	N-CA-C	7.31	126.37	110.80
1	H	288	ALA	N-CA-C	-7.27	102.41	112.30
1	B	178	LEU	N-CA-C	7.21	121.25	109.85
1	G	285	HIS	N-CA-C	7.07	122.03	113.41
1	E	250	SER	N-CA-C	6.83	119.74	111.82
1	J	308	PHE	N-CA-C	6.82	120.82	112.23
1	H	296	LEU	CA-CB-CG	6.77	140.00	116.30
1	I	182	GLN	CA-CB-CG	6.75	127.60	114.10
1	E	63	ILE	N-CA-C	6.70	116.83	110.53
1	C	252	ILE	CB-CA-C	-6.67	103.92	111.80
1	E	178	LEU	N-CA-C	6.64	118.61	109.18
1	I	179	SER	CA-C-N	-6.63	114.15	123.03
1	I	179	SER	C-N-CA	-6.63	114.15	123.03
1	D	300	CYS	N-CA-C	-6.62	105.95	112.97
1	E	273	ILE	N-CA-C	6.61	117.59	111.45
1	J	12	VAL	N-CA-C	6.58	117.53	108.84
1	H	176	ASP	N-CA-C	6.57	118.10	111.07
1	E	101	ILE	CB-CA-C	-6.57	103.02	110.96
1	H	286	ARG	CB-CG-CD	6.50	126.26	111.30
1	E	53	ASP	N-CA-C	-6.33	103.06	113.50
1	A	178	LEU	N-CA-C	6.31	120.32	108.65
1	H	309	LEU	N-CA-C	-6.25	104.47	111.28
1	I	165	LYS	N-CA-C	-6.20	101.02	109.95
1	H	304	PHE	N-CA-C	6.18	123.47	109.81
1	J	297	ILE	CB-CA-C	-6.12	102.18	112.16
1	B	153	ASP	N-CA-C	6.12	123.83	110.80
1	E	101	ILE	N-CA-C	6.11	117.58	108.23
1	C	298	GLN	N-CA-C	-6.08	105.34	112.89
1	G	294	ASP	N-CA-C	6.07	118.34	108.63
1	D	178	LEU	N-CA-C	6.05	119.85	108.65
1	I	12	VAL	N-CA-C	6.02	116.78	108.84
1	C	169	HIS	CB-CA-C	5.98	118.72	110.34
1	A	300	CYS	N-CA-C	-5.97	106.64	112.97
1	E	303	ALA	CA-C-N	5.95	127.14	120.06
1	E	303	ALA	C-N-CA	5.95	127.14	120.06
1	J	28	THR	N-CA-C	5.95	117.76	111.28
1	I	307	GLY	N-CA-C	-5.87	107.06	114.16
1	D	159	GLU	N-CA-C	5.85	117.66	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	155	GLU	N-CA-C	-5.83	105.43	112.54
1	J	124	GLN	N-CA-C	5.78	118.20	109.41
1	A	20	ILE	CA-C-N	-5.73	112.35	122.26
1	A	20	ILE	C-N-CA	-5.73	112.35	122.26
1	C	288	ALA	N-CA-C	-5.73	103.77	112.99
1	J	304	PHE	N-CA-C	5.70	122.41	109.81
1	J	297	ILE	N-CA-C	5.69	119.06	111.44
1	D	304	PHE	CA-C-N	-5.68	113.03	119.28
1	D	304	PHE	C-N-CA	-5.68	113.03	119.28
1	A	304	PHE	CA-C-N	-5.68	113.17	119.19
1	A	304	PHE	C-N-CA	-5.68	113.17	119.19
1	F	20	ILE	CB-CA-C	-5.67	104.05	111.25
1	B	84	SER	CA-C-N	5.66	125.57	119.85
1	B	84	SER	C-N-CA	5.66	125.57	119.85
1	B	300	CYS	N-CA-C	-5.66	106.70	113.21
1	H	305	PRO	N-CA-C	-5.63	106.04	113.65
1	D	46	LYS	CA-C-N	5.62	125.55	119.76
1	D	46	LYS	C-N-CA	5.62	125.55	119.76
1	F	182	GLN	CA-CB-CG	5.60	125.30	114.10
1	E	56	LEU	CB-CA-C	-5.59	100.06	109.50
1	A	307	GLY	N-CA-C	-5.58	107.75	114.66
1	H	299	ARG	N-CA-C	-5.57	107.07	112.97
1	E	287	GLN	N-CA-C	5.55	117.23	108.96
1	H	42	GLN	N-CA-C	5.47	117.71	109.23
1	A	14	VAL	N-CA-C	5.46	115.72	107.75
1	B	303	ALA	CA-C-N	5.43	126.53	120.06
1	B	303	ALA	C-N-CA	5.43	126.53	120.06
1	A	299	ARG	CA-CB-CG	5.40	124.90	114.10
1	H	179	SER	N-CA-C	5.40	122.30	110.80
1	E	252	ILE	N-CA-C	5.39	116.45	111.81
1	C	37	GLY	N-CA-C	5.38	119.79	111.08
1	C	182	GLN	N-CA-C	5.37	121.68	109.81
1	F	154	ASN	N-CA-C	5.36	118.59	111.30
1	A	46	LYS	CA-C-N	5.35	125.36	119.90
1	A	46	LYS	C-N-CA	5.35	125.36	119.90
1	C	151	ASN	N-CA-C	5.34	117.58	110.53
1	C	177	HIS	CA-C-N	-5.31	115.15	122.16
1	C	177	HIS	C-N-CA	-5.31	115.15	122.16
1	C	285	HIS	CA-C-N	-5.30	115.25	122.93
1	C	285	HIS	C-N-CA	-5.30	115.25	122.93
1	H	306	LEU	CA-CB-CG	5.30	134.84	116.30
1	F	301	ARG	N-CA-C	5.29	122.08	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	182	GLN	CB-CG-CD	5.28	121.58	112.60
1	C	165	LYS	N-CA-C	-5.27	103.76	111.30
1	B	139	GLN	N-CA-C	-5.26	105.68	112.68
1	B	285	HIS	CA-C-N	-5.25	115.21	122.30
1	B	285	HIS	C-N-CA	-5.25	115.21	122.30
1	E	307	GLY	N-CA-C	-5.25	107.81	114.16
1	J	179	SER	N-CA-C	-5.19	99.75	110.80
1	G	304	PHE	CA-C-N	-5.18	113.58	119.28
1	G	304	PHE	C-N-CA	-5.18	113.58	119.28
1	F	181	VAL	N-CA-C	5.17	120.10	109.34
1	A	179	SER	N-CA-C	-5.16	101.75	109.95
1	G	297	ILE	N-CA-C	-5.16	104.64	111.09
1	B	46	LYS	CA-C-N	5.15	125.44	119.93
1	B	46	LYS	C-N-CA	5.15	125.44	119.93
1	F	287	GLN	N-CA-C	5.14	116.62	108.96
1	A	301	ARG	NE-CZ-NH2	-5.11	114.60	119.20
1	H	210	LEU	CA-C-N	-5.07	113.70	119.28
1	H	210	LEU	C-N-CA	-5.07	113.70	119.28
1	B	182	GLN	N-CA-C	5.06	120.99	109.81
1	B	151	ASN	N-CA-C	5.05	117.98	109.95
1	C	176	ASP	CA-C-N	5.05	130.75	123.13
1	C	176	ASP	C-N-CA	5.05	130.75	123.13
1	D	306	LEU	N-CA-C	-5.03	106.66	112.89
1	H	290	GLY	N-CA-C	-5.03	101.26	113.18
1	C	84	SER	CA-C-N	5.02	125.47	120.14
1	C	84	SER	C-N-CA	5.02	125.47	120.14
1	G	287	GLN	N-CA-C	5.02	115.93	108.60
1	D	95	PHE	CA-C-N	5.01	124.50	119.19
1	D	95	PHE	C-N-CA	5.01	124.50	119.19

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
1	B	286	ARG	Peptide

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Mol	Chain	Res	Type	Group
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	120	0
1	B	2497	0	2468	119	0
1	C	2497	0	2468	123	0
1	D	2497	0	2468	83	0
1	E	2497	0	2468	123	0
1	F	2497	0	2468	128	0
1	G	2497	0	2468	126	0
1	H	2497	0	2468	135	0
1	I	2497	0	2468	140	0
1	J	2497	0	2468	119	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1126	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 (1126) 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: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:E:239:MET:HE1	1:E:273:ILE:HD13	1.46	0.98
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:239:MET:HE3	1:E:273:ILE:HG21	1.61	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
1:C:298:GLN:C	1:C:301:ARG:HH12	1.90	0.79
2:A:402:BR7:BR	1:C:244:ALA:HA	2.38	0.79
1:E:239:MET:CE	1:E:273:ILE:HG21	2.12	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:A:215:ILE:HD13	1:B:239:MET:HE3	1.64	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: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:E:239:MET:HE2	1:E:239:MET:N	2.00	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:G:215:ILE:HD13	1:H:239:MET:HE3	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:87:THR:HG21	1:B:90:LYS:HZ2	1.51	0.75
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: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: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:I:215:ILE:HD13	1:J:239:MET:HE3	1.71	0.73
1:I:34:LYS:HZ3	1:I:108:GLY:H	1.36	0.72
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: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:E:239:MET:CE	1:E:273:ILE:HD13	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:E:238:LEU:C	1:E:239:MET:HE2	2.18	0.68
1:J:81:VAL:HG21	1:J:85:PRO:HG3	1.75	0.68
1:J:180:SER:OG	1:J:180:SER:O	2.08	0.68
1:J:220:TRP:NE1	1:J:272:SER:OG	2.20	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: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:A:239:MET:HE3	1:E:215:ILE:HD13	1.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HE2	1:E:101:ILE:HD12	1.81	0.62
1:E:93:MET:HB3	1:E:101:ILE:HB	1.82	0.62
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: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: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:B:87:THR:CG2	1:B:90:LYS:HZ2	2.14	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:J:34:LYS:NZ	1:J:109:SER:OG	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:J:286:ARG:O	1:J:287:GLN:HB3	2.00	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:E:299:ARG:C	1:E:301:ARG:H	2.10	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:I:232:LEU:O	1:I:235:SER:OG	2.21	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:B:314:VAL:C	1:B:316:VAL:H	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:37:GLY:C	1:D:38:TYR:HD1	2.11	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:A:93:MET:HE3	1:A:101:ILE:HB	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
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:97:ASP:CG	1:G:99:ARG:NH1	2.62	0.58
1:G:233:GLN:HA	1:G:236:PHE:HD1	1.68	0.58
1:H:208:PHE:O	1:H:245:TYR:OH	2.21	0.58
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:299:ARG:C	1:I:301:ARG:H	2.11	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: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:G:181:VAL:C	1:G:183:PRO:HD3	2.30	0.57
1:B:260:THR:O	1:B:264:GLN:HG3	2.05	0.57
1:J:295:LEU:HA	1:J:298:GLN:HG2	1.86	0.57
1:E:93:MET:HE3	1:E:95:PHE:CE1	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:221:SER:C	1:A:301:ARG:HH12	2.13	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
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:97:ASP:CG	1:D:99:ARG:NH1	2.64	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:E:93:MET:HE3	1:E:95:PHE:CZ	2.41	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:C:156:GLU:H	1:C:156:GLU:CD	2.14	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:H:289:ASN:CG	1:H:292:GLU:HB3	2.31	0.55
1:B:33:TYR:C	1:B:34:LYS:HD3	2.30	0.55
1:B:224:TRP:CD1	1:B:301:ARG:HE	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:49:LYS:NZ	1:I:52:GLY:O	2.30	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:J:153:ASP:CG	1:J:154:ASN:H	2.15	0.55
1:A:292:GLU:HG2	1:A:292:GLU:O	2.06	0.55
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:F:90:LYS:HE3	1:F:102:TYR:CZ	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:299:ARG:HA	1:C:301:ARG:HH11	1.73	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: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
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:A:165:LYS:O	1:A:165:LYS:HG2	2.06	0.53
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: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:E:295:LEU:HA	1:E:298:GLN:CD	2.34	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:223:PHE:HE1	1:G:304:PHE:HE2	1.55	0.53
1:I:34:LYS:HE3	1:I:107:LEU:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:J:286:ARG:HD2	1:J:286:ARG:C	2.34	0.52
1:A:91:ARG:HB3	1:A:103:ASN:HB2	1.91	0.52
1:A:218:ALA:O	1:A:221:SER:OG	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:LEU:CD1	1:B:122:ASP:HA	2.40	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: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: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
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:13:ASP:CG	1:B:143:SER:HB3	2.36	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: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: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:H:41:ALA:C	1:H:42:GLN:HG3	2.35	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:A:299:ARG:C	1:A:301:ARG:H	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:220:TRP:HE1	1:J:272:SER:HG	1.52	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:I:90:LYS:HD2	1:I:90:LYS:C	2.36	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: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
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:C:176:ASP:C	1:C:177:HIS:HD2	2.19	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: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:B:62:GLN:HE22	1:C:68:ASN:CG	2.18	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:C:169:HIS:C	1:C:169:HIS:CD2	2.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:299:ARG:C	1:B:301:ARG:H	2.18	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
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:C:26:VAL:HG13	1:C:114:MET:HE1	1.95	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:289:ASN:CG	1:C:291:VAL:H	2.21	0.48
1:F:62:GLN:NE2	1:G:68:ASN:OD1	2.42	0.48
1:F:123:ARG:C	1:F:124:GLN:HG2	2.39	0.48
1:F:178:LEU:HD11	1:F:181:VAL:HG23	1.95	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
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:J:186:ASN:OD1	1:J:186:ASN:N	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:288:ALA:C	1:H:289:ASN:HD22	2.22	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:F:204:TYR:O	1:F:209:ILE:HG12	2.14	0.47
1:G:136:ASN:CG	1:G:185:GLN:HG3	2.39	0.47
1:G:230:GLU:O	1:G:234:THR:OG1	2.18	0.47
1:I:223:PHE:CZ	1:I:279:LEU:HD21	2.49	0.47
1:J:301:ARG:HD2	1:J:301:ARG:C	2.39	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
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:F:215:ILE:HD13	1:G:239:MET:HE3	1.95	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:G:227:SER:HB3	1:G:230:GLU:CD	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:155:GLU:H	1:D:155:GLU:CD	2.23	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: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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:22:LYS:HZ2	1:I:24:TYR:HB3	1.80	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:123:ARG:C	1:B:124:GLN:HG2	2.40	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:G:90:LYS:HZ2	1:G:104:ALA:CA	2.29	0.46
1:I:78:PHE:O	1:I:81:VAL:HG12	2.15	0.46
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:E:164:GLY:C	1:E:165:LYS:HD2	2.41	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:C:239:MET:HE2	1:C:239:MET:HB2	1.85	0.45
1:G:90:LYS:HZ2	1:G:104:ALA:HB1	1.80	0.45
1:I:36:ASP:OD1	1:I:37:GLY:N	2.49	0.45
1:J:114:MET:HE2	1:J:116:PHE:HZ	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:144:ASP:C	1:E:145:ILE:HG13	2.42	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
1:J:153:ASP:CG	1:J:154:ASN:N	2.74	0.45
1:A:223:PHE:N	1:A:301:ARG:NH1	2.65	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: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:D:227:SER:C	1:D:231:ARG:NH1	2.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:299:ARG:C	1:F:301:ARG:N	2.74	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
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:G:287:GLN:HG2	1:G:288:ALA:N	2.31	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:H:287:GLN:HG3	1:H:290:GLY:C	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:184:ASN:C	1:B:186:ASN:H	2.26	0.43
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:A:87:THR:HG21	1:A:90:LYS:HZ2	1.82	0.43
1:C:154:ASN:HB3	1:C:157:ILE:HG12	1.98	0.43
1:F:260:THR:H	1:F:263:ASP:HB2	1.83	0.43
1:G:18:ILE:HD13	1:G:39:ILE:HG12	1.99	0.43
1:G:18:ILE:HB	1:G:147:VAL:HG22	2.01	0.43
1:I:182:GLN:O	1:I:183:PRO:C	2.61	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:33:TYR:OH	1:E:127:VAL:O	2.36	0.43
1:F:44:THR:HA	1:F:99:ARG:HA	2.00	0.43
1:F:122:ASP:CG	1:F:199:ARG:HE	2.26	0.43
1:F:165:LYS:HD2	1:F:165:LYS:HA	1.57	0.43
1:H:286:ARG:NH1	1:H:297:ILE:HD13	2.34	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:C:287:GLN:HE21	1:C:289:ASN:C	2.27	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
1:C:298:GLN:C	1:C:300:CYS:H	2.26	0.43
1:D:286:ARG:HA	1:D:286:ARG:HD3	1.59	0.43
1:D:288:ALA:HB3	1:D:292:GLU:CD	2.44	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:I:182:GLN:C	1:I:182:GLN:OE1	2.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:314:VAL:C	1:D:316:VAL:H	2.27	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:I:34:LYS:HD3	1:I:108:GLY:C	2.44	0.42
1:J:114:MET:HE2	1:J:116:PHE:CZ	2.54	0.42
1:C:115:ASP:OD2	1:C:117:ARG:NE	2.50	0.42
1:D:227:SER:HB3	1:D:230:GLU:CD	2.44	0.42
1:E:118:LEU:HA	1:E:261:VAL:HG23	2.00	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
1:D:224:TRP:CD1	1:D:301:ARG:HD3	2.55	0.42
1:D:314:VAL:C	1:D:316:VAL:N	2.75	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:136:ASN:CG	1:H:139:GLN:HG3	2.44	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:SER:HA	1:A:85:PRO:HD3	1.86	0.42
1:C:295:LEU:HD23	1:C:298:GLN:CD	2.45	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:E:182:GLN:O	1:E:183:PRO:C	2.62	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: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:26:VAL:HG13	1:A:114:MET:HE1	2.01	0.42
1:A:205:LEU:HD23	1:A:205:LEU:HA	1.82	0.42
1:B:227:SER:HB3	1:B:230:GLU:CD	2.45	0.42
1:E:117:ARG:O	1:E:260:THR:HA	2.20	0.42
1:F:46:LYS:HD2	1:F:46:LYS:C	2.45	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
1:D:299:ARG:C	1:D:301:ARG:H	2.26	0.41
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:H:122:ASP:CG	1:H:199:ARG:HE	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:177:HIS:CD2	1:H:177:HIS:C	2.98	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:J:182:GLN:N	1:J:182:GLN:CD	2.78	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:302:LEU:C	1:G:305:PRO:HD2	2.46	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: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: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
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:I:50:THR:OG1	1:I:54:LYS:O	2.26	0.40
1:A:178:LEU:HB2	1:A:179:SER:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:182:GLN:O	1:B:183:PRO:C	2.64	0.40
1:C:174:ARG:HA	1:C:186:ASN:O	2.21	0.40
1:F:286:ARG:NE	1:F:294:ASP:OD2	2.55	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:F:181:VAL:CG2	1:F:182:GLN:N	2.84	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:204:TYR:HA	1:E:208:PHE:HD1	1.85	0.40
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

