



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 04:27 AM UTC

PDB ID : 1Q23 / pdb_00001q23
Title : Crystal structure of Chloramphenicol acetyltransferase I complexed with Fusidic acid at 2.18 Å resolution
Authors : Roidis, A.; Kokkinidis, M.
Deposited on : 2003-07-23
Resolution : 2.18 Å (reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

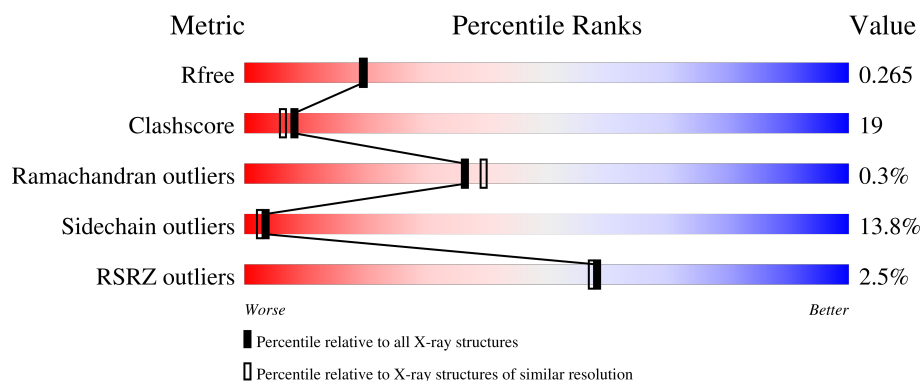
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	219	2% 48% 41% 7% ..
1	B	219	2% 60% 31% 7% ..
1	C	219	61% 24% 11% ..
1	D	219	2% 53% 30% 13% ..
1	E	219	2% 55% 33% 7% ..

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Mol	Chain	Length	Quality of chain
1	F	219	
1	G	219	
1	H	219	
1	I	219	
1	J	219	
1	K	219	
1	L	219	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FUA	A	702	X	-	-	-
3	FUA	B	703	X	-	-	-
3	FUA	C	701	X	-	-	-
3	FUA	D	705	X	-	-	-
3	FUA	E	706	X	-	-	-
3	FUA	F	704	X	-	-	-
3	FUA	G	708	X	-	-	-
3	FUA	H	709	X	-	-	-
3	FUA	I	707	X	-	-	-
3	FUA	J	711	X	-	-	-
3	FUA	K	712	X	-	-	-
3	FUA	L	710	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22280 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.

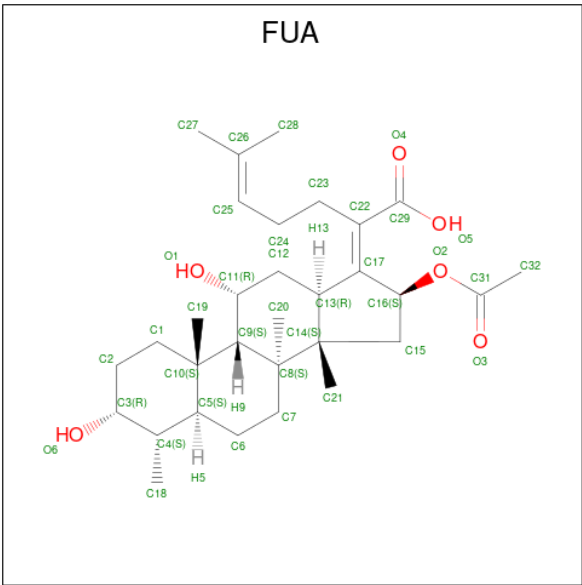
- Molecule 1 is a protein called Chloramphenicol acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1771	1150	291	317	13			
1	B	217	Total	C	N	O	S	0	0	0
			1798	1167	296	322	13			
1	C	213	Total	C	N	O	S	0	0	0
			1763	1144	290	316	13			
1	D	213	Total	C	N	O	S	0	0	0
			1763	1144	290	316	13			
1	E	215	Total	C	N	O	S	0	0	0
			1785	1160	294	318	13			
1	F	212	Total	C	N	O	S	0	0	0
			1759	1142	289	315	13			
1	G	213	Total	C	N	O	S	0	0	0
			1763	1144	290	316	13			
1	H	216	Total	C	N	O	S	0	0	0
			1785	1159	294	319	13			
1	I	215	Total	C	N	O	S	0	0	0
			1785	1160	294	318	13			
1	J	212	Total	C	N	O	S	0	0	0
			1763	1146	289	315	13			
1	K	213	Total	C	N	O	S	0	0	0
			1772	1153	291	315	13			
1	L	210	Total	C	N	O	S	0	0	0
			1746	1135	286	312	13			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is FUSIDIC ACID (CCD ID: FUA) (formula: C₃₁H₄₈O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			37	31	6		
3	B	1	Total	C	O	0	0
			37	31	6		
3	C	1	Total	C	O	0	0
			37	31	6		
3	D	1	Total	C	O	0	0
			37	31	6		
3	E	1	Total	C	O	0	0
			37	31	6		
3	F	1	Total	C	O	0	0
			37	31	6		
3	G	1	Total	C	O	0	0
			37	31	6		
3	H	1	Total	C	O	0	0
			37	31	6		
3	I	1	Total	C	O	0	0
			37	31	6		
3	J	1	Total	C	O	0	0
			37	31	6		
3	K	1	Total	C	O	0	0
			37	31	6		
3	L	1	Total	C	O	0	0
			37	31	6		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	78	Total 78	O 78	0	0
4	B	51	Total 51	O 51	0	0
4	C	68	Total 68	O 68	0	0
4	D	58	Total 58	O 58	0	0
4	E	44	Total 44	O 44	0	0
4	F	43	Total 43	O 43	0	0
4	G	43	Total 43	O 43	0	0
4	H	74	Total 74	O 74	0	0
4	I	42	Total 42	O 42	0	0
4	J	34	Total 34	O 34	0	0
4	K	26	Total 26	O 26	0	0
4	L	21	Total 21	O 21	0	0

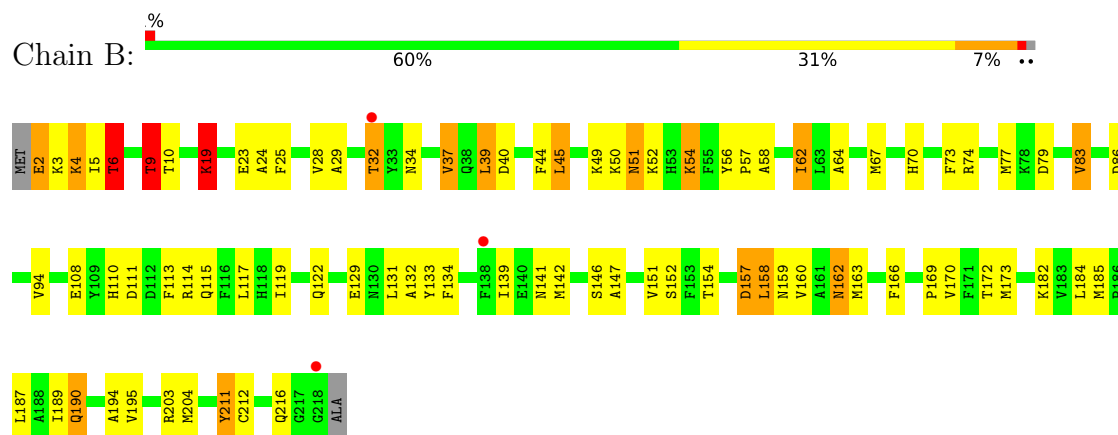
3 Residue-property plots

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.

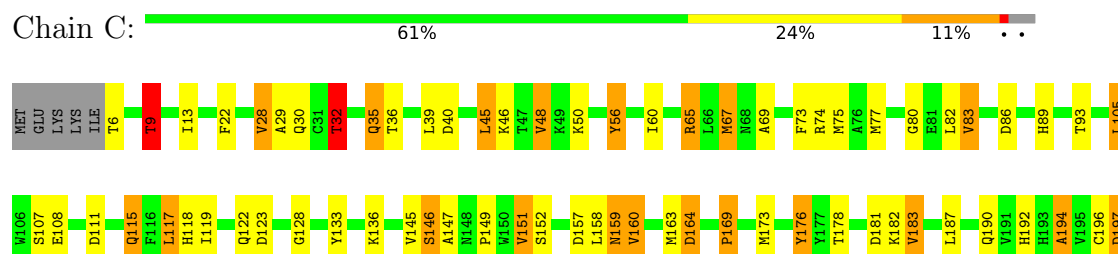
• Molecule 1: Chloramphenicol acetyltransferase

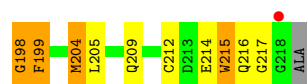


• Molecule 1: Chloramphenicol acetyltransferase

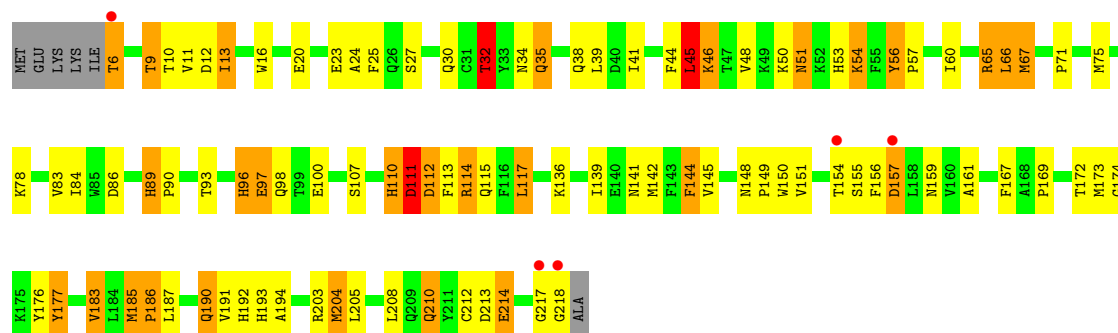


• Molecule 1: Chloramphenicol acetyltransferase

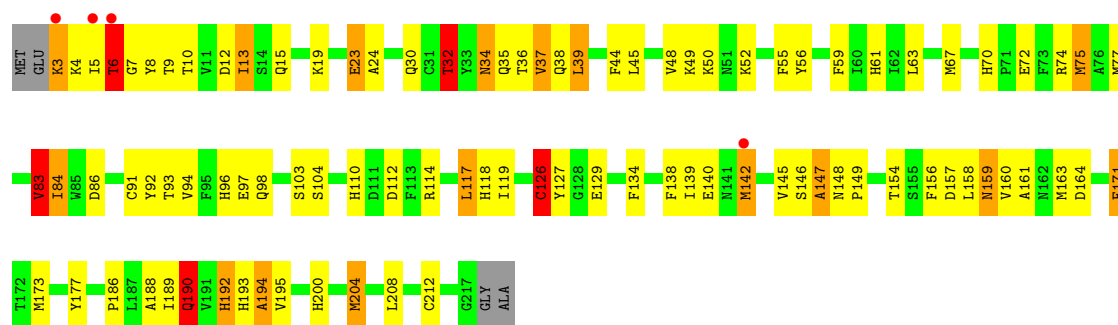




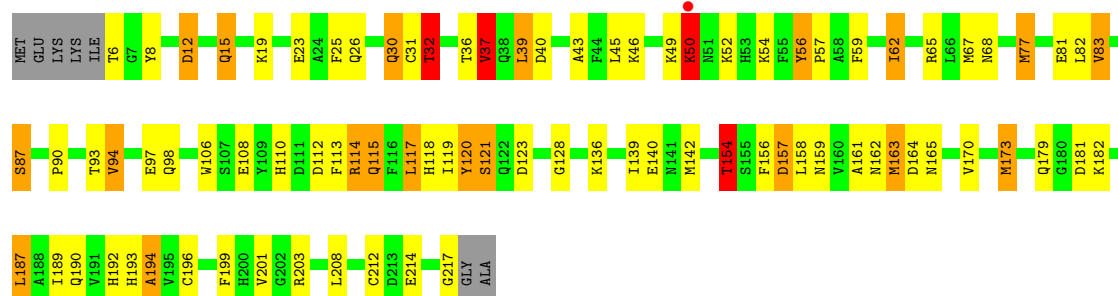
• Molecule 1: Chloramphenicol acetyltransferase



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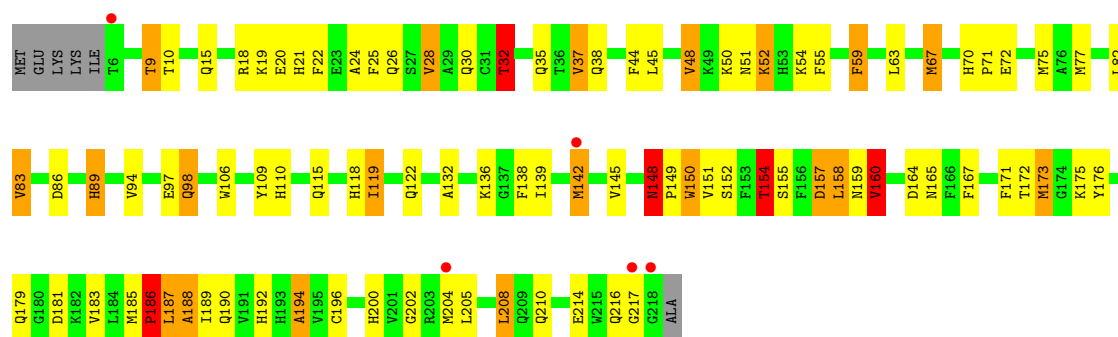


• Molecule 1: Chloramphenicol acetyltransferase

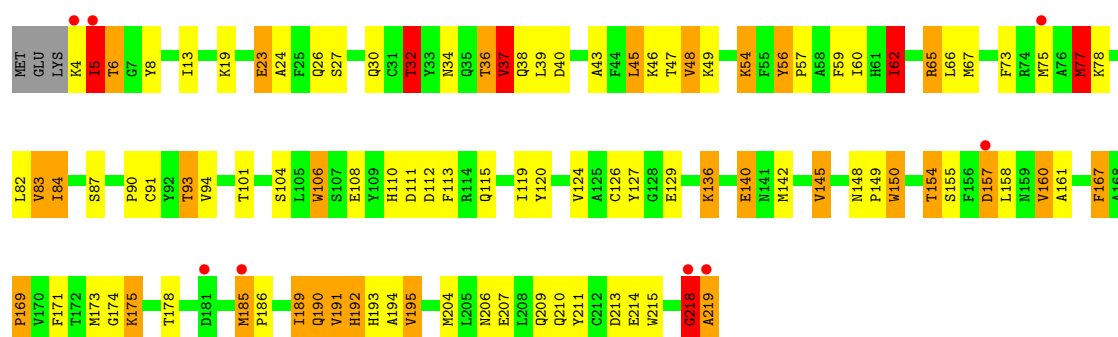


• Molecule 1: Chloramphenicol acetyltransferase

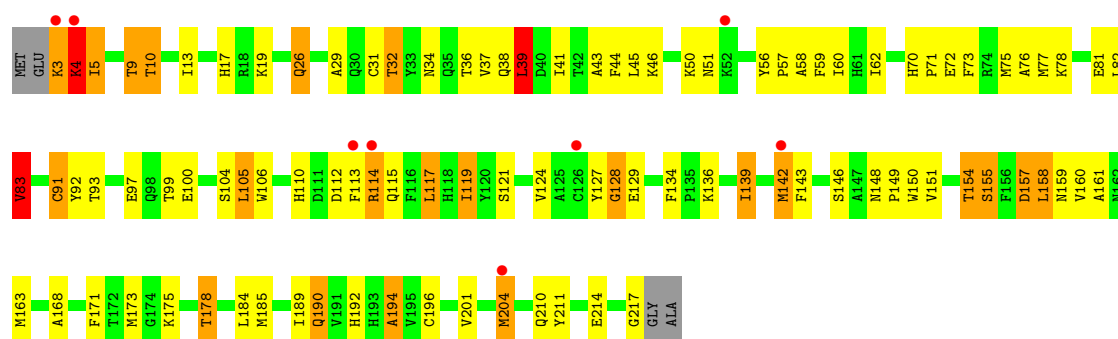




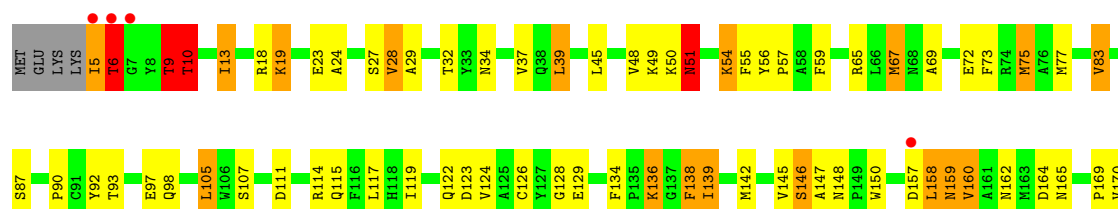
• Molecule 1: Chloramphenicol acetyltransferase



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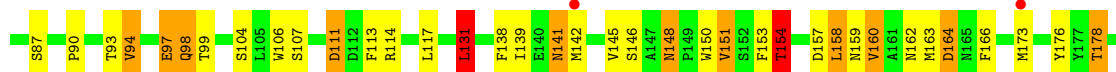
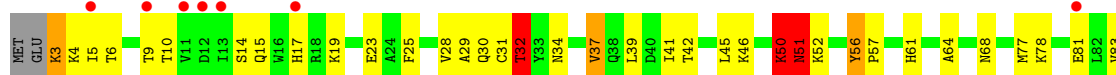


• Molecule 1: Chloramphenicol acetyltransferase

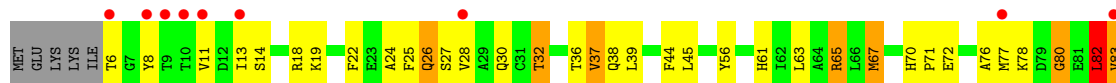




• Molecule 1: Chloramphenicol acetyltransferase



• Molecule 1: Chloramphenicol acetyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	115.35Å 129.20Å 118.07Å 90.00° 108.30° 90.00°	Depositor
Resolution (Å)	111.80 – 2.18 111.80 – 2.18	Depositor EDS
% Data completeness (in resolution range)	99.7 (111.80-2.18) 99.7 (111.80-2.18)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.192 , 0.263 0.200 , 0.265	Depositor DCC
R_{free} test set	9151 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	26.9	Xtriage
Anisotropy	0.702	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.026 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	22280	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.66% 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: CA, FUA

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	1.93	41/1830 (2.2%)	1.69	26/2484 (1.0%)
1	B	1.86	32/1857 (1.7%)	1.66	26/2518 (1.0%)
1	C	1.84	24/1822 (1.3%)	1.60	21/2473 (0.8%)
1	D	1.92	33/1822 (1.8%)	1.69	27/2473 (1.1%)
1	E	1.87	34/1844 (1.8%)	1.59	15/2501 (0.6%)
1	F	1.81	22/1818 (1.2%)	1.63	26/2468 (1.1%)
1	G	1.86	34/1822 (1.9%)	1.71	40/2473 (1.6%)
1	H	1.96	36/1844 (2.0%)	1.69	32/2502 (1.3%)
1	I	1.81	20/1844 (1.1%)	1.72	24/2501 (1.0%)
1	J	1.59	15/1822 (0.8%)	1.58	16/2474 (0.6%)
1	K	1.59	9/1831 (0.5%)	1.55	25/2484 (1.0%)
1	L	1.56	14/1805 (0.8%)	1.49	12/2451 (0.5%)
All	All	1.81	314/21961 (1.4%)	1.63	290/29802 (1.0%)

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	H	0	2
1	I	0	2
1	J	0	1
All	All	0	5

All (314) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	56	TYR	C-O	-11.11	1.14	1.24
1	E	70	HIS	C-O	-10.64	1.16	1.25
1	K	41	ILE	CA-CB	9.79	1.65	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	162	ASN	CG-OD1	9.53	1.41	1.23
1	H	112	ASP	N-CA	9.34	1.58	1.46
1	L	160	VAL	CA-C	8.79	1.62	1.52
1	H	5	ILE	N-CA	8.72	1.56	1.46
1	G	187	LEU	CA-C	8.62	1.62	1.52
1	B	185	MET	CA-C	8.57	1.62	1.53
1	K	29	ALA	CA-CB	8.50	1.66	1.53
1	H	111	ASP	CA-C	8.31	1.63	1.52
1	C	133	TYR	C-O	8.28	1.33	1.24
1	E	83	VAL	CA-C	8.25	1.62	1.52
1	D	151	VAL	CA-CB	8.11	1.65	1.54
1	I	41	ILE	CA-CB	8.09	1.65	1.54
1	H	218	GLY	C-N	7.92	1.44	1.33
1	E	119	ILE	CA-CB	-7.91	1.46	1.54
1	I	91	CYS	C-O	7.84	1.32	1.24
1	E	195	VAL	C-O	-7.83	1.16	1.24
1	H	36	THR	C-N	-7.83	1.23	1.33
1	L	195	VAL	CA-CB	7.73	1.64	1.54
1	F	30	GLN	CA-C	7.65	1.62	1.52
1	E	56	TYR	C-O	-7.64	1.17	1.24
1	I	178	THR	CA-CB	7.57	1.65	1.53
1	E	6	THR	CA-C	-7.57	1.42	1.53
1	J	185	MET	SD-CE	7.56	1.98	1.79
1	G	188	ALA	CA-C	-7.52	1.43	1.52
1	F	43	ALA	CA-C	7.51	1.62	1.52
1	B	194	ALA	CA-CB	-7.50	1.41	1.53
1	F	62	ILE	CA-CB	7.45	1.62	1.54
1	C	133	TYR	N-CA	-7.42	1.37	1.46
1	J	28	VAL	CA-CB	7.39	1.64	1.54
1	G	151	VAL	CA-CB	7.34	1.64	1.54
1	D	157	ASP	CB-CG	7.34	1.70	1.52
1	H	37	VAL	N-CA	-7.22	1.38	1.46
1	H	5	ILE	CA-CB	7.17	1.63	1.54
1	A	156	PHE	CA-C	7.16	1.60	1.52
1	D	60	ILE	CA-CB	7.12	1.63	1.54
1	C	48	VAL	CA-CB	7.12	1.62	1.54
1	J	134	PHE	CA-C	7.12	1.60	1.52
1	A	122	GLN	CA-C	-7.09	1.43	1.52
1	B	62	ILE	CA-C	7.05	1.61	1.52
1	F	170	VAL	CA-CB	-7.05	1.45	1.54
1	I	76	ALA	CA-CB	7.02	1.65	1.53
1	D	48	VAL	CA-CB	6.99	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	36	THR	CA-C	-6.98	1.44	1.52
1	E	77	MET	SD-CE	-6.95	1.62	1.79
1	D	167	PHE	CA-C	6.92	1.61	1.52
1	E	194	ALA	CA-CB	6.91	1.64	1.53
1	G	194	ALA	CA-CB	6.91	1.65	1.53
1	E	61	HIS	CA-C	6.90	1.61	1.52
1	C	194	ALA	CA-CB	6.87	1.64	1.53
1	L	161	ALA	CA-CB	-6.86	1.42	1.53
1	A	170	VAL	CA-CB	-6.84	1.45	1.54
1	H	43	ALA	C-O	6.84	1.31	1.24
1	F	179	GLN	CA-C	6.82	1.60	1.53
1	I	139	ILE	CA-C	6.81	1.60	1.52
1	B	131	LEU	CA-C	6.76	1.62	1.52
1	H	119	ILE	CA-CB	6.75	1.63	1.54
1	A	169	PRO	CA-C	6.73	1.60	1.52
1	B	77	MET	CG-SD	6.69	1.97	1.80
1	E	91	CYS	N-CA	-6.68	1.38	1.46
1	E	188	ALA	CA-CB	6.68	1.65	1.53
1	E	92	TYR	C-O	-6.67	1.15	1.23
1	A	174	GLY	CA-C	6.64	1.60	1.52
1	B	195	VAL	N-CA	6.64	1.52	1.46
1	A	130	ASN	N-CA	6.63	1.54	1.46
1	H	40	ASP	CA-CB	6.63	1.61	1.52
1	A	200	HIS	N-CA	6.63	1.54	1.46
1	A	110	HIS	C-O	6.58	1.31	1.23
1	F	56	TYR	C-O	-6.58	1.15	1.24
1	A	58	ALA	CA-CB	6.55	1.63	1.53
1	H	5	ILE	CA-C	6.54	1.60	1.52
1	H	191	VAL	CA-C	6.52	1.59	1.52
1	G	55	PHE	CA-C	6.51	1.61	1.52
1	E	208	LEU	C-O	-6.50	1.16	1.24
1	E	48	VAL	CA-CB	6.50	1.61	1.54
1	A	69	ALA	CA-CB	-6.45	1.45	1.54
1	I	119	ILE	CA-CB	6.44	1.61	1.54
1	A	45	LEU	C-O	6.43	1.31	1.24
1	D	111	ASP	CB-CG	-6.41	1.36	1.52
1	H	186	PRO	C-O	6.40	1.30	1.23
1	C	89	HIS	CA-C	-6.37	1.47	1.52
1	H	93	THR	C-O	-6.37	1.16	1.23
1	B	184	LEU	N-CA	6.34	1.53	1.45
1	E	193	HIS	C-O	6.34	1.32	1.24
1	G	119	ILE	CA-CB	6.33	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	37	VAL	C-O	-6.30	1.17	1.24
1	K	113	PHE	C-O	6.29	1.31	1.24
1	D	144	PHE	CA-C	6.28	1.60	1.52
1	G	196	CYS	C-O	6.27	1.31	1.23
1	G	20	GLU	CA-C	6.25	1.61	1.52
1	B	74	ARG	CA-C	-6.24	1.44	1.52
1	C	196	CYS	C-O	6.24	1.31	1.23
1	G	77	MET	CG-SD	6.22	1.96	1.80
1	H	108	GLU	C-O	6.22	1.31	1.24
1	J	69	ALA	CA-CB	6.21	1.63	1.53
1	B	158	LEU	C-O	6.20	1.31	1.24
1	I	39	LEU	C-O	6.20	1.31	1.23
1	C	145	VAL	C-O	6.20	1.30	1.24
1	I	163	MET	N-CA	-6.19	1.38	1.46
1	G	63	LEU	C-O	-6.18	1.16	1.24
1	A	182	LYS	CA-C	-6.18	1.45	1.52
1	D	212	CYS	CA-C	6.18	1.60	1.52
1	A	126	CYS	C-O	6.16	1.32	1.24
1	J	196	CYS	CA-C	-6.16	1.45	1.52
1	H	77	MET	CB-CG	6.15	1.71	1.52
1	B	173	MET	SD-CE	6.15	1.95	1.79
1	I	31	CYS	C-O	-6.14	1.16	1.23
1	C	152	SER	CA-CB	6.13	1.60	1.52
1	F	189	ILE	C-O	-6.13	1.17	1.24
1	C	164	ASP	C-O	-6.12	1.16	1.23
1	H	219	ALA	C-O	6.11	1.35	1.23
1	A	58	ALA	C-O	6.10	1.31	1.24
1	F	201	VAL	CA-C	6.09	1.60	1.52
1	C	107	SER	C-O	6.08	1.31	1.23
1	F	8	TYR	CA-C	-6.08	1.45	1.52
1	F	65	ARG	NE-CZ	6.08	1.39	1.33
1	G	25	PHE	C-O	-6.07	1.16	1.24
1	E	34	ASN	CG-ND2	-6.07	1.20	1.33
1	L	36	THR	CA-C	-6.06	1.45	1.52
1	D	23	GLU	C-O	-6.05	1.17	1.24
1	E	23	GLU	C-O	-6.02	1.16	1.24
1	K	77	MET	SD-CE	-6.01	1.64	1.79
1	L	101	THR	CA-C	-5.99	1.45	1.52
1	A	48	VAL	CA-C	5.99	1.60	1.52
1	D	44	PHE	C-O	-5.99	1.17	1.24
1	G	152	SER	CA-C	-5.99	1.46	1.53
1	H	106	TRP	N-CA	-5.98	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	173	MET	SD-CE	5.98	1.94	1.79
1	G	185	MET	SD-CE	-5.98	1.64	1.79
1	H	34	ASN	C-O	5.96	1.31	1.23
1	B	37	VAL	C-O	-5.95	1.18	1.24
1	B	152	SER	N-CA	-5.95	1.39	1.46
1	E	159	ASN	CB-CG	5.95	1.67	1.52
1	A	152	SER	CA-CB	5.94	1.61	1.52
1	F	120	TYR	C-O	5.94	1.30	1.24
1	I	189	ILE	CA-C	5.94	1.60	1.52
1	C	149	PRO	C-O	-5.94	1.17	1.23
1	D	24	ALA	C-O	5.93	1.31	1.24
1	F	87	SER	C-O	5.92	1.31	1.23
1	D	157	ASP	N-CA	5.92	1.53	1.46
1	E	140	GLU	CA-C	5.92	1.60	1.52
1	D	27	SER	CA-CB	5.91	1.63	1.53
1	G	24	ALA	CA-CB	-5.91	1.43	1.53
1	G	158	LEU	CA-C	-5.90	1.45	1.52
1	E	147	ALA	CA-CB	5.89	1.61	1.53
1	A	22	PHE	CE2-CZ	5.88	1.56	1.38
1	G	75	MET	CG-SD	-5.85	1.66	1.80
1	H	210	GLN	C-O	5.85	1.31	1.24
1	L	94	VAL	CA-CB	5.84	1.61	1.54
1	E	171	PHE	N-CA	5.83	1.53	1.46
1	I	72	GLU	CA-C	-5.83	1.44	1.52
1	D	183	VAL	CB-CG2	5.83	1.71	1.52
1	L	28	VAL	CA-CB	5.83	1.63	1.54
1	A	96	HIS	CA-C	5.82	1.60	1.52
1	E	75	MET	SD-CE	5.82	1.94	1.79
1	F	32	THR	CA-CB	-5.80	1.44	1.53
1	A	56	TYR	CA-C	5.79	1.59	1.52
1	H	110	HIS	N-CA	5.79	1.52	1.46
1	C	56	TYR	N-CA	-5.79	1.42	1.46
1	K	104	SER	CA-C	5.79	1.60	1.53
1	C	74	ARG	CA-C	-5.78	1.45	1.53
1	G	217	GLY	C-O	5.77	1.30	1.23
1	B	189	ILE	C-O	-5.77	1.18	1.24
1	A	166	PHE	C-O	5.76	1.30	1.23
1	A	54	LYS	CG-CD	5.76	1.69	1.52
1	G	37	VAL	CB-CG2	-5.75	1.33	1.52
1	H	126	CYS	CA-C	5.75	1.60	1.52
1	K	141	ASN	C-O	5.75	1.30	1.23
1	H	161	ALA	CA-CB	5.74	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	112	ASP	CA-C	5.73	1.60	1.52
1	L	24	ALA	CA-C	5.73	1.60	1.52
1	H	6	THR	CA-C	5.70	1.59	1.52
1	H	209	GLN	CA-C	5.70	1.59	1.52
1	B	54	LYS	CA-C	5.70	1.59	1.52
1	A	94	VAL	CA-CB	5.70	1.61	1.54
1	A	61	HIS	C-O	-5.69	1.17	1.24
1	E	118	HIS	C-O	-5.68	1.17	1.24
1	E	63	LEU	N-CA	5.67	1.53	1.46
1	G	22	PHE	C-O	5.67	1.30	1.24
1	J	55	PHE	N-CA	-5.67	1.39	1.46
1	G	202	GLY	CA-C	5.67	1.58	1.52
1	B	172	THR	C-O	-5.66	1.17	1.24
1	D	145	VAL	CA-CB	-5.64	1.46	1.54
1	A	47	THR	CA-C	-5.63	1.45	1.52
1	B	28	VAL	CB-CG1	5.62	1.71	1.52
1	F	161	ALA	C-O	-5.61	1.17	1.24
1	H	47	THR	N-CA	5.61	1.53	1.46
1	C	69	ALA	CA-C	5.61	1.60	1.52
1	J	183	VAL	CA-C	5.61	1.59	1.52
1	A	11	VAL	CA-CB	-5.60	1.47	1.54
1	D	210	GLN	CA-C	5.60	1.59	1.52
1	B	58	ALA	CA-CB	5.59	1.62	1.53
1	G	172	THR	CA-C	5.59	1.59	1.52
1	B	157	ASP	CA-CB	-5.59	1.43	1.53
1	E	86	ASP	CA-C	-5.58	1.45	1.52
1	I	36	THR	CA-C	5.56	1.59	1.52
1	C	215	TRP	CA-C	5.56	1.59	1.52
1	F	50	LYS	CG-CD	5.56	1.69	1.52
1	H	214	GLU	C-O	-5.56	1.16	1.24
1	K	56	TYR	C-O	-5.55	1.19	1.24
1	E	8	TYR	CA-C	-5.54	1.46	1.52
1	D	172	THR	C-O	-5.52	1.17	1.24
1	H	206	ASN	C-O	5.51	1.30	1.24
1	G	132	ALA	CA-CB	5.51	1.62	1.53
1	A	75	MET	SD-CE	-5.51	1.65	1.79
1	C	159	ASN	CB-CG	5.50	1.65	1.52
1	I	196	CYS	N-CA	5.50	1.52	1.46
1	H	189	ILE	CA-CB	5.50	1.61	1.54
1	B	6	THR	CB-CG2	5.50	1.70	1.52
1	J	6	THR	CB-CG2	5.49	1.70	1.52
1	B	170	VAL	CA-C	5.49	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	133	TYR	CA-C	5.48	1.59	1.52
1	A	178	THR	CA-C	-5.46	1.45	1.52
1	H	167	PHE	C-O	-5.46	1.16	1.24
1	B	45	LEU	CA-C	5.45	1.59	1.52
1	A	132	ALA	CA-CB	5.45	1.62	1.53
1	H	27	SER	CA-C	-5.45	1.45	1.52
1	C	60	ILE	C-O	5.44	1.30	1.24
1	G	179	GLN	CA-C	5.44	1.58	1.52
1	C	197	ASP	CA-CB	5.42	1.62	1.53
1	G	154	THR	CB-CG2	-5.41	1.34	1.52
1	G	70	HIS	CA-C	5.41	1.59	1.52
1	E	55	PHE	C-O	5.41	1.30	1.24
1	I	78	LYS	CE-NZ	5.39	1.65	1.49
1	D	203	ARG	NE-CZ	5.38	1.39	1.33
1	B	166	PHE	C-O	5.37	1.30	1.23
1	D	210	GLN	C-O	5.37	1.30	1.24
1	A	119	ILE	C-O	-5.37	1.17	1.24
1	H	65	ARG	CA-C	5.37	1.59	1.52
1	D	190	GLN	CA-C	-5.36	1.46	1.52
1	A	70	HIS	C-N	-5.36	1.27	1.34
1	D	66	LEU	CA-C	5.36	1.59	1.52
1	A	24	ALA	CA-C	5.35	1.59	1.52
1	J	189	ILE	CA-CB	5.35	1.61	1.54
1	H	211	TYR	CA-CB	5.34	1.61	1.53
1	G	89	HIS	C-O	5.33	1.30	1.24
1	J	13	ILE	CA-CB	5.32	1.61	1.54
1	A	168	ALA	CA-C	5.32	1.59	1.53
1	K	145	VAL	CB-CG1	5.32	1.70	1.52
1	C	197	ASP	CA-C	5.31	1.59	1.52
1	I	117	LEU	C-O	5.30	1.30	1.24
1	D	71	PRO	CA-C	5.29	1.61	1.52
1	C	86	ASP	C-O	5.28	1.30	1.24
1	A	64	ALA	CA-CB	-5.28	1.45	1.53
1	G	183	VAL	N-CA	-5.28	1.39	1.46
1	I	185	MET	N-CA	5.26	1.53	1.46
1	F	196	CYS	N-CA	5.25	1.52	1.46
1	I	76	ALA	CA-C	5.25	1.58	1.52
1	B	204	MET	CA-C	-5.25	1.46	1.52
1	L	170	VAL	CA-C	5.24	1.59	1.52
1	D	155	SER	N-CA	5.24	1.52	1.46
1	J	24	ALA	CA-C	5.24	1.59	1.52
1	F	12	ASP	CA-C	-5.23	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	15	GLN	CA-C	5.23	1.60	1.52
1	G	148	ASN	CA-CB	5.23	1.59	1.53
1	J	165	ASN	CA-C	5.23	1.60	1.52
1	G	59	PHE	CE1-CZ	5.22	1.54	1.38
1	B	23	GLU	N-CA	5.21	1.53	1.46
1	D	177	TYR	N-CA	5.20	1.52	1.45
1	G	109	TYR	N-CA	-5.20	1.39	1.45
1	D	89	HIS	CA-C	-5.20	1.46	1.52
1	L	151	VAL	CA-CB	5.19	1.61	1.54
1	A	185	MET	CA-C	5.19	1.59	1.52
1	J	194	ALA	CA-C	5.18	1.59	1.52
1	B	157	ASP	N-CA	-5.18	1.39	1.45
1	D	11	VAL	CA-C	5.18	1.58	1.52
1	J	191	VAL	C-O	-5.18	1.18	1.23
1	A	151	VAL	CA-CB	5.18	1.61	1.54
1	K	195	VAL	C-O	-5.18	1.16	1.24
1	A	13	ILE	CA-CB	-5.17	1.48	1.54
1	L	185	MET	CA-C	5.16	1.57	1.52
1	J	29	ALA	CA-CB	5.15	1.60	1.53
1	D	191	VAL	CA-C	5.15	1.58	1.52
1	B	24	ALA	CA-CB	5.13	1.61	1.53
1	I	154	THR	N-CA	-5.12	1.39	1.46
1	A	82	LEU	C-O	-5.12	1.18	1.24
1	C	151	VAL	CA-CB	5.11	1.61	1.54
1	I	5	ILE	C-O	-5.11	1.18	1.24
1	H	192	HIS	CA-C	-5.11	1.46	1.52
1	D	75	MET	SD-CE	5.11	1.92	1.79
1	A	28	VAL	CA-C	5.10	1.60	1.52
1	E	36	THR	CA-C	5.10	1.58	1.52
1	C	198	GLY	C-O	-5.09	1.17	1.23
1	A	41	ILE	CA-CB	5.09	1.60	1.54
1	D	10	THR	CA-CB	5.09	1.60	1.53
1	D	151	VAL	CA-C	-5.09	1.46	1.52
1	B	119	ILE	CA-C	5.08	1.59	1.52
1	B	64	ALA	CA-CB	5.07	1.61	1.53
1	F	118	HIS	CA-CB	5.07	1.61	1.53
1	A	191	VAL	N-CA	-5.07	1.40	1.46
1	G	83	VAL	CA-C	5.06	1.58	1.52
1	G	185	MET	CA-C	5.06	1.59	1.52
1	G	82	LEU	CG-CD1	5.06	1.69	1.52
1	E	24	ALA	CA-CB	5.05	1.61	1.53
1	E	103	SER	C-O	5.05	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	86	ASP	CA-C	-5.05	1.46	1.52
1	L	153	PHE	C-O	-5.05	1.17	1.23
1	B	147	ALA	CA-CB	-5.03	1.46	1.53
1	D	90	PRO	CA-CB	5.03	1.60	1.53
1	F	90	PRO	CA-C	-5.03	1.46	1.52
1	H	82	LEU	N-CA	-5.03	1.39	1.46
1	F	199	PHE	CA-C	-5.03	1.46	1.52
1	D	35	GLN	C-O	-5.02	1.18	1.23
1	L	78	LYS	CA-C	5.02	1.58	1.52
1	G	48	VAL	CA-C	5.01	1.59	1.52
1	A	111	ASP	C-O	-5.01	1.18	1.24
1	C	163	MET	SD-CE	5.01	1.92	1.79
1	F	194	ALA	CA-C	-5.01	1.46	1.52
1	E	96	HIS	N-CA	5.01	1.52	1.46
1	E	192	HIS	N-CA	5.01	1.52	1.46
1	L	143	PHE	N-CA	5.01	1.52	1.45
1	E	84	ILE	C-O	-5.00	1.18	1.24

All (290) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	4	LYS	O-C-N	-25.16	95.45	121.87
1	I	4	LYS	N-CA-C	12.04	132.02	113.72
1	I	51	ASN	CA-C-N	-10.72	106.82	123.12
1	I	51	ASN	C-N-CA	-10.72	106.82	123.12
1	C	35	GLN	OE1-CD-NE2	-10.49	112.11	122.60
1	G	51	ASN	CA-C-N	-10.41	109.08	123.03
1	G	51	ASN	C-N-CA	-10.41	109.08	123.03
1	G	98	GLN	OE1-CD-NE2	-10.19	112.41	122.60
1	A	32	THR	N-CA-CB	-9.71	96.49	111.05
1	A	129	GLU	N-CA-C	-9.56	99.47	112.94
1	B	157	ASP	N-CA-C	9.49	123.90	108.99
1	H	83	VAL	N-CA-CB	-9.30	99.50	112.52
1	F	32	THR	N-CA-CB	-9.09	96.86	110.85
1	I	51	ASN	O-C-N	-8.46	110.98	122.23
1	H	6	THR	N-CA-C	8.41	123.00	108.02
1	B	19	LYS	N-CA-C	8.39	120.04	111.07
1	D	51	ASN	N-CA-C	-8.34	103.12	113.38
1	D	32	THR	N-CA-CB	-8.33	97.71	111.20
1	B	131	LEU	N-CA-C	8.30	123.19	112.89
1	G	32	THR	N-CA-CB	-8.25	97.84	111.20
1	E	6	THR	N-CA-C	-8.17	98.42	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	VAL	N-CA-C	-8.09	96.93	108.58
1	C	32	THR	N-CA-CB	-7.97	98.28	111.20
1	I	51	ASN	N-CA-C	-7.96	99.37	110.35
1	I	26	GLN	N-CA-C	-7.93	103.18	113.17
1	J	138	PHE	N-CA-C	7.92	121.32	108.41
1	K	160	VAL	N-CA-CB	-7.63	102.21	110.53
1	L	93	THR	N-CA-C	7.54	122.11	110.20
1	G	186	PRO	CA-N-CD	-7.52	101.48	112.00
1	D	86	ASP	N-CA-C	-7.49	103.19	111.36
1	F	154	THR	N-CA-CB	-7.37	98.89	110.46
1	J	51	ASN	CA-C-N	-7.37	111.29	123.37
1	J	51	ASN	C-N-CA	-7.37	111.29	123.37
1	C	46	LYS	N-CA-C	-7.32	102.69	111.69
1	D	214	GLU	CB-CA-C	7.30	122.58	109.29
1	A	201	VAL	CA-C-N	7.29	128.22	119.99
1	A	201	VAL	C-N-CA	7.29	128.22	119.99
1	G	150	TRP	CA-C-N	-7.28	112.20	122.75
1	G	150	TRP	C-N-CA	-7.28	112.20	122.75
1	G	158	LEU	CB-CA-C	-7.26	98.39	110.29
1	K	195	VAL	CB-CA-C	-7.25	102.21	111.20
1	B	115	GLN	N-CA-C	-7.24	102.18	111.02
1	G	44	PHE	N-CA-C	-7.24	102.78	111.69
1	J	10	THR	N-CA-CB	-7.19	99.28	110.57
1	C	35	GLN	CG-CD-NE2	7.17	127.15	116.40
1	F	83	VAL	N-CA-CB	-7.12	100.50	112.47
1	K	51	ASN	N-CA-C	-7.06	101.06	110.24
1	G	132	ALA	N-CA-C	7.04	119.39	110.24
1	F	67	MET	N-CA-C	-7.02	103.63	111.28
1	L	160	VAL	N-CA-CB	-7.01	101.68	110.31
1	G	86	ASP	N-CA-C	-6.95	103.71	111.28
1	E	83	VAL	N-CA-CB	-6.92	100.81	112.44
1	K	32	THR	N-CA-CB	-6.92	99.99	111.20
1	C	28	VAL	N-CA-CB	-6.92	100.20	110.58
1	L	63	LEU	N-CA-C	-6.88	103.86	111.36
1	F	212	CYS	N-CA-C	-6.86	103.88	111.36
1	K	164	ASP	N-CA-C	-6.83	100.17	110.28
1	L	26	GLN	N-CA-C	-6.82	104.96	113.28
1	H	32	THR	N-CA-CB	-6.82	100.16	111.20
1	G	98	GLN	CG-CD-NE2	6.79	126.58	116.40
1	L	82	LEU	N-CA-C	6.79	119.56	109.59
1	I	168	ALA	N-CA-C	-6.78	99.79	109.62
1	A	121	SER	N-CA-C	-6.75	103.72	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	83	VAL	N-CA-CB	-6.73	101.14	112.44
1	A	121	SER	CA-CB-OG	-6.71	97.69	111.10
1	I	196	CYS	N-CA-C	6.70	119.82	108.90
1	A	28	VAL	CA-C-N	-6.69	111.88	122.79
1	A	28	VAL	C-N-CA	-6.69	111.88	122.79
1	L	37	VAL	CB-CA-C	6.67	120.50	110.90
1	G	51	ASN	N-CA-C	-6.66	99.40	109.79
1	H	145	VAL	CA-C-N	-6.60	112.45	122.81
1	H	145	VAL	C-N-CA	-6.60	112.45	122.81
1	G	208	LEU	N-CA-C	-6.58	104.03	111.07
1	D	111	ASP	CB-CA-C	-6.53	97.80	110.46
1	F	154	THR	CB-CA-C	6.49	122.17	109.72
1	H	218	GLY	CA-C-O	-6.48	109.29	120.57
1	K	154	THR	CB-CA-C	6.48	122.70	109.55
1	D	96	HIS	CA-C-N	6.46	128.84	120.44
1	D	96	HIS	C-N-CA	6.46	128.84	120.44
1	G	63	LEU	N-CA-C	-6.45	104.25	111.28
1	A	181	ASP	N-CA-C	6.45	120.86	113.19
1	F	46	LYS	N-CA-C	-6.43	104.19	111.07
1	J	160	VAL	N-CA-CB	-6.43	102.40	110.31
1	E	37	VAL	CA-CB-CG1	6.42	121.31	110.40
1	D	213	ASP	N-CA-C	-6.41	104.72	112.54
1	H	140	GLU	N-CA-C	6.40	120.93	113.18
1	C	169	PRO	CA-C-O	-6.40	114.13	121.56
1	D	217	GLY	N-CA-C	6.36	123.80	115.40
1	G	145	VAL	CA-C-N	-6.36	112.70	122.62
1	G	145	VAL	C-N-CA	-6.36	112.70	122.62
1	B	203	ARG	N-CA-C	-6.35	104.36	111.28
1	E	32	THR	N-CA-CB	-6.34	101.55	111.05
1	B	70	HIS	CA-C-N	6.33	125.95	119.56
1	B	70	HIS	C-N-CA	6.33	125.95	119.56
1	K	98	GLN	N-CA-C	-6.32	103.69	111.40
1	B	29	ALA	CA-C-N	-6.31	111.92	120.82
1	B	29	ALA	C-N-CA	-6.31	111.92	120.82
1	A	160	VAL	N-CA-CB	-6.31	103.84	110.72
1	I	154	THR	N-CA-C	-6.27	105.67	113.38
1	J	170	VAL	N-CA-C	6.27	116.90	107.75
1	G	83	VAL	N-CA-CB	-6.26	101.92	112.44
1	H	150	TRP	CA-C-N	-6.25	114.10	122.98
1	H	150	TRP	C-N-CA	-6.25	114.10	122.98
1	G	94	VAL	N-CA-C	-6.25	99.05	108.17
1	D	110	HIS	CA-C-N	6.19	129.41	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	110	HIS	C-N-CA	6.19	129.41	120.38
1	D	185	MET	CA-C-N	-6.16	113.62	119.90
1	D	185	MET	C-N-CA	-6.16	113.62	119.90
1	G	173	MET	CA-C-N	-6.16	115.38	122.83
1	G	173	MET	C-N-CA	-6.16	115.38	122.83
1	J	10	THR	CB-CA-C	6.16	120.38	109.72
1	D	112	ASP	N-CA-C	-6.16	98.48	108.52
1	D	214	GLU	N-CA-CB	-6.15	101.49	110.53
1	I	201	VAL	N-CA-C	-6.15	104.30	111.00
1	B	49	LYS	N-CA-C	6.14	117.64	111.07
1	G	149	PRO	CB-CA-C	-6.14	102.23	110.88
1	C	105	LEU	CB-CA-C	-6.13	98.49	109.71
1	H	215	TRP	N-CA-C	-6.13	100.57	110.32
1	H	87	SER	CA-CB-OG	-6.13	98.84	111.10
1	I	201	VAL	CB-CA-C	-6.13	104.03	112.24
1	G	21	HIS	N-CA-C	-6.13	103.93	111.40
1	A	83	VAL	N-CA-CB	-6.09	102.22	112.44
1	K	178	THR	N-CA-C	6.08	119.81	110.20
1	D	136	LYS	N-CA-C	-6.06	105.06	112.88
1	D	65	ARG	NE-CZ-NH2	-6.06	113.75	119.20
1	G	154	THR	CA-CB-CG2	6.05	120.79	110.50
1	I	83	VAL	N-CA-CB	-6.04	100.63	111.92
1	K	6	THR	N-CA-C	6.02	118.54	110.35
1	D	203	ARG	N-CA-C	-6.02	104.72	111.28
1	K	14	SER	N-CA-C	6.00	118.59	111.33
1	H	120	TYR	N-CA-C	-5.97	104.77	111.28
1	B	9	THR	CB-CA-C	5.97	120.63	109.71
1	J	203	ARG	N-CA-C	-5.96	104.86	111.36
1	A	75	MET	CG-SD-CE	5.96	114.01	100.90
1	H	178	THR	OG1-CB-CG2	-5.94	97.42	109.30
1	H	160	VAL	CG1-CB-CG2	5.91	123.81	110.80
1	E	32	THR	CA-CB-CG2	5.91	120.55	110.50
1	L	144	PHE	N-CA-C	5.91	118.53	108.90
1	H	213	ASP	N-CA-C	5.91	118.67	111.82
1	G	50	LYS	N-CA-C	-5.87	104.96	111.36
1	C	212	CYS	N-CA-C	5.87	117.75	111.36
1	H	207	GLU	N-CA-CB	5.86	119.25	110.22
1	G	97	GLU	CA-C-N	5.86	128.45	120.54
1	G	97	GLU	C-N-CA	5.86	128.45	120.54
1	J	139	ILE	N-CA-C	5.86	117.59	109.45
1	A	154	THR	N-CA-CB	-5.84	101.33	110.44
1	A	74	ARG	CD-NE-CZ	5.84	132.57	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	48	VAL	N-CA-CB	-5.83	101.84	110.58
1	J	159	ASN	CA-C-N	5.81	128.88	120.98
1	J	159	ASN	C-N-CA	5.81	128.88	120.98
1	A	32	THR	N-CA-C	-5.80	100.94	109.81
1	J	9	THR	CB-CA-C	5.80	119.30	109.50
1	H	195	VAL	CB-CA-C	-5.79	104.97	110.65
1	C	67	MET	CG-SD-CE	-5.79	88.17	100.90
1	K	37	VAL	CB-CA-C	5.76	119.91	110.69
1	E	39	LEU	CB-CA-C	-5.76	99.80	109.65
1	A	165	ASN	N-CA-C	5.74	119.59	112.47
1	A	210	GLN	N-CA-C	5.73	117.99	111.11
1	B	163	MET	N-CA-C	5.72	120.25	113.16
1	K	4	LYS	N-CA-C	5.72	118.06	107.99
1	F	154	THR	CA-CB-CG2	5.70	120.19	110.50
1	E	126	CYS	CB-CA-C	-5.70	101.89	110.90
1	E	37	VAL	N-CA-CB	-5.69	101.40	111.93
1	H	174	GLY	N-CA-C	5.67	120.92	112.41
1	I	151	VAL	CB-CA-C	-5.67	102.71	110.77
1	J	75	MET	N-CA-C	5.65	118.84	110.48
1	C	160	VAL	N-CA-CB	-5.65	102.53	110.26
1	B	37	VAL	N-CA-CB	-5.64	101.49	111.93
1	I	4	LYS	N-CA-CB	-5.63	105.37	113.65
1	A	70	HIS	CA-C-O	5.63	124.84	119.72
1	G	9	THR	CB-CA-C	5.62	120.11	109.37
1	I	97	GLU	N-CA-CB	5.62	118.98	110.28
1	A	197	ASP	CA-C-N	5.61	126.21	119.98
1	A	197	ASP	C-N-CA	5.61	126.21	119.98
1	C	128	GLY	N-CA-C	5.61	120.84	114.67
1	D	214	GLU	CA-CB-CG	5.59	125.29	114.10
1	F	121	SER	N-CA-CB	5.58	118.42	110.16
1	H	160	VAL	N-CA-CB	-5.58	102.86	110.56
1	H	48	VAL	N-CA-C	5.57	116.35	110.72
1	F	140	GLU	CA-C-N	-5.57	114.85	122.87
1	F	140	GLU	C-N-CA	-5.57	114.85	122.87
1	J	69	ALA	N-CA-C	-5.56	105.27	113.61
1	B	83	VAL	CA-CB-CG1	5.55	119.83	110.40
1	F	128	GLY	N-CA-C	5.55	120.56	114.40
1	C	183	VAL	CB-CA-C	5.54	119.04	110.96
1	E	117	LEU	CB-CA-C	-5.53	101.60	110.79
1	K	160	VAL	CB-CA-C	5.53	118.34	111.15
1	B	39	LEU	CA-C-N	-5.52	114.30	122.41
1	B	39	LEU	C-N-CA	-5.52	114.30	122.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	194	ALA	CA-C-N	-5.51	115.61	121.84
1	I	194	ALA	C-N-CA	-5.51	115.61	121.84
1	F	39	LEU	CB-CA-C	-5.51	100.22	109.53
1	G	205	LEU	N-CA-C	5.51	117.36	111.36
1	H	62	ILE	CB-CG1-CD1	-5.51	102.24	113.80
1	D	9	THR	OG1-CB-CG2	-5.49	98.31	109.30
1	B	25	PHE	N-CA-C	-5.48	106.59	113.28
1	H	115	GLN	N-CA-C	-5.47	105.39	111.36
1	F	37	VAL	N-CA-CB	-5.47	102.24	112.36
1	G	148	ASN	CB-CA-C	5.47	119.67	111.14
1	L	80	GLY	N-CA-C	5.45	123.58	113.76
1	I	4	LYS	CA-C-O	5.44	126.39	119.16
1	G	67	MET	N-CA-C	-5.43	105.46	111.71
1	B	151	VAL	CB-CA-C	-5.43	101.71	110.28
1	H	36	THR	CA-C-N	-5.43	114.55	122.58
1	H	36	THR	C-N-CA	-5.43	114.55	122.58
1	G	160	VAL	CA-C-O	-5.42	115.43	121.23
1	C	133	TYR	N-CA-C	-5.41	105.28	111.07
1	L	151	VAL	CB-CA-C	5.41	117.47	110.12
1	D	111	ASP	N-CA-CB	-5.40	101.60	110.14
1	H	191	VAL	CB-CA-C	-5.39	102.06	110.52
1	E	61	HIS	N-CA-C	5.38	117.57	111.11
1	K	6	THR	CA-C-N	-5.38	117.64	122.43
1	K	6	THR	C-N-CA	-5.38	117.64	122.43
1	K	154	THR	N-CA-CB	-5.38	102.05	110.44
1	G	32	THR	N-CA-C	-5.37	101.36	109.85
1	E	74	ARG	N-CA-C	-5.35	104.17	111.56
1	K	31	CYS	N-CA-C	5.35	116.97	108.79
1	K	97	GLU	N-CA-C	5.34	119.28	112.87
1	G	205	LEU	CA-C-N	5.34	127.75	120.54
1	G	205	LEU	C-N-CA	5.34	127.75	120.54
1	A	37	VAL	N-CA-CB	-5.34	102.05	111.93
1	D	90	PRO	CB-CA-C	-5.32	104.13	111.21
1	L	115	GLN	N-CA-C	5.32	119.49	112.89
1	C	80	GLY	CA-C-N	-5.32	114.96	122.94
1	C	80	GLY	C-N-CA	-5.32	114.96	122.94
1	F	40	ASP	CA-C-N	-5.32	114.73	122.28
1	F	40	ASP	C-N-CA	-5.32	114.73	122.28
1	G	136	LYS	CB-CA-C	-5.32	101.73	110.72
1	H	60	ILE	N-CA-C	-5.31	105.20	110.62
1	F	187	LEU	CA-C-N	-5.30	113.91	122.81
1	F	187	LEU	C-N-CA	-5.30	113.91	122.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	171	PHE	CB-CA-C	-5.30	99.84	109.38
1	D	45	LEU	N-CA-C	5.29	117.05	111.28
1	B	83	VAL	CA-C-O	-5.29	116.12	121.67
1	E	94	VAL	N-CA-C	-5.29	100.45	108.17
1	A	37	VAL	CG1-CB-CG2	5.29	122.43	110.80
1	D	97	GLU	N-CA-CB	-5.29	102.34	110.01
1	D	157	ASP	OD1-CG-OD2	-5.26	110.27	122.90
1	L	151	VAL	N-CA-C	5.26	115.62	107.78
1	G	10	THR	N-CA-C	-5.26	101.89	110.20
1	C	9	THR	CB-CA-C	5.25	118.81	109.72
1	H	124	VAL	N-CA-C	-5.25	105.41	110.72
1	A	77	MET	CG-SD-CE	-5.25	89.35	100.90
1	E	190	GLN	CA-C-N	-5.22	115.40	122.92
1	E	190	GLN	C-N-CA	-5.22	115.40	122.92
1	I	160	VAL	N-CA-C	5.22	116.32	109.58
1	D	56	TYR	CA-C-O	5.22	124.04	119.08
1	G	157	ASP	CA-C-O	-5.22	114.69	120.33
1	E	161	ALA	N-CA-C	5.22	116.97	111.28
1	B	113	PHE	N-CA-C	5.21	117.37	111.11
1	H	84	ILE	N-CA-CB	-5.21	104.22	111.41
1	K	131	LEU	N-CA-C	5.20	118.73	112.38
1	K	94	VAL	CA-C-N	-5.20	115.39	122.93
1	K	94	VAL	C-N-CA	-5.20	115.39	122.93
1	F	94	VAL	CB-CA-C	5.19	117.91	110.33
1	A	66	LEU	N-CA-C	5.18	116.93	111.28
1	B	211	TYR	CB-CA-C	-5.18	100.42	110.46
1	B	110	HIS	O-C-N	5.17	129.27	123.27
1	C	117	LEU	N-CA-C	-5.17	105.82	111.82
1	F	68	ASN	N-CA-C	5.17	119.22	113.02
1	J	48	VAL	CB-CA-C	-5.16	105.10	112.22
1	D	157	ASP	CB-CG-OD2	5.16	130.26	118.40
1	K	61	HIS	N-CA-C	-5.16	105.84	111.82
1	F	214	GLU	N-CA-C	5.15	119.56	113.28
1	C	199	PHE	N-CA-C	5.14	117.28	111.11
1	C	77	MET	CA-C-N	-5.14	115.75	123.00
1	C	77	MET	C-N-CA	-5.14	115.75	123.00
1	B	110	HIS	CA-C-N	5.13	127.88	120.38
1	B	110	HIS	C-N-CA	5.13	127.88	120.38
1	C	22	PHE	N-CA-C	-5.13	104.96	111.11
1	L	32	THR	N-CA-C	-5.11	101.77	109.85
1	F	203	ARG	CA-C-N	-5.11	113.03	120.29
1	F	203	ARG	C-N-CA	-5.11	113.03	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	173	MET	CA-C-N	-5.11	117.89	122.43
1	F	173	MET	C-N-CA	-5.11	117.89	122.43
1	I	161	ALA	CA-C-N	-5.10	115.62	123.07
1	I	161	ALA	C-N-CA	-5.10	115.62	123.07
1	G	115	GLN	CA-CB-CG	5.09	124.29	114.10
1	H	186	PRO	CB-CA-C	-5.09	104.43	111.21
1	F	163	MET	N-CA-C	-5.08	106.50	113.30
1	K	51	ASN	CA-C-N	-5.07	115.99	122.79
1	K	51	ASN	C-N-CA	-5.07	115.99	122.79
1	I	143	PHE	N-CA-C	-5.04	101.71	109.52
1	I	41	ILE	N-CA-C	5.03	117.02	112.29
1	K	64	ALA	N-CA-C	-5.01	105.90	111.36
1	J	83	VAL	N-CA-CB	-5.01	104.03	112.44
1	B	83	VAL	CA-CB-CG2	5.01	118.91	110.40
1	H	136	LYS	CB-CA-C	-5.01	102.68	110.94
1	A	82	LEU	CB-CG-CD2	-5.01	95.68	110.70
1	G	154	THR	N-CA-CB	-5.00	102.63	110.44

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	218	GLY	Peptide
1	H	5	ILE	Peptide
1	I	3	LYS	Peptide
1	I	4	LYS	Mainchain
1	J	6	THR	Peptide

5.2 Too-close contacts

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	1771	0	1658	64	0
1	B	1798	0	1690	47	0
1	C	1763	0	1647	50	0
1	D	1763	0	1647	71	0
1	E	1785	0	1681	73	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1759	0	1644	59	0
1	G	1763	0	1647	68	0
1	H	1785	0	1676	82	0
1	I	1785	0	1681	80	0
1	J	1763	0	1652	91	0
1	K	1772	0	1670	65	0
1	L	1746	0	1633	79	0
2	A	1	0	0	0	0
3	A	37	0	44	8	0
3	B	37	0	44	9	0
3	C	37	0	44	4	0
3	D	37	0	44	10	0
3	E	37	0	44	3	0
3	F	37	0	44	8	0
3	G	37	0	43	6	0
3	H	37	0	43	4	0
3	I	37	0	44	16	0
3	J	37	0	44	10	0
3	K	37	0	44	10	0
3	L	37	0	44	4	0
4	A	78	0	0	6	0
4	B	51	0	0	7	0
4	C	68	0	0	10	0
4	D	58	0	0	7	0
4	E	44	0	0	8	0
4	F	43	0	0	5	0
4	G	43	0	0	6	0
4	H	74	0	0	10	0
4	I	42	0	0	8	0
4	J	34	0	0	9	0
4	K	26	0	0	7	0
4	L	21	0	0	7	0
All	All	22280	0	20452	813	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 19.