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	9	40
1	B	305/307 (99%)	280 (92%)	19 (6%)	6 (2%)	6	32
1	C	305/307 (99%)	281 (92%)	20 (7%)	4 (1%)	9	40
1	D	305/307 (99%)	273 (90%)	23 (8%)	9 (3%)	3	26
1	E	305/307 (99%)	277 (91%)	26 (8%)	2 (1%)	18	53
1	F	305/307 (99%)	280 (92%)	20 (7%)	5 (2%)	7	36
1	G	305/307 (99%)	280 (92%)	18 (6%)	7 (2%)	5	30
1	H	305/307 (99%)	280 (92%)	19 (6%)	6 (2%)	6	32
1	I	305/307 (99%)	276 (90%)	25 (8%)	4 (1%)	9	40
1	J	305/307 (99%)	279 (92%)	24 (8%)	2 (1%)	18	53
All	All	3050/3070 (99%)	2784 (91%)	217 (7%)	49 (2%)	7	36

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
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

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

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	274/274 (100%)	254 (93%)	20 (7%)	13	39
1	B	274/274 (100%)	266 (97%)	8 (3%)	37	58
1	C	274/274 (100%)	262 (96%)	12 (4%)	25	49
1	D	274/274 (100%)	259 (94%)	15 (6%)	19	45
1	E	274/274 (100%)	261 (95%)	13 (5%)	23	48
1	F	274/274 (100%)	259 (94%)	15 (6%)	19	45
1	G	274/274 (100%)	263 (96%)	11 (4%)	28	51
1	H	274/274 (100%)	261 (95%)	13 (5%)	23	48
1	I	274/274 (100%)	257 (94%)	17 (6%)	16	43
1	J	274/274 (100%)	253 (92%)	21 (8%)	12	37
All	All	2740/2740 (100%)	2595 (95%)	145 (5%)	20	46

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	SER
1	A	21	ASN
1	A	32	THR
1	A	118	LEU
1	A	124	GLN
1	A	137	ASN
1	A	138	GLN
1	A	145	ILE
1	A	156	GLU
1	A	163	ARG
1	A	178	LEU
1	A	184	ASN
1	A	186	ASN
1	A	187	GLU
1	A	212	LEU
1	A	240	LEU
1	A	292	GLU
1	A	297	ILE
1	A	298	GLN
1	A	299	ARG
1	B	118	LEU
1	B	163	ARG
1	B	173	ILE

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Mol	Chain	Res	Type
1	B	212	LEU
1	B	240	LEU
1	B	286	ARG
1	B	298	GLN
1	B	299	ARG
1	C	32	THR
1	C	50	THR
1	C	54	LYS
1	C	145	ILE
1	C	163	ARG
1	C	169	HIS
1	C	177	HIS
1	C	212	LEU
1	C	240	LEU
1	C	250	SER
1	C	255	ARG
1	C	291	VAL
1	D	29	LEU
1	D	38	TYR
1	D	90	LYS
1	D	124	GLN
1	D	145	ILE
1	D	150	GLU
1	D	156	GLU
1	D	158	ASP
1	D	167	SER
1	D	182	GLN
1	D	212	LEU
1	D	255	ARG
1	D	286	ARG
1	D	302	LEU
1	D	316	VAL
1	E	29	LEU
1	E	32	THR
1	E	50	THR
1	E	64	GLU
1	E	65	ARG
1	E	123	ARG
1	E	141	ARG
1	E	174	ARG
1	E	179	SER
1	E	212	LEU

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Mol	Chain	Res	Type
1	E	240	LEU
1	E	302	LEU
1	E	306	LEU
1	F	32	THR
1	F	50	THR
1	F	90	LYS
1	F	138	GLN
1	F	145	ILE
1	F	173	ILE
1	F	212	LEU
1	F	230	GLU
1	F	233	GLN
1	F	240	LEU
1	F	292	GLU
1	F	293	ASP
1	F	297	ILE
1	F	299	ARG
1	F	302	LEU
1	G	46	LYS
1	G	54	LYS
1	G	89	ASN
1	G	123	ARG
1	G	212	LEU
1	G	233	GLN
1	G	240	LEU
1	G	295	LEU
1	G	296	LEU
1	G	297	ILE
1	G	316	VAL
1	H	42	GLN
1	H	90	LYS
1	H	124	GLN
1	H	145	ILE
1	H	173	ILE
1	H	177	HIS
1	H	226	GLU
1	H	240	LEU
1	H	296	LEU
1	H	297	ILE
1	H	306	LEU
1	H	309	LEU
1	H	314	VAL

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Mol	Chain	Res	Type
1	I	32	THR
1	I	65	ARG
1	I	129	GLU
1	I	145	ILE
1	I	157	ILE
1	I	173	ILE
1	I	180	SER
1	I	182	GLN
1	I	184	ASN
1	I	194	ARG
1	I	212	LEU
1	I	230	GLU
1	I	239	MET
1	I	240	LEU
1	I	264	GLN
1	I	299	ARG
1	I	315	LEU
1	J	32	THR
1	J	49	LYS
1	J	56	LEU
1	J	90	LYS
1	J	99	ARG
1	J	124	GLN
1	J	145	ILE
1	J	151	ASN
1	J	173	ILE
1	J	180	SER
1	J	187	GLU
1	J	212	LEU
1	J	233	GLN
1	J	240	LEU
1	J	286	ARG
1	J	291	VAL
1	J	295	LEU
1	J	297	ILE
1	J	306	LEU
1	J	309	LEU
1	J	317	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	60	ASN
1	A	89	ASN
1	A	154	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
1	C	287	GLN
1	D	62	GLN
1	D	177	HIS
1	D	182	GLN
1	D	184	ASN
1	D	251	ASN
1	D	287	GLN
1	E	62	GLN
1	E	186	ASN
1	F	136	ASN
1	F	138	GLN
1	F	151	ASN
1	F	182	GLN
1	G	138	GLN
1	G	139	GLN
1	G	182	GLN
1	G	251	ASN
1	G	285	HIS
1	H	42	GLN
1	H	125	GLN
1	H	139	GLN
1	H	251	ASN
1	H	289	ASN
1	I	42	GLN
1	I	233	GLN
1	I	264	GLN
1	J	124	GLN
1	J	177	HIS

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Mol	Chain	Res	Type
1	J	185	GLN
1	J	233	GLN
1	J	251	ASN
1	J	287	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	H	401	-	13,16,16	3.70	9 (69%)	23,30,30	3.70	14 (60%)
2	BR7	A	402	-	13,16,16	3.99	10 (76%)	23,30,30	3.74	14 (60%)
2	BR7	J	401	-	13,16,16	3.64	8 (61%)	23,30,30	3.51	13 (56%)
2	BR7	F	401	-	13,16,16	3.66	8 (61%)	23,30,30	3.73	15 (65%)
2	BR7	A	401	-	13,16,16	3.63	9 (69%)	23,30,30	3.53	14 (60%)
2	BR7	E	401	-	13,16,16	3.72	11 (84%)	23,30,30	4.26	12 (52%)
2	BR7	G	401	-	13,16,16	3.81	9 (69%)	23,30,30	3.58	15 (65%)
2	BR7	I	401	-	13,16,16	3.81	9 (69%)	23,30,30	3.40	10 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BR7	D	401	-	13,16,16	3.82	9 (69%)	23,30,30	4.11	13 (56%)
2	BR7	C	401	-	13,16,16	3.90	10 (76%)	23,30,30	4.07	14 (60%)
2	BR7	F	402	-	13,16,16	3.88	10 (76%)	23,30,30	3.73	14 (60%)
2	BR7	B	401	-	13,16,16	3.86	11 (84%)	23,30,30	4.38	12 (52%)

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

All (113) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	402	BR7	C09-C10	-10.49	1.37	1.53
2	C	401	BR7	C09-C10	-10.37	1.38	1.53
2	F	402	BR7	C09-C10	-10.34	1.38	1.53
2	I	401	BR7	C09-C10	-10.31	1.38	1.53
2	D	401	BR7	C09-C10	-10.30	1.38	1.53
2	H	401	BR7	C09-C10	-10.26	1.38	1.53
2	G	401	BR7	C09-C10	-10.16	1.38	1.53
2	B	401	BR7	C09-C10	-10.07	1.38	1.53
2	F	401	BR7	C09-C10	-10.00	1.38	1.53
2	A	401	BR7	C09-C10	-9.76	1.38	1.53
2	J	401	BR7	C09-C10	-9.74	1.38	1.53
2	E	401	BR7	C09-C10	-9.61	1.39	1.53
2	J	401	BR7	C11-C02	-4.55	1.47	1.53
2	E	401	BR7	C11-C02	-4.51	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	BR7	C11-C02	-4.49	1.47	1.53
2	D	401	BR7	C03-C02	-4.45	1.47	1.53
2	B	401	BR7	C03-C02	-4.31	1.47	1.53
2	I	401	BR7	C11-C02	-4.29	1.47	1.53
2	G	401	BR7	C11-C02	-4.25	1.48	1.53
2	I	401	BR7	C03-C02	-4.22	1.48	1.53
2	H	401	BR7	C03-C02	-4.15	1.48	1.53
2	C	401	BR7	C03-C02	-4.09	1.48	1.53
2	G	401	BR7	C03-C02	-4.08	1.48	1.53
2	A	401	BR7	C11-C02	-4.07	1.48	1.53
2	C	401	BR7	C11-C02	-4.06	1.48	1.53
2	D	401	BR7	C11-C02	-4.05	1.48	1.53
2	F	401	BR7	C11-C02	-4.04	1.48	1.53
2	A	402	BR7	C11-C02	-3.97	1.48	1.53
2	A	401	BR7	C03-C02	-3.89	1.48	1.53
2	F	402	BR7	C11-C02	-3.87	1.48	1.53
2	E	401	BR7	C03-C02	-3.85	1.48	1.53
2	J	401	BR7	C03-C02	-3.83	1.48	1.53
2	F	402	BR7	C03-C02	-3.82	1.48	1.53
2	F	401	BR7	C03-C02	-3.81	1.48	1.53
2	H	401	BR7	C11-C02	-3.79	1.48	1.53
2	A	402	BR7	C03-C02	-3.58	1.48	1.53
2	A	402	BR7	C08-C02	-3.51	1.49	1.53
2	C	401	BR7	C08-C02	-3.44	1.49	1.53
2	A	402	BR7	C-C04	-3.36	1.49	1.53
2	F	402	BR7	C08-C02	-3.17	1.49	1.53
2	J	401	BR7	C08-C02	-3.10	1.49	1.53
2	F	401	BR7	C08-C02	-3.09	1.49	1.53
2	G	401	BR7	C08-C02	-3.06	1.49	1.53
2	B	401	BR7	C03-C04	-3.02	1.49	1.53
2	F	402	BR7	C-C04	-3.02	1.49	1.53
2	C	401	BR7	C03-C04	-3.00	1.49	1.53
2	F	402	BR7	C05-C04	-2.98	1.47	1.54
2	A	402	BR7	C06-C04	-2.92	1.49	1.53
2	D	401	BR7	C08-C02	-2.91	1.49	1.53
2	I	401	BR7	C08-C02	-2.91	1.49	1.53
2	E	401	BR7	C-C04	-2.90	1.49	1.53
2	A	401	BR7	C08-C02	-2.90	1.49	1.53
2	A	402	BR7	C05-C04	-2.87	1.48	1.54
2	H	401	BR7	C08-C02	-2.85	1.49	1.53
2	D	401	BR7	C03-C04	-2.84	1.49	1.53
2	A	402	BR7	C-C10	-2.83	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	401	BR7	C-C04	-2.81	1.49	1.53
2	G	401	BR7	C03-C04	-2.78	1.50	1.53
2	B	401	BR7	C-C04	-2.78	1.50	1.53
2	E	401	BR7	C08-C02	-2.76	1.50	1.53
2	C	401	BR7	C06-C04	-2.74	1.50	1.53
2	J	401	BR7	C06-C04	-2.70	1.50	1.53
2	B	401	BR7	C08-C02	-2.66	1.50	1.53
2	E	401	BR7	C05-C04	-2.64	1.48	1.54
2	A	401	BR7	C-C04	-2.62	1.50	1.53
2	F	402	BR7	C06-C04	-2.62	1.50	1.53
2	F	402	BR7	C03-C04	-2.61	1.50	1.53
2	E	401	BR7	C03-C04	-2.58	1.50	1.53
2	F	401	BR7	C03-C04	-2.57	1.50	1.53
2	I	401	BR7	C06-C04	-2.56	1.50	1.53
2	I	401	BR7	C05-C04	-2.51	1.48	1.54
2	D	401	BR7	C01-C02	-2.49	1.48	1.54
2	F	402	BR7	C01-C02	-2.47	1.49	1.54
2	D	401	BR7	C05-C04	-2.45	1.49	1.54
2	J	401	BR7	C05-C04	-2.45	1.49	1.54
2	E	401	BR7	C06-C04	-2.44	1.50	1.53
2	G	401	BR7	C01-C02	-2.44	1.49	1.54
2	A	401	BR7	C06-C04	-2.44	1.50	1.53
2	C	401	BR7	C05-C04	-2.43	1.49	1.54
2	F	401	BR7	C-C04	-2.43	1.50	1.53
2	B	401	BR7	C-C10	-2.42	1.49	1.53
2	I	401	BR7	C01-C02	-2.40	1.49	1.54
2	B	401	BR7	C01-C02	-2.40	1.49	1.54
2	H	401	BR7	C05-C04	-2.38	1.49	1.54
2	A	402	BR7	C01-C02	-2.38	1.49	1.54
2	A	402	BR7	C03-C04	-2.34	1.50	1.53
2	H	401	BR7	C-C04	-2.33	1.50	1.53
2	I	401	BR7	C-C04	-2.33	1.50	1.53
2	A	401	BR7	C05-C04	-2.32	1.49	1.54
2	G	401	BR7	C05-C04	-2.29	1.49	1.54
2	F	402	BR7	C-C10	-2.26	1.50	1.53
2	H	401	BR7	C03-C04	-2.25	1.50	1.53
2	A	401	BR7	C-C10	-2.25	1.50	1.53
2	C	401	BR7	C-C10	-2.25	1.50	1.53
2	H	401	BR7	C06-C04	-2.24	1.50	1.53
2	B	401	BR7	C05-C04	-2.23	1.49	1.54
2	I	401	BR7	C03-C04	-2.22	1.50	1.53
2	B	401	BR7	C06-C04	-2.21	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	BR7	C01-C02	-2.21	1.49	1.54
2	F	401	BR7	C01-C02	-2.20	1.49	1.54
2	C	401	BR7	C-C04	-2.17	1.50	1.53
2	F	401	BR7	C05-C04	-2.16	1.49	1.54
2	G	401	BR7	C-C10	-2.15	1.50	1.53
2	H	401	BR7	C01-C02	-2.15	1.49	1.54
2	E	401	BR7	C01-C02	-2.14	1.49	1.54
2	D	401	BR7	C-C04	-2.14	1.50	1.53
2	J	401	BR7	C-C04	-2.12	1.50	1.53
2	E	401	BR7	C-C10	-2.11	1.50	1.53
2	A	401	BR7	C01-C02	-2.09	1.49	1.54
2	B	401	BR7	C11-C10	-2.07	1.50	1.53
2	J	401	BR7	C01-C02	-2.06	1.49	1.54
2	D	401	BR7	C06-C04	-2.05	1.51	1.53
2	E	401	BR7	C11-C10	-2.02	1.50	1.53