All (813) 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:E:139:ILE:H	1:E:142:MET:CE	1.31	1.37

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:67:MET:HE2	1:E:171:PHE:CE1	1.70	1.26
1:H:218:GLY:HA2	1:H:219:ALA:O	1.36	1.24
1:E:67:MET:CE	1:E:171:PHE:HE1	1.49	1.24
1:I:171:PHE:CZ	1:I:204:MET:HE1	1.73	1.23
1:J:67:MET:HA	1:J:67:MET:CE	1.71	1.20
1:G:139:ILE:H	1:G:142:MET:CE	1.58	1.16
1:D:67:MET:HE3	1:D:169:PRO:HG2	1.23	1.13
1:D:154:THR:O	1:F:154:THR:HG23	1.46	1.12
1:A:171:PHE:CZ	1:A:204:MET:HE1	1.84	1.12
1:L:67:MET:HE3	1:L:169:PRO:HG2	1.14	1.11
1:A:154:THR:HG23	1:B:154:THR:O	1.50	1.11
1:D:67:MET:CE	1:D:169:PRO:HG2	1.82	1.08
1:E:139:ILE:N	1:E:142:MET:CE	2.16	1.08
1:A:6:THR:HG21	4:A:837:HOH:O	1.52	1.08
1:K:138:PHE:HA	1:K:142:MET:HE1	1.27	1.08
1:K:154:THR:HG23	1:L:154:THR:O	1.53	1.07
1:H:154:THR:CG2	1:I:154:THR:O	2.02	1.07
1:C:67:MET:CE	1:C:73:PHE:HB3	1.85	1.06
1:C:67:MET:HE1	1:C:169:PRO:HG2	1.11	1.06
1:J:67:MET:HE2	1:J:67:MET:CA	1.84	1.06
1:C:146:SER:HB3	4:C:709:HOH:O	1.53	1.06
1:K:139:ILE:H	1:K:142:MET:CE	1.69	1.05
1:H:154:THR:HG23	1:I:154:THR:O	1.54	1.05
1:G:154:THR:HG23	1:H:154:THR:O	1.54	1.05
1:J:171:PHE:HZ	1:J:204:MET:CE	1.71	1.03
1:E:139:ILE:HG12	1:E:142:MET:HE3	1.41	1.03
1:F:114:ARG:HD3	4:F:729:HOH:O	1.58	1.02
1:C:67:MET:CE	1:C:169:PRO:HG2	1.89	1.01
1:I:171:PHE:CE2	1:I:204:MET:HE1	1.95	1.01
1:D:154:THR:HG23	1:E:154:THR:O	1.60	1.00
1:C:40:ASP:OD1	1:C:182:LYS:HD2	1.60	1.00
1:J:67:MET:HE1	1:J:73:PHE:CD1	1.97	0.99
1:E:139:ILE:H	1:E:142:MET:HE3	1.22	0.99
1:H:8:TYR:CE2	1:H:78:LYS:HE2	1.97	0.99
1:E:145:VAL:HG11	1:E:173:MET:HE3	1.44	0.98
1:G:139:ILE:HG12	1:G:142:MET:HE3	1.42	0.98
1:E:139:ILE:H	1:E:142:MET:HE1	1.25	0.98
1:K:139:ILE:H	1:K:142:MET:HE3	1.29	0.98
1:J:171:PHE:CZ	1:J:204:MET:CE	2.47	0.97
1:J:67:MET:HE1	1:J:73:PHE:CG	2.00	0.96
1:C:115:GLN:O	1:C:119:ILE:CD1	2.13	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:MET:HE3	1:C:73:PHE:HB3	1.47	0.96
1:E:139:ILE:O	1:E:142:MET:SD	2.22	0.96
1:H:218:GLY:HA2	1:H:219:ALA:C	1.90	0.96
1:C:115:GLN:O	1:C:119:ILE:HD12	1.65	0.95
1:E:67:MET:HE2	1:E:171:PHE:HE1	0.79	0.95
1:I:139:ILE:HG13	1:I:142:MET:SD	2.07	0.95
1:A:171:PHE:HZ	1:A:204:MET:HE1	1.24	0.94
1:J:115:GLN:O	1:J:119:ILE:HD12	1.67	0.94
1:F:123:ASP:OD1	1:F:136:LYS:HE2	1.66	0.94
1:G:159:ASN:HB3	1:H:32:THR:HG22	1.49	0.94
1:E:67:MET:CE	1:E:171:PHE:CE1	2.39	0.94
1:H:67:MET:HE3	1:H:73:PHE:HB3	1.49	0.94
1:E:154:THR:HG23	1:F:154:THR:O	1.68	0.93
1:F:192:HIS:HD1	1:F:194:ALA:H	1.13	0.93
1:H:56:TYR:HE1	1:H:173:MET:HE1	1.32	0.93
1:G:32:THR:HG22	1:I:159:ASN:HB3	1.49	0.93
1:A:159:ASN:HB3	1:B:32:THR:HG22	1.51	0.92
1:G:138:PHE:HA	1:G:142:MET:HE1	1.48	0.92
1:L:106:TRP:CD1	1:L:142:MET:CE	2.53	0.92
1:E:138:PHE:HA	1:E:142:MET:HE1	1.50	0.92
1:H:75:MET:SD	1:H:195:VAL:HB	2.09	0.92
1:I:171:PHE:CZ	1:I:204:MET:CE	2.53	0.91
1:L:11:VAL:CG1	1:L:82:LEU:HB3	2.00	0.91
1:L:67:MET:CE	1:L:169:PRO:HG2	1.99	0.91
1:E:145:VAL:CG1	1:E:173:MET:HE3	2.00	0.90
1:I:134:PHE:CE1	3:I:707:FUA:H282	2.06	0.90
1:H:56:TYR:CE1	1:H:173:MET:HE1	2.07	0.90
1:E:34:ASN:ND2	1:E:190:GLN:HB3	1.88	0.89
1:K:138:PHE:CA	1:K:142:MET:HE1	2.01	0.88
1:D:157:ASP:OD2	1:F:157:ASP:HB2	1.74	0.88
1:L:162:ASN:CG	4:L:723:HOH:O	2.14	0.88
1:G:154:THR:O	1:I:154:THR:HG23	1.72	0.88
1:J:93:THR:HG21	3:J:711:FUA:H22	1.54	0.88
1:H:106:TRP:HB3	1:H:142:MET:CE	2.03	0.88
1:G:38:GLN:HE22	1:G:186:PRO:HG3	1.38	0.88
1:J:67:MET:HA	1:J:67:MET:HE2	0.90	0.87
1:E:192:HIS:HD1	1:E:194:ALA:H	1.21	0.87
1:I:171:PHE:HZ	1:I:204:MET:HE1	1.38	0.87
1:K:99:THR:HG21	1:K:131:LEU:HD11	1.57	0.85
1:L:8:TYR:HB2	1:L:83:VAL:HG13	1.57	0.85
1:L:204:MET:HE1	1:L:205:LEU:HD23	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:ASP:OD2	1:J:65:ARG:HD2	1.75	0.85
1:J:171:PHE:CZ	1:J:204:MET:HE1	2.10	0.85
1:B:67:MET:HE3	1:B:73:PHE:HB3	1.59	0.85
1:E:171:PHE:CZ	1:E:204:MET:HE1	2.11	0.85
1:G:139:ILE:CG1	1:G:142:MET:HE3	2.06	0.85
1:E:171:PHE:CE2	1:E:204:MET:HE1	2.12	0.84
1:C:65:ARG:HD2	4:C:765:HOH:O	1.77	0.84
1:D:159:ASN:HB3	1:E:32:THR:HG22	1.60	0.84
1:J:5:ILE:HA	4:J:740:HOH:O	1.78	0.83
1:G:139:ILE:N	1:G:142:MET:CE	2.41	0.83
1:C:67:MET:HE1	1:C:73:PHE:HB3	1.59	0.83
1:H:192:HIS:HD1	1:H:194:ALA:H	1.27	0.83
1:D:210:GLN:O	1:D:214:GLU:HB3	1.78	0.82
1:H:155:SER:CB	1:I:155:SER:HB2	2.09	0.82
1:I:171:PHE:HZ	1:I:204:MET:CE	1.90	0.82
1:J:75:MET:HE3	1:J:195:VAL:HB	1.61	0.82
1:D:32:THR:HG21	4:D:709:HOH:O	1.78	0.82
1:F:59:PHE:CD2	1:F:173:MET:SD	2.73	0.82
1:I:3:LYS:N	4:I:748:HOH:O	2.12	0.82
1:A:106:TRP:CD1	1:A:142:MET:CE	2.62	0.82
1:G:192:HIS:HD1	1:G:194:ALA:H	1.25	0.82
1:A:154:THR:CG2	1:B:154:THR:O	2.28	0.81
1:A:123:ASP:OD1	1:A:136:LYS:NZ	2.13	0.81
1:A:192:HIS:HD1	1:A:194:ALA:H	1.28	0.81
1:G:171:PHE:CE2	1:G:204:MET:HE1	2.16	0.81
1:K:192:HIS:HD1	1:K:194:ALA:H	1.29	0.81
1:H:113:PHE:H	1:H:219:ALA:HB1	1.44	0.80
1:H:155:SER:HB2	1:I:155:SER:HB2	1.62	0.80
1:D:157:ASP:OD2	1:F:157:ASP:CB	2.29	0.80
1:A:67:MET:HE2	1:A:67:MET:HA	1.64	0.80
1:G:15:GLN:HE21	1:G:15:GLN:HA	1.46	0.80
1:D:56:TYR:HB3	1:D:57:PRO:CD	2.12	0.80
1:J:146:SER:HB3	3:J:711:FUA:H3	1.63	0.80
1:G:139:ILE:H	1:G:142:MET:HE1	1.47	0.80
1:A:106:TRP:CD1	1:A:142:MET:HE3	2.17	0.79
1:E:139:ILE:N	1:E:142:MET:HE1	1.86	0.79
1:F:77:MET:CE	1:F:81:GLU:C	2.56	0.79
1:L:11:VAL:HG12	1:L:82:LEU:HB3	1.65	0.79
1:L:106:TRP:CD1	1:L:142:MET:HE3	2.18	0.79
1:C:40:ASP:OD1	1:C:182:LYS:CD	2.30	0.79
1:D:6:THR:HG23	4:D:733:HOH:O	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:139:ILE:H	1:G:142:MET:HE3	1.46	0.78
1:J:192:HIS:HD1	1:J:194:ALA:H	1.29	0.78
1:I:192:HIS:HD1	1:I:194:ALA:H	1.31	0.78
1:L:67:MET:HE3	1:L:169:PRO:CG	2.06	0.78
1:B:67:MET:HE3	1:B:73:PHE:CB	2.14	0.78
1:E:138:PHE:CA	1:E:142:MET:HE1	2.14	0.78
1:H:32:THR:HG21	4:H:731:HOH:O	1.83	0.77
1:B:50:LYS:HG3	1:B:51:ASN:ND2	2.00	0.77
1:E:38:GLN:HE22	1:E:186:PRO:HG3	1.48	0.77
1:H:145:VAL:CG1	1:H:173:MET:HE2	2.15	0.77
1:D:110:HIS:HD2	1:D:112:ASP:H	1.33	0.77
1:L:22:PHE:CZ	1:L:82:LEU:HD12	2.19	0.77
1:B:2:GLU:N	4:B:714:HOH:O	2.17	0.76
1:F:114:ARG:NH2	1:F:217:GLY:O	2.19	0.76
1:B:56:TYR:HB3	1:B:57:PRO:CD	2.13	0.76
1:H:149:PRO:O	1:H:175:LYS:HG2	1.86	0.76
1:K:139:ILE:HG12	1:K:142:MET:HE3	1.68	0.76
1:H:106:TRP:HB3	1:H:142:MET:HE2	1.67	0.76
1:D:41:ILE:HG21	1:D:185:MET:HE2	1.68	0.75
1:G:158:LEU:HD11	3:G:708:FUA:H72	1.67	0.75
1:C:192:HIS:HD1	1:C:194:ALA:H	1.34	0.75
1:I:139:ILE:CG1	1:I:142:MET:SD	2.75	0.75
1:K:139:ILE:CG1	1:K:142:MET:HE3	2.17	0.75
1:D:114:ARG:HH21	1:D:218:GLY:HA3	1.51	0.75
1:G:139:ILE:O	1:G:142:MET:SD	2.46	0.74
1:J:93:THR:CG2	3:J:711:FUA:H22	2.17	0.74
1:A:123:ASP:CG	1:A:136:LYS:HZ1	1.95	0.74
1:J:171:PHE:CE2	1:J:204:MET:HE1	2.22	0.74
1:K:3:LYS:CB	4:K:720:HOH:O	2.36	0.73
1:B:32:THR:HG21	4:B:707:HOH:O	1.87	0.73
1:J:65:ARG:HD3	4:J:727:HOH:O	1.89	0.73
1:E:157:ASP:OD1	4:E:744:HOH:O	2.07	0.73
1:J:72:GLU:HA	1:J:75:MET:HE2	1.70	0.73
1:J:171:PHE:HZ	1:J:204:MET:HE3	1.51	0.72
1:L:204:MET:CE	1:L:205:LEU:HD23	2.20	0.72
1:J:67:MET:CE	1:J:67:MET:CA	2.55	0.72
1:D:13:ILE:HD12	1:D:16:TRP:CE3	2.24	0.72
1:F:110:HIS:HD2	1:F:119:ILE:HD13	1.54	0.72
3:B:703:FUA:C28	1:C:29:ALA:HB2	2.20	0.72
1:C:119:ILE:HD12	1:C:119:ILE:H	1.53	0.72
1:E:129:GLU:CB	4:E:729:HOH:O	2.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:ARG:HD2	1:J:111:ASP:OD2	1.89	0.72
1:J:56:TYR:CD1	1:J:173:MET:HE1	2.25	0.72
1:I:26:GLN:NE2	4:I:749:HOH:O	2.23	0.71
3:B:703:FUA:H282	1:C:29:ALA:HB2	1.72	0.71
1:F:77:MET:CE	1:F:77:MET:HA	2.20	0.71
1:I:106:TRP:CD1	1:I:142:MET:HE1	2.25	0.71
1:E:171:PHE:CZ	1:E:204:MET:CE	2.73	0.71
3:F:704:FUA:C12	3:F:704:FUA:H232	2.20	0.71
1:H:167:PHE:O	1:H:169:PRO:HD3	1.91	0.71
1:I:9:THR:HG23	4:I:721:HOH:O	1.90	0.71
1:B:67:MET:HE2	1:B:169:PRO:HG2	1.73	0.71
1:K:3:LYS:HB3	4:K:720:HOH:O	1.89	0.71
1:K:139:ILE:N	1:K:142:MET:CE	2.49	0.70
1:D:148:ASN:ND2	1:D:150:TRP:HE3	1.89	0.70
1:D:114:ARG:NH2	1:D:218:GLY:HA3	2.05	0.70
1:J:9:THR:HG23	4:J:712:HOH:O	1.92	0.70
1:L:11:VAL:HG11	1:L:82:LEU:HB3	1.71	0.70
1:J:13:ILE:HG22	1:J:19:LYS:HE3	1.74	0.70
1:H:218:GLY:CA	1:H:219:ALA:O	2.30	0.70
1:E:159:ASN:HB3	1:F:32:THR:HG22	1.72	0.70
1:J:90:PRO:HD2	1:J:107:SER:O	1.92	0.69
1:F:114:ARG:CD	4:F:729:HOH:O	2.27	0.69
1:C:204:MET:C	1:C:204:MET:HE2	2.17	0.69
3:I:707:FUA:H122	3:I:707:FUA:H283	1.72	0.69
1:B:56:TYR:HB3	1:B:57:PRO:HD3	1.72	0.69
1:F:77:MET:CE	1:F:82:LEU:N	2.56	0.69
1:D:13:ILE:HD12	1:D:16:TRP:HE3	1.57	0.68
1:I:139:ILE:O	1:I:142:MET:SD	2.51	0.68
1:A:32:THR:HG22	1:C:159:ASN:HB3	1.76	0.68
1:E:129:GLU:HB2	4:E:729:HOH:O	1.92	0.68
1:F:110:HIS:HD2	1:F:119:ILE:CD1	2.06	0.68
1:H:67:MET:HE2	1:H:169:PRO:HB2	1.74	0.68
1:J:139:ILE:H	1:J:142:MET:HE3	1.58	0.68
1:K:106:TRP:CD1	1:K:142:MET:HE2	2.28	0.68
1:E:9:THR:HG22	4:E:725:HOH:O	1.93	0.67
1:E:171:PHE:HZ	1:E:204:MET:CE	2.07	0.67
1:I:134:PHE:HE1	3:I:707:FUA:H282	1.57	0.67
1:H:23:GLU:HG2	4:H:727:HOH:O	1.94	0.67
3:D:705:FUA:H232	3:D:705:FUA:C12	2.25	0.67
1:E:6:THR:HB	1:E:7:GLY:O	1.94	0.67
1:J:67:MET:CE	1:J:73:PHE:CG	2.78	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:56:TYR:HB3	1:I:57:PRO:HD3	1.77	0.67
1:C:32:THR:HG21	4:C:726:HOH:O	1.92	0.67
1:D:148:ASN:HD22	1:D:150:TRP:HE3	1.43	0.67
1:G:38:GLN:HE22	1:G:186:PRO:CG	2.08	0.67
1:H:56:TYR:HE1	1:H:173:MET:CE	2.05	0.67
1:G:138:PHE:CA	1:G:142:MET:HE1	2.23	0.67
1:A:171:PHE:HZ	1:A:204:MET:CE	2.02	0.67
3:B:703:FUA:H232	3:B:703:FUA:C12	2.25	0.67
1:J:157:ASP:OD1	1:L:157:ASP:OD2	2.12	0.66
1:B:50:LYS:CG	1:B:51:ASN:ND2	2.58	0.66
1:F:77:MET:HE1	1:F:82:LEU:N	2.10	0.66
1:J:56:TYR:CE1	1:J:173:MET:CE	2.78	0.66
1:D:13:ILE:CD1	1:D:16:TRP:CE3	2.78	0.66
1:B:114:ARG:HG3	1:B:114:ARG:HH11	1.59	0.66
3:I:707:FUA:H283	3:I:707:FUA:H232	1.76	0.66
1:B:162:ASN:HB3	4:B:712:HOH:O	1.96	0.66
1:H:77:MET:HE2	1:H:77:MET:CA	2.26	0.66
1:K:3:LYS:N	4:K:733:HOH:O	2.29	0.66
1:D:67:MET:CE	1:D:169:PRO:CG	2.68	0.65
1:G:110:HIS:HD2	1:G:119:ILE:CD1	2.09	0.65
1:D:204:MET:HE3	1:D:205:LEU:N	2.11	0.65
1:D:34:ASN:OD1	1:D:157:ASP:OD1	2.12	0.65
3:I:707:FUA:H232	3:I:707:FUA:C28	2.26	0.65
1:J:19:LYS:HE2	1:J:23:GLU:OE2	1.95	0.65
1:J:171:PHE:CZ	1:J:204:MET:HE3	2.29	0.65
1:I:32:THR:HG21	4:I:708:HOH:O	1.97	0.65
1:G:171:PHE:HE2	1:G:204:MET:HE1	1.58	0.65
1:H:218:GLY:CA	1:H:219:ALA:C	2.65	0.65
1:H:65:ARG:HH22	1:H:219:ALA:HB2	1.62	0.64
1:K:111:ASP:OD1	1:K:111:ASP:N	2.30	0.64
1:A:106:TRP:HB3	1:A:142:MET:HE2	1.79	0.64
1:G:171:PHE:CZ	1:G:204:MET:HE1	2.33	0.64
1:J:67:MET:SD	1:J:73:PHE:HB3	2.38	0.64
1:D:32:THR:HG22	1:F:159:ASN:HB3	1.79	0.64
1:F:77:MET:HA	1:F:77:MET:HE2	1.80	0.63
1:J:67:MET:CE	1:J:73:PHE:CD1	2.79	0.63
1:H:113:PHE:H	1:H:219:ALA:CB	2.11	0.63
1:A:67:MET:HE2	1:A:67:MET:CA	2.28	0.63
1:I:56:TYR:HB3	1:I:57:PRO:CD	2.29	0.63
1:C:119:ILE:HD12	1:C:119:ILE:N	2.13	0.63
1:B:67:MET:CE	1:B:73:PHE:HB3	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:34:ASN:ND2	1:E:190:GLN:CB	2.62	0.63
1:J:105:LEU:H	1:J:105:LEU:HD23	1.63	0.63
1:E:139:ILE:HG12	1:E:142:MET:CE	2.24	0.62
1:H:75:MET:SD	1:H:195:VAL:CB	2.87	0.62
1:F:77:MET:HE1	1:F:81:GLU:C	2.23	0.62
1:L:204:MET:HE2	1:L:205:LEU:N	2.13	0.62
1:E:148:ASN:N	1:E:149:PRO:CD	2.63	0.62
1:K:139:ILE:HD12	1:K:141:ASN:OD1	1.99	0.62
1:L:44:PHE:HB2	1:L:212:CYS:O	1.99	0.62
1:I:134:PHE:HE1	3:I:707:FUA:C28	2.12	0.62
1:L:146:SER:OG	3:L:710:FUA:H3	1.99	0.62
1:A:56:TYR:HD1	1:A:173:MET:CE	2.13	0.62
1:G:38:GLN:NE2	1:G:186:PRO:HD3	2.15	0.62
1:G:139:ILE:N	1:G:142:MET:HE1	2.10	0.62
1:A:56:TYR:CD1	1:A:173:MET:HE2	2.35	0.62
1:L:22:PHE:CZ	1:L:82:LEU:CD1	2.83	0.62
1:L:67:MET:HB3	1:L:88:VAL:HG21	1.81	0.62
1:F:57:PRO:HG3	1:F:120:TYR:CE2	2.35	0.61
1:I:134:PHE:CE1	3:I:707:FUA:C28	2.82	0.61
1:F:56:TYR:HB3	1:F:57:PRO:HD3	1.82	0.61
1:I:149:PRO:O	1:I:175:LYS:HG3	2.00	0.61
1:E:148:ASN:N	1:E:149:PRO:HD3	2.15	0.61
1:H:113:PHE:N	1:H:219:ALA:HB1	2.14	0.61
1:E:110:HIS:HD2	1:E:112:ASP:H	1.47	0.61
1:G:155:SER:HB2	1:H:155:SER:HB2	1.82	0.61
1:H:56:TYR:HB3	1:H:57:PRO:HD3	1.81	0.61
1:J:105:LEU:HD23	1:J:105:LEU:N	2.14	0.61
1:H:8:TYR:CD2	1:H:78:LYS:HE2	2.35	0.61
1:L:98:GLN:HG2	4:L:725:HOH:O	2.00	0.61
1:E:59:PHE:HD2	1:E:173:MET:HE2	1.65	0.61
1:B:159:ASN:HB3	1:C:32:THR:HG22	1.83	0.61
1:G:158:LEU:HD13	1:G:160:VAL:HG23	1.81	0.61
1:A:133:TYR:CE2	3:A:702:FUA:H272	2.35	0.60
1:G:15:GLN:HA	1:G:15:GLN:NE2	2.16	0.60
1:L:179:GLN:O	1:L:179:GLN:HG3	2.00	0.60
1:E:139:ILE:N	1:E:142:MET:HE3	1.99	0.60
1:A:215:TRP:CZ2	1:A:217:GLY:HA2	2.37	0.60
1:G:210:GLN:O	1:G:214:GLU:HG3	2.00	0.60
1:H:30:GLN:NE2	4:H:761:HOH:O	2.35	0.60
1:B:114:ARG:HH11	1:B:114:ARG:CG	2.14	0.60
1:K:148:ASN:C	1:K:148:ASN:HD22	2.10	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:101:THR:HG21	1:I:17:HIS:HB3	1.83	0.59
1:K:106:TRP:CD1	1:K:142:MET:CE	2.85	0.59
1:E:139:ILE:N	1:E:142:MET:SD	2.74	0.59
1:J:157:ASP:OD2	1:K:157:ASP:OD2	2.20	0.59
1:B:51:ASN:N	1:B:51:ASN:HD22	2.00	0.59
1:I:62:ILE:HG23	1:I:211:TYR:HD1	1.66	0.59
1:J:159:ASN:HB3	1:K:32:THR:HG22	1.83	0.59
1:B:67:MET:HE3	1:B:73:PHE:CG	2.38	0.59
1:C:9:THR:HG22	4:C:712:HOH:O	2.00	0.59
1:A:123:ASP:CG	1:A:136:LYS:NZ	2.56	0.59
1:B:4:LYS:HE2	1:B:108:GLU:OE1	2.02	0.59
1:B:67:MET:CE	1:B:73:PHE:CG	2.86	0.59
3:D:705:FUA:C22	3:D:705:FUA:H283	2.32	0.59
1:F:115:GLN:O	1:F:119:ILE:HD12	2.03	0.59
1:C:159:ASN:ND2	4:C:768:HOH:O	2.07	0.59
1:L:139:ILE:HG12	1:L:142:MET:SD	2.41	0.59
1:E:13:ILE:HG22	1:E:19:LYS:HG3	1.85	0.59
1:I:190:GLN:C	1:I:190:GLN:HE21	2.10	0.59
1:G:110:HIS:CD2	1:G:119:ILE:CD1	2.86	0.58
1:G:187:LEU:HD22	1:G:208:LEU:HD21	1.82	0.58
1:H:91:CYS:HB2	1:H:142:MET:HE2	1.85	0.58
1:J:56:TYR:HE1	1:J:173:MET:CE	2.15	0.58
1:H:67:MET:CE	1:H:169:PRO:HG2	2.34	0.58
1:H:106:TRP:CB	1:H:142:MET:CE	2.81	0.58
1:I:106:TRP:CG	1:I:142:MET:HE1	2.39	0.58
1:I:26:GLN:HA	1:I:26:GLN:HE21	1.69	0.58
1:D:154:THR:CG2	1:E:154:THR:O	2.46	0.58
1:G:30:GLN:HE22	1:G:164:ASP:HA	1.69	0.58
1:L:106:TRP:CG	1:L:142:MET:HE3	2.38	0.58
1:H:23:GLU:CG	4:H:727:HOH:O	2.52	0.58
1:I:4:LYS:HE2	1:I:4:LYS:HA	1.86	0.57
1:D:12:ASP:O	1:J:10:THR:HG23	2.04	0.57
1:D:56:TYR:HB3	1:D:57:PRO:HD2	1.86	0.57
1:G:32:THR:HG21	4:G:725:HOH:O	2.03	0.57
1:J:148:ASN:ND2	1:J:150:TRP:HE3	2.01	0.57
1:G:171:PHE:HZ	1:G:204:MET:SD	2.27	0.57
1:L:26:GLN:OE1	1:L:26:GLN:HA	2.02	0.57
1:J:56:TYR:HD1	1:J:173:MET:HE1	1.65	0.57
1:J:93:THR:HG21	3:J:711:FUA:C2	2.32	0.57
1:F:110:HIS:CD2	1:F:119:ILE:HD13	2.38	0.57
1:G:154:THR:CG2	1:H:154:THR:O	2.44	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ARG:NH2	1:L:80:GLY:O	2.38	0.56
1:A:117:LEU:O	1:A:117:LEU:HD22	2.06	0.56
1:G:106:TRP:CD1	1:G:142:MET:HE2	2.40	0.56
1:H:23:GLU:HG3	1:H:24:ALA:N	2.15	0.56
1:J:157:ASP:OD2	1:K:157:ASP:CG	2.47	0.56
1:K:3:LYS:CG	4:K:720:HOH:O	2.52	0.56
1:L:145:VAL:HG11	1:L:173:MET:CE	2.34	0.56
1:L:11:VAL:HG13	1:L:11:VAL:O	2.06	0.56
1:G:118:HIS:O	1:G:122:GLN:HG3	2.05	0.56
1:H:106:TRP:CG	1:H:142:MET:HE3	2.40	0.56
1:F:110:HIS:CD2	1:F:119:ILE:CD1	2.88	0.56
1:J:75:MET:HE3	1:J:195:VAL:CB	2.35	0.56
1:F:56:TYR:HB3	1:F:57:PRO:CD	2.36	0.56
1:G:67:MET:HE1	1:G:204:MET:SD	2.46	0.56
1:G:154:THR:HG21	1:H:38:GLN:OE1	2.06	0.56
1:E:93:THR:HG21	3:E:706:FUA:H22	1.88	0.56
1:I:146:SER:CB	3:I:707:FUA:H3	2.35	0.56
1:K:139:ILE:HG13	1:K:142:MET:HG3	1.88	0.56
1:K:90:PRO:HD2	1:K:107:SER:O	2.06	0.56
1:A:30:GLN:NE2	4:A:802:HOH:O	2.38	0.55
1:B:3:LYS:H	1:I:10:THR:HB	1.69	0.55
1:C:30:GLN:HE22	1:C:164:ASP:HA	1.70	0.55
1:D:56:TYR:HB3	1:D:57:PRO:HD3	1.88	0.55
1:E:67:MET:HE1	1:E:171:PHE:CE1	2.35	0.55
1:L:76:ALA:HA	4:L:729:HOH:O	2.05	0.55
1:I:105:LEU:HD11	1:I:127:TYR:HB2	1.86	0.55
1:D:157:ASP:OD2	1:F:157:ASP:HB3	2.05	0.55
1:I:93:THR:CG2	3:I:707:FUA:H22	2.37	0.55
1:K:148:ASN:HD21	1:K:151:VAL:HG13	1.71	0.55
1:A:114:ARG:HH11	1:A:218:GLY:HA2	1.72	0.55
1:E:138:PHE:C	1:E:142:MET:HE1	2.32	0.55
3:I:707:FUA:H122	3:I:707:FUA:C28	2.37	0.55
1:J:56:TYR:CD1	1:J:173:MET:CE	2.89	0.55
1:K:139:ILE:HG13	1:K:142:MET:CG	2.36	0.55
1:K:187:LEU:HG	1:K:188:ALA:N	2.18	0.55
1:D:12:ASP:O	1:J:10:THR:CG2	2.55	0.55
1:B:114:ARG:CG	1:B:114:ARG:NH1	2.68	0.55
1:H:148:ASN:OD1	1:H:150:TRP:HE3	1.90	0.54
1:H:8:TYR:CE2	1:H:78:LYS:CE	2.83	0.54
1:H:190:GLN:HE21	1:H:190:GLN:C	2.15	0.54
1:J:49:LYS:O	1:J:51:ASN:O	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:MET:HE1	1:A:204:MET:SD	2.47	0.54
1:D:46:LYS:HE2	4:D:749:HOH:O	2.07	0.54
1:H:155:SER:HB3	1:I:155:SER:HB2	1.89	0.54
1:A:56:TYR:CD1	1:A:173:MET:CE	2.91	0.54
1:E:154:THR:CG2	1:F:154:THR:O	2.51	0.54
1:E:104:SER:HB2	1:E:134:PHE:CE2	2.42	0.54
1:K:148:ASN:HD21	1:K:151:VAL:CG1	2.19	0.54
1:L:71:PRO:HD3	4:L:714:HOH:O	2.08	0.54
1:H:67:MET:HE1	1:H:73:PHE:CD2	2.43	0.54
1:G:67:MET:CE	1:G:204:MET:SD	2.96	0.53
1:A:139:ILE:HG13	1:A:142:MET:HG3	1.89	0.53
1:E:34:ASN:HD22	1:E:190:GLN:HB3	1.67	0.53
1:K:25:PHE:O	1:K:30:GLN:HG3	2.08	0.53
1:K:150:TRP:HB3	1:L:206:ASN:HD21	1.74	0.53
1:H:145:VAL:HG12	1:H:173:MET:HE2	1.90	0.53
1:K:34:ASN:ND2	1:K:158:LEU:H	2.06	0.53
1:L:22:PHE:CE2	1:L:82:LEU:HD11	2.43	0.53
1:C:67:MET:HE3	1:C:73:PHE:CB	2.30	0.53
1:K:148:ASN:ND2	1:K:151:VAL:HG13	2.23	0.53
1:J:50:LYS:C	1:J:51:ASN:O	2.48	0.53
1:L:145:VAL:CG1	1:L:173:MET:CE	2.87	0.53
1:C:115:GLN:O	1:C:119:ILE:HD13	2.05	0.52
1:F:77:MET:HE3	1:F:82:LEU:HA	1.90	0.52
3:F:704:FUA:H232	3:F:704:FUA:H121	1.92	0.52
1:G:158:LEU:HD11	3:G:708:FUA:C7	2.38	0.52
1:L:18:ARG:O	1:L:19:LYS:C	2.52	0.52
1:H:54:LYS:HG3	4:H:768:HOH:O	2.08	0.52
1:I:124:VAL:O	1:I:128:GLY:N	2.41	0.52
1:J:123:ASP:OD1	1:J:136:LYS:HE3	2.10	0.52
1:A:59:PHE:CD2	1:A:173:MET:SD	3.03	0.52
1:I:34:ASN:ND2	1:I:158:LEU:H	2.07	0.52
1:K:3:LYS:CA	4:K:733:HOH:O	2.58	0.52
1:I:34:ASN:ND2	1:I:190:GLN:HB2	2.24	0.52
3:A:702:FUA:H122	3:A:702:FUA:H25	1.91	0.52
1:K:139:ILE:HG13	1:K:142:MET:HE3	1.91	0.52
1:G:106:TRP:CD1	1:G:142:MET:CE	2.92	0.52
1:D:144:PHE:CZ	3:D:705:FUA:H231	2.44	0.52
3:E:706:FUA:H232	3:E:706:FUA:C12	2.40	0.52
1:J:148:ASN:HD22	1:J:150:TRP:HE3	1.57	0.52
1:E:44:PHE:HB2	1:E:212:CYS:HB3	1.91	0.52
1:L:113:PHE:O	1:L:114:ARG:C	2.52	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:93:THR:HG21	3:H:709:FUA:H22	1.93	0.51
3:K:712:FUA:H282	3:K:712:FUA:H232	1.91	0.51
1:L:30:GLN:HE22	1:L:164:ASP:HA	1.75	0.51
1:G:26:GLN:NE2	4:G:740:HOH:O	2.43	0.51
1:I:91:CYS:SG	1:I:104:SER:HB3	2.50	0.51
1:J:59:PHE:CZ	1:J:185:MET:HE1	2.46	0.51
1:B:51:ASN:HD22	1:B:51:ASN:H	1.56	0.51
1:J:56:TYR:CE1	1:J:147:ALA:HB2	2.46	0.51
1:B:146:SER:HB3	3:B:703:FUA:H22	1.91	0.51
1:I:92:TYR:OH	1:I:105:LEU:HD23	2.11	0.51
1:C:204:MET:HE2	1:C:205:LEU:N	2.26	0.51
1:D:154:THR:O	1:F:154:THR:CG2	2.39	0.51
1:E:19:LYS:O	1:E:23:GLU:HG3	2.11	0.51
1:L:8:TYR:HB2	1:L:83:VAL:CG1	2.36	0.51
1:L:67:MET:CE	1:L:169:PRO:CG	2.79	0.51
1:L:204:MET:HE2	1:L:204:MET:C	2.35	0.51
1:J:92:TYR:CE1	1:J:105:LEU:HD21	2.45	0.51
1:A:37:VAL:CG2	1:C:151:VAL:HG13	2.41	0.51
1:C:9:THR:CG2	4:C:712:HOH:O	2.57	0.51
1:I:159:ASN:ND2	4:I:726:HOH:O	2.16	0.51
1:J:139:ILE:N	1:J:142:MET:HE3	2.26	0.51
1:H:46:LYS:NZ	4:H:734:HOH:O	2.44	0.51
3:I:707:FUA:H283	3:I:707:FUA:C23	2.40	0.51
1:L:145:VAL:HG11	1:L:173:MET:HE2	1.93	0.51
1:L:162:ASN:ND2	4:L:723:HOH:O	2.36	0.51
4:J:724:HOH:O	1:K:159:ASN:ND2	2.25	0.50
1:G:139:ILE:N	1:G:142:MET:HE3	2.20	0.50
1:L:84:ILE:HG22	1:L:85:TRP:O	2.12	0.50
1:F:19:LYS:O	1:F:23:GLU:HG3	2.11	0.50
1:I:13:ILE:O	1:I:13:ILE:CG2	2.59	0.50
3:I:707:FUA:C28	3:I:707:FUA:C23	2.89	0.50
1:E:97:GLU:HG3	4:E:750:HOH:O	2.10	0.50
1:H:154:THR:HG21	1:I:154:THR:O	2.05	0.50
1:F:77:MET:HG3	1:F:165:ASN:CG	2.36	0.50
1:K:139:ILE:N	1:K:142:MET:HE3	2.12	0.50
1:G:28:VAL:HG12	4:G:742:HOH:O	2.11	0.50
1:I:136:LYS:NZ	4:I:717:HOH:O	2.42	0.50
1:H:106:TRP:CB	1:H:142:MET:HE3	2.42	0.50
1:I:58:ALA:HA	1:I:113:PHE:CE1	2.46	0.50
1:J:158:LEU:HD11	3:J:711:FUA:H72	1.93	0.50
1:A:56:TYR:HD1	1:A:173:MET:HE1	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:49:LYS:O	1:F:50:LYS:C	2.55	0.50
1:A:56:TYR:CE1	1:A:173:MET:HE2	2.47	0.49
1:E:156:PHE:C	1:E:157:ASP:OD1	2.55	0.49
1:J:204:MET:SD	1:J:204:MET:C	2.95	0.49
1:D:25:PHE:O	1:D:30:GLN:HG3	2.12	0.49
1:G:139:ILE:HG13	1:G:142:MET:CG	2.41	0.49
1:J:146:SER:CB	3:J:711:FUA:H3	2.40	0.49
1:H:167:PHE:O	1:H:169:PRO:CD	2.58	0.49
1:A:106:TRP:CG	1:A:142:MET:HE3	2.46	0.49
3:B:703:FUA:H232	3:B:703:FUA:H121	1.94	0.49
1:D:110:HIS:CD2	1:D:112:ASP:H	2.22	0.49
1:E:177:TYR:HE2	1:E:186:PRO:HD3	1.76	0.49
1:F:113:PHE:CZ	1:F:117:LEU:HG	2.47	0.49
1:A:72:GLU:OE2	4:A:868:HOH:O	2.18	0.49
1:C:93:THR:HG21	3:C:701:FUA:H22	1.95	0.49
1:C:215:TRP:CZ2	1:C:217:GLY:HA2	2.48	0.49
1:C:176:TYR:CD1	1:C:176:TYR:C	2.91	0.49
1:J:32:THR:HG22	1:L:159:ASN:HB3	1.94	0.49
1:K:139:ILE:O	1:K:142:MET:SD	2.71	0.49
1:I:56:TYR:O	1:I:60:ILE:HG13	2.13	0.49
1:G:52:LYS:HE2	4:G:735:HOH:O	2.12	0.49
1:H:106:TRP:CD1	1:H:142:MET:HE3	2.47	0.49
1:K:106:TRP:CG	1:K:142:MET:HE2	2.47	0.49
1:B:9:THR:HG23	4:B:721:HOH:O	2.12	0.48
1:D:13:ILE:HD11	1:D:16:TRP:CE3	2.48	0.48
3:G:708:FUA:H121	3:G:708:FUA:H232	1.94	0.48
1:H:75:MET:SD	1:H:195:VAL:CG1	3.01	0.48
1:K:159:ASN:HB3	1:L:32:THR:CG2	2.43	0.48
1:A:34:ASN:ND2	1:A:158:LEU:H	2.10	0.48
1:B:162:ASN:CA	4:B:712:HOH:O	2.60	0.48
1:E:32:THR:HG21	4:E:707:HOH:O	2.13	0.48
1:I:99:THR:O	1:I:100:GLU:HB2	2.13	0.48
1:D:139:ILE:HG13	1:D:142:MET:HG3	1.94	0.48
1:C:204:MET:HE2	1:C:205:LEU:HA	1.95	0.48
1:A:41:ILE:O	1:A:42:THR:C	2.56	0.48
1:A:48:VAL:HG13	1:A:53:HIS:O	2.14	0.48
1:D:115:GLN:HE21	1:J:214:GLU:HG3	1.79	0.48
1:A:39:LEU:HD22	1:A:209:GLN:OE1	2.14	0.48
1:I:13:ILE:O	1:I:13:ILE:HG22	2.12	0.48
1:B:6:THR:HG21	1:B:141:ASN:HD21	1.78	0.48
1:B:51:ASN:ND2	1:B:51:ASN:N	2.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:GLU:OE2	4:D:727:HOH:O	2.20	0.48
1:I:77:MET:HE1	1:I:82:LEU:HB2	1.96	0.48
1:A:32:THR:HG21	4:A:812:HOH:O	2.14	0.48
1:F:77:MET:HA	1:F:77:MET:HE3	1.96	0.48
1:K:68:ASN:OD1	1:K:87:SER:HA	2.13	0.48
1:J:39:LEU:O	1:J:184:LEU:HA	2.14	0.48
1:K:50:LYS:C	1:K:51:ASN:O	2.54	0.48
1:F:93:THR:CG2	3:F:704:FUA:H22	2.44	0.48
1:E:30:GLN:HE22	1:E:164:ASP:HA	1.78	0.47
1:K:32:THR:HG21	4:K:714:HOH:O	2.13	0.47
1:K:176:TYR:HA	1:K:184:LEU:O	2.14	0.47
1:C:67:MET:CE	1:C:73:PHE:CB	2.76	0.47
1:A:62:ILE:HD13	1:A:211:TYR:HD2	1.80	0.47
1:F:162:ASN:O	3:F:704:FUA:H321	2.14	0.47
1:J:5:ILE:N	4:J:740:HOH:O	2.47	0.47
1:L:38:GLN:NE2	1:L:177:TYR:OH	2.46	0.47
1:E:49:LYS:O	1:E:50:LYS:C	2.56	0.47
1:F:163:MET:O	1:F:164:ASP:C	2.56	0.47
1:L:65:ARG:NH2	1:L:211:TYR:CD2	2.81	0.47
1:F:93:THR:HG21	3:F:704:FUA:H22	1.95	0.47
1:F:187:LEU:CD2	1:F:208:LEU:HD21	2.44	0.47
1:L:148:ASN:OD1	1:L:151:VAL:HG13	2.15	0.47
1:A:30:GLN:HE22	1:A:164:ASP:HA	1.80	0.47
1:G:139:ILE:HG13	1:G:142:MET:SD	2.55	0.47
1:J:145:VAL:CG1	1:J:173:MET:HE2	2.44	0.47
1:D:174:GLY:HA3	1:D:186:PRO:HB2	1.96	0.47
1:G:139:ILE:HG13	1:G:142:MET:HG3	1.95	0.47
1:G:157:ASP:OD1	1:H:157:ASP:HB2	2.15	0.47
1:H:185:MET:HB3	1:H:185:MET:HE3	1.72	0.47
1:I:110:HIS:CD2	1:I:119:ILE:HD13	2.49	0.47
1:K:51:ASN:OD1	1:K:51:ASN:N	2.46	0.47
1:L:11:VAL:CG1	1:L:11:VAL:O	2.63	0.47
1:L:106:TRP:CD1	1:L:142:MET:HE1	2.45	0.47
1:L:150:TRP:HB2	1:L:151:VAL:HG12	1.97	0.47
1:F:26:GLN:NE2	4:F:717:HOH:O	2.48	0.47
1:B:159:ASN:ND2	4:C:768:HOH:O	2.33	0.47
1:C:30:GLN:NE2	4:C:708:HOH:O	2.47	0.47
1:K:56:TYR:HB3	1:K:57:PRO:CD	2.45	0.47
3:K:712:FUA:H232	3:K:712:FUA:C28	2.45	0.47
1:L:61:HIS:O	1:L:65:ARG:HG3	2.14	0.47
1:D:45:LEU:HD12	1:D:183:VAL:HG11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:MET:HE2	1:D:204:MET:HB3	1.61	0.47
1:E:12:ASP:OD2	1:E:15:GLN:HG2	2.15	0.47
1:L:138:PHE:HA	1:L:142:MET:HE1	1.96	0.47
3:D:705:FUA:H151	3:D:705:FUA:H203	1.50	0.46
1:F:123:ASP:OD1	1:F:136:LYS:CE	2.53	0.46
1:B:34:ASN:CB	1:B:157:ASP:HB3	2.45	0.46
1:G:38:GLN:HE22	1:G:186:PRO:CD	2.29	0.46
1:J:56:TYR:HB3	1:J:57:PRO:CD	2.45	0.46
1:G:176:TYR:N	4:G:736:HOH:O	2.25	0.46
1:H:90:PRO:O	1:H:106:TRP:HA	2.15	0.46
1:K:17:HIS:N	1:K:17:HIS:ND1	2.62	0.46
1:K:99:THR:HG21	1:K:131:LEU:CD1	2.39	0.46
1:K:146:SER:HB3	3:K:712:FUA:H3	1.97	0.46
1:C:123:ASP:OD1	1:C:136:LYS:NZ	2.47	0.46
1:D:110:HIS:HD2	1:D:112:ASP:N	2.09	0.46
1:A:54:LYS:HD3	4:A:818:HOH:O	2.16	0.46
1:I:92:TYR:CZ	1:I:105:LEU:HD23	2.50	0.46
1:L:187:LEU:HD22	1:L:208:LEU:HD21	1.96	0.46
1:J:77:MET:HE3	1:J:77:MET:HB3	1.77	0.46
1:A:133:TYR:HE2	3:A:702:FUA:H272	1.77	0.46
1:A:159:ASN:OD1	1:B:159:ASN:ND2	2.48	0.46
1:D:6:THR:CG2	4:D:733:HOH:O	2.54	0.46
1:D:9:THR:HG23	4:D:730:HOH:O	2.16	0.46
1:E:156:PHE:O	1:E:157:ASP:OD1	2.34	0.46
1:G:59:PHE:CD2	1:G:173:MET:HE3	2.50	0.46
1:F:187:LEU:HD22	1:F:208:LEU:HD21	1.98	0.46
1:H:26:GLN:NE2	4:H:761:HOH:O	2.47	0.46
1:I:93:THR:HG21	3:I:707:FUA:H22	1.97	0.46
1:L:164:ASP:HB2	4:L:723:HOH:O	2.15	0.46
1:B:146:SER:CB	3:B:703:FUA:H3	2.46	0.46
1:D:89:HIS:O	1:D:142:MET:HA	2.15	0.46
1:D:96:HIS:O	1:D:100:GLU:N	2.49	0.46
1:E:126:CYS:HB3	1:E:127:TYR:CD2	2.51	0.46
1:I:148:ASN:HB3	1:I:173:MET:O	2.16	0.46
1:J:124:VAL:O	1:J:128:GLY:N	2.47	0.46
1:L:204:MET:HE1	1:L:205:LEU:CD2	2.39	0.46
1:G:171:PHE:CZ	1:G:204:MET:CE	2.98	0.46
3:J:711:FUA:H72	3:J:711:FUA:H212	1.57	0.46
1:L:187:LEU:HD22	1:L:208:LEU:CD2	2.45	0.46
3:A:702:FUA:H203	3:A:702:FUA:H151	1.71	0.45
1:C:192:HIS:HD1	1:C:194:ALA:N	2.08	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:35:GLN:HG3	4:E:731:HOH:O	2.15	0.45
1:H:59:PHE:O	1:H:62:ILE:HG22	2.15	0.45
1:D:159:ASN:OD1	4:D:761:HOH:O	2.21	0.45
1:E:75:MET:HA	1:E:83:VAL:O	2.16	0.45
1:E:145:VAL:HG11	1:E:173:MET:CE	2.30	0.45
3:L:710:FUA:H232	3:L:710:FUA:C12	2.47	0.45
3:B:703:FUA:H151	3:B:703:FUA:H203	1.42	0.45
1:L:204:MET:HE2	1:L:205:LEU:CA	2.46	0.45
1:A:13:ILE:HG22	1:A:19:LYS:HG3	1.99	0.45
1:B:34:ASN:ND2	1:B:190:GLN:HB2	2.32	0.45
1:B:67:MET:HE1	1:B:73:PHE:CG	2.52	0.45
1:F:77:MET:HE3	1:F:82:LEU:CA	2.47	0.45
1:G:18:ARG:O	1:G:19:LYS:C	2.59	0.45
1:G:175:LYS:HA	4:G:736:HOH:O	2.16	0.45
1:J:92:TYR:HA	1:J:145:VAL:O	2.17	0.45
3:H:709:FUA:O2	3:H:709:FUA:C29	2.64	0.45
1:I:59:PHE:CD2	1:I:173:MET:HE3	2.52	0.45
1:J:138:PHE:CE2	3:J:711:FUA:H283	2.52	0.45
3:F:704:FUA:H232	3:F:704:FUA:H122	1.96	0.45
1:I:114:ARG:HH22	1:I:217:GLY:C	2.25	0.45
1:J:34:ASN:HD21	1:J:158:LEU:H	1.64	0.45
1:J:37:VAL:HG23	4:J:726:HOH:O	2.15	0.45
1:J:65:ARG:NH1	1:J:211:TYR:CE2	2.85	0.45
1:A:34:ASN:OD1	1:A:157:ASP:OD2	2.35	0.45
1:B:67:MET:CE	1:B:73:PHE:CB	2.91	0.45
3:C:701:FUA:H203	3:C:701:FUA:H151	1.14	0.45
1:I:37:VAL:HG12	1:I:38:GLN:N	2.32	0.45
1:J:105:LEU:N	1:J:105:LEU:CD2	2.80	0.45
1:C:75:MET:HA	1:C:83:VAL:O	2.17	0.45
1:F:25:PHE:O	1:F:30:GLN:HA	2.17	0.45
1:H:45:LEU:HD22	1:H:49:LYS:HD2	1.99	0.45
1:J:162:ASN:ND2	1:J:164:ASP:H	2.15	0.45
1:K:146:SER:HB3	3:K:712:FUA:H22	1.99	0.45
1:K:204:MET:SD	1:K:204:MET:C	3.00	0.45
1:C:45:LEU:HD12	1:C:183:VAL:HG11	1.99	0.45
1:F:77:MET:HE3	1:F:82:LEU:N	2.31	0.45
1:F:106:TRP:O	1:F:136:LYS:HE3	2.16	0.45
1:I:75:MET:HA	1:I:83:VAL:O	2.16	0.45
1:K:166:PHE:CZ	3:K:712:FUA:H211	2.52	0.45
1:L:72:GLU:HG3	1:L:200:HIS:HB3	1.99	0.45
1:L:116:PHE:O	1:L:117:LEU:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:ILE:HG13	1:B:142:MET:HG2	1.97	0.44
3:G:708:FUA:H151	3:G:708:FUA:H203	1.83	0.44
1:I:56:TYR:N	1:I:57:PRO:HD2	2.32	0.44
1:B:162:ASN:CB	4:B:712:HOH:O	2.62	0.44
1:E:9:THR:CG2	1:E:84:ILE:HB	2.46	0.44
1:A:159:ASN:ND2	4:C:768:HOH:O	2.09	0.44
1:D:214:GLU:HG3	1:J:115:GLN:NE2	2.32	0.44
3:D:705:FUA:H212	3:D:705:FUA:H72	1.65	0.44
1:I:70:HIS:HB2	1:I:73:PHE:CD1	2.52	0.44
1:A:106:TRP:CG	1:A:142:MET:CE	2.99	0.44
3:D:705:FUA:C12	3:D:705:FUA:C23	2.95	0.44
1:F:12:ASP:OD1	1:F:15:GLN:HG2	2.18	0.44
1:H:65:ARG:HH22	1:H:219:ALA:CB	2.28	0.44
1:L:117:LEU:O	1:L:117:LEU:HD12	2.17	0.44
1:C:56:TYR:CE1	1:C:147:ALA:HB2	2.53	0.44
1:C:118:HIS:O	1:C:122:GLN:HG3	2.17	0.44
1:F:36:THR:HG22	1:F:37:VAL:N	2.32	0.44
1:G:110:HIS:HD2	1:G:119:ILE:HD12	1.81	0.44
1:A:57:PRO:HB3	1:A:120:TYR:CD2	2.52	0.44
1:D:30:GLN:HE21	1:D:192:HIS:HE2	1.66	0.44
1:J:159:ASN:HD22	1:L:159:ASN:ND2	2.15	0.44
1:G:35:GLN:O	1:G:188:ALA:HA	2.17	0.44
1:L:72:GLU:OE1	1:L:203:ARG:NH2	2.51	0.44
1:L:92:TYR:HA	1:L:145:VAL:O	2.16	0.44
1:D:111:ASP:OD2	1:J:65:ARG:CD	2.58	0.44
3:D:705:FUA:H232	3:D:705:FUA:H121	1.97	0.44
1:E:9:THR:HG23	1:E:84:ILE:HB	2.00	0.44
1:G:139:ILE:HG13	1:G:142:MET:HE3	1.96	0.44
1:A:49:LYS:O	1:A:50:LYS:C	2.61	0.44
3:C:701:FUA:H212	3:C:701:FUA:H72	1.72	0.44
1:I:77:MET:CE	1:I:82:LEU:HD13	2.48	0.44
1:J:34:ASN:ND2	1:J:158:LEU:H	2.16	0.44
1:J:67:MET:SD	1:J:169:PRO:HG2	2.58	0.44
1:C:197:ASP:O	1:C:198:GLY:C	2.61	0.43
3:K:712:FUA:H151	3:K:712:FUA:H203	1.43	0.43
1:A:171:PHE:CE2	1:A:204:MET:HE1	2.44	0.43
1:E:104:SER:CB	1:E:134:PHE:CE2	3.01	0.43
1:F:156:PHE:C	1:F:156:PHE:CD2	2.95	0.43
1:G:38:GLN:HE22	1:G:186:PRO:HD3	1.81	0.43
1:K:93:THR:HG23	1:K:146:SER:HA	1.99	0.43
1:A:56:TYR:CE1	1:A:147:ALA:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:ASP:HB3	1:C:209:GLN:HE22	1.81	0.43
1:D:149:PRO:HD2	1:D:150:TRP:CZ3	2.53	0.43
1:G:158:LEU:HD23	1:G:158:LEU:HA	1.68	0.43
1:G:187:LEU:HD22	1:G:208:LEU:CD2	2.46	0.43
1:I:134:PHE:CZ	3:I:707:FUA:H282	2.52	0.43
1:J:138:PHE:CD1	1:J:138:PHE:O	2.72	0.43
3:K:712:FUA:H72	3:K:712:FUA:H212	1.62	0.43
1:C:204:MET:C	1:C:204:MET:CE	2.91	0.43
1:H:127:TYR:CD2	1:H:136:LYS:HG2	2.53	0.43
1:I:26:GLN:NE2	1:I:26:GLN:HA	2.33	0.43
1:K:162:ASN:O	3:K:712:FUA:H321	2.17	0.43
1:L:145:VAL:CG1	1:L:173:MET:HE2	2.47	0.43
1:I:34:ASN:HD21	1:I:158:LEU:H	1.67	0.43
1:J:171:PHE:CE2	1:J:204:MET:CE	2.93	0.43
1:C:198:GLY:O	1:C:199:PHE:C	2.56	0.43
1:D:177:TYR:HE2	1:D:186:PRO:HD3	1.83	0.43
1:H:8:TYR:CD1	1:H:8:TYR:C	2.96	0.43
1:I:19:LYS:HD2	4:I:727:HOH:O	2.18	0.43
1:J:54:LYS:HG3	1:J:57:PRO:HG3	2.01	0.43
1:C:204:MET:HE2	1:C:205:LEU:CA	2.49	0.43
1:K:158:LEU:HD11	3:K:712:FUA:H72	2.01	0.43
1:K:159:ASN:HB3	1:L:32:THR:HG22	2.01	0.43
1:B:50:LYS:HG2	1:B:51:ASN:ND2	2.32	0.43
1:F:30:GLN:NE2	4:F:717:HOH:O	2.52	0.43
1:B:6:THR:CG2	1:B:141:ASN:HD21	2.32	0.43
1:D:176:TYR:HA	1:D:185:MET:HA	2.00	0.43
1:G:72:GLU:HG3	1:G:200:HIS:HB3	2.01	0.43
1:L:30:GLN:HG3	1:L:192:HIS:CE1	2.54	0.43
1:B:19:LYS:HE2	1:B:19:LYS:HB2	1.55	0.42
3:H:709:FUA:H72	3:H:709:FUA:H212	1.66	0.42
1:I:139:ILE:HG12	1:I:142:MET:SD	2.59	0.42
1:A:146:SER:HB3	3:A:702:FUA:H22	2.01	0.42
1:A:148:ASN:ND2	1:A:150:TRP:HE3	2.17	0.42
3:H:709:FUA:H283	1:I:29:ALA:HB2	2.00	0.42
1:D:113:PHE:O	1:D:117:LEU:HB2	2.20	0.42
1:E:147:ALA:C	1:E:149:PRO:CD	2.93	0.42
1:J:56:TYR:CE1	1:J:173:MET:HE3	2.53	0.42
1:K:93:THR:HG21	3:K:712:FUA:H22	2.01	0.42
1:E:139:ILE:C	1:E:142:MET:SD	2.99	0.42
1:G:89:HIS:O	1:G:142:MET:HA	2.19	0.42
1:H:67:MET:CE	1:H:73:PHE:HB3	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:157:ASP:CG	1:I:157:ASP:OD2	2.63	0.42
1:I:171:PHE:HZ	1:I:204:MET:SD	2.42	0.42
1:H:36:THR:HG22	1:H:37:VAL:N	2.34	0.42
1:L:8:TYR:CD2	1:L:8:TYR:N	2.86	0.42
1:L:133:TYR:CZ	1:L:134:PHE:HE1	2.37	0.42
1:B:9:THR:CG2	4:B:721:HOH:O	2.68	0.42
1:B:50:LYS:CG	1:B:51:ASN:HD22	2.30	0.42
1:D:176:TYR:HB3	1:D:185:MET:HB2	2.01	0.42
3:D:705:FUA:C23	3:D:705:FUA:C28	2.98	0.42
3:F:704:FUA:H72	3:F:704:FUA:H212	1.76	0.42
1:H:56:TYR:HB3	1:H:57:PRO:CD	2.49	0.42
1:I:70:HIS:HA	1:I:71:PRO:HD2	1.87	0.42
1:K:153:PHE:O	1:K:186:PRO:HB3	2.20	0.42
1:L:56:TYR:CE1	1:L:147:ALA:HB2	2.55	0.42
1:L:162:ASN:OD1	4:L:723:HOH:O	2.22	0.42
1:F:77:MET:HG3	1:F:165:ASN:OD1	2.20	0.42
1:F:110:HIS:CD2	1:F:119:ILE:HD11	2.55	0.42
1:H:67:MET:HE2	1:H:169:PRO:CB	2.44	0.42
1:H:157:ASP:OD1	1:I:157:ASP:OD2	2.38	0.42
3:J:711:FUA:H151	3:J:711:FUA:H203	1.47	0.42
1:C:13:ILE:HD11	1:C:82:LEU:HD23	2.00	0.42
1:D:25:PHE:HB2	1:D:194:ALA:HA	2.01	0.42
1:F:30:GLN:HE22	1:F:164:ASP:HA	1.85	0.42
1:D:65:ARG:CD	1:J:111:ASP:OD2	2.64	0.42
1:E:160:VAL:HA	1:F:31:CYS:HB3	2.02	0.42
1:I:39:LEU:O	1:I:184:LEU:HA	2.20	0.42
1:A:108:GLU:OE1	1:A:110:HIS:NE2	2.51	0.42
1:D:156:PHE:CD2	1:D:156:PHE:C	2.98	0.42
1:E:3:LYS:N	4:E:748:HOH:O	2.53	0.42
3:F:704:FUA:H151	3:F:704:FUA:H203	1.53	0.42
1:H:13:ILE:HD12	1:H:13:ILE:HG23	1.74	0.42
1:H:140:GLU:HG2	4:H:778:HOH:O	2.20	0.42
3:D:705:FUA:H232	3:D:705:FUA:H122	2.01	0.41
1:E:104:SER:O	1:E:134:PHE:HD2	2.03	0.41
1:I:148:ASN:ND2	1:I:150:TRP:HE3	2.18	0.41
1:K:56:TYR:HB3	1:K:57:PRO:HD3	2.02	0.41
1:A:133:TYR:HE2	3:A:702:FUA:C27	2.32	0.41
1:D:54:LYS:HZ3	1:D:54:LYS:HG2	1.59	0.41
1:H:175:LYS:HD2	1:H:175:LYS:C	2.44	0.41
1:J:105:LEU:HD23	1:J:105:LEU:C	2.44	0.41
1:K:148:ASN:ND2	1:K:150:TRP:HE3	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:MET:HE1	1:C:205:LEU:HD23	2.00	0.41
1:D:38:GLN:OE1	1:F:154:THR:HG21	2.20	0.41
1:E:72:GLU:HG3	1:E:200:HIS:HB3	2.02	0.41
1:F:32:THR:HG21	4:F:705:HOH:O	2.18	0.41
3:G:708:FUA:H232	3:G:708:FUA:C12	2.51	0.41
1:J:158:LEU:HD11	3:J:711:FUA:C7	2.50	0.41
1:L:171:PHE:CE2	1:L:189:ILE:HD13	2.54	0.41
1:B:134:PHE:CE1	3:B:703:FUA:H273	2.55	0.41
1:C:119:ILE:CD1	1:C:119:ILE:H	2.26	0.41
1:D:66:LEU:HD11	1:D:208:LEU:HA	2.01	0.41
1:G:187:LEU:HD12	1:G:187:LEU:HA	1.89	0.41
1:I:115:GLN:O	1:I:119:ILE:HD12	2.20	0.41
1:A:6:THR:CG2	4:A:837:HOH:O	2.34	0.41
1:A:17:HIS:HD2	4:C:750:HOH:O	2.03	0.41
1:D:84:ILE:HD13	1:J:9:THR:HG21	2.02	0.41
1:D:93:THR:HG21	3:D:705:FUA:H22	2.01	0.41
1:E:93:THR:CG2	3:E:706:FUA:H22	2.49	0.41
1:G:165:ASN:HA	1:G:167:PHE:CE1	2.56	0.41
3:G:708:FUA:C5	3:G:708:FUA:H202	2.50	0.41
1:H:66:LEU:HD23	4:H:715:HOH:O	2.20	0.41
3:I:707:FUA:H151	3:I:707:FUA:H203	1.72	0.41
1:K:34:ASN:HD21	1:K:158:LEU:H	1.68	0.41
3:A:702:FUA:H212	3:A:702:FUA:H72	1.71	0.41
1:C:93:THR:CG2	3:C:701:FUA:H22	2.51	0.41
1:D:110:HIS:HE1	4:J:725:HOH:O	2.02	0.41
1:J:123:ASP:OD1	1:J:136:LYS:CE	2.68	0.41
1:K:163:MET:O	1:K:164:ASP:C	2.62	0.41
1:L:204:MET:CE	1:L:204:MET:C	2.93	0.41
1:H:104:SER:OG	4:H:783:HOH:O	2.22	0.41
1:A:67:MET:HE2	1:A:67:MET:N	2.35	0.41
1:J:189:ILE:HD12	1:J:190:GLN:N	2.36	0.41
1:K:150:TRP:HB3	1:L:206:ASN:ND2	2.34	0.41
1:A:8:TYR:HB2	1:A:83:VAL:HG13	2.02	0.41
1:A:25:PHE:HB2	1:A:194:ALA:HA	2.03	0.41
1:B:40:ASP:OD1	1:B:182:LYS:HG2	2.20	0.41
1:D:157:ASP:HB2	1:E:157:ASP:OD2	2.21	0.41
1:F:112:ASP:HB3	1:F:115:GLN:HB2	2.01	0.41
1:F:139:ILE:HG13	1:F:142:MET:HG2	2.03	0.41
1:H:204:MET:HE3	1:H:204:MET:HB3	1.96	0.41
1:K:148:ASN:C	1:K:148:ASN:ND2	2.79	0.41
1:L:145:VAL:CG1	1:L:173:MET:HE3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ASP:OD2	1:A:40:ASP:C	2.63	0.41
1:A:75:MET:HA	1:A:83:VAL:O	2.21	0.41
1:H:77:MET:HE3	1:H:77:MET:HB2	1.45	0.41
1:J:9:THR:CG2	4:J:712:HOH:O	2.62	0.41
1:J:138:PHE:CD1	1:J:138:PHE:C	2.98	0.41
1:L:93:THR:HG21	3:L:710:FUA:H22	2.02	0.41
1:L:204:MET:CE	1:L:205:LEU:HA	2.51	0.41
1:A:67:MET:CE	1:A:204:MET:SD	3.09	0.40
3:A:702:FUA:H121	3:A:702:FUA:H232	2.03	0.40
1:B:62:ILE:HG23	1:B:211:TYR:HD1	1.85	0.40
1:D:141:ASN:OD1	1:D:141:ASN:N	2.52	0.40
1:H:67:MET:CE	1:H:169:PRO:CB	3.00	0.40
1:I:4:LYS:HE2	1:I:4:LYS:CA	2.51	0.40
1:I:70:HIS:HB2	1:I:73:PHE:CE1	2.56	0.40
1:L:70:HIS:HA	1:L:71:PRO:HD2	1.70	0.40
1:G:71:PRO:O	1:G:72:GLU:C	2.62	0.40
1:J:18:ARG:O	1:J:19:LYS:C	2.63	0.40
3:L:710:FUA:H212	3:L:710:FUA:H72	1.63	0.40
3:B:703:FUA:H72	3:B:703:FUA:H212	1.79	0.40
1:C:214:GLU:O	1:C:215:TRP:C	2.64	0.40
1:D:51:ASN:HB3	1:D:53:HIS:CD2	2.57	0.40
1:H:23:GLU:CG	1:H:24:ALA:N	2.83	0.40
4:J:724:HOH:O	1:L:159:ASN:OD1	2.22	0.40
1:D:161:ALA:HB2	1:E:163:MET:SD	2.61	0.40
3:I:707:FUA:H232	3:I:707:FUA:C12	2.52	0.40
1:K:25:PHE:HB2	1:K:194:ALA:HA	2.03	0.40
1:L:25:PHE:HB2	1:L:194:ALA:HA	2.03	0.40
1:B:44:PHE:HB2	1:B:212:CYS:O	2.21	0.40
1:G:38:GLN:NE2	1:G:186:PRO:HG3	2.20	0.40
1:G:148:ASN:HD22	1:G:150:TRP:HE3	1.70	0.40
1:I:43:ALA:O	1:I:44:PHE:C	2.61	0.40
1:I:81:GLU:HB2	4:I:739:HOH:O	2.20	0.40
1:K:3:LYS:HG2	4:K:720:HOH:O	2.21	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	212/219 (97%)	205 (97%)	6 (3%)	1 (0%)	24	25
1	B	215/219 (98%)	206 (96%)	8 (4%)	1 (0%)	24	25
1	C	211/219 (96%)	202 (96%)	9 (4%)	0	100	100
1	D	211/219 (96%)	207 (98%)	4 (2%)	0	100	100
1	E	213/219 (97%)	202 (95%)	11 (5%)	0	100	100
1	F	210/219 (96%)	201 (96%)	8 (4%)	1 (0%)	24	25
1	G	211/219 (96%)	206 (98%)	5 (2%)	0	100	100
1	H	214/219 (98%)	208 (97%)	6 (3%)	0	100	100
1	I	213/219 (97%)	206 (97%)	6 (3%)	1 (0%)	24	25
1	J	210/219 (96%)	202 (96%)	6 (3%)	2 (1%)	12	10
1	K	211/219 (96%)	202 (96%)	8 (4%)	1 (0%)	24	25
1	L	208/219 (95%)	200 (96%)	8 (4%)	0	100	100
All	All	2539/2628 (97%)	2447 (96%)	85 (3%)	7 (0%)	36	39