All (160) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	B	401	BR7	C-C04-C03	-8.11	100.99	108.54
2	A	402	BR7	C-C10-C11	-7.85	106.15	110.55
2	A	402	BR7	BR-C10-C	-7.37	101.75	108.52
2	D	401	BR7	C-C10-C09	7.30	114.63	110.55
2	B	401	BR7	C06-C04-C03	7.21	115.25	108.54
2	E	401	BR7	C-C10-C09	7.05	114.50	110.55
2	C	401	BR7	C-C04-C03	-6.94	102.07	108.54
2	E	401	BR7	C-C04-C03	-6.88	102.13	108.54
2	A	402	BR7	C-C10-C09	6.82	114.36	110.55
2	A	402	BR7	BR-C10-C09	6.67	114.65	108.52
2	B	401	BR7	C-C10-C09	6.66	114.28	110.55
2	C	401	BR7	C06-C04-C03	6.50	114.59	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	BR7	C-C10-C09	6.48	114.18	110.55
2	G	401	BR7	C08-C02-C03	6.03	114.16	108.54
2	J	401	BR7	C06-C04-C03	6.03	114.15	108.54
2	E	401	BR7	C06-C04-C03	5.85	113.99	108.54
2	I	401	BR7	C06-C04-C03	5.83	113.97	108.54
2	E	401	BR7	BR-C10-C09	5.77	113.83	108.52
2	H	401	BR7	C-C10-C09	5.71	113.75	110.55
2	J	401	BR7	BR-C10-C09	5.70	113.76	108.52
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	F	402	BR7	C06-C04-C03	5.62	113.78	108.54
2	G	401	BR7	C-C10-C09	5.53	113.64	110.55
2	B	401	BR7	BR-C10-C09	5.52	113.59	108.52
2	D	401	BR7	C06-C04-C03	5.50	113.66	108.54
2	H	401	BR7	C06-C04-C03	5.48	113.65	108.54
2	A	401	BR7	BR-C10-C09	5.46	113.54	108.52
2	A	402	BR7	C06-C04-C03	5.33	113.50	108.54
2	G	401	BR7	BR-C10-C09	5.31	113.40	108.52
2	D	401	BR7	C08-C02-C03	5.26	113.44	108.54
2	F	402	BR7	C08-C02-C03	5.12	113.31	108.54
2	A	401	BR7	C06-C04-C03	5.10	113.29	108.54
2	F	401	BR7	C08-C02-C03	5.05	113.25	108.54
2	A	402	BR7	C-C04-C03	-4.90	103.97	108.54
2	C	401	BR7	BR-C10-C09	4.85	112.97	108.52
2	A	401	BR7	C-C10-C09	4.83	113.25	110.55
2	F	402	BR7	BR-C10-C09	4.69	112.83	108.52
2	C	401	BR7	C08-C02-C03	4.62	112.85	108.54
2	J	401	BR7	C-C04-C03	-4.48	104.37	108.54
2	H	401	BR7	C08-C02-C03	4.47	112.70	108.54
2	I	401	BR7	C-C04-C03	-4.42	104.42	108.54
2	G	401	BR7	C06-C04-C03	4.39	112.63	108.54
2	F	401	BR7	C-C04-C03	-4.34	104.50	108.54
2	A	401	BR7	C-C04-C03	-4.31	104.52	108.54
2	I	401	BR7	C08-C02-C03	4.30	112.55	108.54
2	G	401	BR7	C-C04-C03	-4.25	104.58	108.54
2	F	401	BR7	C06-C04-C03	4.21	112.47	108.54
2	I	401	BR7	C-C10-C09	4.19	112.89	110.55
2	F	402	BR7	BR-C10-C	-4.16	104.70	108.52
2	J	401	BR7	C08-C02-C03	4.14	112.39	108.54
2	E	401	BR7	C08-C02-C03	4.12	112.38	108.54
2	F	402	BR7	C-C04-C03	-4.11	104.71	108.54
2	H	401	BR7	C-C04-C03	-4.11	104.72	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	BR7	C08-C02-C03	4.09	112.35	108.54
2	F	401	BR7	C11-C10-C09	-4.08	108.27	110.55
2	F	401	BR7	BR-C10-C09	4.04	112.23	108.52
2	D	401	BR7	C-C04-C03	-4.00	104.81	108.54
2	A	401	BR7	C08-C02-C03	3.95	112.22	108.54
2	J	401	BR7	C10-C11-C02	3.86	113.70	107.39
2	H	401	BR7	C-C04-C06	-3.81	104.99	108.54
2	I	401	BR7	BR-C10-C09	3.79	112.01	108.52
2	F	401	BR7	C07-C06-C04	3.75	112.71	110.73
2	J	401	BR7	C11-C02-C03	-3.69	105.11	108.54
2	E	401	BR7	C11-C10-C09	-3.45	108.62	110.55
2	H	401	BR7	BR-C10-C11	3.44	111.68	108.52
2	F	402	BR7	BR-C10-C11	3.42	111.66	108.52
2	A	401	BR7	BR-C10-C	-3.41	105.39	108.52
2	A	401	BR7	C10-C11-C02	3.39	112.93	107.39
2	A	402	BR7	C08-C02-C03	3.39	111.69	108.54
2	I	401	BR7	C-C04-C06	-3.35	105.42	108.54
2	F	401	BR7	C-C04-C06	-3.31	105.46	108.54
2	G	401	BR7	C-C04-C06	-3.30	105.47	108.54
2	I	401	BR7	C10-C11-C02	3.26	112.72	107.39
2	D	401	BR7	C10-C11-C02	3.23	112.67	107.39
2	D	401	BR7	C-C04-C06	-3.21	105.55	108.54
2	E	401	BR7	C10-C11-C02	3.20	112.63	107.39
2	F	401	BR7	C10-C11-C02	3.20	112.62	107.39
2	J	401	BR7	C-C04-C06	-3.17	105.59	108.54
2	H	401	BR7	C10-C11-C02	3.11	112.48	107.39
2	F	402	BR7	C-C04-C06	-3.10	105.65	108.54
2	A	402	BR7	C11-C10-C09	-3.05	108.84	110.55
2	B	401	BR7	C10-C-C04	3.04	112.35	107.39
2	G	401	BR7	C07-C08-C02	-3.03	109.13	110.73
2	J	401	BR7	C11-C10-C09	-3.02	108.86	110.55
2	C	401	BR7	C10-C11-C02	2.99	112.28	107.39
2	A	401	BR7	C11-C02-C03	-2.99	105.76	108.54
2	G	401	BR7	C07-C06-C04	2.98	112.31	110.73
2	G	401	BR7	C10-C11-C02	2.95	112.21	107.39
2	I	401	BR7	C11-C02-C08	-2.91	105.83	108.54
2	A	401	BR7	C11-C10-C09	-2.90	108.92	110.55
2	G	401	BR7	C11-C02-C08	-2.89	105.84	108.54
2	F	402	BR7	C11-C10-C09	-2.87	108.94	110.55
2	A	401	BR7	C-C04-C06	-2.79	105.94	108.54
2	C	401	BR7	C10-C-C04	2.76	111.91	107.39
2	J	401	BR7	C-C10-C09	2.74	112.08	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	402	BR7	C07-C08-C02	-2.74	109.29	110.73
2	G	401	BR7	C05-C04-C06	2.70	114.22	110.55
2	D	401	BR7	C07-C08-C02	-2.70	109.31	110.73
2	G	401	BR7	C11-C10-C09	-2.70	109.04	110.55
2	C	401	BR7	C07-C08-C02	-2.70	109.31	110.73
2	G	401	BR7	C11-C02-C03	-2.69	106.04	108.54
2	B	401	BR7	C-C04-C06	-2.63	106.09	108.54
2	B	401	BR7	C10-C11-C02	2.63	111.68	107.39
2	F	402	BR7	C10-C11-C02	2.60	111.64	107.39
2	F	402	BR7	C11-C02-C08	-2.59	106.13	108.54
2	C	401	BR7	C-C04-C06	-2.58	106.14	108.54
2	E	401	BR7	C07-C08-C02	-2.56	109.38	110.73
2	A	402	BR7	C11-C02-C08	-2.54	106.18	108.54
2	H	401	BR7	C11-C10-C09	-2.49	109.16	110.55
2	D	401	BR7	C11-C10-C09	-2.46	109.17	110.55
2	D	401	BR7	BR-C10-C09	2.45	110.77	108.52
2	F	402	BR7	C10-C-C04	2.42	111.35	107.39
2	E	401	BR7	C01-C02-C11	-2.40	107.30	110.55
2	A	402	BR7	C07-C08-C02	-2.40	109.47	110.73
2	F	401	BR7	C11-C02-C03	-2.35	106.35	108.54
2	H	401	BR7	C11-C02-C03	-2.35	106.35	108.54
2	D	401	BR7	C07-C06-C04	2.34	111.97	110.73
2	A	402	BR7	BR-C10-C11	2.31	110.64	108.52
2	H	401	BR7	C11-C02-C08	-2.31	106.39	108.54
2	F	401	BR7	C11-C02-C08	-2.30	106.40	108.54
2	J	401	BR7	C11-C02-C08	-2.30	106.40	108.54
2	C	401	BR7	C05-C04-C	2.30	113.67	110.55
2	E	401	BR7	C10-C-C04	2.29	111.13	107.39
2	F	401	BR7	C10-C-C04	2.28	111.12	107.39
2	E	401	BR7	C11-C02-C08	-2.28	106.42	108.54
2	H	401	BR7	C10-C-C04	2.28	111.11	107.39
2	H	401	BR7	C07-C06-C04	2.26	111.92	110.73
2	A	401	BR7	C11-C02-C08	-2.24	106.46	108.54
2	I	401	BR7	C10-C-C04	2.23	111.04	107.39
2	C	401	BR7	C11-C02-C03	-2.21	106.48	108.54
2	A	402	BR7	C10-C11-C02	2.18	110.96	107.39
2	A	401	BR7	BR-C10-C11	2.18	110.52	108.52
2	J	401	BR7	C01-C02-C03	2.17	113.49	110.55
2	B	401	BR7	C01-C02-C11	-2.16	107.62	110.55
2	F	401	BR7	C07-C08-C02	-2.16	109.59	110.73
2	H	401	BR7	BR-C10-C09	2.14	110.49	108.52
2	D	401	BR7	C10-C-C04	2.11	110.85	107.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	BR7	C11-C02-C03	-2.11	106.58	108.54
2	F	401	BR7	C05-C04-C06	2.10	113.41	110.55
2	C	401	BR7	C11-C10-C09	-2.10	109.38	110.55
2	J	401	BR7	C10-C-C04	2.09	110.81	107.39
2	A	401	BR7	C10-C-C04	2.08	110.80	107.39
2	C	401	BR7	C11-C02-C08	-2.07	106.61	108.54
2	G	401	BR7	C10-C-C04	2.06	110.76	107.39
2	A	402	BR7	C-C04-C06	-2.05	106.63	108.54
2	B	401	BR7	C11-C10-C09	-2.02	109.42	110.55
2	A	402	BR7	C10-C-C04	2.02	110.69	107.39
2	B	401	BR7	BR-C10-C	-2.00	106.68	108.52

There are no chirality outliers.

There are no torsion outliers.

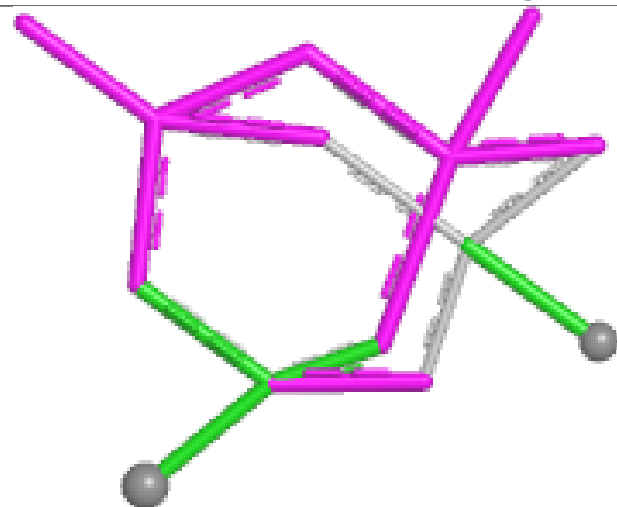
There are no ring outliers.

8 monomers are involved in 20 short contacts:

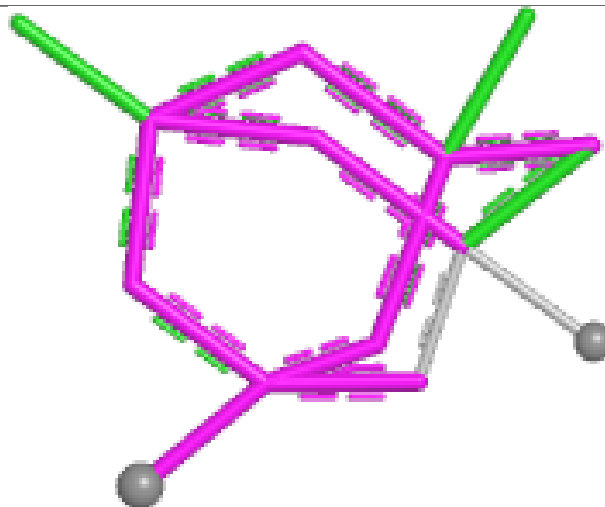
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	402	BR7	2	0
2	J	401	BR7	2	0
2	E	401	BR7	2	0
2	G	401	BR7	3	0
2	I	401	BR7	1	0
2	C	401	BR7	5	0
2	F	402	BR7	1	0
2	B	401	BR7	4	0