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	50	LYS
1	I	128	GLY
1	J	51	ASN
1	F	52	LYS
1	A	165	ASN
1	B	132	ALA
1	J	27	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	190/194 (98%)	170 (90%)	20 (10%)	6	5
1	B	193/194 (100%)	167 (86%)	26 (14%)	4	3
1	C	189/194 (97%)	161 (85%)	28 (15%)	3	2
1	D	189/194 (97%)	166 (88%)	23 (12%)	5	3
1	E	192/194 (99%)	170 (88%)	22 (12%)	5	4
1	F	189/194 (97%)	163 (86%)	26 (14%)	3	2
1	G	189/194 (97%)	170 (90%)	19 (10%)	7	6
1	H	191/194 (98%)	163 (85%)	28 (15%)	3	2
1	I	192/194 (99%)	169 (88%)	23 (12%)	5	4
1	J	190/194 (98%)	157 (83%)	33 (17%)	2	1
1	K	191/194 (98%)	153 (80%)	38 (20%)	1	1
1	L	188/194 (97%)	160 (85%)	28 (15%)	3	2
All	All	2283/2328 (98%)	1969 (86%)	314 (14%)	3	2

All (314) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	10	THR
1	A	32	THR
1	A	39	LEU
1	A	45	LEU
1	A	46	LYS
1	A	50	LYS
1	A	52	LYS
1	A	54	LYS
1	A	62	ILE
1	A	83	VAL
1	A	114	ARG
1	A	117	LEU
1	A	142	MET

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Mol	Chain	Res	Type
1	A	154	THR
1	A	160	VAL
1	A	175	LYS
1	A	189	ILE
1	A	190	GLN
1	A	193	HIS
1	B	2	GLU
1	B	4	LYS
1	B	5	ILE
1	B	6	THR
1	B	9	THR
1	B	10	THR
1	B	19	LYS
1	B	32	THR
1	B	37	VAL
1	B	39	LEU
1	B	45	LEU
1	B	51	ASN
1	B	52	LYS
1	B	54	LYS
1	B	79	ASP
1	B	83	VAL
1	B	94	VAL
1	B	111	ASP
1	B	117	LEU
1	B	122	GLN
1	B	129	GLU
1	B	158	LEU
1	B	160	VAL
1	B	187	LEU
1	B	190	GLN
1	B	216	GLN
1	C	6	THR
1	C	9	THR
1	C	28	VAL
1	C	32	THR
1	C	35	GLN
1	C	39	LEU
1	C	45	LEU
1	C	48	VAL
1	C	50	LYS
1	C	65	ARG

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Mol	Chain	Res	Type
1	C	83	VAL
1	C	105	LEU
1	C	108	GLU
1	C	111	ASP
1	C	115	GLN
1	C	117	LEU
1	C	146	SER
1	C	157	ASP
1	C	158	LEU
1	C	160	VAL
1	C	173	MET
1	C	176	TYR
1	C	178	THR
1	C	181	ASP
1	C	187	LEU
1	C	190	GLN
1	C	204	MET
1	C	216	GLN
1	D	6	THR
1	D	13	ILE
1	D	32	THR
1	D	35	GLN
1	D	39	LEU
1	D	45	LEU
1	D	46	LYS
1	D	50	LYS
1	D	54	LYS
1	D	67	MET
1	D	78	LYS
1	D	83	VAL
1	D	97	GLU
1	D	98	GLN
1	D	107	SER
1	D	111	ASP
1	D	114	ARG
1	D	117	LEU
1	D	186	PRO
1	D	187	LEU
1	D	190	GLN
1	D	193	HIS
1	D	204	MET
1	E	3	LYS

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Mol	Chain	Res	Type
1	E	4	LYS
1	E	5	ILE
1	E	6	THR
1	E	10	THR
1	E	13	ILE
1	E	32	THR
1	E	37	VAL
1	E	39	LEU
1	E	45	LEU
1	E	52	LYS
1	E	83	VAL
1	E	98	GLN
1	E	114	ARG
1	E	117	LEU
1	E	126	CYS
1	E	142	MET
1	E	146	SER
1	E	158	LEU
1	E	189	ILE
1	E	190	GLN
1	E	204	MET
1	F	6	THR
1	F	32	THR
1	F	37	VAL
1	F	39	LEU
1	F	45	LEU
1	F	50	LYS
1	F	54	LYS
1	F	62	ILE
1	F	77	MET
1	F	83	VAL
1	F	87	SER
1	F	94	VAL
1	F	97	GLU
1	F	98	GLN
1	F	108	GLU
1	F	114	ARG
1	F	115	GLN
1	F	117	LEU
1	F	121	SER
1	F	154	THR
1	F	157	ASP

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Mol	Chain	Res	Type
1	F	158	LEU
1	F	181	ASP
1	F	182	LYS
1	F	190	GLN
1	F	193	HIS
1	G	9	THR
1	G	28	VAL
1	G	32	THR
1	G	37	VAL
1	G	45	LEU
1	G	48	VAL
1	G	52	LYS
1	G	54	LYS
1	G	83	VAL
1	G	98	GLN
1	G	142	MET
1	G	148	ASN
1	G	154	THR
1	G	160	VAL
1	G	181	ASP
1	G	186	PRO
1	G	189	ILE
1	G	190	GLN
1	G	216	GLN
1	H	4	LYS
1	H	5	ILE
1	H	6	THR
1	H	19	LYS
1	H	23	GLU
1	H	32	THR
1	H	37	VAL
1	H	39	LEU
1	H	45	LEU
1	H	48	VAL
1	H	54	LYS
1	H	62	ILE
1	H	77	MET
1	H	83	VAL
1	H	84	ILE
1	H	94	VAL
1	H	129	GLU
1	H	154	THR

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Mol	Chain	Res	Type
1	H	157	ASP
1	H	158	LEU
1	H	160	VAL
1	H	169	PRO
1	H	175	LYS
1	H	185	MET
1	H	189	ILE
1	H	190	GLN
1	H	191	VAL
1	H	193	HIS
1	I	5	ILE
1	I	9	THR
1	I	10	THR
1	I	32	THR
1	I	39	LEU
1	I	45	LEU
1	I	46	LYS
1	I	50	LYS
1	I	83	VAL
1	I	105	LEU
1	I	114	ARG
1	I	117	LEU
1	I	121	SER
1	I	129	GLU
1	I	142	MET
1	I	155	SER
1	I	157	ASP
1	I	158	LEU
1	I	178	THR
1	I	190	GLN
1	I	204	MET
1	I	210	GLN
1	I	214	GLU
1	J	5	ILE
1	J	6	THR
1	J	9	THR
1	J	10	THR
1	J	19	LYS
1	J	28	VAL
1	J	39	LEU
1	J	45	LEU
1	J	54	LYS

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Mol	Chain	Res	Type
1	J	67	MET
1	J	83	VAL
1	J	87	SER
1	J	97	GLU
1	J	98	GLN
1	J	105	LEU
1	J	114	ARG
1	J	117	LEU
1	J	122	GLN
1	J	126	CYS
1	J	129	GLU
1	J	136	LYS
1	J	146	SER
1	J	158	LEU
1	J	160	VAL
1	J	173	MET
1	J	175	LYS
1	J	178	THR
1	J	181	ASP
1	J	182	LYS
1	J	189	ILE
1	J	190	GLN
1	J	204	MET
1	J	214	GLU
1	K	3	LYS
1	K	5	ILE
1	K	9	THR
1	K	10	THR
1	K	15	GLN
1	K	19	LYS
1	K	23	GLU
1	K	28	VAL
1	K	32	THR
1	K	37	VAL
1	K	39	LEU
1	K	42	THR
1	K	45	LEU
1	K	46	LYS
1	K	50	LYS
1	K	51	ASN
1	K	52	LYS
1	K	78	LYS

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Mol	Chain	Res	Type
1	K	81	GLU
1	K	83	VAL
1	K	94	VAL
1	K	97	GLU
1	K	98	GLN
1	K	111	ASP
1	K	114	ARG
1	K	117	LEU
1	K	131	LEU
1	K	148	ASN
1	K	151	VAL
1	K	154	THR
1	K	158	LEU
1	K	160	VAL
1	K	173	MET
1	K	178	THR
1	K	182	LYS
1	K	187	LEU
1	K	190	GLN
1	K	203	ARG
1	L	6	THR
1	L	13	ILE
1	L	14	SER
1	L	27	SER
1	L	37	VAL
1	L	39	LEU
1	L	45	LEU
1	L	65	ARG
1	L	67	MET
1	L	77	MET
1	L	82	LEU
1	L	83	VAL
1	L	94	VAL
1	L	105	LEU
1	L	108	GLU
1	L	115	GLN
1	L	117	LEU
1	L	118	HIS
1	L	122	GLN
1	L	136	LYS
1	L	142	MET
1	L	151	VAL

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Mol	Chain	Res	Type
1	L	158	LEU
1	L	160	VAL
1	L	181	ASP
1	L	182	LYS
1	L	190	GLN
1	L	204	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	34	ASN
1	A	122	GLN
1	A	148	ASN
1	A	159	ASN
1	A	190	GLN
1	B	34	ASN
1	B	51	ASN
1	B	159	ASN
1	B	210	GLN
1	C	30	GLN
1	C	34	ASN
1	C	38	GLN
1	C	190	GLN
1	D	30	GLN
1	D	35	GLN
1	D	51	ASN
1	D	110	HIS
1	D	115	GLN
1	D	190	GLN
1	E	15	GLN
1	E	26	GLN
1	E	30	GLN
1	E	34	ASN
1	E	38	GLN
1	E	98	GLN
1	E	110	HIS
1	E	148	ASN
1	E	190	GLN
1	F	26	GLN
1	F	30	GLN
1	F	34	ASN

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Mol	Chain	Res	Type
1	F	35	GLN
1	F	53	HIS
1	F	110	HIS
1	F	190	GLN
1	G	15	GLN
1	G	26	GLN
1	G	30	GLN
1	G	38	GLN
1	G	98	GLN
1	G	110	HIS
1	G	148	ASN
1	G	190	GLN
1	G	210	GLN
1	H	26	GLN
1	H	30	GLN
1	H	34	ASN
1	H	98	GLN
1	H	190	GLN
1	I	26	GLN
1	I	30	GLN
1	I	34	ASN
1	I	98	GLN
1	I	148	ASN
1	I	159	ASN
1	I	190	GLN
1	J	15	GLN
1	J	30	GLN
1	J	34	ASN
1	J	38	GLN
1	J	159	ASN
1	J	162	ASN
1	K	26	GLN
1	K	30	GLN
1	K	34	ASN
1	K	38	GLN
1	K	98	GLN
1	K	148	ASN
1	K	159	ASN
1	K	162	ASN
1	K	165	ASN
1	K	190	GLN
1	L	15	GLN

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Mol	Chain	Res	Type
1	L	30	GLN
1	L	35	GLN
1	L	179	GLN
1	L	190	GLN
1	L	206	ASN
1	L	210	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	FUA	I	707	-	39,40,40	1.70	8 (20%)	50,64,64	5.22	34 (68%)
3	FUA	F	704	-	39,40,40	1.91	8 (20%)	50,64,64	5.17	30 (60%)
3	FUA	D	705	-	39,40,40	2.03	8 (20%)	50,64,64	5.56	33 (66%)
3	FUA	J	711	-	39,40,40	1.75	8 (20%)	50,64,64	5.99	36 (72%)
3	FUA	B	703	-	39,40,40	2.15	12 (30%)	50,64,64	5.76	34 (68%)
3	FUA	A	702	-	39,40,40	2.27	11 (28%)	50,64,64	5.33	37 (74%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FUA	G	708	-	39,40,40	1.65	6 (15%)	50,64,64	5.19	37 (74%)
3	FUA	C	701	-	39,40,40	2.15	11 (28%)	50,64,64	5.89	35 (70%)
3	FUA	K	712	-	39,40,40	1.80	5 (12%)	50,64,64	5.53	28 (56%)
3	FUA	L	710	-	39,40,40	1.80	7 (17%)	50,64,64	5.26	31 (62%)
3	FUA	E	706	-	39,40,40	1.88	7 (17%)	50,64,64	5.29	34 (68%)
3	FUA	H	709	-	39,40,40	2.00	9 (23%)	50,64,64	5.99	37 (74%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUA	I	707	-	2/2/15/16	5/16/92/92	0/4/4/4
3	FUA	F	704	-	3/3/15/16	4/16/92/92	0/4/4/4
3	FUA	D	705	-	2/2/15/16	7/16/92/92	0/4/4/4
3	FUA	J	711	-	2/2/15/16	5/16/92/92	0/4/4/4
3	FUA	B	703	-	4/4/15/16	7/16/92/92	0/4/4/4
3	FUA	A	702	-	3/3/15/16	4/16/92/92	0/4/4/4
3	FUA	G	708	-	4/4/15/16	1/16/92/92	0/4/4/4
3	FUA	C	701	-	3/3/15/16	6/16/92/92	0/4/4/4
3	FUA	K	712	-	3/3/15/16	6/16/92/92	0/4/4/4
3	FUA	L	710	-	3/3/15/16	6/16/92/92	0/4/4/4
3	FUA	E	706	-	4/4/15/16	7/16/92/92	0/4/4/4
3	FUA	H	709	-	3/3/15/16	8/16/92/92	0/4/4/4

All (100) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	705	FUA	C14-C8	-7.68	1.46	1.59
3	A	702	FUA	C14-C8	-6.94	1.47	1.59
3	B	703	FUA	C14-C8	-6.81	1.47	1.59
3	L	710	FUA	O2-C31	6.36	1.49	1.35
3	C	701	FUA	C14-C8	-6.30	1.48	1.59
3	F	704	FUA	C14-C8	-6.12	1.48	1.59
3	J	711	FUA	C14-C8	-5.88	1.49	1.59
3	K	712	FUA	C14-C8	-5.85	1.49	1.59
3	A	702	FUA	C8-C9	-5.70	1.47	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	712	FUA	O2-C31	5.62	1.47	1.35
3	L	710	FUA	C14-C8	-5.60	1.49	1.59
3	E	706	FUA	C14-C8	-5.33	1.50	1.59
3	H	709	FUA	O2-C31	5.32	1.47	1.35
3	C	701	FUA	O2-C31	5.31	1.46	1.35
3	H	709	FUA	C14-C8	-5.23	1.50	1.59
3	F	704	FUA	C8-C9	-5.11	1.48	1.56
3	G	708	FUA	O2-C31	5.08	1.46	1.35
3	E	706	FUA	O2-C16	-5.02	1.36	1.45
3	J	711	FUA	O2-C31	4.99	1.46	1.35
3	A	702	FUA	O2-C31	4.90	1.46	1.35
3	F	704	FUA	O2-C31	4.87	1.46	1.35
3	I	707	FUA	C8-C9	-4.76	1.48	1.56
3	A	702	FUA	C14-C13	-4.71	1.43	1.57
3	D	705	FUA	O2-C31	4.49	1.45	1.35
3	B	703	FUA	O2-C31	4.46	1.45	1.35
3	E	706	FUA	O2-C31	4.25	1.44	1.35
3	B	703	FUA	C1-C10	-4.19	1.46	1.54
3	J	711	FUA	C8-C9	-4.14	1.49	1.56
3	I	707	FUA	O2-C31	4.13	1.44	1.35
3	D	705	FUA	C8-C9	-4.13	1.49	1.56
3	C	701	FUA	C7-C6	-4.08	1.45	1.53
3	G	708	FUA	C14-C8	-4.05	1.52	1.59
3	C	701	FUA	C19-C10	3.87	1.60	1.54
3	B	703	FUA	O2-C16	-3.86	1.38	1.45
3	H	709	FUA	C4-C5	-3.81	1.46	1.54
3	I	707	FUA	C14-C8	-3.71	1.52	1.59
3	H	709	FUA	C14-C13	-3.65	1.46	1.57
3	C	701	FUA	C8-C9	-3.57	1.50	1.56
3	B	703	FUA	C6-C5	-3.55	1.47	1.53
3	C	701	FUA	C6-C5	-3.47	1.48	1.53
3	A	702	FUA	C15-C14	-3.37	1.48	1.54
3	G	708	FUA	C9-C11	3.33	1.59	1.54
3	E	706	FUA	C14-C13	-3.31	1.47	1.57
3	F	704	FUA	C19-C10	3.19	1.59	1.54
3	D	705	FUA	C10-C9	-3.17	1.52	1.57
3	K	712	FUA	C10-C9	-3.17	1.52	1.57
3	E	706	FUA	C8-C9	-3.15	1.51	1.56
3	E	706	FUA	C1-C10	-3.11	1.48	1.54
3	A	702	FUA	C10-C5	-3.10	1.50	1.56
3	C	701	FUA	C12-C13	3.09	1.60	1.54
3	C	701	FUA	C14-C13	-3.05	1.48	1.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	709	FUA	C10-C9	-3.01	1.52	1.57
3	A	702	FUA	C7-C6	-2.94	1.47	1.53
3	D	705	FUA	C14-C13	-2.90	1.48	1.57
3	J	711	FUA	O2-C16	-2.88	1.40	1.45
3	B	703	FUA	C8-C9	-2.86	1.51	1.56
3	H	709	FUA	C18-C4	2.83	1.59	1.53
3	B	703	FUA	C20-C8	2.82	1.59	1.54
3	I	707	FUA	C19-C10	2.77	1.58	1.54
3	K	712	FUA	O2-C16	-2.75	1.40	1.45
3	K	712	FUA	C8-C9	-2.74	1.52	1.56
3	B	703	FUA	C12-C11	2.71	1.57	1.52
3	I	707	FUA	C10-C9	-2.65	1.52	1.57
3	G	708	FUA	C2-C3	2.64	1.56	1.52
3	H	709	FUA	C8-C9	-2.62	1.52	1.56
3	I	707	FUA	C1-C10	-2.62	1.49	1.54
3	B	703	FUA	C19-C10	2.61	1.58	1.54
3	E	706	FUA	C19-C10	2.56	1.58	1.54
3	B	703	FUA	C7-C8	-2.56	1.49	1.54
3	F	704	FUA	O6-C3	2.54	1.48	1.43
3	H	709	FUA	O2-C16	-2.53	1.41	1.45
3	A	702	FUA	C1-C10	-2.53	1.49	1.54
3	C	701	FUA	C10-C5	-2.52	1.51	1.56
3	D	705	FUA	C1-C10	-2.44	1.49	1.54
3	L	710	FUA	C12-C13	2.42	1.58	1.54
3	D	705	FUA	C12-C11	2.41	1.57	1.52
3	L	710	FUA	C19-C10	2.40	1.58	1.54
3	A	702	FUA	C7-C8	-2.38	1.50	1.54
3	B	703	FUA	C7-C6	-2.38	1.48	1.53
3	J	711	FUA	C10-C5	-2.35	1.52	1.56
3	I	707	FUA	C14-C13	-2.32	1.50	1.57
3	L	710	FUA	C29-C22	-2.31	1.44	1.47
3	A	702	FUA	C2-C3	2.30	1.55	1.52
3	J	711	FUA	C14-C13	-2.28	1.50	1.57
3	D	705	FUA	O2-C16	-2.25	1.41	1.45
3	H	709	FUA	C10-C5	-2.23	1.52	1.56
3	I	707	FUA	O2-C16	-2.22	1.41	1.45
3	L	710	FUA	C12-C11	2.17	1.56	1.52
3	F	704	FUA	C2-C3	2.16	1.55	1.52
3	G	708	FUA	C10-C5	-2.12	1.52	1.56
3	J	711	FUA	C6-C5	-2.11	1.50	1.53
3	F	704	FUA	C29-C22	-2.10	1.44	1.47
3	L	710	FUA	C10-C9	-2.10	1.53	1.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	701	FUA	C7-C8	-2.08	1.50	1.54
3	A	702	FUA	C9-C11	-2.08	1.51	1.54
3	F	704	FUA	C14-C13	-2.07	1.51	1.57
3	B	703	FUA	C14-C13	-2.06	1.51	1.57
3	J	711	FUA	C10-C9	-2.03	1.53	1.57
3	G	708	FUA	C8-C9	-2.01	1.53	1.56
3	C	701	FUA	C4-C5	-2.01	1.50	1.54

All (406) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	709	FUA	C21-C14-C8	-21.01	94.81	112.23
3	J	711	FUA	C21-C14-C8	-19.12	96.38	112.23
3	K	712	FUA	C21-C14-C8	-15.93	99.03	112.23
3	B	703	FUA	C19-C10-C1	-15.30	83.99	108.31
3	L	710	FUA	C21-C14-C8	-14.54	100.17	112.23
3	J	711	FUA	C20-C8-C14	-14.31	90.96	110.83
3	D	705	FUA	C19-C10-C5	-14.29	91.97	111.18
3	K	712	FUA	C19-C10-C1	-13.95	86.13	108.31
3	C	701	FUA	C19-C10-C5	-13.76	92.68	111.18
3	D	705	FUA	C1-C10-C5	13.12	124.94	107.77
3	J	711	FUA	C19-C10-C5	-13.12	93.55	111.18
3	C	701	FUA	C20-C8-C14	-12.69	93.21	110.83
3	H	709	FUA	C1-C10-C5	12.58	124.23	107.77
3	F	704	FUA	C19-C10-C1	-12.18	88.94	108.31
3	E	706	FUA	C19-C10-C1	-11.95	89.31	108.31
3	C	701	FUA	C6-C5-C10	11.86	125.89	111.66
3	G	708	FUA	C19-C10-C5	-11.82	95.28	111.18
3	B	703	FUA	O6-C3-C4	-11.61	86.81	110.62
3	E	706	FUA	C6-C5-C10	11.41	125.35	111.66
3	K	712	FUA	C20-C8-C14	-11.40	94.99	110.83
3	I	707	FUA	C19-C10-C1	-11.39	90.20	108.31
3	C	701	FUA	C1-C10-C5	11.36	122.64	107.77
3	F	704	FUA	C21-C14-C8	-11.35	102.82	112.23
3	L	710	FUA	C20-C8-C14	-11.17	95.31	110.83
3	D	705	FUA	C6-C5-C10	11.14	125.03	111.66
3	G	708	FUA	C1-C10-C5	11.11	122.31	107.77
3	A	702	FUA	C19-C10-C5	-11.11	96.25	111.18
3	B	703	FUA	C1-C10-C5	11.11	122.30	107.77
3	F	704	FUA	C6-C5-C10	11.02	124.88	111.66
3	B	703	FUA	C20-C8-C14	-10.99	95.56	110.83
3	C	701	FUA	O6-C3-C4	-10.91	88.24	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	FUA	C19-C10-C1	-10.89	91.00	108.31
3	A	702	FUA	C1-C10-C5	10.81	121.91	107.77
3	D	705	FUA	C20-C8-C14	-10.79	95.85	110.83
3	D	705	FUA	C21-C14-C8	-10.64	103.41	112.23
3	B	703	FUA	C6-C5-C10	10.60	124.38	111.66
3	L	710	FUA	C19-C10-C5	-10.54	97.01	111.18
3	A	702	FUA	C21-C14-C8	-10.46	103.56	112.23
3	G	708	FUA	C19-C10-C1	-10.44	91.72	108.31
3	C	701	FUA	C20-C8-C7	-10.27	90.96	107.83
3	I	707	FUA	C1-C10-C5	10.24	121.17	107.77
3	J	711	FUA	C1-C10-C5	10.24	121.16	107.77
3	I	707	FUA	C21-C14-C8	-10.18	103.79	112.23
3	J	711	FUA	C6-C5-C10	10.01	123.67	111.66
3	H	709	FUA	C19-C10-C5	-10.00	97.73	111.18
3	H	709	FUA	C6-C5-C10	9.99	123.64	111.66
3	E	706	FUA	C1-C10-C5	9.98	120.83	107.77
3	F	704	FUA	C1-C10-C5	9.87	120.68	107.77
3	C	701	FUA	C13-C12-C11	9.86	126.20	111.90
3	A	702	FUA	O6-C3-C4	-9.78	90.56	110.62
3	G	708	FUA	C6-C5-C10	9.68	123.27	111.66
3	C	701	FUA	C19-C10-C1	-9.64	92.98	108.31
3	B	703	FUA	C10-C5-C4	9.63	124.89	113.20
3	K	712	FUA	C1-C10-C5	9.57	120.29	107.77
3	H	709	FUA	C19-C10-C9	-9.52	89.62	113.19
3	B	703	FUA	C21-C14-C8	-9.46	104.39	112.23
3	E	706	FUA	O6-C3-C4	-9.44	91.26	110.62
3	F	704	FUA	C10-C5-C4	9.34	124.53	113.20
3	I	707	FUA	C20-C8-C14	-9.32	97.88	110.83
3	L	710	FUA	C19-C10-C1	-9.27	93.57	108.31
3	L	710	FUA	C6-C5-C10	9.06	122.53	111.66
3	G	708	FUA	C20-C8-C9	-9.00	91.51	111.90
3	B	703	FUA	C20-C8-C7	-8.97	93.09	107.83
3	K	712	FUA	C6-C5-C10	8.91	122.36	111.66
3	E	706	FUA	C20-C8-C9	-8.86	91.81	111.90
3	D	705	FUA	O6-C3-C4	-8.86	92.46	110.62
3	L	710	FUA	C19-C10-C9	-8.83	91.32	113.19
3	F	704	FUA	C20-C8-C14	-8.81	98.59	110.83
3	D	705	FUA	C20-C8-C9	-8.76	92.03	111.90
3	C	701	FUA	C18-C4-C3	8.74	121.57	111.35
3	G	708	FUA	C21-C14-C8	-8.71	105.01	112.23
3	D	705	FUA	C7-C8-C9	8.67	128.57	108.91
3	L	710	FUA	C20-C8-C7	-8.61	93.69	107.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	705	FUA	C19-C10-C1	-8.60	94.63	108.31
3	A	702	FUA	C6-C5-C10	8.59	121.96	111.66
3	G	708	FUA	C18-C4-C5	8.50	126.71	112.95
3	K	712	FUA	C7-C8-C9	8.49	128.16	108.91
3	H	709	FUA	C20-C8-C9	-8.45	92.74	111.90
3	F	704	FUA	C20-C8-C9	-8.41	92.84	111.90
3	A	702	FUA	C20-C8-C9	-8.40	92.85	111.90
3	B	703	FUA	O5-C29-C22	8.36	140.05	115.83
3	J	711	FUA	C19-C10-C9	-8.35	92.52	113.19
3	I	707	FUA	C20-C8-C9	-8.33	93.01	111.90
3	I	707	FUA	C19-C10-C5	-8.31	100.01	111.18
3	A	702	FUA	C20-C8-C14	-8.29	99.31	110.83
3	H	709	FUA	C18-C4-C3	8.29	121.05	111.35
3	I	707	FUA	C10-C5-C4	8.25	123.21	113.20
3	C	701	FUA	O5-C29-C22	8.23	139.67	115.83
3	F	704	FUA	C19-C10-C9	-8.21	92.86	113.19
3	L	710	FUA	C1-C10-C5	8.21	118.50	107.77
3	H	709	FUA	O6-C3-C4	-8.16	93.88	110.62
3	E	706	FUA	C19-C10-C5	-8.07	100.33	111.18
3	E	706	FUA	C20-C8-C7	-8.07	94.58	107.83
3	F	704	FUA	O6-C3-C4	-8.06	94.09	110.62
3	F	704	FUA	C7-C8-C9	7.89	126.81	108.91
3	K	712	FUA	C10-C5-C4	7.86	122.74	113.20
3	H	709	FUA	C7-C8-C9	7.80	126.60	108.91
3	B	703	FUA	C18-C4-C5	7.76	125.51	112.95
3	I	707	FUA	C19-C10-C9	-7.76	93.98	113.19
3	K	712	FUA	C19-C10-C9	-7.75	93.99	113.19
3	G	708	FUA	C19-C10-C9	-7.75	93.99	113.19
3	E	706	FUA	C7-C8-C9	7.72	126.43	108.91
3	E	706	FUA	C10-C5-C4	7.71	122.55	113.20
3	H	709	FUA	C20-C8-C14	-7.66	100.19	110.83
3	G	708	FUA	C7-C8-C9	7.61	126.17	108.91
3	G	708	FUA	C20-C8-C7	-7.61	95.33	107.83
3	C	701	FUA	C7-C8-C9	7.60	126.15	108.91
3	A	702	FUA	C7-C8-C9	7.59	126.13	108.91
3	E	706	FUA	C20-C8-C14	-7.52	100.38	110.83
3	E	706	FUA	C19-C10-C9	-7.47	94.69	113.19
3	I	707	FUA	C6-C5-C10	7.42	120.56	111.66
3	B	703	FUA	C7-C8-C9	7.35	125.58	108.91
3	L	710	FUA	O6-C3-C4	-7.31	95.63	110.62
3	L	710	FUA	C13-C12-C11	7.30	122.49	111.90
3	J	711	FUA	O6-C3-C4	-7.24	95.77	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	707	FUA	O6-C3-C4	-7.19	95.88	110.62
3	C	701	FUA	C21-C14-C8	-7.16	106.29	112.23
3	A	702	FUA	C10-C5-C4	7.16	121.88	113.20
3	E	706	FUA	C14-C8-C9	7.10	121.77	109.30
3	J	711	FUA	C7-C8-C9	7.05	124.89	108.91
3	A	702	FUA	C19-C10-C9	-7.01	95.82	113.19
3	H	709	FUA	C19-C10-C1	-7.01	97.16	108.31
3	G	708	FUA	O6-C3-C4	-6.91	96.44	110.62
3	H	709	FUA	C20-C8-C7	-6.90	96.49	107.83
3	I	707	FUA	C13-C12-C11	6.90	121.91	111.90
3	E	706	FUA	C13-C12-C11	6.89	121.89	111.90
3	K	712	FUA	C20-C8-C9	-6.85	96.36	111.90
3	K	712	FUA	O5-C29-C22	6.83	135.63	115.83
3	G	708	FUA	C1-C2-C3	6.79	124.33	111.59
3	I	707	FUA	C7-C8-C9	6.79	124.31	108.91
3	J	711	FUA	C19-C10-C1	-6.76	97.55	108.31
3	C	701	FUA	C14-C8-C9	6.76	121.18	109.30
3	B	703	FUA	C21-C14-C13	-6.70	95.88	112.91
3	J	711	FUA	C20-C8-C7	-6.69	96.83	107.83
3	I	707	FUA	O6-C3-C2	-6.69	93.63	109.99
3	K	712	FUA	C20-C8-C7	-6.67	96.86	107.83
3	A	702	FUA	C20-C8-C7	-6.66	96.89	107.83
3	H	709	FUA	O5-C29-C22	6.65	135.10	115.83
3	B	703	FUA	C19-C10-C9	-6.61	96.83	113.19
3	E	706	FUA	C21-C14-C13	-6.52	96.34	112.91
3	L	710	FUA	C7-C8-C9	6.51	123.67	108.91
3	J	711	FUA	C16-O2-C31	-6.44	107.44	117.00
3	I	707	FUA	O5-C29-C22	6.43	134.45	115.83
3	L	710	FUA	C14-C8-C9	6.41	120.56	109.30
3	K	712	FUA	C13-C12-C11	6.39	121.16	111.90
3	K	712	FUA	C19-C10-C5	-6.32	102.68	111.18
3	G	708	FUA	C20-C8-C14	-6.32	102.05	110.83
3	J	711	FUA	C10-C5-C4	6.29	120.83	113.20
3	H	709	FUA	C21-C14-C15	-6.27	91.77	108.66
3	L	710	FUA	C10-C5-C4	6.25	120.78	113.20
3	K	712	FUA	C1-C2-C3	6.24	123.30	111.59
3	K	712	FUA	C18-C4-C5	6.24	123.04	112.95
3	J	711	FUA	O2-C31-C32	6.23	122.20	111.09
3	H	709	FUA	C8-C9-C11	6.22	124.15	110.65
3	F	704	FUA	C20-C8-C7	-6.20	97.65	107.83
3	H	709	FUA	C18-C4-C5	6.16	122.91	112.95
3	D	705	FUA	C19-C10-C9	-6.12	98.02	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	707	FUA	C21-C14-C13	-6.12	97.36	112.91
3	G	708	FUA	C13-C12-C11	6.10	120.75	111.90
3	J	711	FUA	O5-C29-C22	6.10	133.49	115.83
3	K	712	FUA	O6-C3-C4	-6.05	98.22	110.62
3	E	706	FUA	C1-C10-C9	6.03	122.70	109.16
3	E	706	FUA	C21-C14-C8	-6.01	107.25	112.23
3	K	712	FUA	C8-C9-C11	5.96	123.59	110.65
3	D	705	FUA	C1-C2-C3	5.96	122.78	111.59
3	G	708	FUA	C21-C14-C13	-5.93	97.84	112.91
3	A	702	FUA	C21-C14-C13	-5.91	97.89	112.91
3	I	707	FUA	C1-C2-C3	5.91	122.67	111.59
3	D	705	FUA	C8-C9-C11	5.90	123.45	110.65
3	E	706	FUA	O5-C29-C22	5.89	132.89	115.83
3	F	704	FUA	C1-C2-C3	5.85	122.57	111.59
3	F	704	FUA	C19-C10-C5	-5.80	103.39	111.18
3	I	707	FUA	C20-C8-C7	-5.74	98.40	107.83
3	L	710	FUA	C1-C2-C3	5.73	122.34	111.59
3	A	702	FUA	C13-C12-C11	5.73	120.21	111.90
3	K	712	FUA	O4-C29-C22	-5.71	106.71	122.44
3	C	701	FUA	C10-C5-C4	5.67	120.08	113.20
3	F	704	FUA	C1-C10-C9	5.64	121.84	109.16
3	H	709	FUA	O6-C3-C2	-5.63	96.22	109.99
3	F	704	FUA	C8-C9-C11	5.63	122.86	110.65
3	F	704	FUA	C21-C14-C13	-5.61	98.66	112.91
3	G	708	FUA	C8-C9-C11	5.61	122.81	110.65
3	J	711	FUA	O4-C29-C22	-5.60	107.02	122.44
3	I	707	FUA	C8-C9-C11	5.59	122.78	110.65
3	B	703	FUA	C1-C10-C9	5.58	121.69	109.16
3	J	711	FUA	C1-C2-C3	5.57	122.04	111.59
3	I	707	FUA	O4-C29-C22	-5.55	107.15	122.44
3	B	703	FUA	C19-C10-C5	-5.55	103.72	111.18
3	L	710	FUA	C8-C9-C11	5.53	122.65	110.65
3	J	711	FUA	C8-C9-C11	5.52	122.63	110.65
3	C	701	FUA	C1-C2-C3	5.47	121.85	111.59
3	B	703	FUA	C1-C2-C3	5.44	121.80	111.59
3	A	702	FUA	C14-C8-C9	5.43	118.84	109.30
3	A	702	FUA	C18-C4-C5	5.43	121.73	112.95
3	D	705	FUA	O5-C29-C22	5.41	131.50	115.83
3	G	708	FUA	C5-C10-C9	5.41	120.90	108.19
3	K	712	FUA	O6-C3-C2	-5.40	96.79	109.99
3	L	710	FUA	C18-C4-C5	5.40	121.69	112.95
3	C	701	FUA	C8-C9-C11	5.39	122.35	110.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	703	FUA	C20-C8-C9	-5.39	99.68	111.90
3	L	710	FUA	C20-C8-C9	-5.35	99.76	111.90
3	D	705	FUA	C18-C4-C3	5.33	117.58	111.35
3	B	703	FUA	C14-C8-C9	5.33	118.66	109.30
3	C	701	FUA	O4-C29-C22	-5.32	107.77	122.44
3	D	705	FUA	C18-C4-C5	5.31	121.55	112.95
3	J	711	FUA	C13-C12-C11	5.30	119.58	111.90
3	J	711	FUA	C5-C10-C9	5.29	120.63	108.19
3	J	711	FUA	C20-C8-C9	-5.27	99.95	111.90
3	A	702	FUA	O5-C29-C22	5.27	131.09	115.83
3	B	703	FUA	O5-C29-O4	-5.26	111.38	123.90
3	F	704	FUA	C14-C8-C9	5.25	118.53	109.30
3	H	709	FUA	C1-C2-C3	5.24	121.42	111.59
3	B	703	FUA	O4-C29-C22	-5.21	108.08	122.44
3	L	710	FUA	C18-C4-C3	5.21	117.45	111.35
3	J	711	FUA	C18-C4-C3	5.14	117.36	111.35
3	I	707	FUA	C5-C10-C9	5.11	120.19	108.19
3	D	705	FUA	C5-C10-C9	5.10	120.17	108.19
3	H	709	FUA	C7-C8-C14	5.06	115.15	110.78
3	C	701	FUA	C21-C14-C13	-5.06	100.06	112.91
3	E	706	FUA	C1-C2-C3	5.05	121.06	111.59
3	L	710	FUA	C5-C10-C9	5.04	120.04	108.19
3	D	705	FUA	C21-C14-C13	-5.04	100.10	112.91
3	F	704	FUA	O4-C29-C22	-5.04	108.56	122.44
3	D	705	FUA	C8-C9-C10	-5.02	111.03	116.42
3	A	702	FUA	C1-C2-C3	5.01	121.00	111.59
3	E	706	FUA	C10-C9-C11	5.00	125.29	114.94
3	C	701	FUA	C18-C4-C5	5.00	121.04	112.95
3	C	701	FUA	C19-C10-C9	-4.97	100.87	113.19
3	C	701	FUA	C16-O2-C31	4.96	124.36	117.00
3	H	709	FUA	C10-C5-C4	4.92	119.17	113.20
3	A	702	FUA	C15-C14-C8	4.91	121.64	116.84
3	D	705	FUA	C20-C8-C7	-4.89	99.80	107.83
3	D	705	FUA	C21-C14-C15	-4.87	95.55	108.66
3	D	705	FUA	C13-C12-C11	4.86	118.95	111.90
3	B	703	FUA	C7-C6-C5	4.85	121.38	113.14
3	L	710	FUA	C1-C10-C9	4.84	120.04	109.16
3	D	705	FUA	C14-C8-C9	4.83	117.79	109.30
3	J	711	FUA	C14-C8-C9	4.82	117.77	109.30
3	J	711	FUA	O6-C3-C2	-4.80	98.25	109.99
3	G	708	FUA	C14-C8-C9	4.80	117.73	109.30
3	I	707	FUA	C14-C8-C9	4.77	117.69	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	701	FUA	O5-C29-O4	-4.77	112.55	123.90
3	K	712	FUA	C5-C10-C9	4.75	119.36	108.19
3	D	705	FUA	C10-C5-C4	4.72	118.93	113.20
3	K	712	FUA	C21-C14-C13	-4.70	100.97	112.91
3	C	701	FUA	O2-C31-C32	4.68	119.43	111.09
3	A	702	FUA	C21-C14-C15	-4.63	96.19	108.66
3	H	709	FUA	O5-C29-O4	-4.60	112.95	123.90
3	C	701	FUA	C1-C10-C9	4.55	119.39	109.16
3	F	704	FUA	O1-C11-C9	-4.55	99.04	111.11
3	E	706	FUA	O4-C29-C22	-4.54	109.94	122.44
3	H	709	FUA	C5-C10-C9	4.53	118.83	108.19
3	A	702	FUA	O4-C29-C22	-4.47	110.11	122.44
3	A	702	FUA	C18-C4-C3	4.47	116.58	111.35
3	A	702	FUA	C8-C9-C11	4.43	120.27	110.65
3	J	711	FUA	O2-C31-O3	-4.40	114.49	122.99
3	K	712	FUA	C14-C8-C9	4.40	117.04	109.30
3	J	711	FUA	C15-C14-C8	4.38	121.11	116.84
3	H	709	FUA	C21-C14-C13	-4.34	101.88	112.91
3	G	708	FUA	C10-C9-C11	4.34	123.92	114.94
3	D	705	FUA	C10-C9-C11	4.33	123.91	114.94
3	G	708	FUA	C15-C14-C8	4.33	121.07	116.84
3	F	704	FUA	C13-C12-C11	4.31	118.15	111.90
3	F	704	FUA	O5-C29-C22	4.30	128.28	115.83
3	G	708	FUA	C21-C14-C15	-4.28	97.14	108.66
3	J	711	FUA	C10-C9-C11	4.27	123.77	114.94
3	E	706	FUA	C16-O2-C31	4.26	123.32	117.00
3	B	703	FUA	C21-C14-C15	-4.25	97.21	108.66
3	E	706	FUA	O1-C11-C12	4.24	120.39	109.86
3	K	712	FUA	C1-C10-C9	4.23	118.67	109.16
3	C	701	FUA	C20-C8-C9	-4.22	102.33	111.90
3	A	702	FUA	C1-C10-C9	4.20	118.61	109.16
3	B	703	FUA	C8-C9-C11	4.18	119.72	110.65
3	I	707	FUA	C7-C8-C14	4.12	114.34	110.78
3	D	705	FUA	O4-C29-C22	-4.11	111.11	122.44
3	I	707	FUA	C18-C4-C5	4.09	119.57	112.95
3	L	710	FUA	C6-C7-C8	4.08	119.90	112.85
3	A	702	FUA	C5-C10-C9	4.08	117.79	108.19
3	J	711	FUA	C6-C7-C8	4.03	119.81	112.85
3	B	703	FUA	C13-C12-C11	3.99	117.69	111.90
3	F	704	FUA	C6-C5-C4	-3.99	108.05	114.27
3	L	710	FUA	C21-C14-C13	-3.99	102.79	112.91
3	D	705	FUA	C24-C23-C22	3.97	121.18	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	707	FUA	C18-C4-C3	3.95	115.97	111.35
3	G	708	FUA	C10-C5-C4	3.94	117.98	113.20
3	H	709	FUA	O4-C29-C22	-3.88	111.75	122.44
3	A	702	FUA	C10-C9-C11	3.86	122.94	114.94
3	H	709	FUA	C15-C14-C8	3.86	120.61	116.84
3	I	707	FUA	C21-C14-C15	-3.84	98.33	108.66
3	B	703	FUA	O1-C11-C12	3.81	119.32	109.86
3	G	708	FUA	C8-C9-C10	-3.78	112.36	116.42
3	L	710	FUA	O2-C31-C32	3.78	117.83	111.09
3	J	711	FUA	C21-C14-C13	-3.77	103.33	112.91
3	H	709	FUA	O2-C16-C17	3.76	119.31	108.30
3	H	709	FUA	C13-C12-C11	3.75	117.33	111.90
3	B	703	FUA	O1-C11-C9	-3.74	101.19	111.11
3	J	711	FUA	C21-C14-C15	-3.73	98.62	108.66
3	E	706	FUA	C21-C14-C15	-3.70	98.69	108.66
3	E	706	FUA	C18-C4-C5	3.70	118.94	112.95
3	E	706	FUA	C28-C26-C27	3.70	123.09	114.59
3	J	711	FUA	C7-C8-C14	3.69	113.96	110.78
3	B	703	FUA	C18-C4-C3	-3.68	107.05	111.35
3	H	709	FUA	O2-C16-C15	3.63	119.47	110.81
3	B	703	FUA	C10-C9-C11	3.63	122.46	114.94
3	G	708	FUA	C24-C23-C22	3.62	120.43	112.72
3	D	705	FUA	O1-C11-C9	-3.62	101.51	111.11
3	E	706	FUA	O1-C11-C9	-3.61	101.53	111.11
3	C	701	FUA	C10-C9-C11	3.61	122.41	114.94
3	B	703	FUA	O6-C3-C2	-3.60	101.20	109.99
3	A	702	FUA	C7-C6-C5	3.58	119.23	113.14
3	L	710	FUA	C10-C9-C11	3.55	122.30	114.94
3	I	707	FUA	C15-C14-C8	3.55	120.31	116.84
3	I	707	FUA	C6-C7-C8	3.49	118.88	112.85
3	A	702	FUA	C24-C25-C26	-3.49	116.00	127.64
3	A	702	FUA	O6-C3-C2	-3.48	101.48	109.99
3	K	712	FUA	C10-C9-C11	3.48	122.14	114.94
3	C	701	FUA	C21-C14-C15	-3.40	99.50	108.66
3	J	711	FUA	C18-C4-C5	3.38	118.42	112.95
3	J	711	FUA	C8-C9-C10	-3.32	112.85	116.42
3	A	702	FUA	O2-C31-O3	-3.32	116.59	122.99
3	I	707	FUA	C1-C10-C9	3.29	116.55	109.16
3	D	705	FUA	O2-C31-C32	3.27	116.92	111.09
3	H	709	FUA	C24-C25-C26	3.24	138.46	127.64
3	I	707	FUA	O2-C16-C15	3.23	118.51	110.81
3	J	711	FUA	C1-C10-C9	3.20	116.35	109.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	709	FUA	O1-C11-C9	-3.19	102.63	111.11
3	E	706	FUA	C7-C6-C5	3.09	118.39	113.14
3	E	706	FUA	C8-C9-C11	3.07	117.32	110.65
3	C	701	FUA	C5-C10-C9	3.03	115.31	108.19
3	H	709	FUA	C14-C8-C9	3.03	114.62	109.30
3	B	703	FUA	C6-C5-C4	-3.03	109.55	114.27
3	F	704	FUA	C5-C10-C9	3.01	115.28	108.19
3	I	707	FUA	C10-C9-C11	3.01	121.17	114.94
3	K	712	FUA	C7-C6-C5	2.98	118.19	113.14
3	B	703	FUA	C12-C11-C9	2.96	119.38	112.30
3	F	704	FUA	O2-C31-C32	2.96	116.36	111.09
3	A	702	FUA	O2-C31-C32	2.89	116.23	111.09
3	E	706	FUA	O6-C3-C2	-2.87	102.97	109.99
3	E	706	FUA	O5-C29-O4	-2.86	117.09	123.90
3	G	708	FUA	C16-O2-C31	2.86	121.23	117.00
3	G	708	FUA	C1-C10-C9	2.85	115.56	109.16
3	D	705	FUA	O5-C29-O4	-2.82	117.17	123.90
3	E	706	FUA	C12-C11-C9	2.82	119.04	112.30
3	C	701	FUA	C14-C15-C16	2.78	110.65	103.38
3	A	702	FUA	O1-C11-C9	-2.76	103.78	111.11
3	F	704	FUA	O6-C3-C2	-2.76	103.25	109.99
3	F	704	FUA	C24-C25-C26	-2.72	118.56	127.64
3	E	706	FUA	C5-C10-C9	2.69	114.52	108.19
3	L	710	FUA	C28-C26-C27	2.69	120.78	114.59
3	G	708	FUA	O2-C31-C32	2.67	115.86	111.09
3	C	701	FUA	C7-C6-C5	2.67	117.68	113.14
3	G	708	FUA	O1-C11-C12	2.65	116.45	109.86
3	K	712	FUA	O5-C29-O4	-2.65	117.59	123.90
3	K	712	FUA	C8-C9-C10	-2.65	113.58	116.42
3	I	707	FUA	C7-C6-C5	2.64	117.62	113.14
3	C	701	FUA	O6-C3-C2	-2.63	103.56	109.99
3	G	708	FUA	C6-C7-C8	2.61	117.36	112.85
3	H	709	FUA	C16-O2-C31	2.59	120.83	117.00
3	H	709	FUA	C23-C24-C25	2.56	124.68	112.02
3	H	709	FUA	O2-C31-C32	2.55	115.64	111.09
3	B	703	FUA	O2-C16-C15	-2.55	104.75	110.81
3	G	708	FUA	O5-C29-C22	2.54	123.20	115.83
3	L	710	FUA	O1-C11-C12	2.54	116.17	109.86
3	I	707	FUA	O5-C29-O4	-2.51	117.93	123.90
3	E	706	FUA	C6-C5-C4	-2.51	110.36	114.27
3	B	703	FUA	C5-C10-C9	2.50	114.07	108.19
3	J	711	FUA	C24-C25-C26	-2.47	119.42	127.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	708	FUA	O1-C11-C9	2.46	117.64	111.11
3	H	709	FUA	C1-C10-C9	2.46	114.68	109.16
3	A	702	FUA	C16-O2-C31	-2.44	113.37	117.00
3	L	710	FUA	C2-C1-C10	2.44	116.86	112.74
3	C	701	FUA	C6-C5-C4	-2.42	110.49	114.27
3	G	708	FUA	O5-C29-O4	-2.40	118.19	123.90
3	D	705	FUA	O6-C3-C2	-2.40	104.13	109.99
3	H	709	FUA	C10-C9-C11	2.39	119.88	114.94
3	F	704	FUA	C7-C6-C5	2.38	117.18	113.14
3	H	709	FUA	C7-C6-C5	2.37	117.17	113.14
3	F	704	FUA	C10-C9-C11	2.33	119.76	114.94
3	A	702	FUA	C28-C26-C27	2.32	119.94	114.59
3	C	701	FUA	C6-C7-C8	2.32	116.86	112.85
3	F	704	FUA	C18-C4-C5	-2.32	109.21	112.95
3	C	701	FUA	C24-C23-C22	-2.31	107.80	112.72
3	G	708	FUA	C7-C8-C14	2.30	112.77	110.78
3	G	708	FUA	O2-C31-O3	-2.30	118.56	122.99
3	D	705	FUA	C6-C7-C8	2.29	116.80	112.85
3	L	710	FUA	C14-C15-C16	2.29	109.37	103.38
3	A	702	FUA	O5-C29-O4	-2.28	118.46	123.90
3	I	707	FUA	O1-C11-C9	-2.26	105.11	111.11
3	B	703	FUA	C23-C24-C25	2.25	123.16	112.02
3	A	702	FUA	C28-C26-C25	-2.25	115.90	122.66
3	J	711	FUA	C24-C23-C22	-2.23	107.97	112.72
3	D	705	FUA	C16-O2-C31	-2.21	113.71	117.00
3	I	707	FUA	O2-C31-C32	2.19	115.00	111.09
3	K	712	FUA	C21-C14-C15	-2.15	102.86	108.66
3	D	705	FUA	C28-C26-C27	2.15	119.53	114.59
3	A	702	FUA	C14-C15-C16	2.14	108.98	103.38
3	G	708	FUA	C7-C6-C5	2.13	116.75	113.14
3	L	710	FUA	O6-C3-C2	-2.10	104.85	109.99
3	C	701	FUA	O1-C11-C12	2.07	115.01	109.86
3	J	711	FUA	O1-C11-C12	2.04	114.94	109.86
3	L	710	FUA	O4-C29-C22	-2.04	116.82	122.44
3	G	708	FUA	O2-C16-C17	2.04	114.27	108.30
3	F	704	FUA	C12-C11-C9	2.03	117.15	112.30
3	G	708	FUA	O6-C3-C2	2.02	114.92	109.99
3	E	706	FUA	O2-C31-C32	2.01	114.67	111.09
3	L	710	FUA	C8-C9-C10	-2.00	114.27	116.42

All (36) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	702	FUA	C10
3	A	702	FUA	C13
3	A	702	FUA	C9
3	B	703	FUA	C4
3	B	703	FUA	C5
3	B	703	FUA	C13
3	B	703	FUA	C9
3	C	701	FUA	C9
3	C	701	FUA	C13
3	C	701	FUA	C4
3	D	705	FUA	C13
3	D	705	FUA	C9
3	E	706	FUA	C4
3	E	706	FUA	C5
3	E	706	FUA	C13
3	E	706	FUA	C9
3	F	704	FUA	C4
3	F	704	FUA	C13
3	F	704	FUA	C9
3	G	708	FUA	C9
3	G	708	FUA	C10
3	G	708	FUA	C13
3	G	708	FUA	C4
3	H	709	FUA	C9
3	H	709	FUA	C13
3	H	709	FUA	C4
3	I	707	FUA	C13
3	I	707	FUA	C9
3	J	711	FUA	C13
3	J	711	FUA	C9
3	K	712	FUA	C10
3	K	712	FUA	C13
3	K	712	FUA	C9
3	L	710	FUA	C10
3	L	710	FUA	C13
3	L	710	FUA	C9

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	FUA	C23-C22-C29-O4
3	A	702	FUA	C23-C22-C29-O5
3	B	703	FUA	C17-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
3	B	703	FUA	C23-C22-C29-O4
3	C	701	FUA	C17-C16-O2-C31
3	C	701	FUA	C23-C22-C29-O4
3	C	701	FUA	C23-C22-C29-O5
3	D	705	FUA	C29-C22-C23-C24
3	D	705	FUA	C23-C22-C29-O4
3	D	705	FUA	C23-C22-C29-O5
3	D	705	FUA	C23-C24-C25-C26
3	E	706	FUA	C23-C22-C29-O4
3	E	706	FUA	C23-C22-C29-O5
3	F	704	FUA	C23-C22-C29-O4
3	F	704	FUA	C23-C22-C29-O5
3	H	709	FUA	C17-C22-C23-C24
3	H	709	FUA	C29-C22-C23-C24
3	H	709	FUA	C23-C22-C29-O4
3	H	709	FUA	C23-C22-C29-O5
3	H	709	FUA	C23-C24-C25-C26
3	I	707	FUA	C17-C22-C23-C24
3	I	707	FUA	C29-C22-C23-C24
3	I	707	FUA	C23-C22-C29-O4
3	I	707	FUA	C23-C22-C29-O5
3	I	707	FUA	C23-C24-C25-C26
3	J	711	FUA	C23-C22-C29-O4
3	J	711	FUA	C23-C22-C29-O5
3	K	712	FUA	C23-C22-C29-O4
3	K	712	FUA	C23-C22-C29-O5
3	K	712	FUA	C23-C24-C25-C26
3	L	710	FUA	C29-C22-C23-C24
3	L	710	FUA	C23-C22-C29-O4
3	L	710	FUA	C23-C22-C29-O5
3	E	706	FUA	C32-C31-O2-C16
3	A	702	FUA	C32-C31-O2-C16
3	H	709	FUA	C22-C23-C24-C25
3	C	701	FUA	C32-C31-O2-C16
3	E	706	FUA	O3-C31-O2-C16
3	A	702	FUA	O3-C31-O2-C16
3	K	712	FUA	C29-C22-C23-C24
3	C	701	FUA	O3-C31-O2-C16
3	D	705	FUA	C17-C22-C23-C24
3	K	712	FUA	C17-C22-C23-C24
3	L	710	FUA	C17-C22-C23-C24
3	B	703	FUA	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
3	B	703	FUA	C23-C22-C29-O5
3	B	703	FUA	C29-C22-C23-C24
3	C	701	FUA	C15-C16-O2-C31
3	F	704	FUA	C29-C22-C23-C24
3	J	711	FUA	C29-C22-C23-C24
3	B	703	FUA	C32-C31-O2-C16
3	B	703	FUA	O3-C31-O2-C16
3	D	705	FUA	C32-C31-O2-C16
3	G	708	FUA	C17-C22-C29-O5
3	L	710	FUA	C17-C22-C29-O4
3	L	710	FUA	C17-C22-C29-O5
3	E	706	FUA	C29-C22-C23-C24
3	D	705	FUA	O3-C31-O2-C16
3	H	709	FUA	O3-C31-O2-C16
3	E	706	FUA	C15-C16-O2-C31
3	H	709	FUA	C32-C31-O2-C16
3	F	704	FUA	C17-C22-C23-C24
3	J	711	FUA	C17-C22-C23-C24
3	K	712	FUA	C22-C23-C24-C25
3	E	706	FUA	C17-C16-O2-C31
3	J	711	FUA	C23-C24-C25-C26

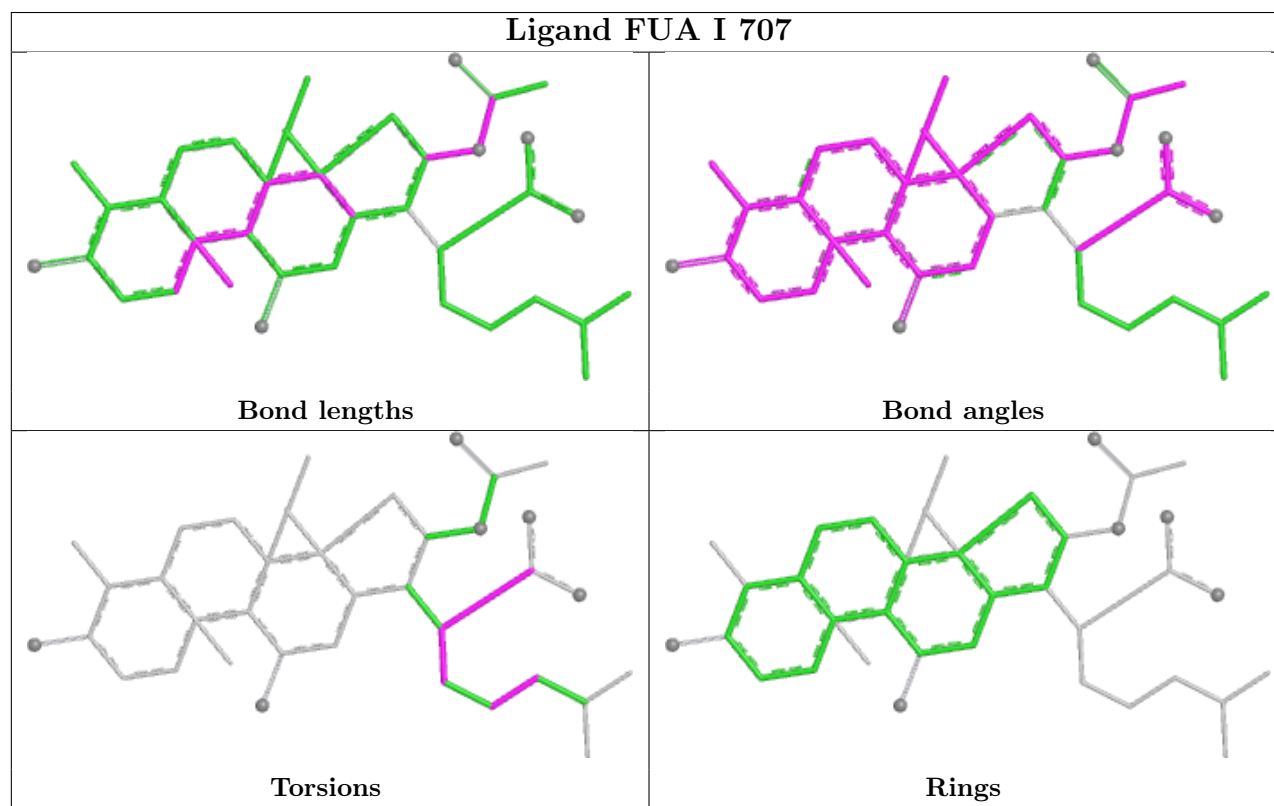
There are no ring outliers.