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

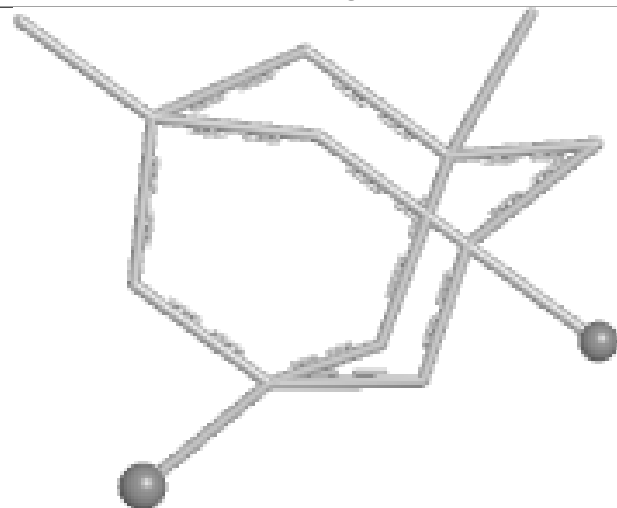
Ligand BR7 H 401



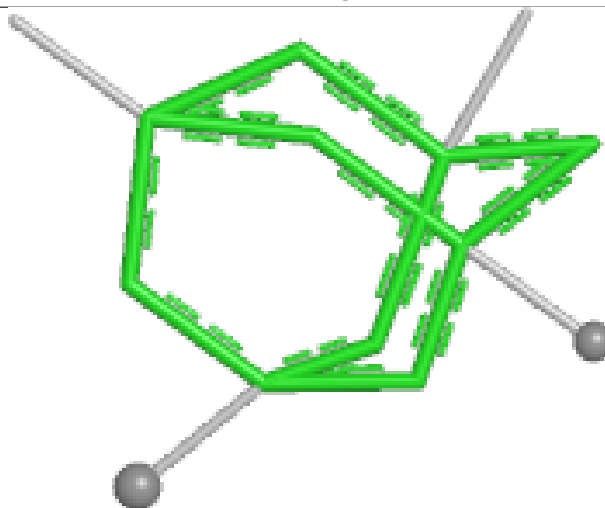
Bond lengths



Bond angles

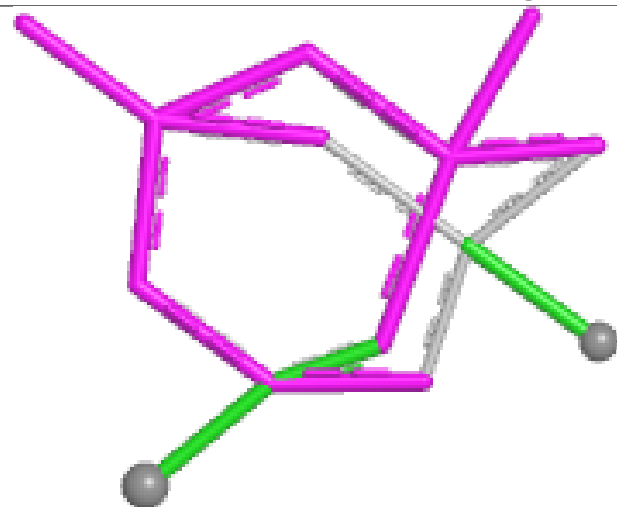


Torsions

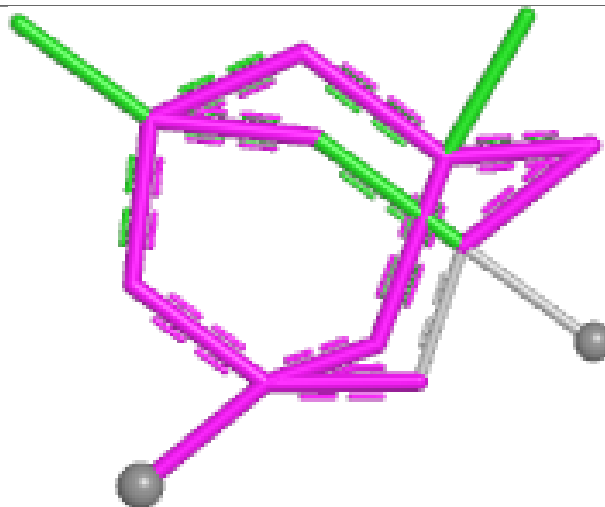


Rings

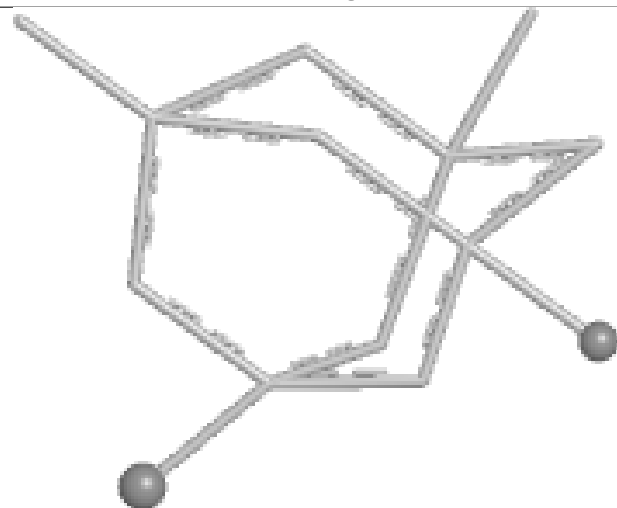
Ligand BR7 A 402



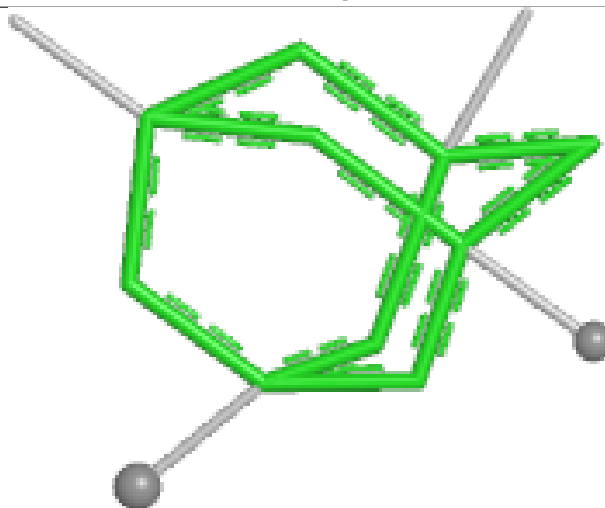
Bond lengths



Bond angles

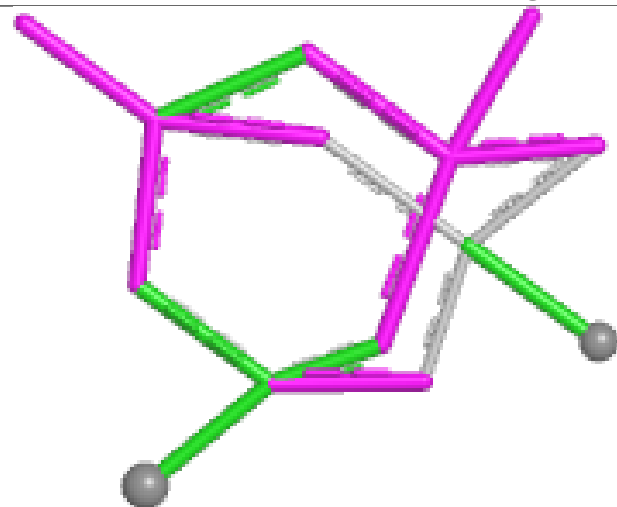


Torsions

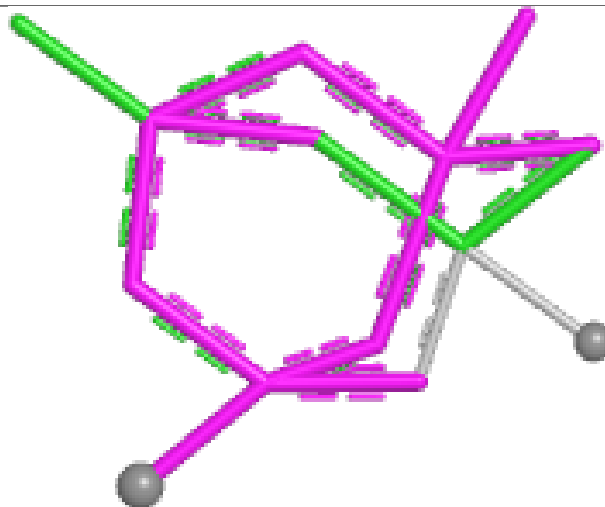


Rings

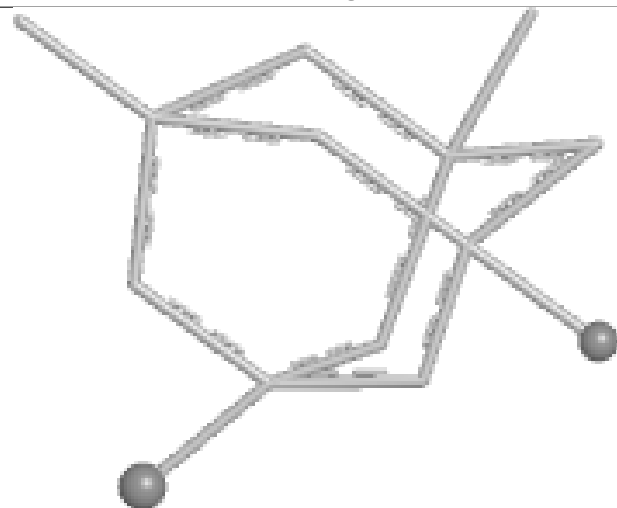
Ligand BR7 J 401



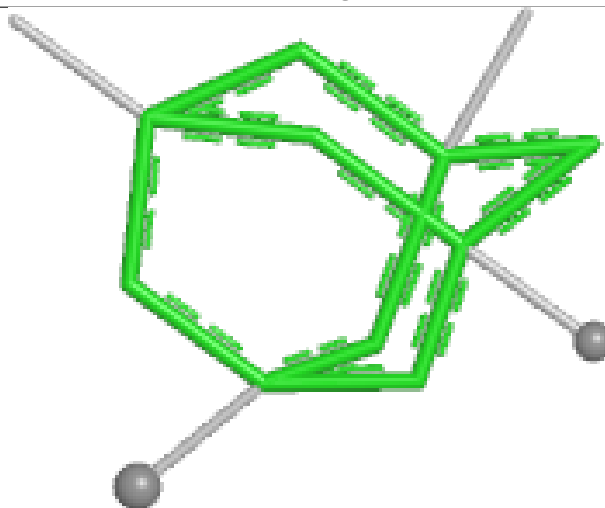
Bond lengths



Bond angles

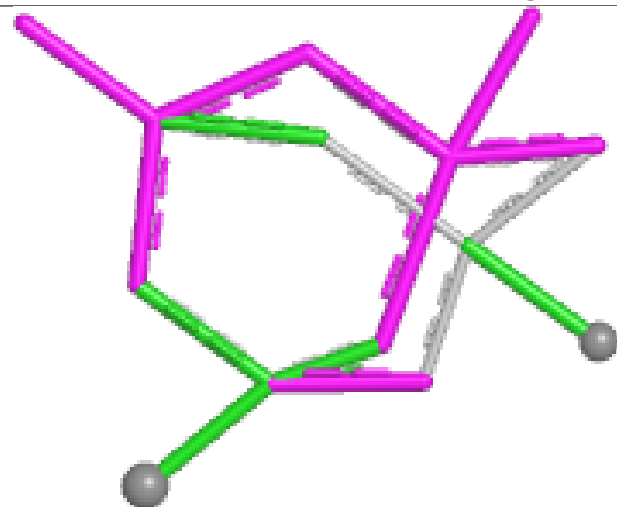


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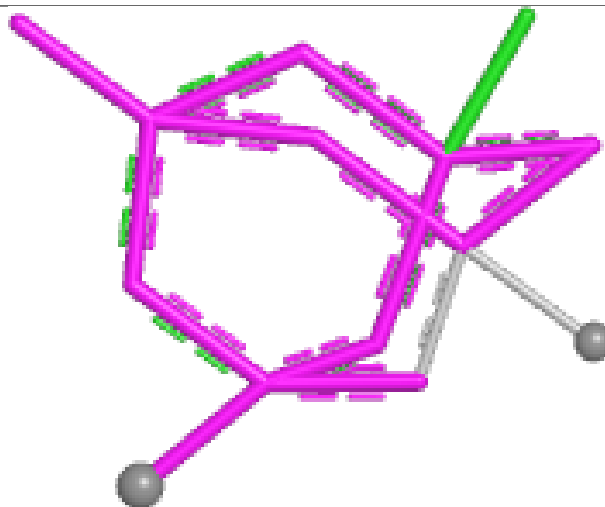


Rings

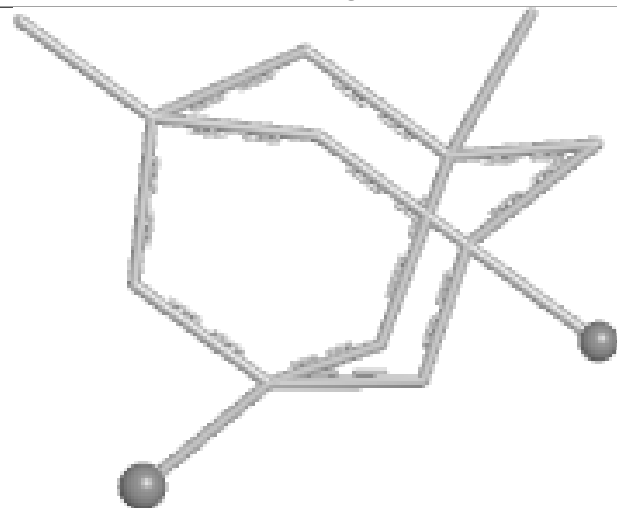
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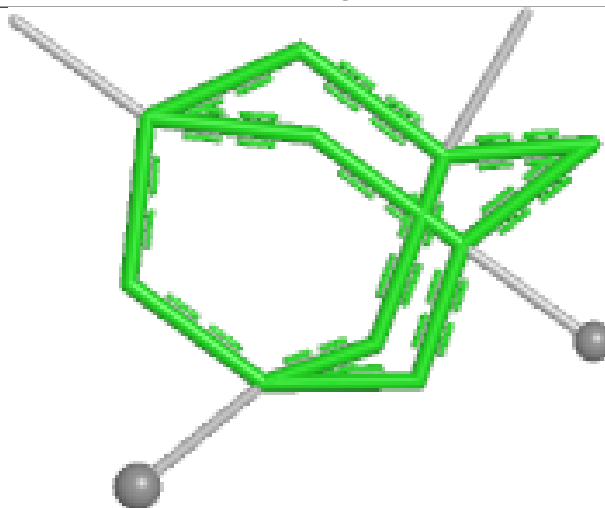
Bond lengths



Bond angles

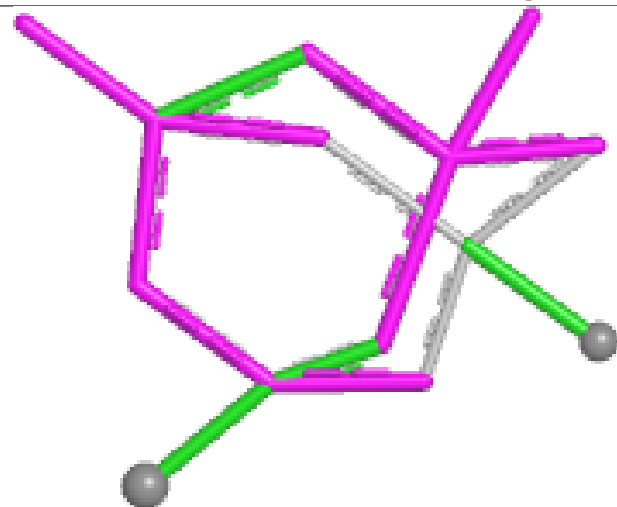


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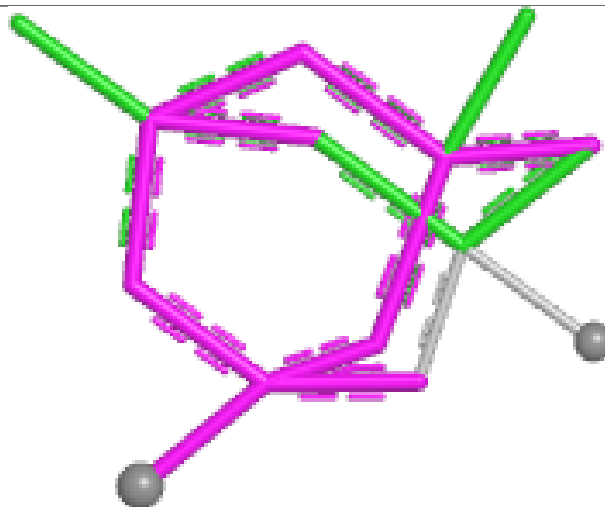


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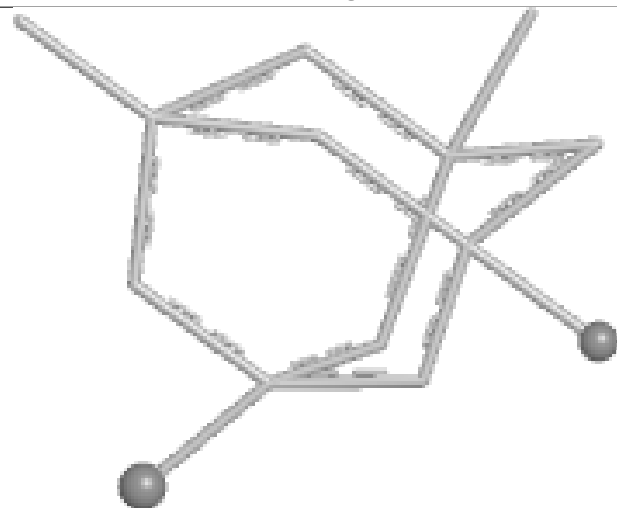
Ligand BR7 A 401