12 monomers are involved in 92 short contacts:

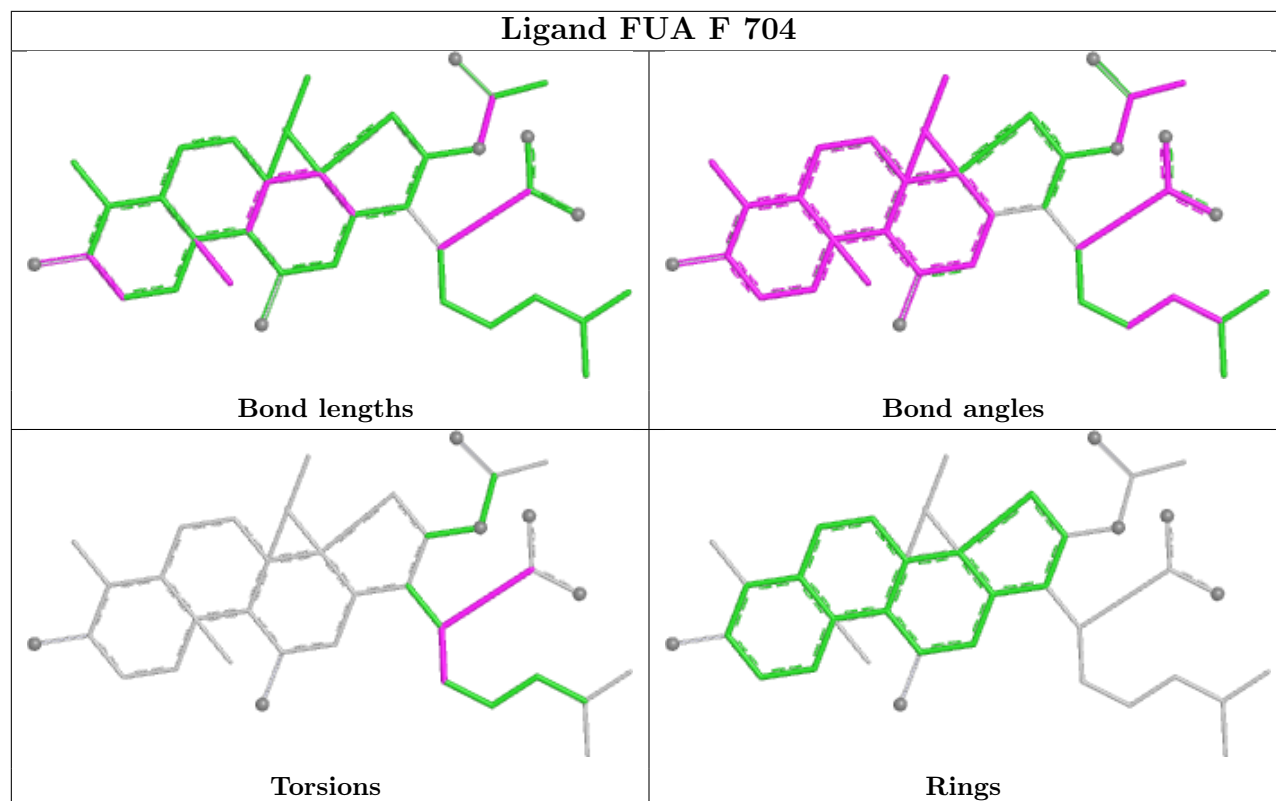
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	707	FUA	16	0
3	F	704	FUA	8	0
3	D	705	FUA	10	0
3	J	711	FUA	10	0
3	B	703	FUA	9	0
3	A	702	FUA	8	0
3	G	708	FUA	6	0
3	C	701	FUA	4	0
3	K	712	FUA	10	0
3	L	710	FUA	4	0
3	E	706	FUA	3	0
3	H	709	FUA	4	0

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

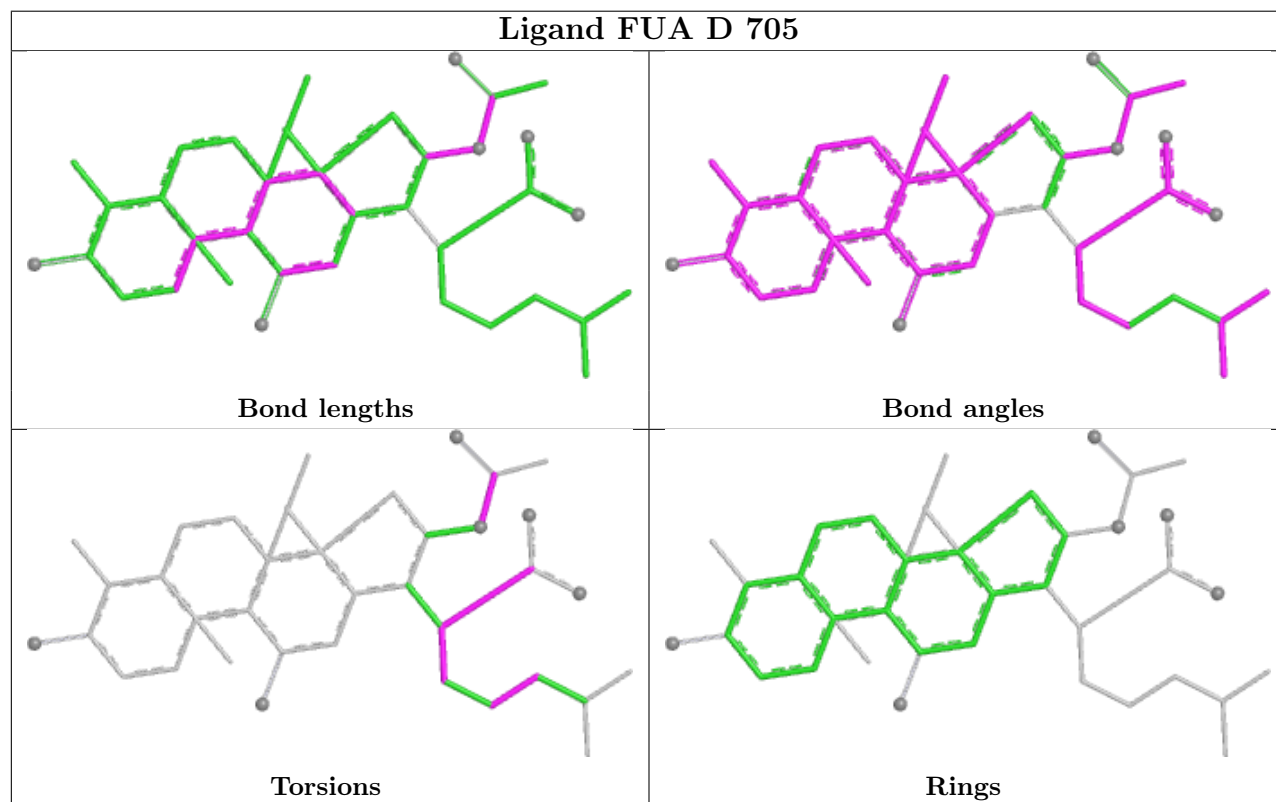
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.