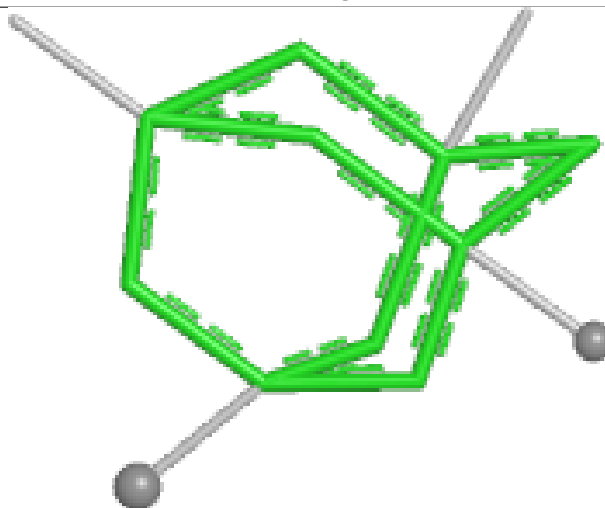
Bond lengths



Bond angles

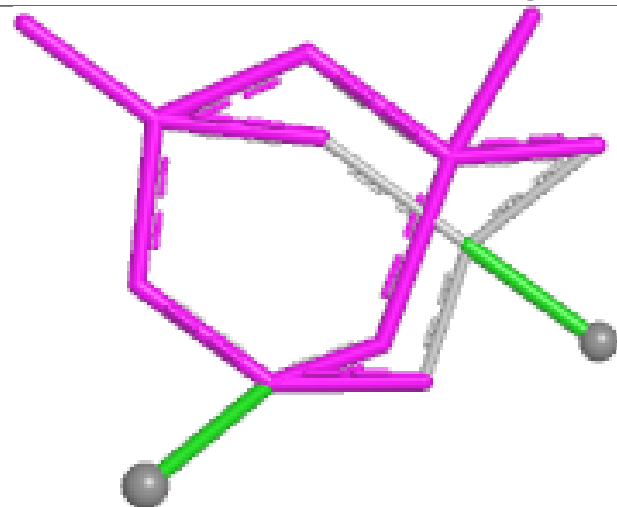


Torsions



Rings

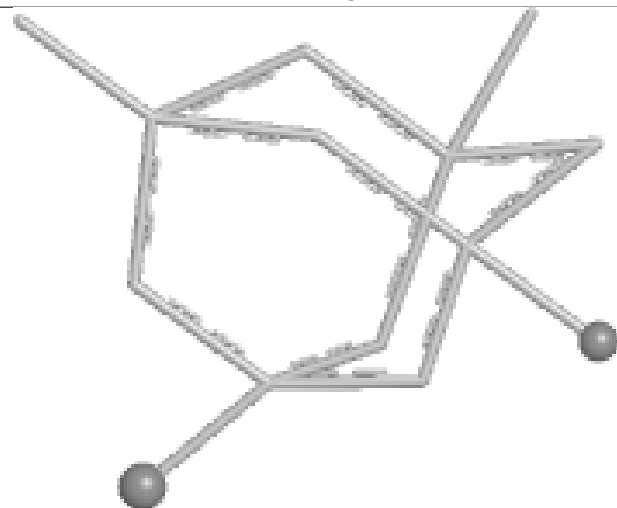
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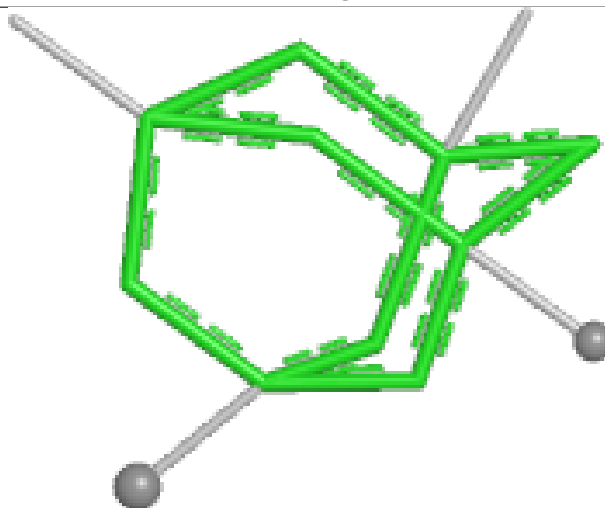
Bond lengths



Bond angles

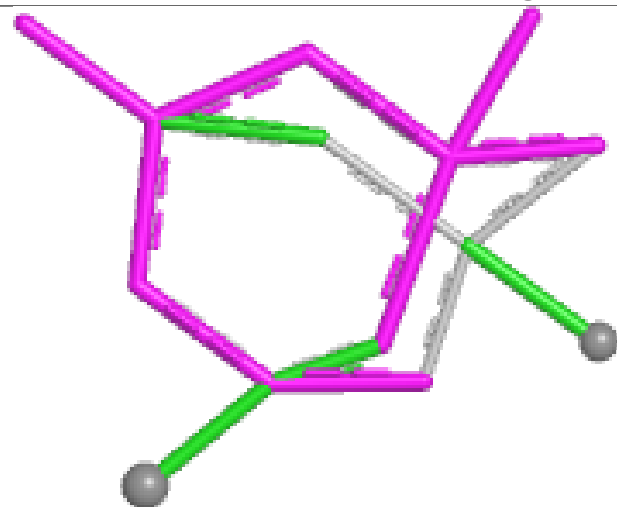


Torsions



Rings

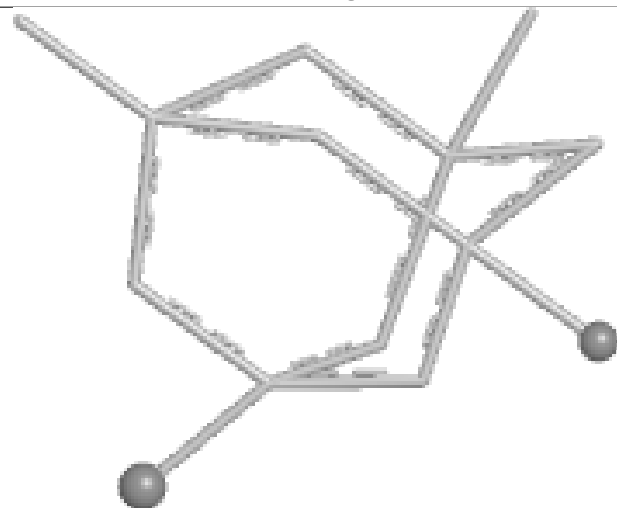
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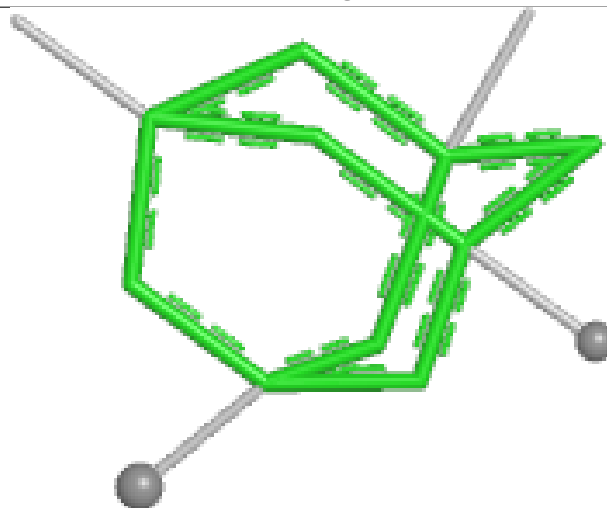
Bond lengths



Bond angles

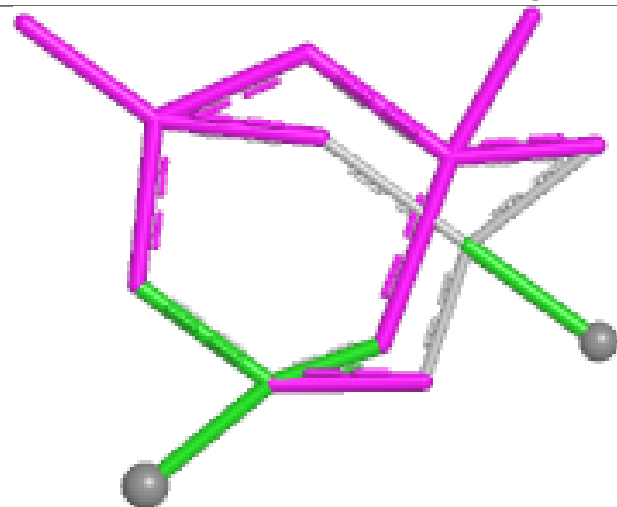


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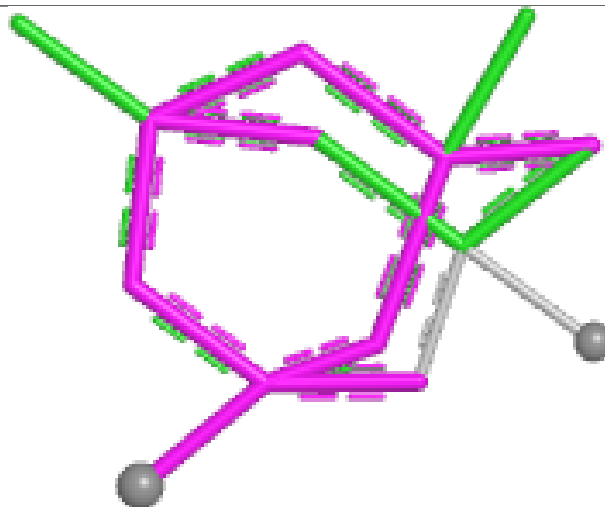


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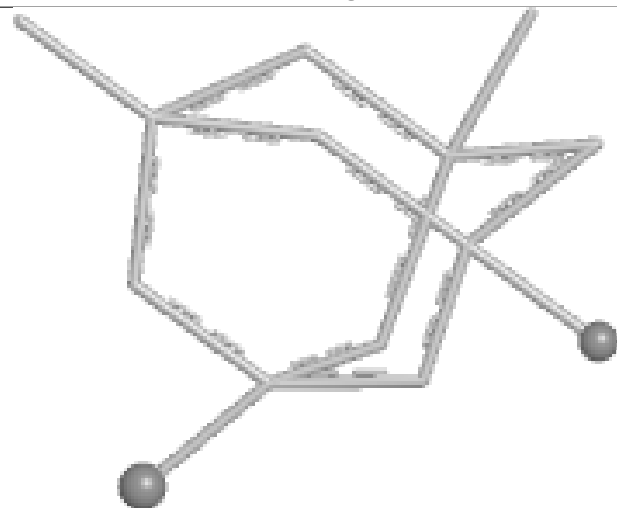
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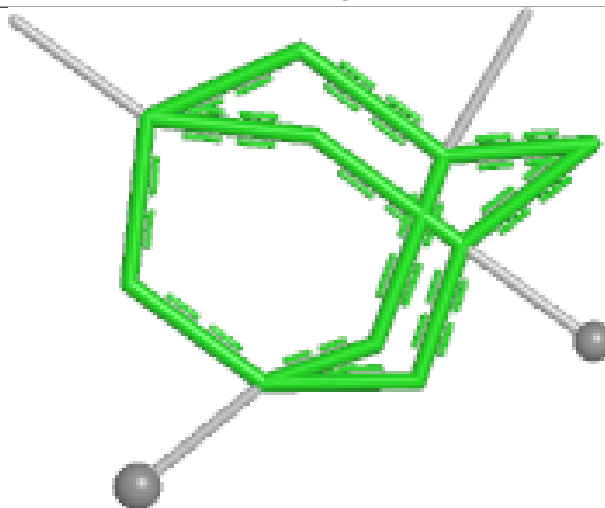
Bond lengths



Bond angles

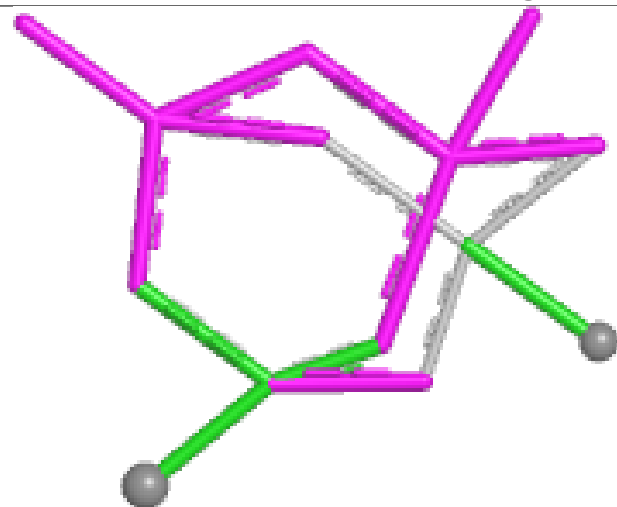


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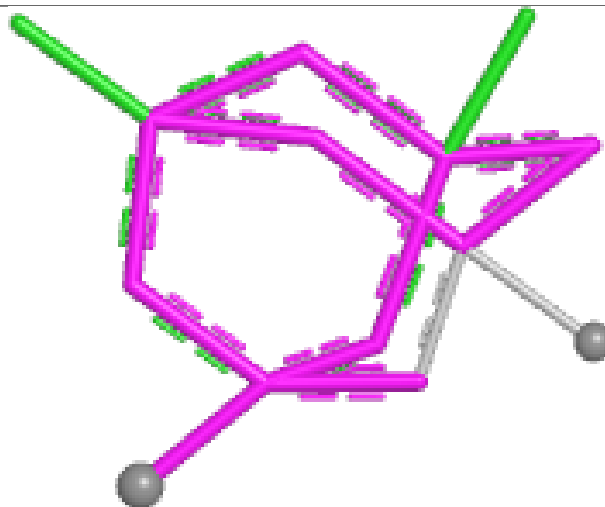


Rings

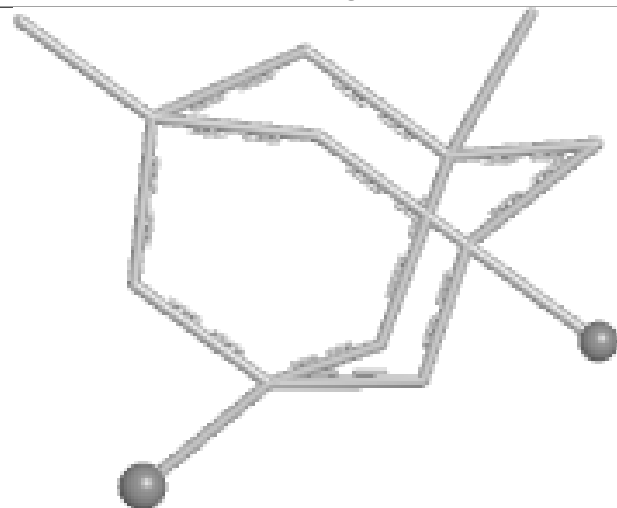
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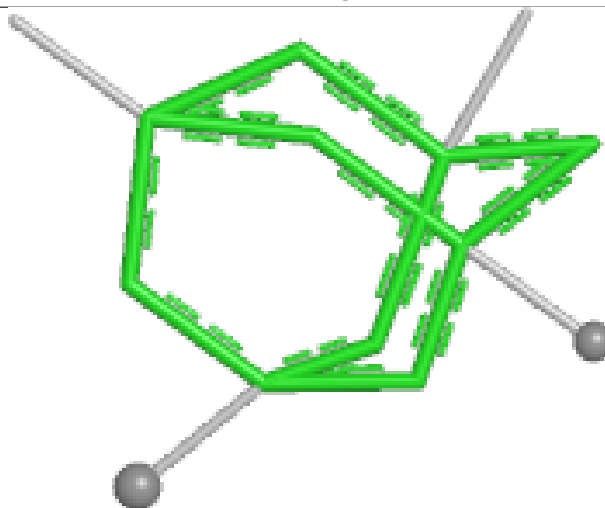
Bond lengths



Bond angles

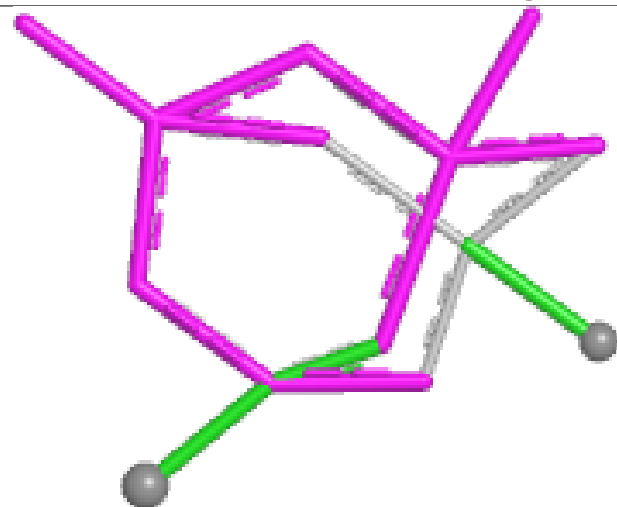


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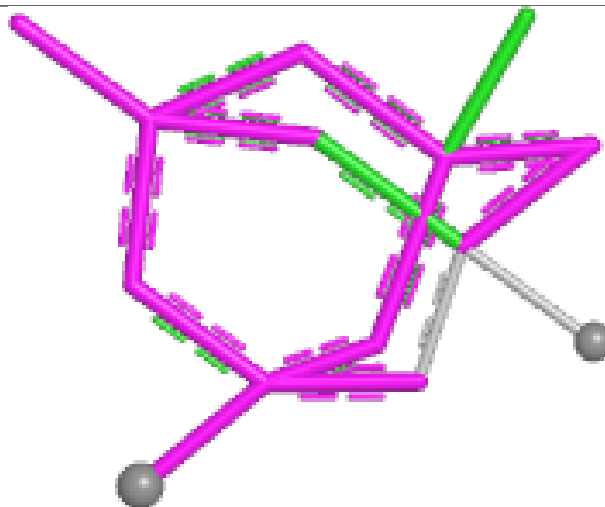


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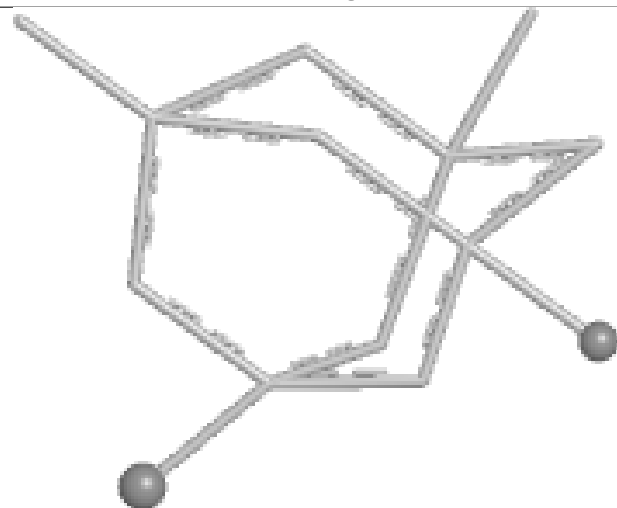
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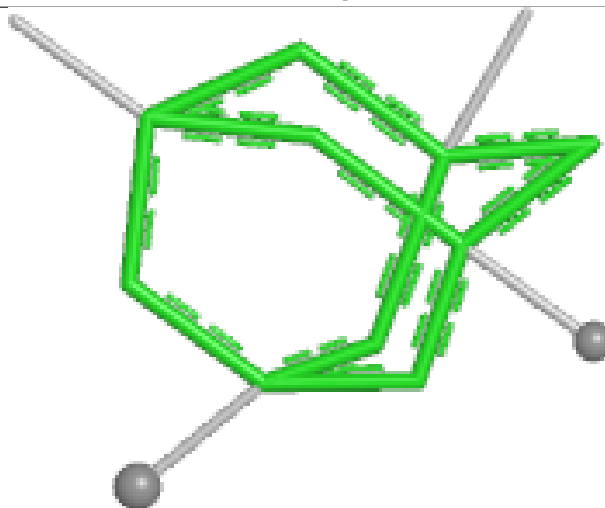
Bond lengths



Bond angles

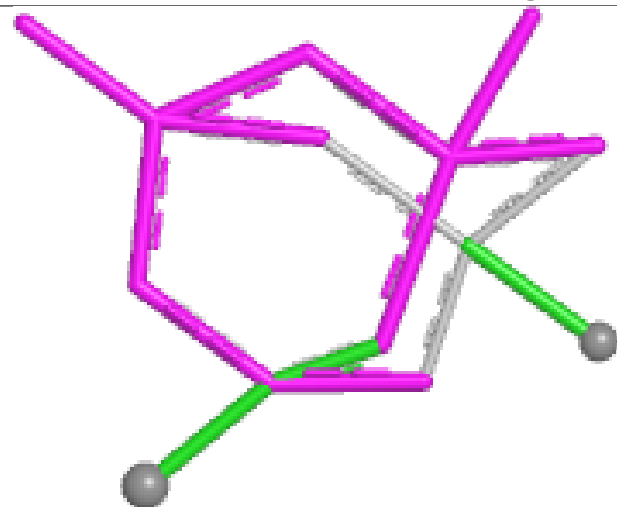


Torsions

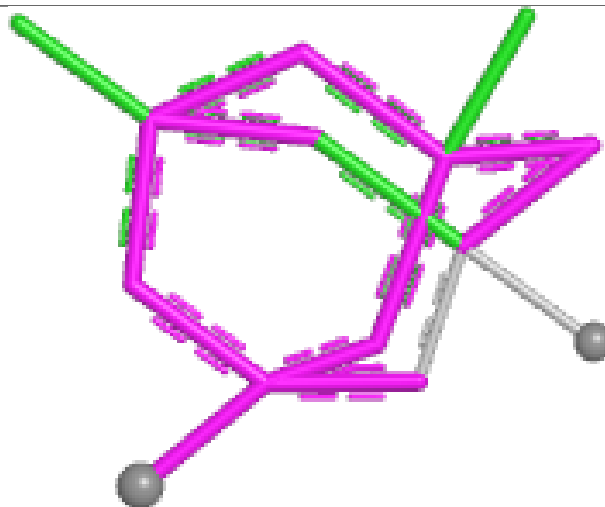


Rings

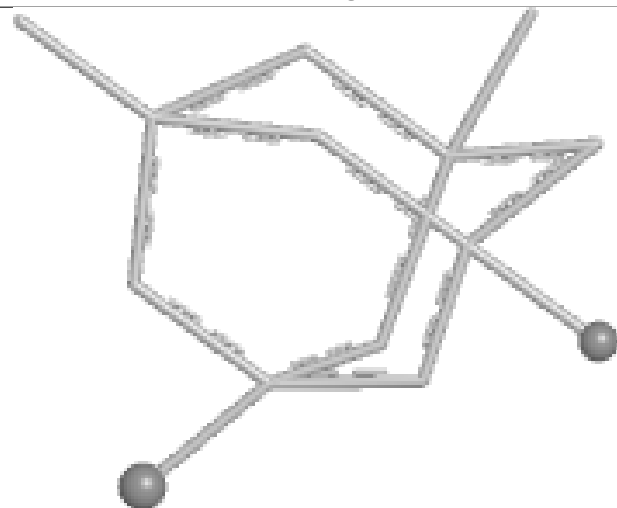
Ligand BR7 F 402



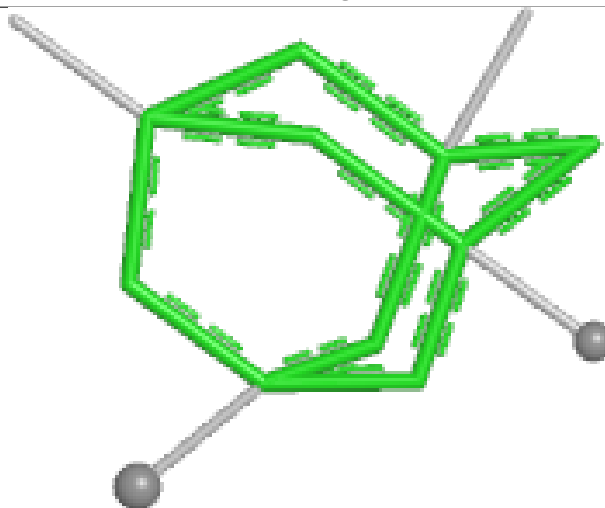
Bond lengths



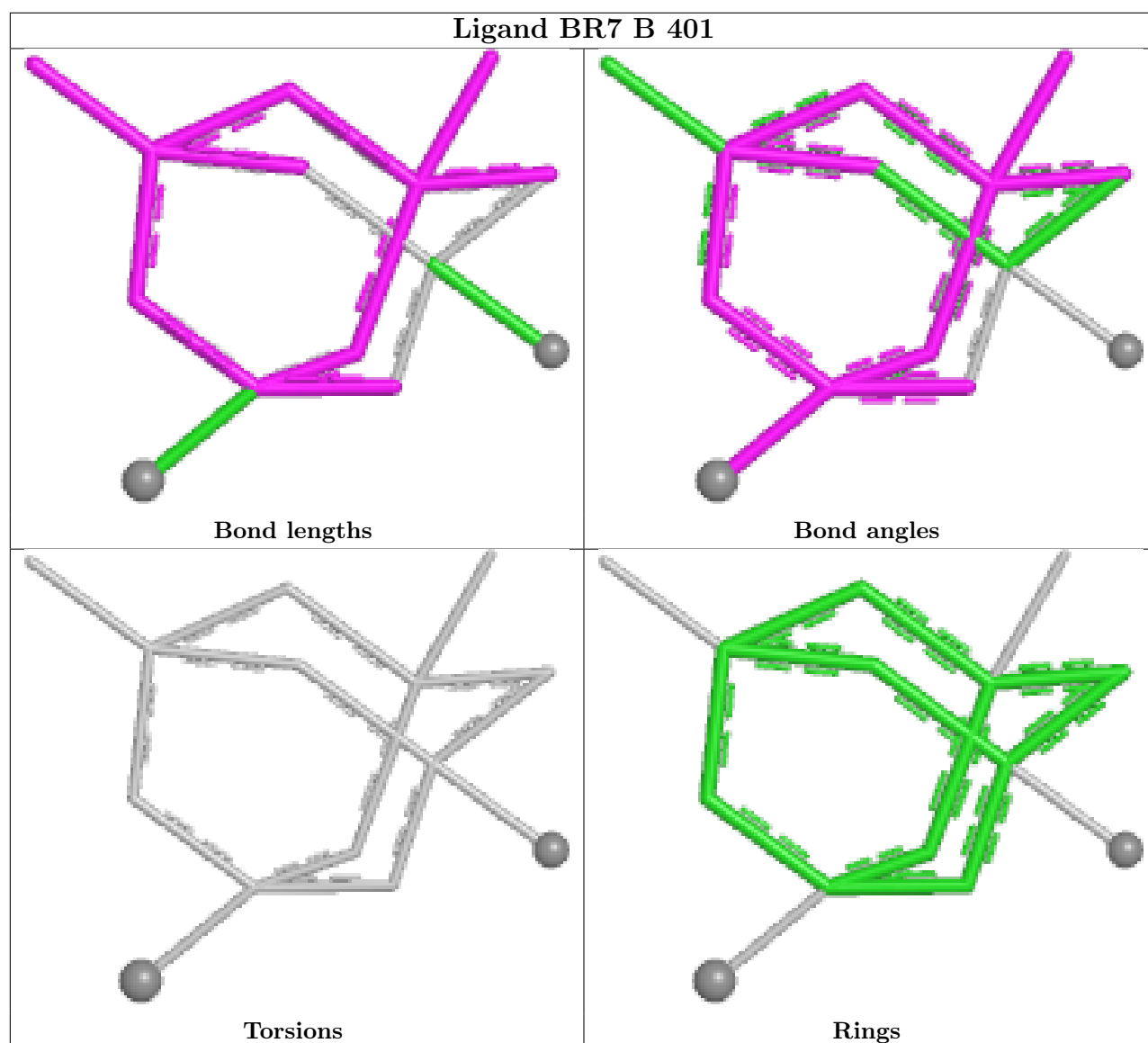
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	307/307 (100%)	0.53	23 (7%) 20 19	89, 136, 232, 324	0
1	B	307/307 (100%)	1.05	59 (19%) 3 5	78, 123, 237, 352	0
1	C	307/307 (100%)	0.67	31 (10%) 12 15	71, 119, 234, 291	0
1	D	307/307 (100%)	0.70	40 (13%) 7 10	73, 121, 228, 325	0
1	E	307/307 (100%)	0.78	43 (14%) 6 9	83, 129, 235, 381	0
1	F	307/307 (100%)	0.74	38 (12%) 8 11	84, 138, 250, 372	0
1	G	307/307 (100%)	0.98	59 (19%) 3 5	78, 122, 221, 324	0
1	H	307/307 (100%)	0.80	39 (12%) 8 11	79, 133, 250, 378	0
1	I	307/307 (100%)	0.85	41 (13%) 7 10	76, 131, 234, 327	0
1	J	307/307 (100%)	0.71	41 (13%) 7 10	91, 139, 272, 347	0
All	All	3070/3070 (100%)	0.78	414 (13%) 7 10	71, 129, 243, 381	0

All (414) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	290	GLY	11.2
1	C	312	GLY	10.6
1	E	291	VAL	10.4
1	C	313	CYS	10.3
1	E	289	ASN	8.7
1	F	176	ASP	8.3
1	B	31	GLN	8.1
1	I	251	ASN	7.9
1	F	226	GLU	7.9
1	C	306	LEU	7.7
1	H	185	GLN	7.6
1	C	314	VAL	7.6
1	H	308	PHE	7.4

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Mol	Chain	Res	Type	RSRZ
1	G	255	ARG	7.3
1	C	309	LEU	7.1
1	I	252	ILE	6.8
1	B	114	MET	6.6
1	B	112	ASN	6.6
1	I	208	PHE	6.5
1	H	138	GLN	6.4
1	B	255	ARG	6.4
1	I	248	TYR	6.3
1	B	113	ASP	6.2
1	I	253	LEU	6.2
1	J	82	VAL	6.1
1	I	245	TYR	6.1
1	A	176	ASP	6.0
1	D	226	GLU	5.8
1	E	255	ARG	5.8
1	H	311	ILE	5.7
1	B	116	PHE	5.7
1	B	206	TRP	5.5
1	H	137	ASN	5.4
1	I	52	GLY	5.4
1	D	89	ASN	5.4
1	H	181	VAL	5.4
1	B	256	LEU	5.3
1	G	253	LEU	5.3
1	G	285	HIS	5.3
1	H	180	SER	5.2
1	B	28	THR	5.2
1	F	225	LEU	5.2
1	C	311	ILE	5.2
1	I	206	TRP	5.0
1	J	230	GLU	5.0
1	H	306	LEU	5.0
1	D	251	ASN	4.9
1	D	233	GLN	4.9
1	C	251	ASN	4.9
1	F	317	ILE	4.8
1	I	179	SER	4.8
1	B	183	PRO	4.7
1	F	59	GLU	4.7
1	C	308	PHE	4.5
1	B	122	ASP	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	254	PRO	4.5
1	F	89	ASN	4.4
1	D	250	SER	4.4
1	G	228	PHE	4.4
1	B	185	GLN	4.4
1	J	308	PHE	4.4
1	F	251	ASN	4.3
1	F	88	GLY	4.3
1	F	252	ILE	4.3
1	F	224	TRP	4.3
1	G	126	PHE	4.3
1	H	140	LEU	4.3
1	B	288	ALA	4.3
1	F	11	PRO	4.2
1	H	312	GLY	4.2
1	E	77	GLU	4.2
1	B	181	VAL	4.2
1	D	317	ILE	4.2
1	C	307	GLY	4.1
1	G	282	PHE	4.1
1	J	305	PRO	4.1
1	B	102	TYR	4.1
1	H	307	GLY	4.1
1	D	204	TYR	4.1
1	C	316	VAL	4.1
1	C	137	ASN	4.1
1	B	150	GLU	4.0
1	H	302	LEU	4.0
1	A	183	PRO	4.0
1	B	29	LEU	3.9
1	D	38	TYR	3.9
1	G	64	GLU	3.9
1	G	229	SER	3.9
1	F	175	TYR	3.9
1	H	183	PRO	3.9
1	G	181	VAL	3.9
1	G	75	ALA	3.9
1	F	90	LYS	3.9
1	J	129	GLU	3.8
1	E	285	HIS	3.8
1	H	288	ALA	3.8
1	B	194	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	J	90	LYS	3.8
1	D	88	GLY	3.7
1	D	230	GLU	3.7
1	G	133	PHE	3.7
1	G	251	ASN	3.7
1	C	180	SER	3.7
1	G	178	LEU	3.7
1	D	249	THR	3.6
1	G	183	PRO	3.6
1	I	64	GLU	3.6
1	B	115	ASP	3.6
1	H	303	ALA	3.6
1	C	187	GLU	3.6
1	A	175	TYR	3.6
1	I	230	GLU	3.6
1	G	43	TRP	3.6
1	F	315	LEU	3.6
1	G	160	TRP	3.5
1	C	315	LEU	3.5
1	H	187	GLU	3.5
1	B	118	LEU	3.5
1	C	188	PHE	3.5
1	G	65	ARG	3.5
1	C	310	ALA	3.5
1	I	291	VAL	3.5
1	H	309	LEU	3.5
1	H	184	ASN	3.5
1	F	247	SER	3.4
1	C	252	ILE	3.4
1	E	11	PRO	3.4
1	A	306	LEU	3.4
1	F	231	ARG	3.4
1	B	184	ASN	3.4
1	F	60	ASN	3.4
1	H	123	ARG	3.4
1	B	44	THR	3.3
1	I	296	LEU	3.3
1	G	156	GLU	3.3
1	J	224	TRP	3.3
1	J	81	VAL	3.3
1	G	232	LEU	3.3
1	F	253	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	I	108	GLY	3.3
1	E	152	ALA	3.3
1	G	308	PHE	3.3
1	G	281	ILE	3.3
1	C	111	SER	3.3
1	A	303	ALA	3.2
1	F	174	ARG	3.2
1	J	11	PRO	3.2
1	G	89	ASN	3.2
1	H	182	GLN	3.2
1	A	150	GLU	3.2
1	E	287	GLN	3.2
1	D	18	ILE	3.2
1	G	252	ILE	3.2
1	J	225	LEU	3.2
1	B	73	VAL	3.2
1	I	210	LEU	3.2
1	J	250	SER	3.2
1	I	250	SER	3.1
1	J	83	GLY	3.1
1	I	249	THR	3.1
1	B	103	ASN	3.1
1	F	222	VAL	3.1
1	J	79	ILE	3.1
1	F	105	ARG	3.1
1	H	233	GLN	3.1
1	I	181	VAL	3.1
1	I	227	SER	3.1
1	G	226	GLU	3.1
1	D	208	PHE	3.1
1	I	300	CYS	3.1
1	I	35	VAL	3.1
1	E	63	ILE	3.1
1	E	288	ALA	3.1
1	H	150	GLU	3.1
1	D	11	PRO	3.1
1	F	227	SER	3.0
1	D	203	TYR	3.0
1	J	184	ASN	3.0
1	B	257	PRO	3.0
1	E	82	VAL	3.0
1	H	255	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	19	PHE	3.0
1	B	253	LEU	3.0
1	D	205	LEU	3.0
1	B	101	ILE	3.0
1	I	205	LEU	3.0
1	B	126	PHE	3.0
1	I	304	PHE	3.0
1	J	291	VAL	3.0
1	F	117	ARG	3.0
1	A	177	HIS	2.9
1	F	177	HIS	2.9
1	D	297	ILE	2.9
1	E	257	PRO	2.9
1	H	241	THR	2.9
1	J	298	GLN	2.9
1	E	151	ASN	2.9
1	J	233	GLN	2.9
1	G	297	ILE	2.9
1	B	196	ASP	2.9
1	B	199	ARG	2.9
1	D	299	ARG	2.9
1	G	317	ILE	2.9
1	B	58	VAL	2.9
1	B	160	TRP	2.9
1	G	73	VAL	2.9
1	E	258	TYR	2.9
1	G	302	LEU	2.9
1	H	305	PRO	2.9
1	I	203	TYR	2.9
1	B	71	LEU	2.8
1	I	204	TYR	2.8
1	D	113	ASP	2.8
1	A	11	PRO	2.8
1	B	258	TYR	2.8
1	E	25	GLY	2.8
1	E	83	GLY	2.8
1	G	86	ASP	2.8
1	B	74	PRO	2.8
1	G	150	GLU	2.8
1	I	290	GLY	2.8
1	J	315	LEU	2.7
1	G	85	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	152	ALA	2.7
1	J	303	ALA	2.7
1	D	177	HIS	2.7
1	G	82	VAL	2.7
1	A	120	PRO	2.7
1	D	253	LEU	2.7
1	C	172	ASP	2.7
1	D	206	TRP	2.7
1	B	125	GLN	2.7
1	E	233	GLN	2.7
1	G	238	LEU	2.7
1	E	133	PHE	2.7
1	G	179	SER	2.7
1	C	152	ALA	2.7
1	D	105	ARG	2.7
1	D	255	ARG	2.7
1	E	123	ARG	2.7
1	E	64	GLU	2.7
1	G	84	SER	2.7
1	C	153	ASP	2.7
1	G	288	ALA	2.7
1	B	90	LYS	2.7
1	I	286	ARG	2.6
1	F	230	GLU	2.6
1	I	180	SER	2.6
1	G	213	GLY	2.6
1	D	202	SER	2.6
1	B	42	GLN	2.6
1	G	233	GLN	2.6
1	A	204	TYR	2.6
1	E	259	THR	2.6
1	B	186	ASN	2.6
1	C	173	ILE	2.6
1	E	158	ASP	2.6
1	G	230	GLU	2.6
1	A	180	SER	2.6
1	J	21	ASN	2.6
1	J	153	ASP	2.6
1	A	291	VAL	2.6
1	A	295	LEU	2.6
1	F	75	ALA	2.6
1	B	290	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	179	SER	2.5
1	C	291	VAL	2.5
1	G	53	ASP	2.5
1	G	265	MET	2.5
1	A	158	ASP	2.5
1	C	148	TYR	2.5
1	E	167	SER	2.5
1	C	226	GLU	2.5
1	F	206	TRP	2.5
1	E	308	PHE	2.5
1	D	13	ASP	2.5
1	G	176	ASP	2.5
1	I	207	SER	2.5
1	D	248	TYR	2.5
1	G	316	VAL	2.5
1	J	64	GLU	2.5
1	G	151	ASN	2.5
1	J	183	PRO	2.5
1	E	13	ASP	2.5
1	H	179	SER	2.5
1	I	24	TYR	2.5
1	B	119	PHE	2.4
1	D	184	ASN	2.4
1	J	138	GLN	2.4
1	E	250	SER	2.4
1	G	61	THR	2.4
1	A	258	TYR	2.4
1	B	248	TYR	2.4
1	C	30	GLU	2.4
1	C	317	ILE	2.4
1	J	85	PRO	2.4
1	A	259	THR	2.4
1	B	13	ASP	2.4
1	D	61	THR	2.4
1	F	246	ALA	2.4
1	A	60	ASN	2.4
1	J	289	ASN	2.4
1	H	52	GLY	2.4
1	B	202	SER	2.4
1	E	65	ARG	2.4
1	D	302	LEU	2.4
1	I	53	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	59	GLU	2.4
1	I	91	ARG	2.4
1	D	183	PRO	2.4
1	J	229	SER	2.4
1	B	291	VAL	2.4
1	H	314	VAL	2.4
1	J	306	LEU	2.4
1	I	49	LYS	2.4
1	D	207	SER	2.3
1	H	315	LEU	2.3
1	J	39	ILE	2.3
1	J	86	ASP	2.3
1	F	229	SER	2.3
1	B	72	TRP	2.3
1	H	186	ASN	2.3
1	F	314	VAL	2.3
1	D	125	GLN	2.3
1	E	263	ASP	2.3
1	F	13	ASP	2.3
1	E	317	ILE	2.3
1	G	76	LEU	2.3
1	H	188	PHE	2.3
1	G	314	VAL	2.3
1	D	139	GLN	2.3
1	J	13	ASP	2.3
1	C	302	LEU	2.3
1	H	75	ALA	2.3
1	G	298	GLN	2.3
1	B	312	GLY	2.3
1	G	184	ASN	2.3
1	F	221	SER	2.3
1	J	307	GLY	2.3
1	C	140	LEU	2.2
1	A	226	GLU	2.2
1	J	309	LEU	2.2
1	E	228	PHE	2.2
1	J	304	PHE	2.2
1	B	207	SER	2.2
1	G	161	TRP	2.2
1	G	174	ARG	2.2
1	J	156	GLU	2.2
1	E	183	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	68	ASN	2.2
1	I	303	ALA	2.2
1	A	302	LEU	2.2
1	F	76	LEU	2.2
1	I	111	SER	2.2
1	B	22	LYS	2.2
1	H	151	ASN	2.2
1	H	176	ASP	2.2
1	E	239	MET	2.2
1	F	255	ARG	2.2
1	D	121	PHE	2.2
1	B	286	ARG	2.1
1	I	219	SER	2.1
1	E	81	VAL	2.1
1	E	198	VAL	2.1
1	A	85	PRO	2.1
1	B	315	LEU	2.1
1	G	239	MET	2.1
1	E	78	PHE	2.1
1	B	182	GLN	2.1
1	C	280	ILE	2.1
1	D	173	ILE	2.1
1	G	215	ILE	2.1
1	F	144	ASP	2.1
1	I	176	ASP	2.1
1	H	21	ASN	2.1
1	J	251	ASN	2.1
1	B	100	VAL	2.1
1	E	253	LEU	2.1
1	G	269	GLY	2.1
1	E	163	ARG	2.1
1	B	180	SER	2.1
1	F	46	LYS	2.1
1	B	298	GLN	2.1
1	J	154	ASN	2.1
1	E	302	LEU	2.1
1	F	232	LEU	2.1
1	A	157	ILE	2.1
1	G	157	ILE	2.1
1	D	227	SER	2.1
1	B	26	VAL	2.1
1	G	271	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	284	HIS	2.0
1	C	183	PRO	2.0
1	H	13	ASP	2.0
1	G	152	ALA	2.0
1	G	197	ALA	2.0
1	I	109	SER	2.0
1	J	109	SER	2.0
1	D	25	GLY	2.0
1	D	52	GLY	2.0
1	J	88	GLY	2.0
1	E	305	PRO	2.0
1	E	150	GLU	2.0
1	E	206	TRP	2.0
1	B	293	ASP	2.0
1	F	244	ALA	2.0
1	I	121	PHE	2.0
1	I	202	SER	2.0
1	J	152	ALA	2.0
1	H	287	GLN	2.0
1	A	93	MET	2.0
1	E	299	ARG	2.0
1	J	159	GLU	2.0
1	I	276	ALA	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

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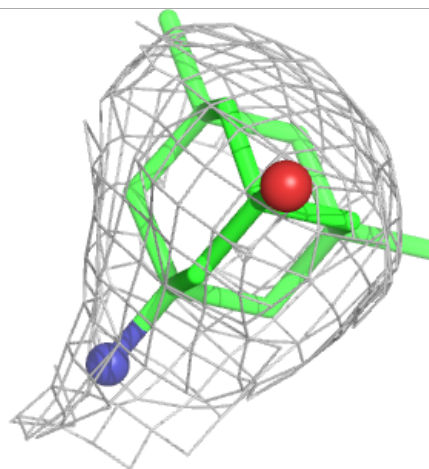
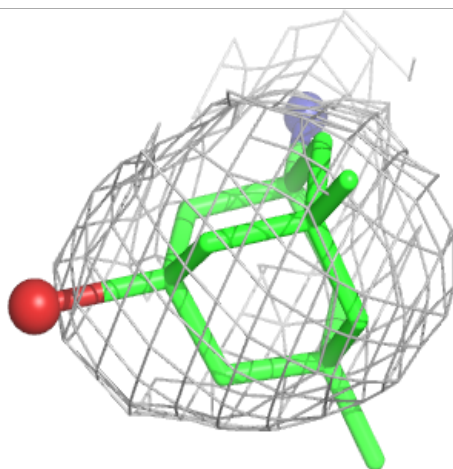
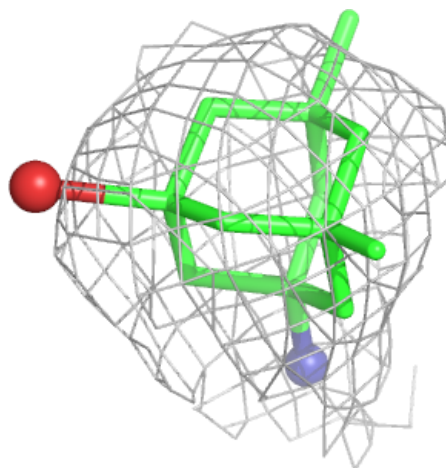
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BR7	F	401	14/14	0.88	0.14	99,129,135,272	0
2	BR7	J	401	14/14	0.90	0.11	98,112,125,194	0
2	BR7	C	401	14/14	0.91	0.12	111,127,145,217	0
2	BR7	B	401	14/14	0.92	0.12	104,108,119,265	0
2	BR7	A	401	14/14	0.92	0.13	112,142,147,354	0
2	BR7	G	401	14/14	0.94	0.10	77,115,131,268	0
2	BR7	F	402	14/14	0.94	0.17	110,131,138,389	0
2	BR7	D	401	14/14	0.95	0.10	98,111,119,277	0
2	BR7	H	401	14/14	0.95	0.09	129,141,153,250	0
2	BR7	I	401	14/14	0.95	0.10	86,100,119,321	0
2	BR7	E	401	14/14	0.95	0.11	84,110,120,309	0
2	BR7	A	402	14/14	0.96	0.13	98,109,129,224	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.

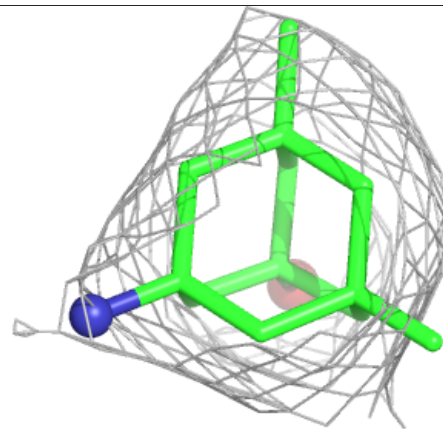
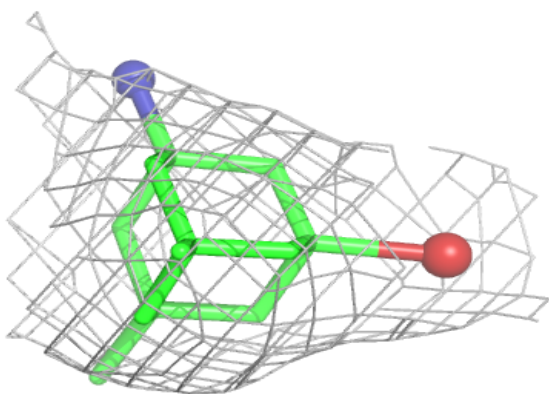
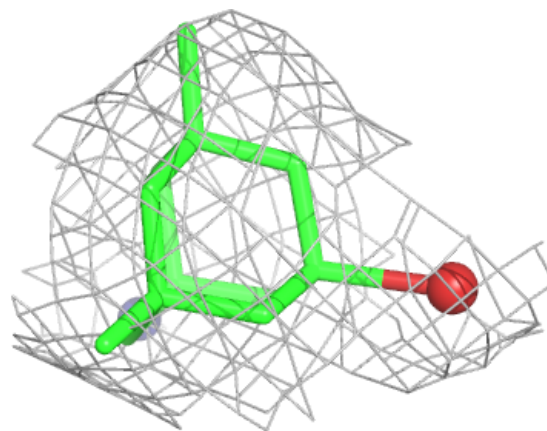
Electron density around BR7 F 401:

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



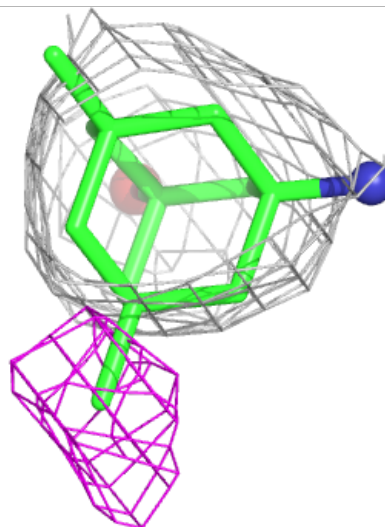
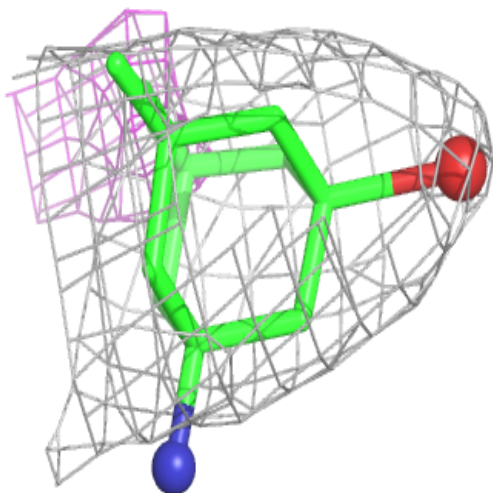
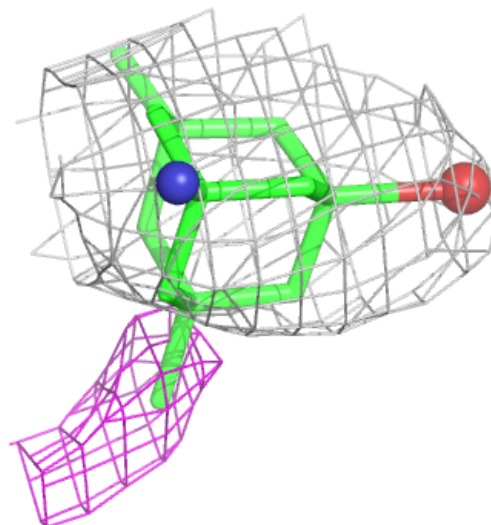
Electron density around BR7 J 401:

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



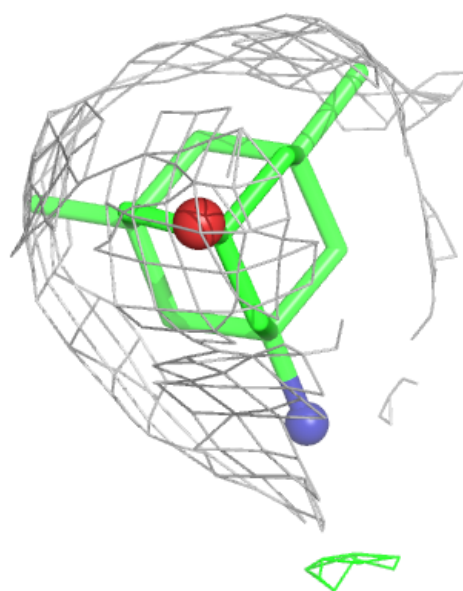
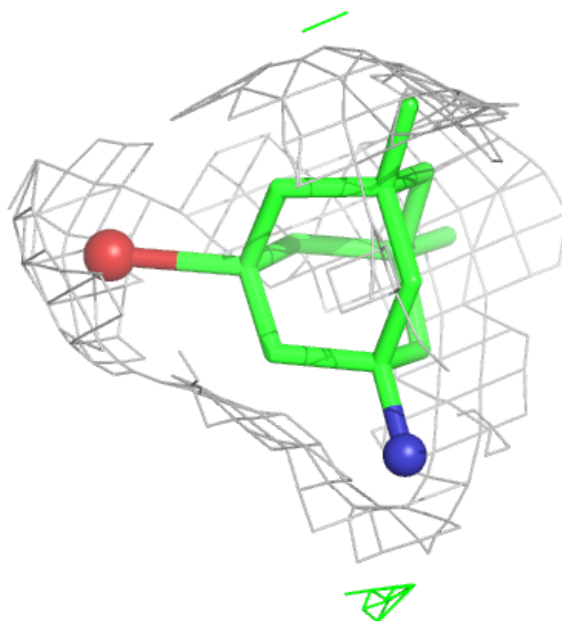
Electron density around BR7 C 401:

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



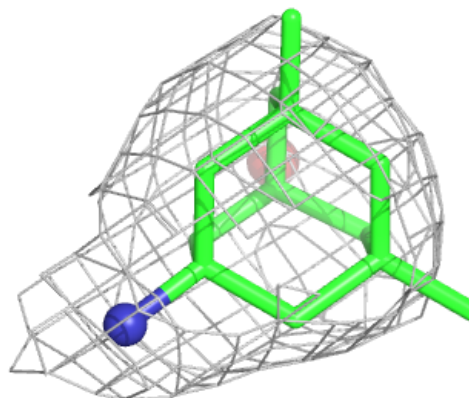
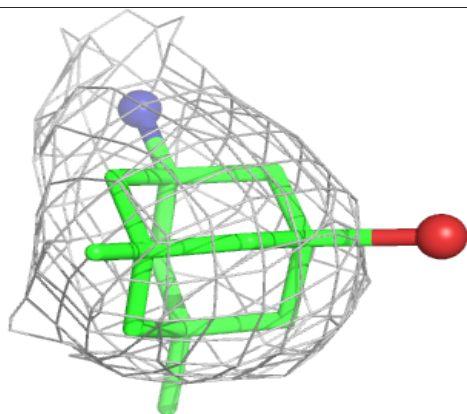
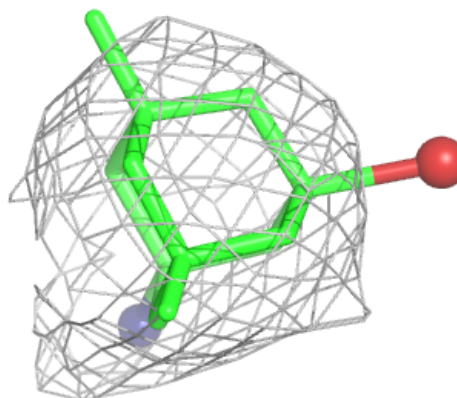
Electron density around BR7 B 401:

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



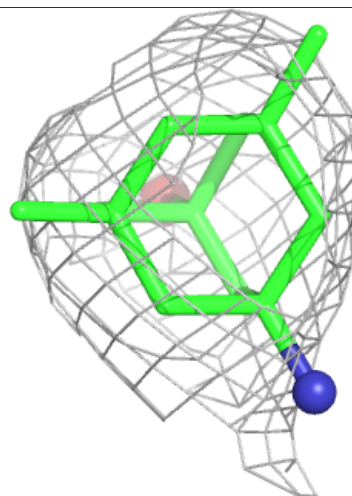
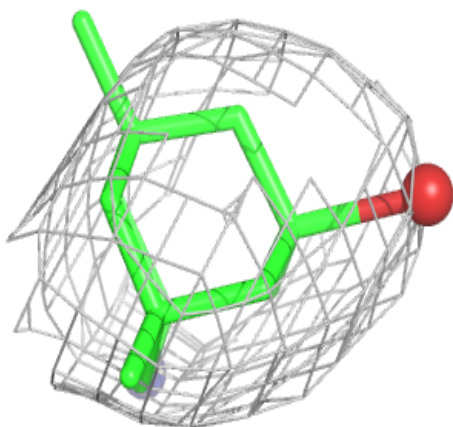
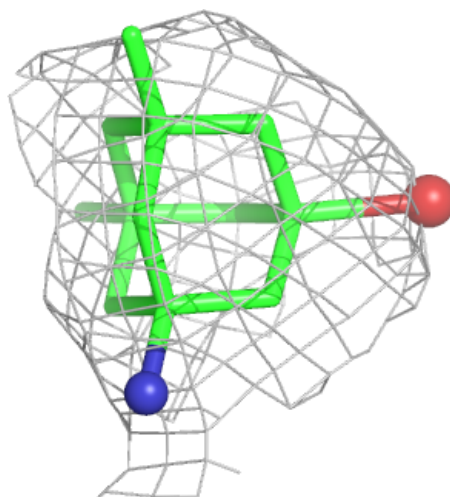
Electron density around BR7 A 401:

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



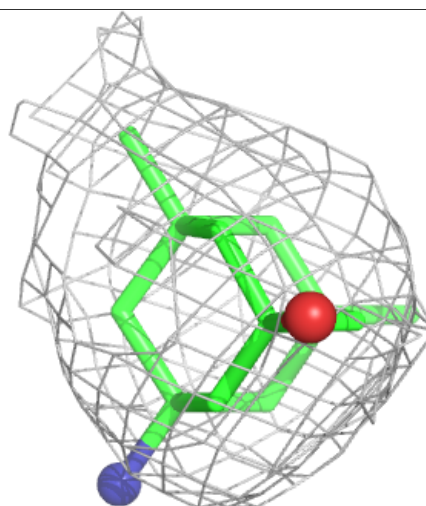
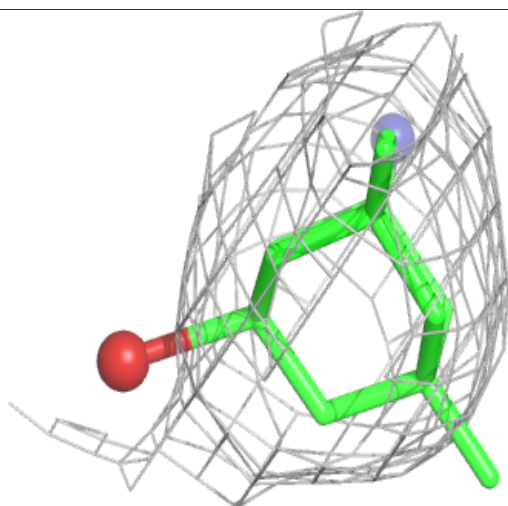
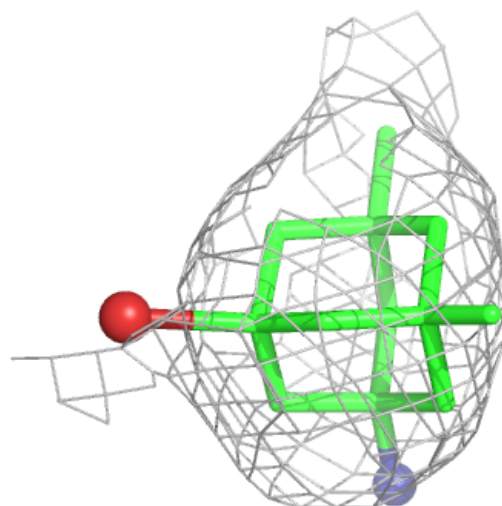
Electron density around BR7 G 401:

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



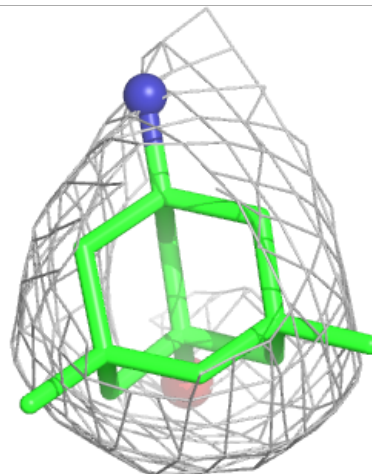
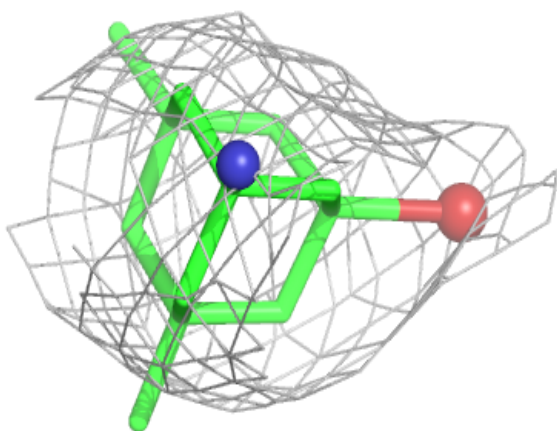
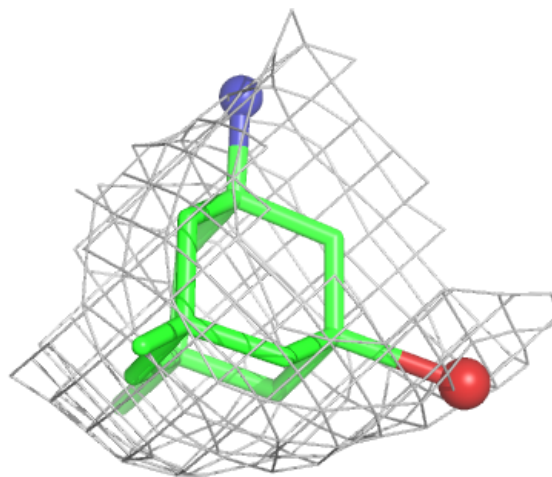
Electron density around BR7 F 402:

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



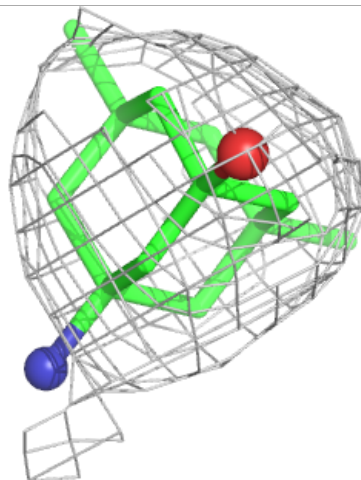
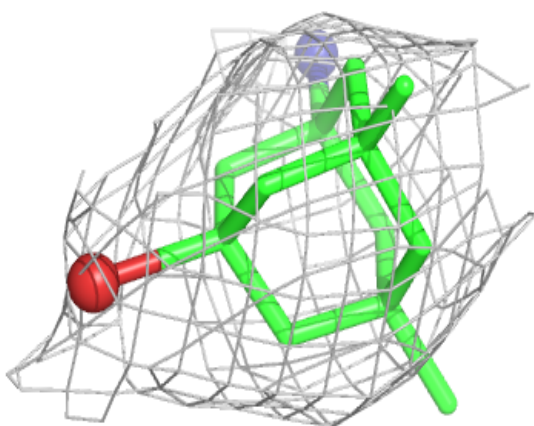
Electron density around BR7 D 401:

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



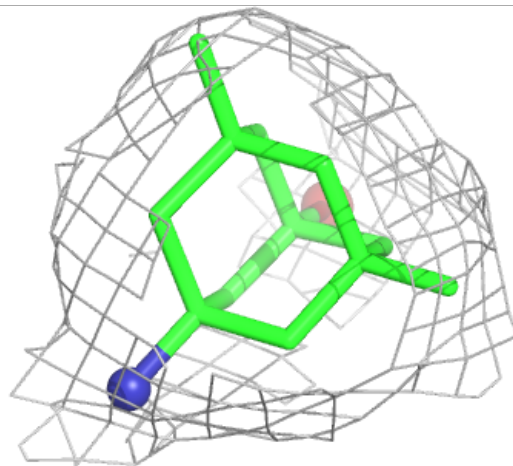
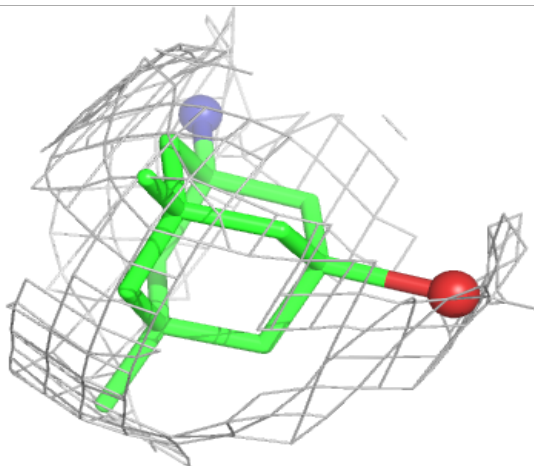
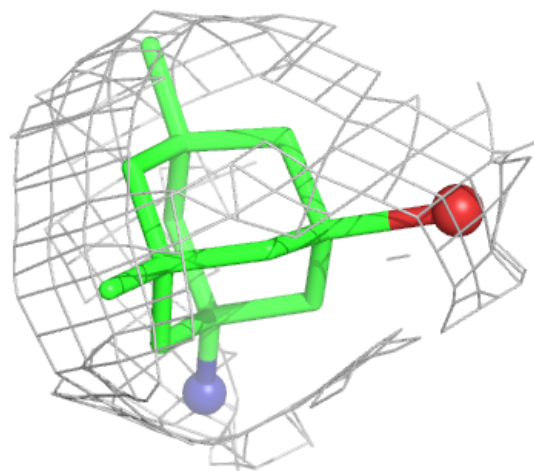
Electron density around BR7 H 401:

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



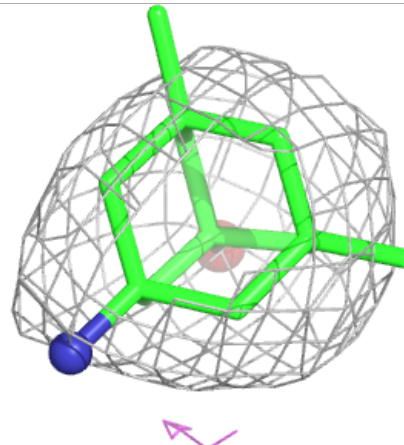
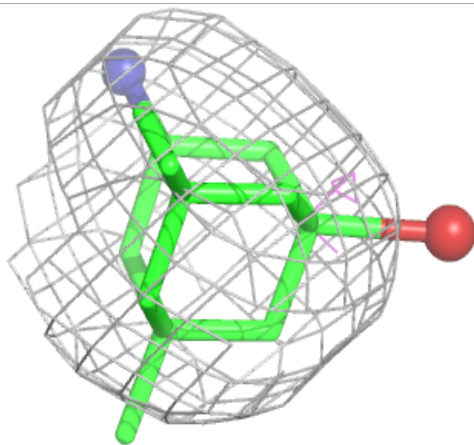
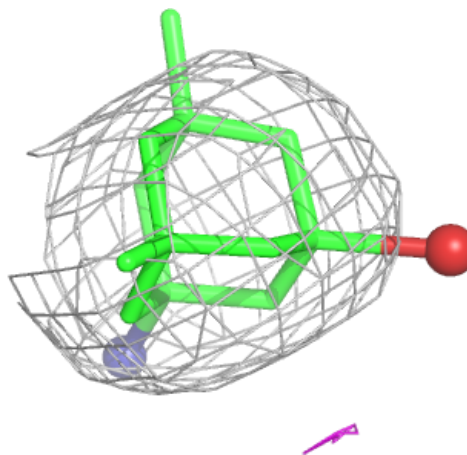
Electron density around BR7 I 401:

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



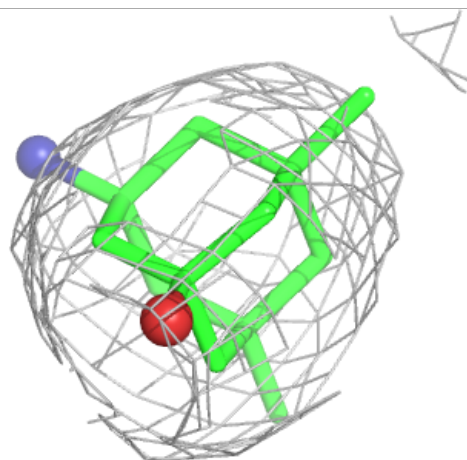
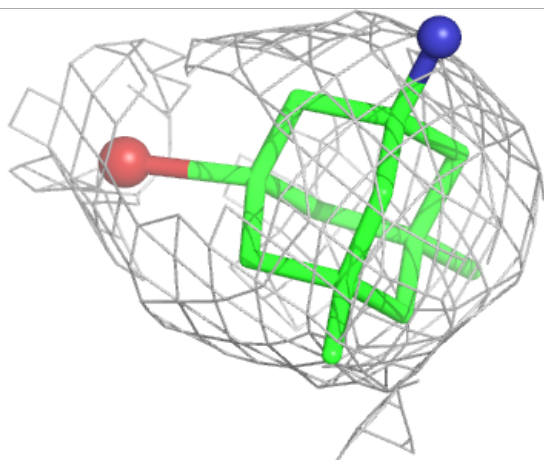
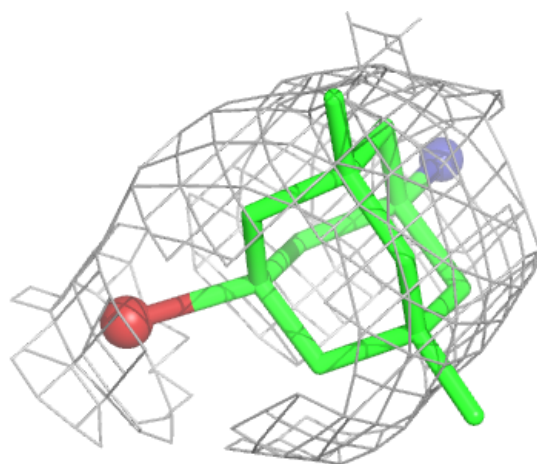
Electron density around BR7 E 401:

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



Electron density around BR7 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.