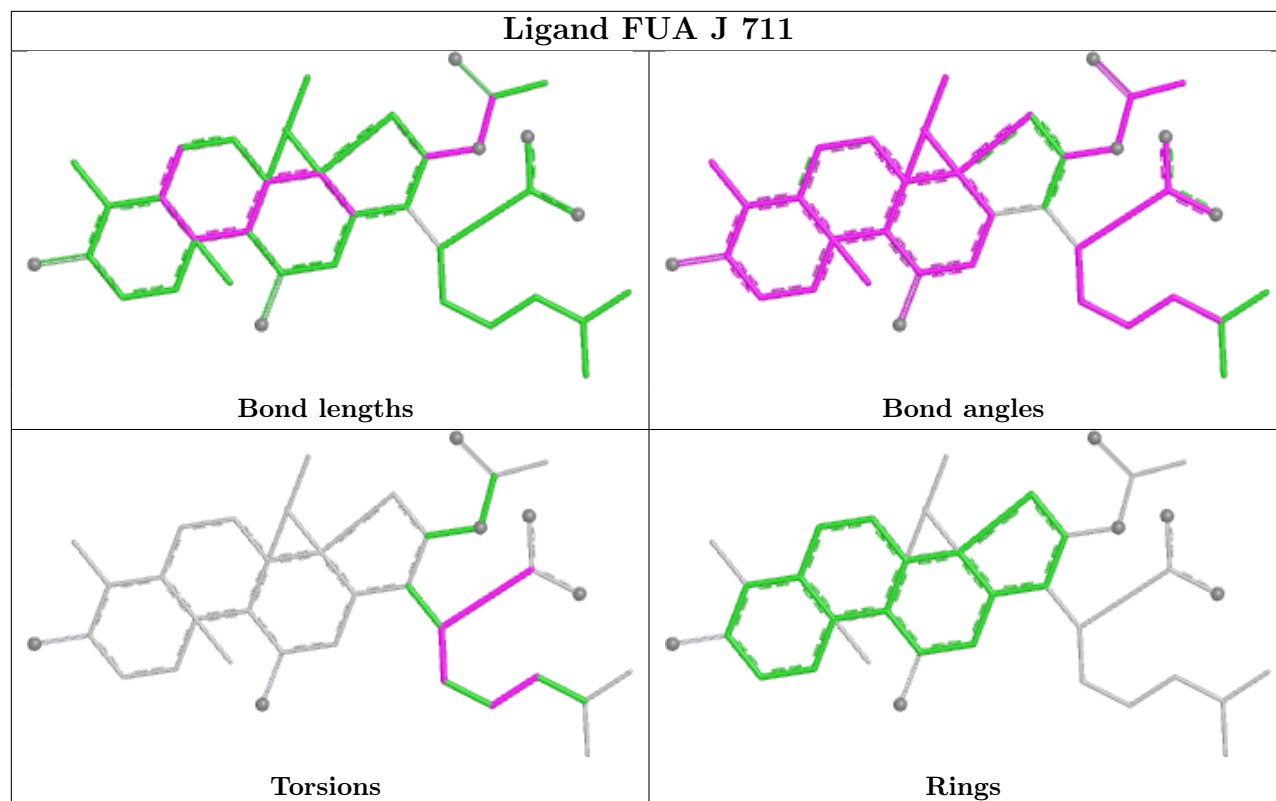
Ligand FUA F 704



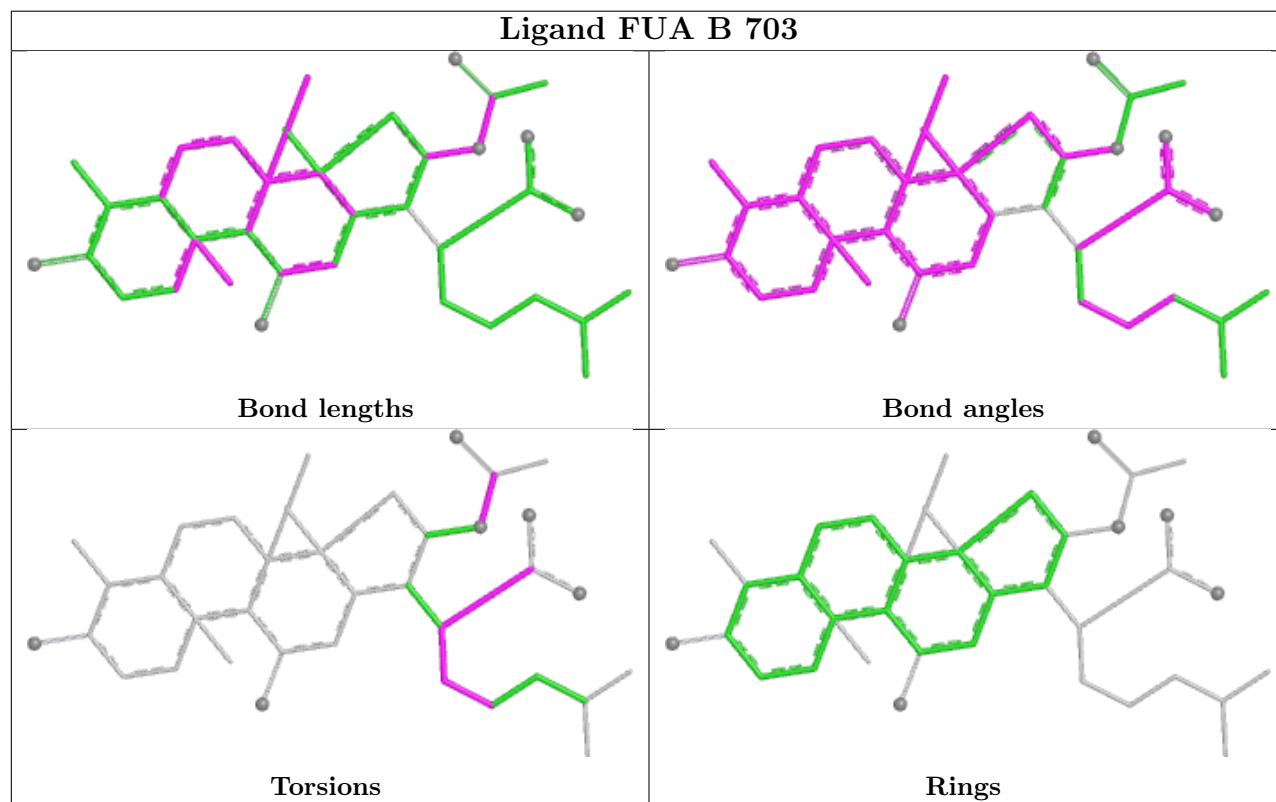
Ligand FUA D 705



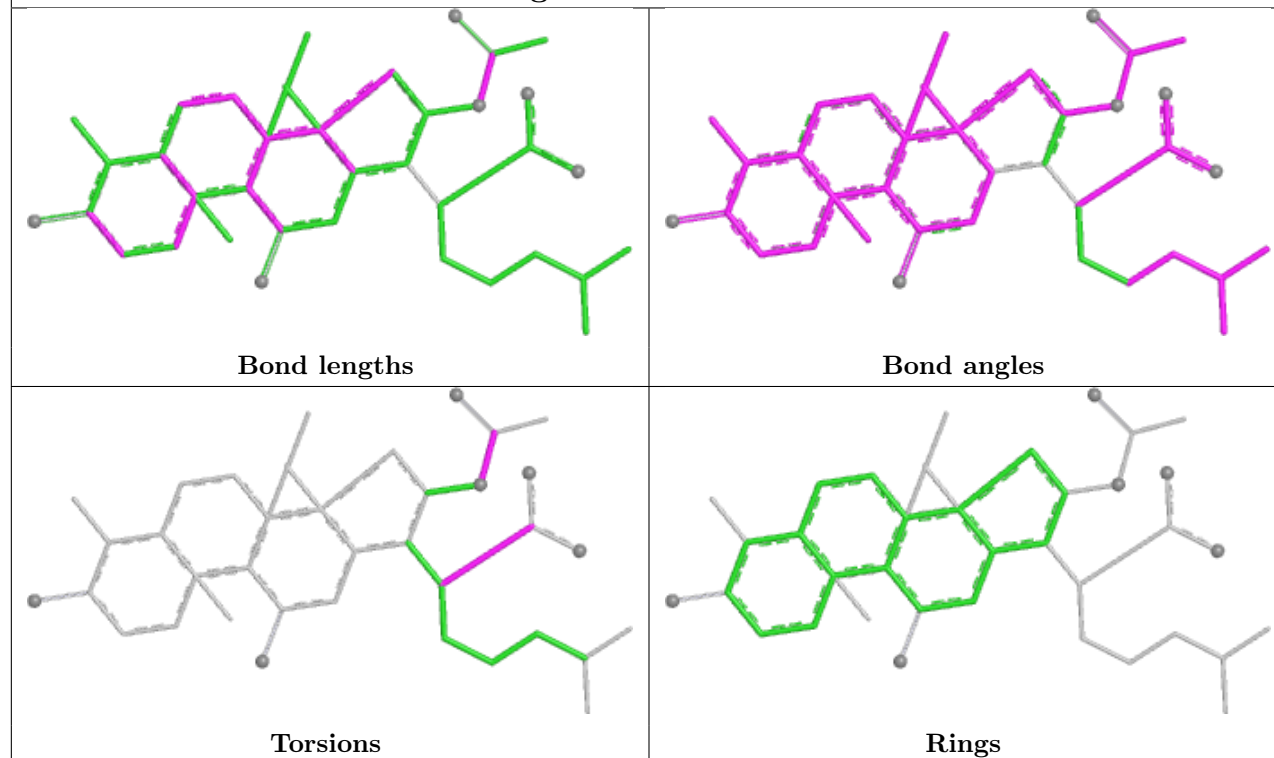
Ligand FUA J 711



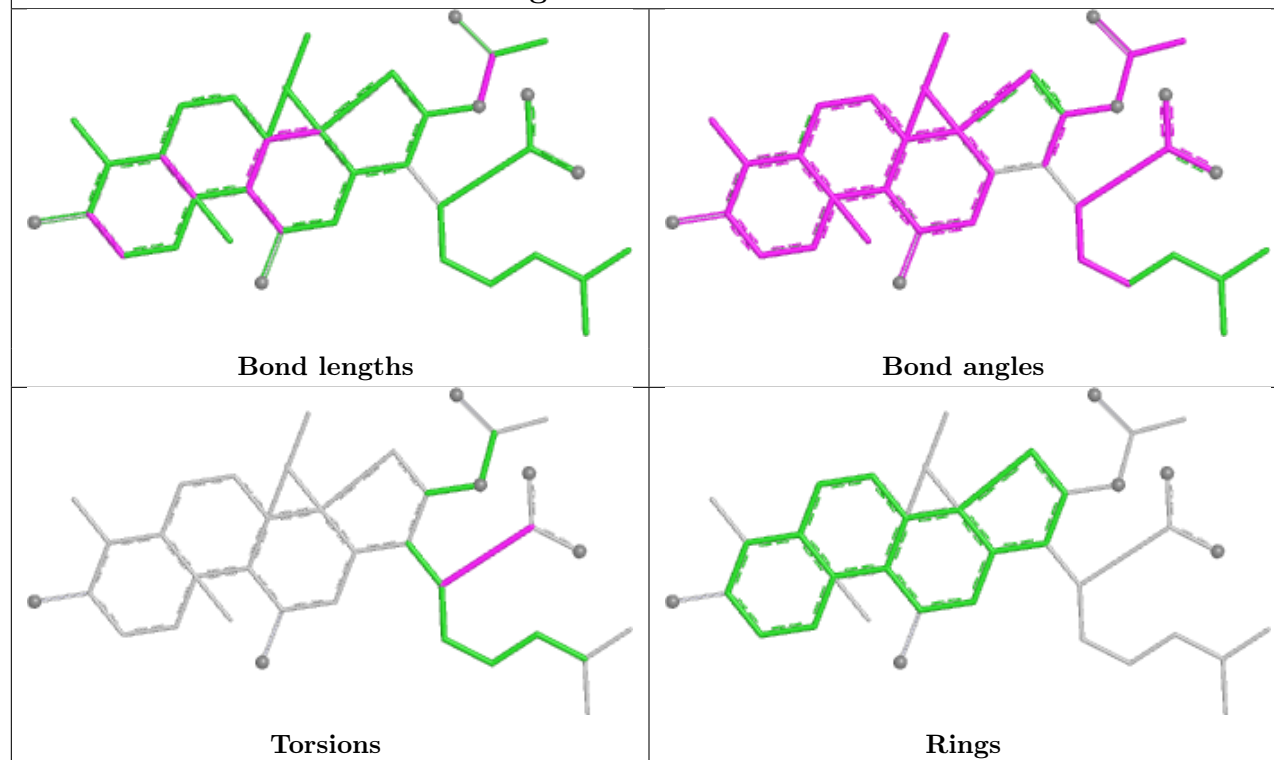
Ligand FUA B 703



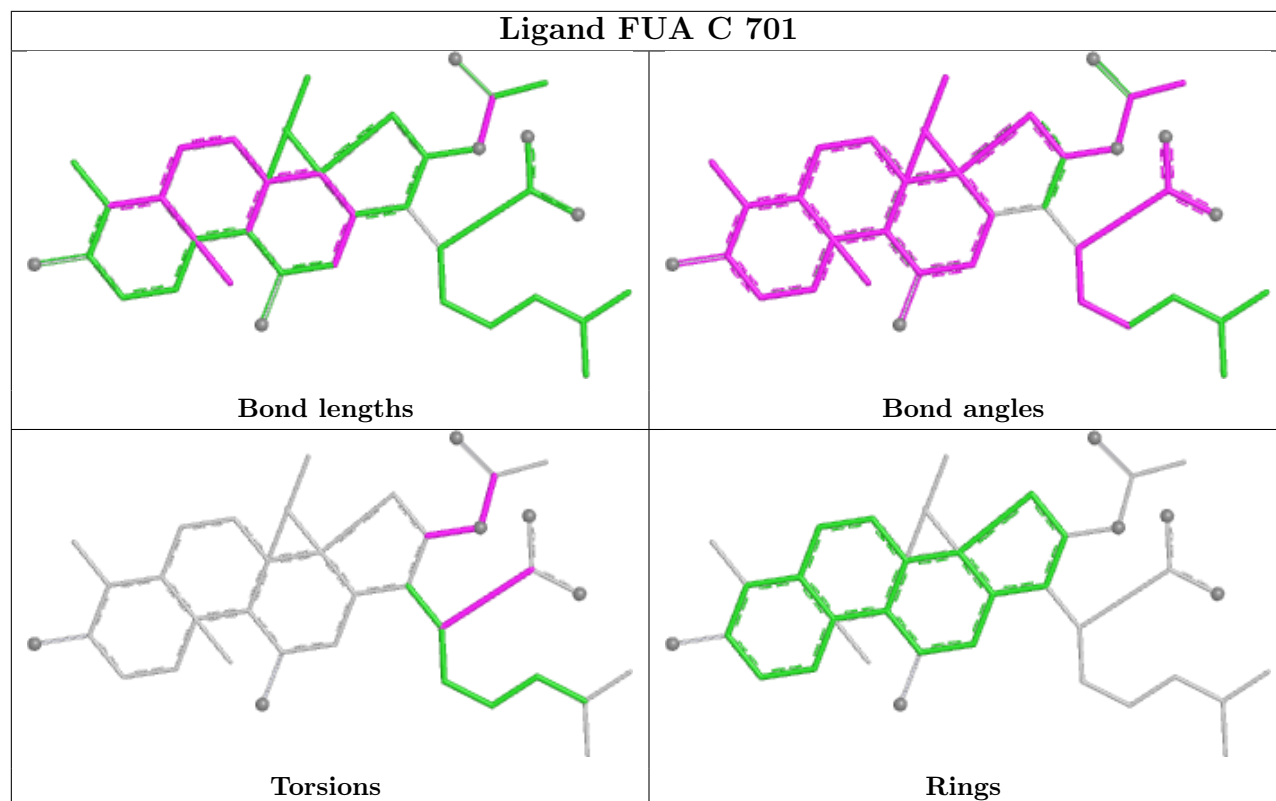
Ligand FUA A 702



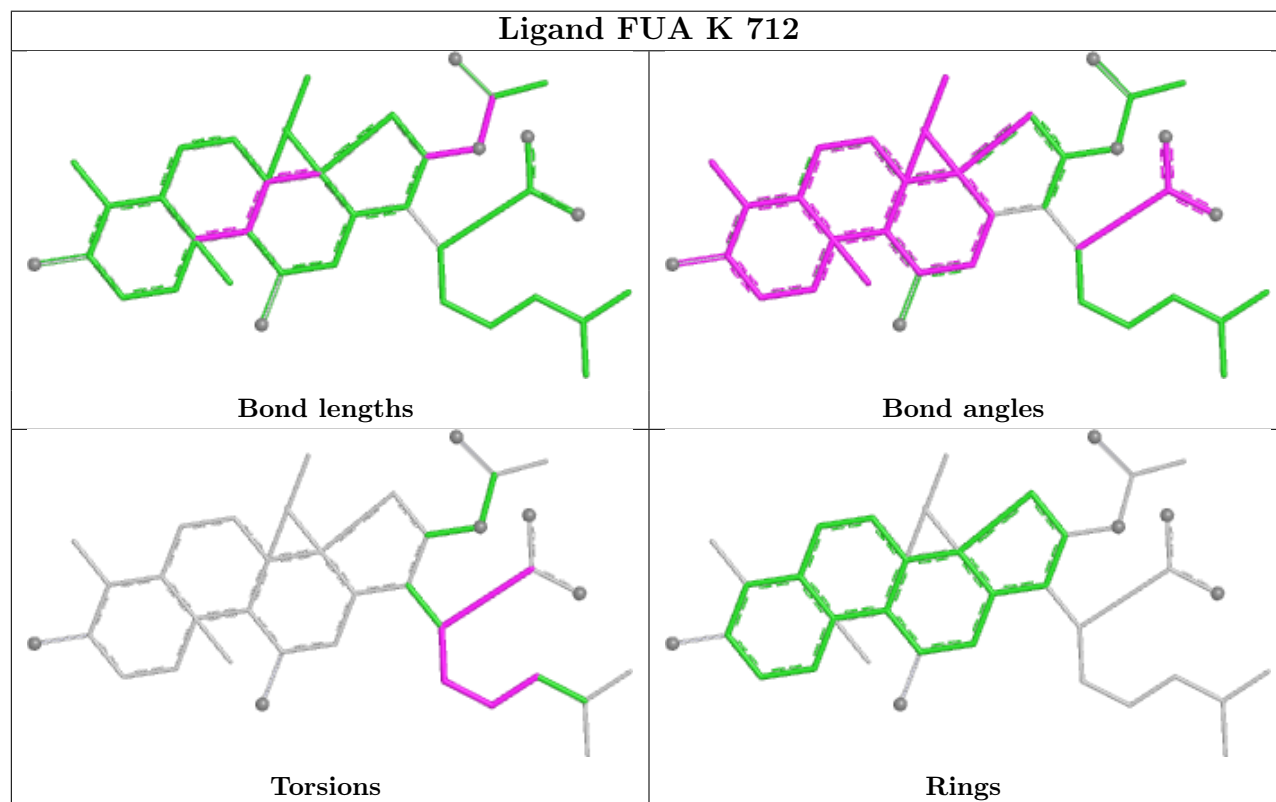
Ligand FUA G 708



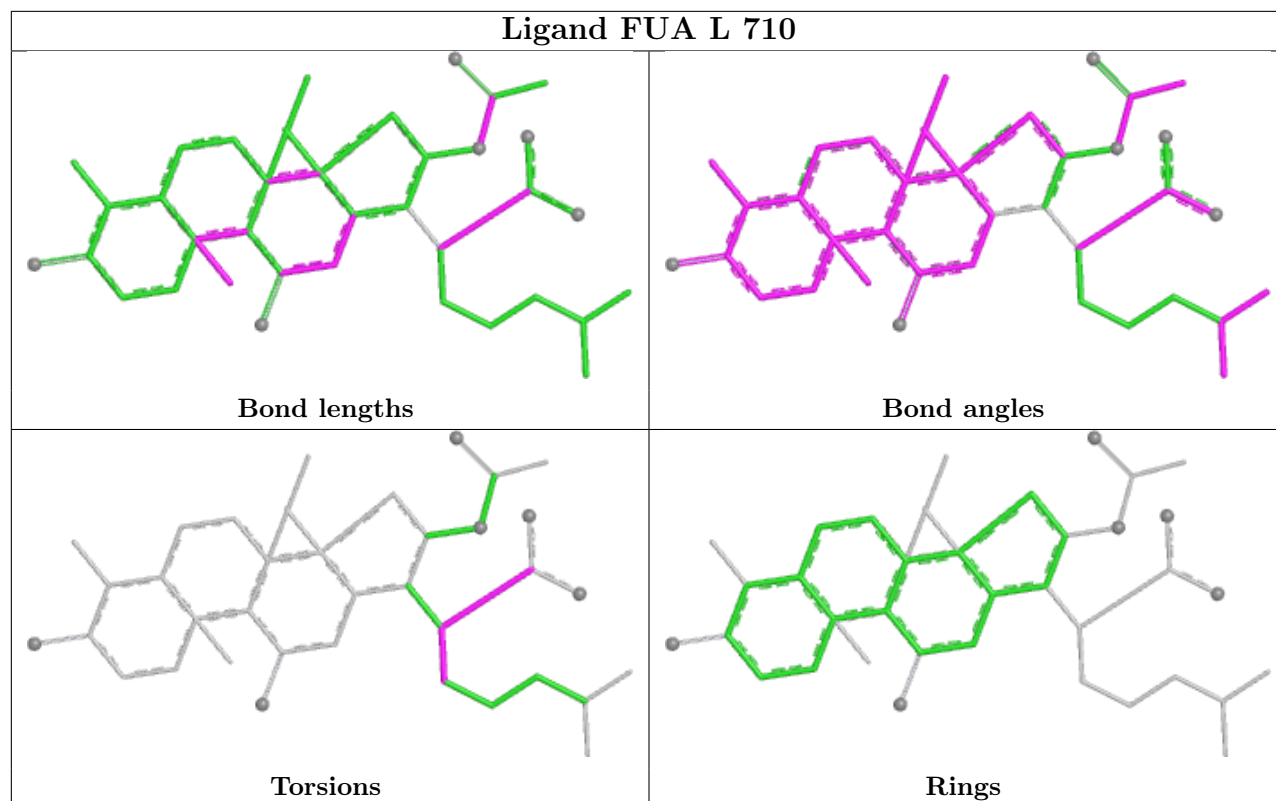
Ligand FUA C 701



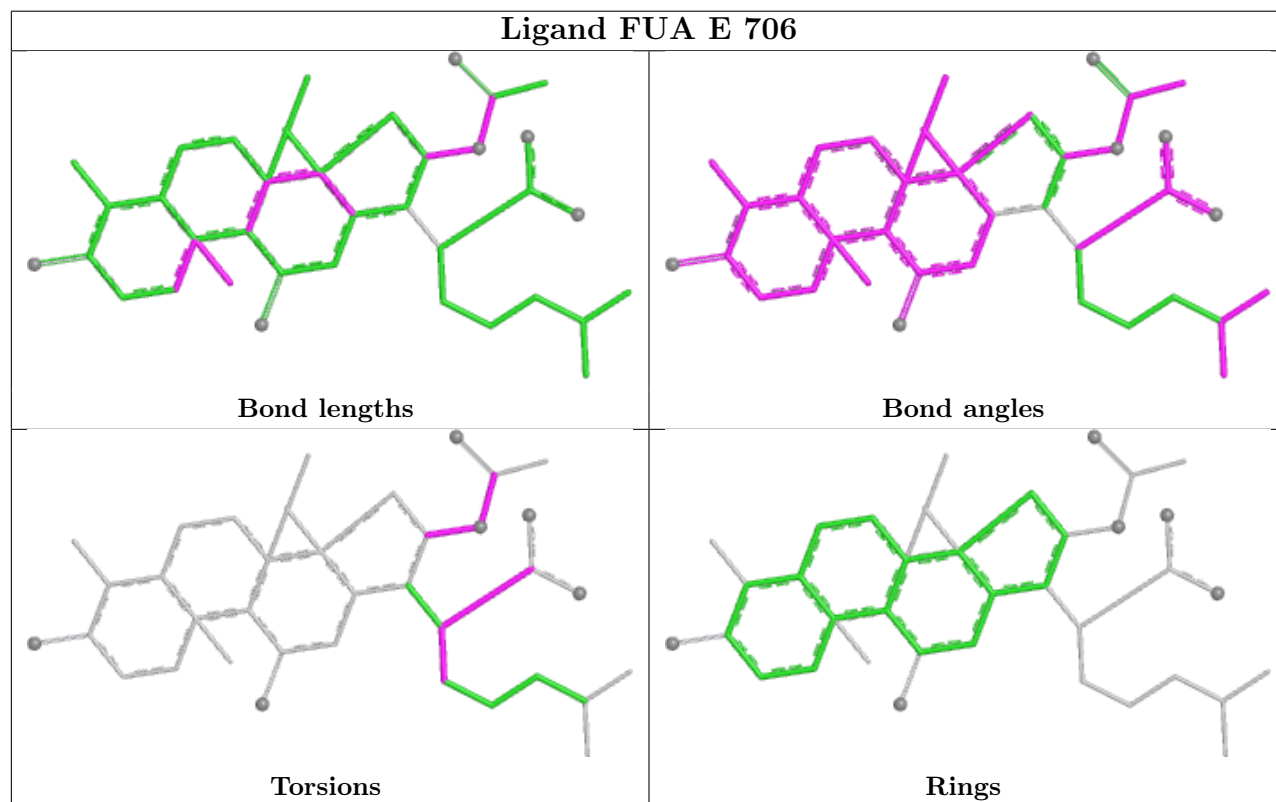
Ligand FUA K 712

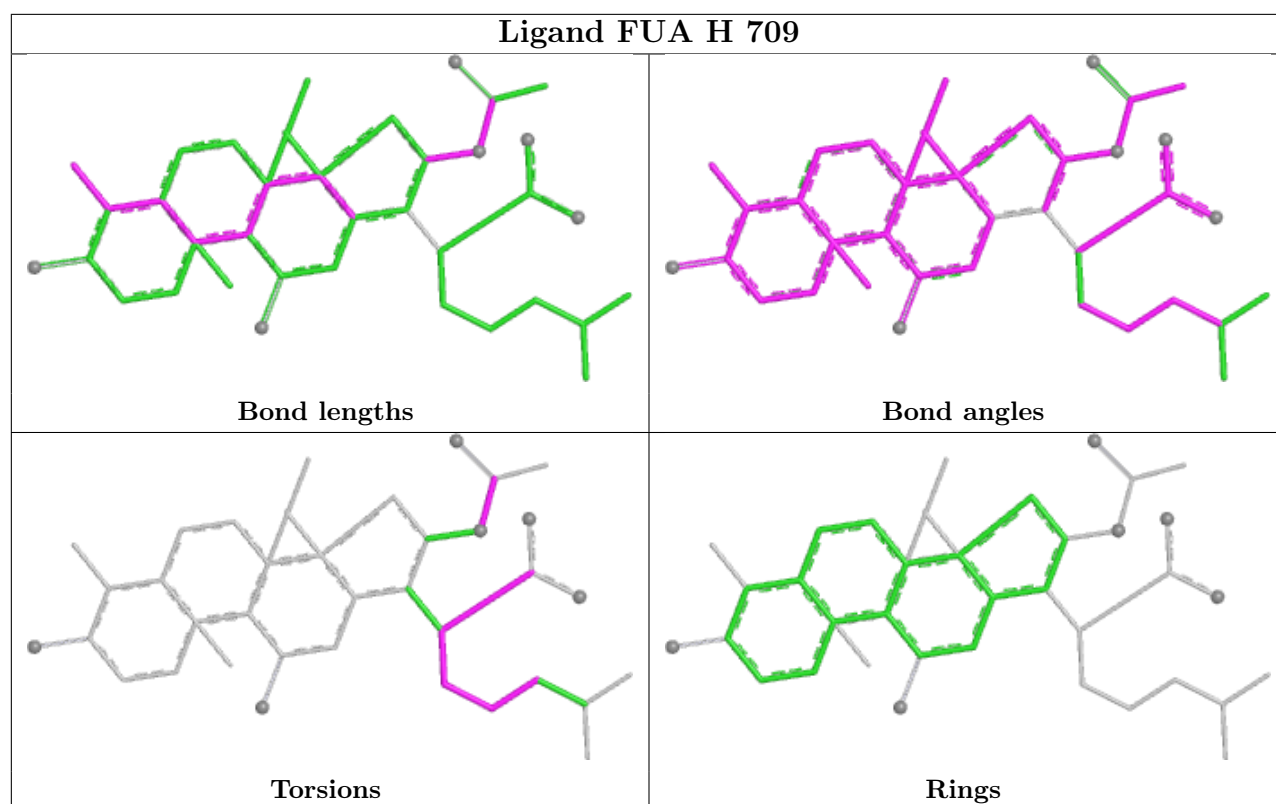


Ligand FUA L 710



Ligand FUA E 706





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	214/219 (97%)	-0.31	3 (1%) 73 73	14, 24, 41, 64	0
1	B	217/219 (99%)	-0.04	3 (1%) 73 73	17, 28, 50, 71	0
1	C	213/219 (97%)	-0.19	1 (0%) 87 86	16, 27, 48, 63	0
1	D	213/219 (97%)	-0.23	5 (2%) 61 60	18, 26, 44, 70	0
1	E	215/219 (98%)	-0.11	4 (1%) 66 65	19, 30, 47, 66	0
1	F	212/219 (96%)	-0.07	1 (0%) 87 86	19, 29, 49, 56	0
1	G	213/219 (97%)	0.02	5 (2%) 61 60	21, 30, 47, 57	0
1	H	216/219 (98%)	-0.18	8 (3%) 45 44	14, 26, 40, 63	0
1	I	215/219 (98%)	0.18	8 (3%) 45 44	19, 32, 51, 68	0
1	J	212/219 (96%)	0.20	4 (1%) 66 65	25, 36, 55, 60	0
1	K	213/219 (97%)	0.44	9 (4%) 40 40	28, 39, 57, 64	0
1	L	210/219 (95%)	0.56	12 (5%) 29 28	26, 42, 63, 75	0
All	All	2563/2628 (97%)	0.02	63 (2%) 58 57	14, 31, 52, 75	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	5	ILE	7.0
1	D	217	GLY	5.6
1	H	218	GLY	5.0
1	C	218	GLY	4.7
1	I	3	LYS	4.5
1	A	5	ILE	4.5
1	J	6	THR	4.3
1	L	13	ILE	4.2
1	I	4	LYS	4.2
1	B	218	GLY	4.0
1	L	6	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	218	GLY	3.8
1	E	142	MET	3.8
1	L	138	PHE	3.4
1	L	83	VAL	3.4
1	E	5	ILE	3.4
1	L	77	MET	3.3
1	G	204	MET	3.3
1	K	142	MET	3.2
1	I	142	MET	3.2
1	A	204	MET	3.1
1	H	4	LYS	2.9
1	G	218	GLY	2.9
1	F	50	LYS	2.9
1	L	142	MET	2.8
1	A	218	GLY	2.8
1	L	8	TYR	2.8
1	L	118	HIS	2.7
1	D	6	THR	2.6
1	L	9	THR	2.6
1	H	181	ASP	2.6
1	K	13	ILE	2.6
1	I	204	MET	2.6
1	J	5	ILE	2.6
1	J	157	ASP	2.5
1	G	142	MET	2.5
1	D	154	THR	2.5
1	G	6	THR	2.5
1	B	138	PHE	2.5
1	L	10	THR	2.5
1	H	185	MET	2.5
1	K	12	ASP	2.4
1	G	217	GLY	2.4
1	K	9	THR	2.4
1	E	3	LYS	2.4
1	K	173	MET	2.4
1	H	157	ASP	2.4
1	H	75	MET	2.4
1	I	114	ARG	2.4
1	H	219	ALA	2.3
1	I	126	CYS	2.3
1	K	5	ILE	2.3
1	E	6	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	11	VAL	2.2
1	B	32	THR	2.2
1	K	81	GLU	2.1
1	I	113	PHE	2.1
1	D	157	ASP	2.1
1	L	11	VAL	2.1
1	L	28	VAL	2.1
1	K	17	HIS	2.0
1	J	7	GLY	2.0
1	I	52	LYS	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](#)

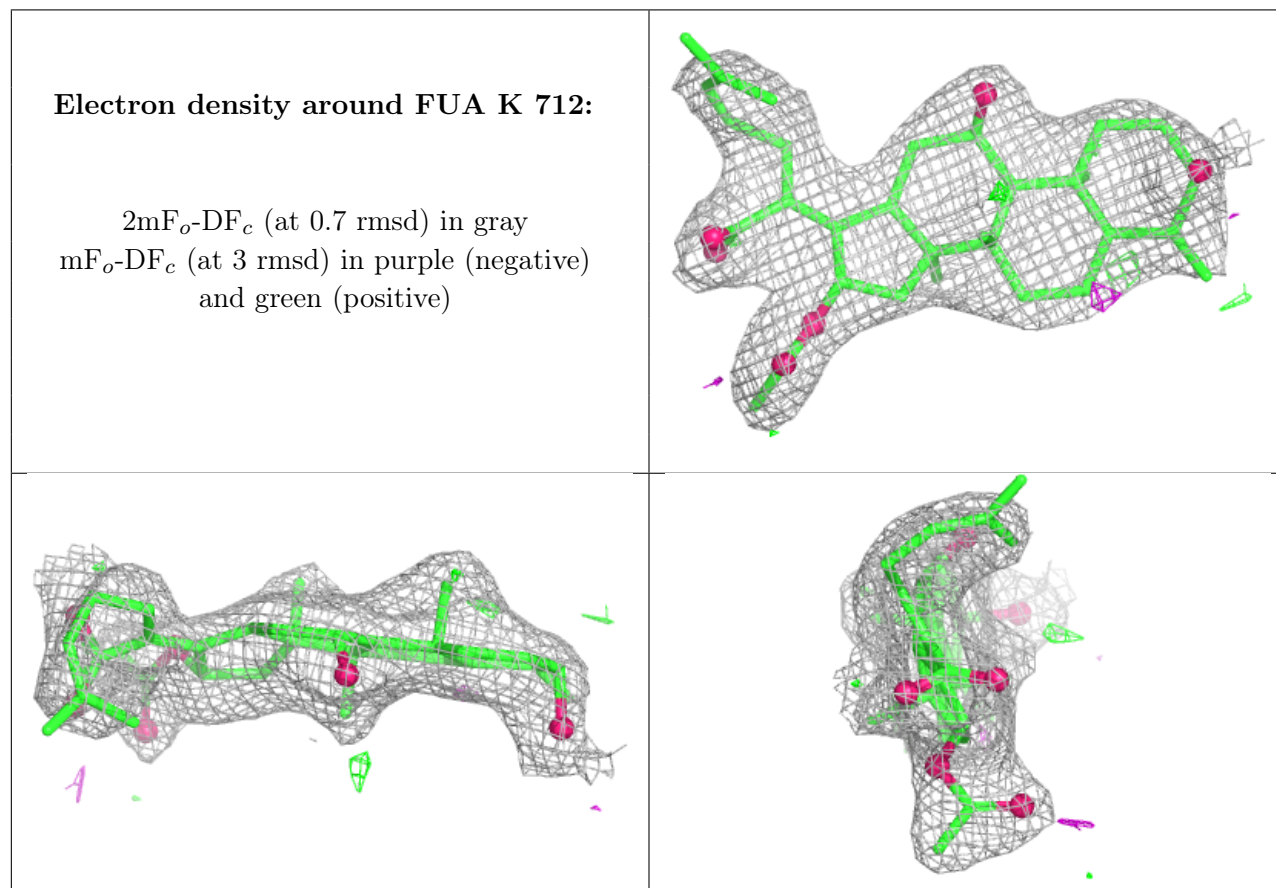
There are no oligosaccharides in this entry.

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.

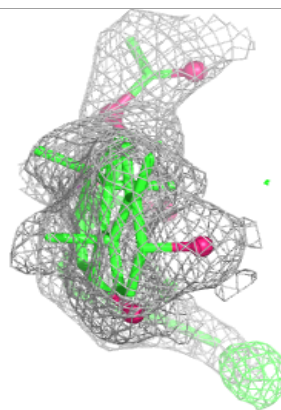
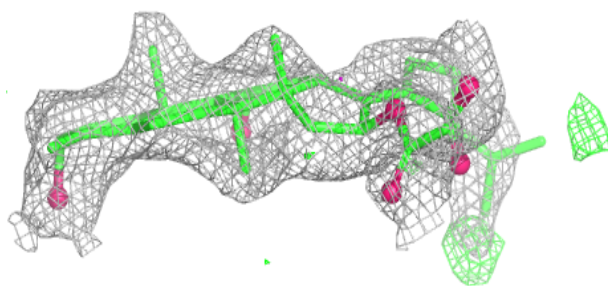
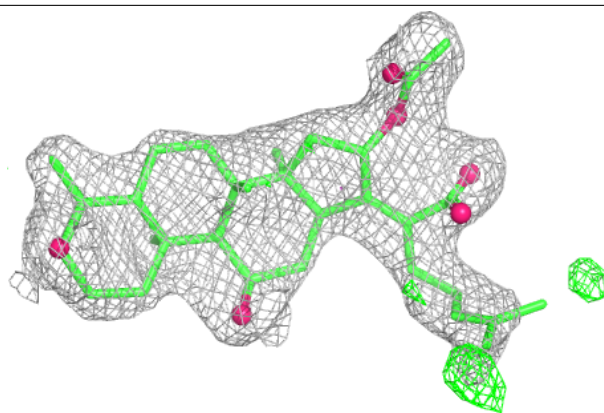
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	FUA	K	712	37/37	0.84	0.16	42,55,72,74	0
3	FUA	L	710	37/37	0.85	0.16	33,59,71,72	0
3	FUA	G	708	37/37	0.86	0.15	43,55,68,70	0
3	FUA	I	707	37/37	0.86	0.13	36,42,51,55	0
3	FUA	H	709	37/37	0.89	0.12	28,38,60,60	0
3	FUA	J	711	37/37	0.89	0.13	43,50,60,64	0
3	FUA	E	706	37/37	0.90	0.12	33,42,51,57	0
3	FUA	F	704	37/37	0.90	0.11	27,40,55,55	0
3	FUA	C	701	37/37	0.90	0.12	31,41,52,55	0
3	FUA	D	705	37/37	0.90	0.12	31,37,58,62	0
3	FUA	B	703	37/37	0.91	0.11	25,35,57,59	0
3	FUA	A	702	37/37	0.92	0.10	19,34,40,44	0
2	CA	A	801	1/1	0.98	0.15	5,5,5,5	1

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.

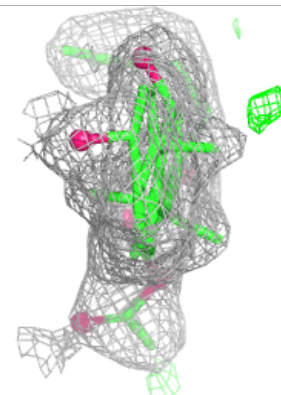
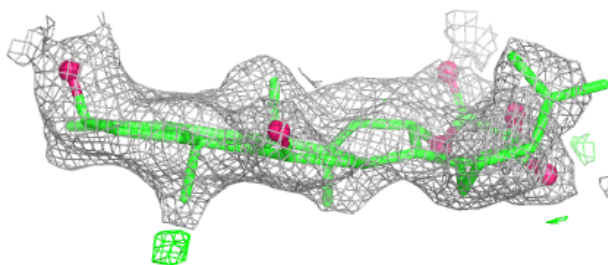
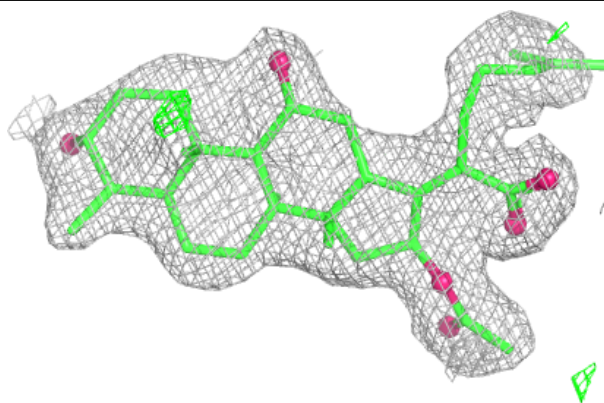


Electron density around FUA L 710:

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

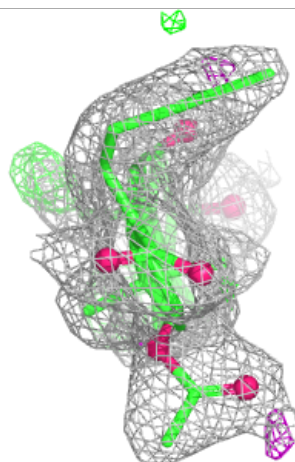
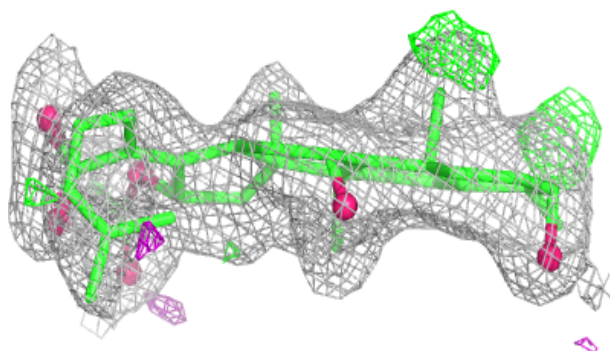
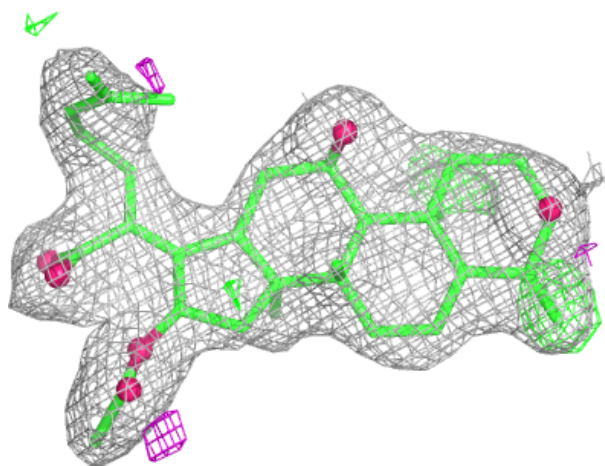
**Electron density around FUA G 708:**

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



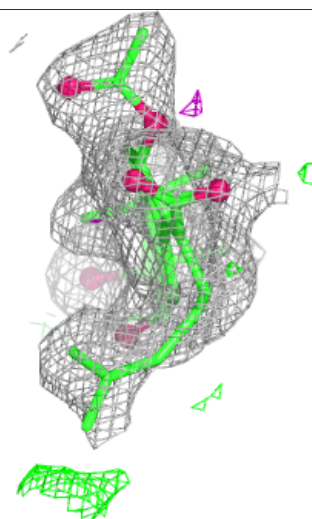
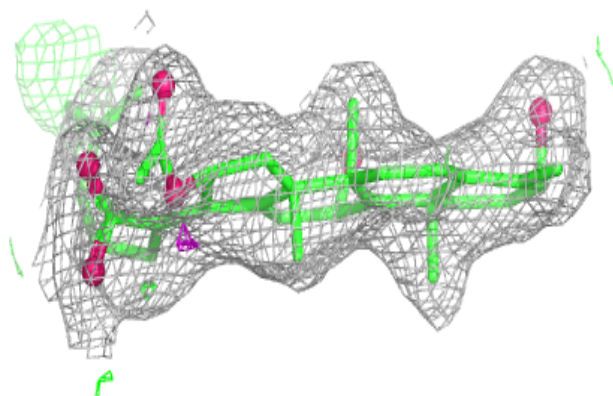
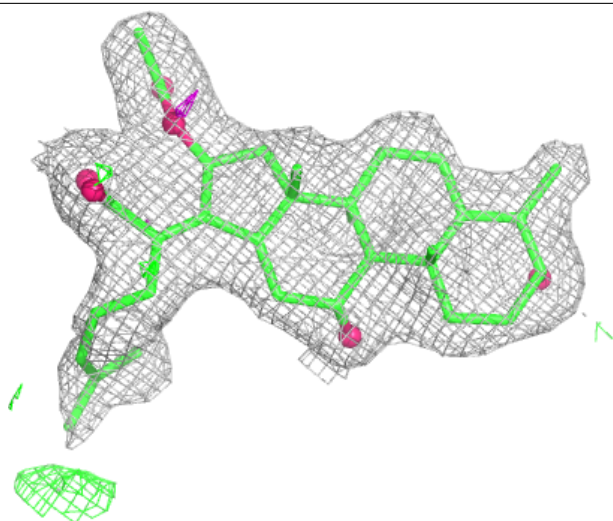
Electron density around FUA I 707:

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



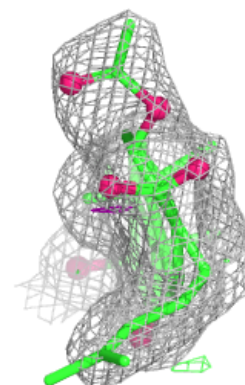
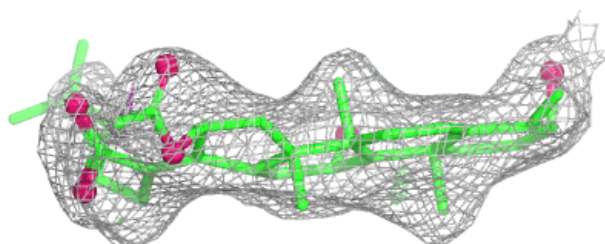
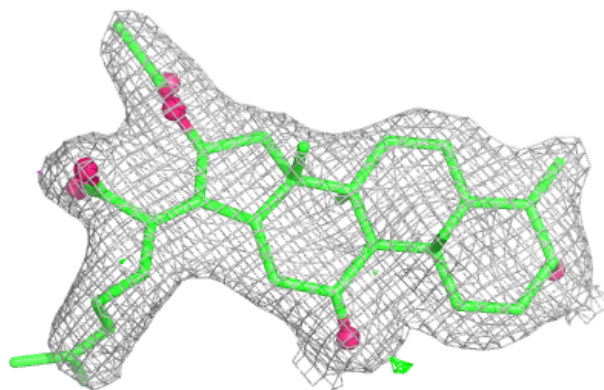
Electron density around FUA H 709:

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

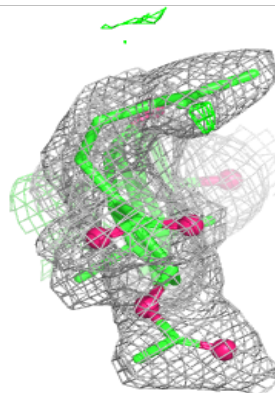
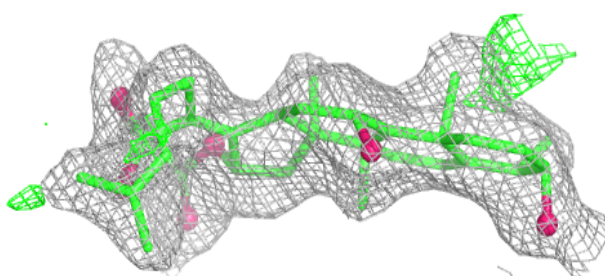
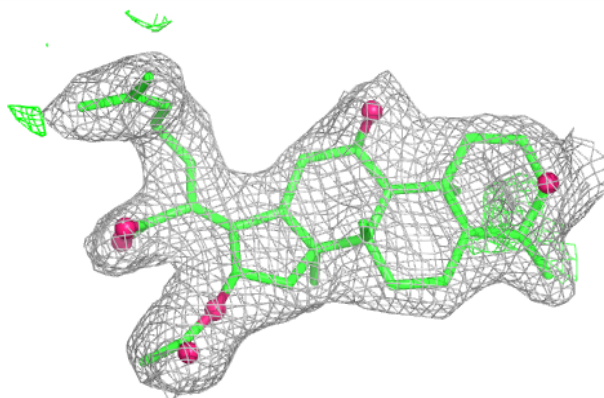


Electron density around FUA J 711:

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

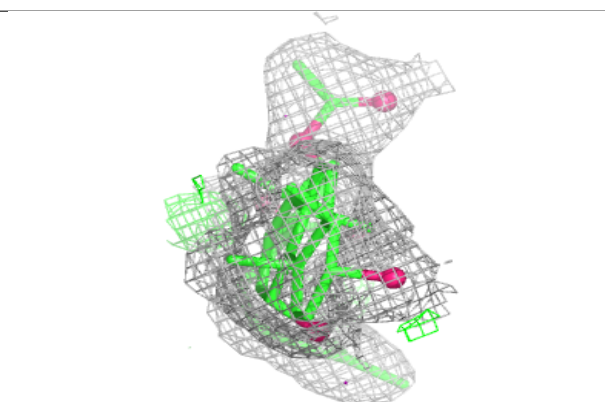
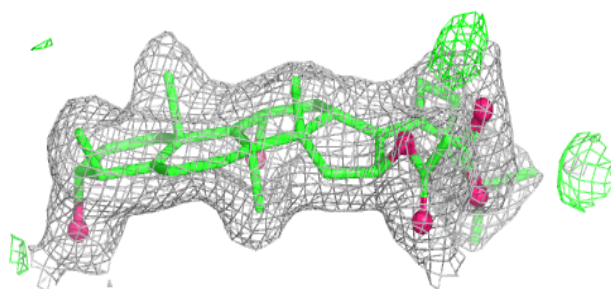
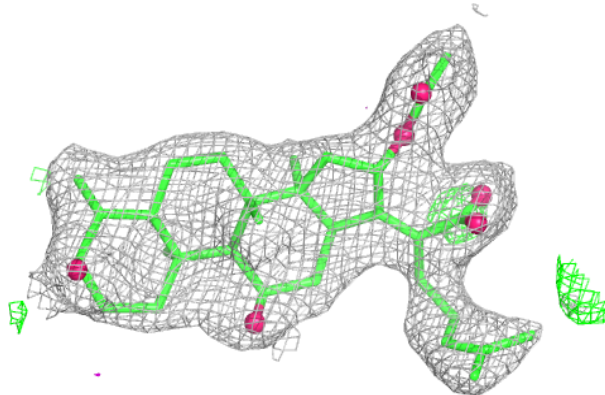
**Electron density around FUA E 706:**

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

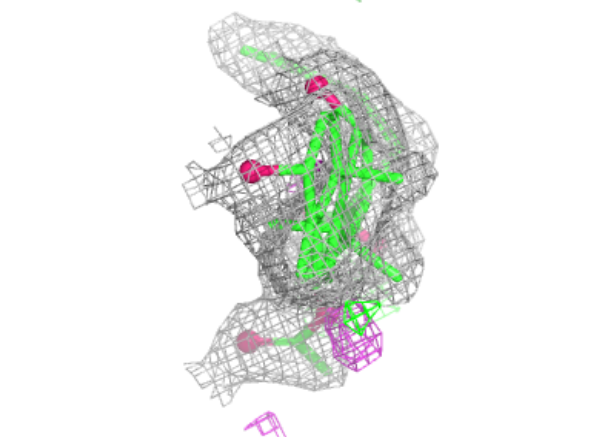
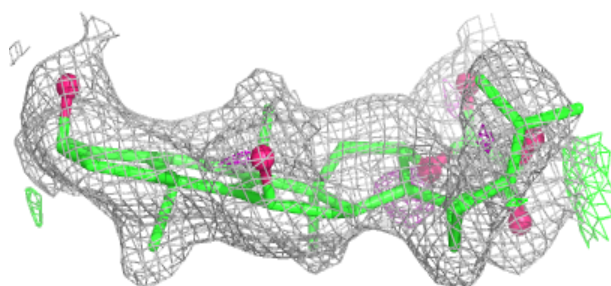
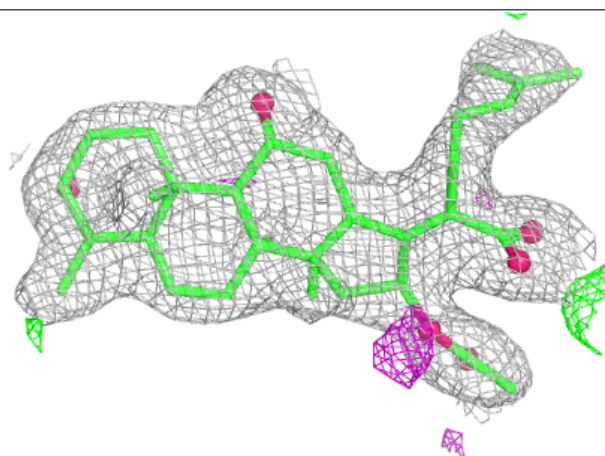


Electron density around FUA F 704:

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

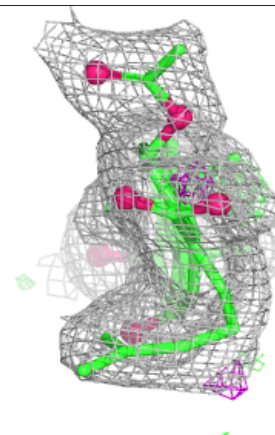
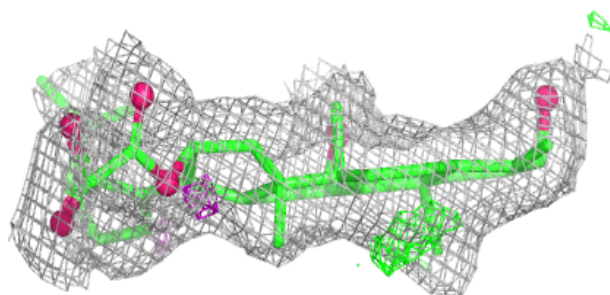
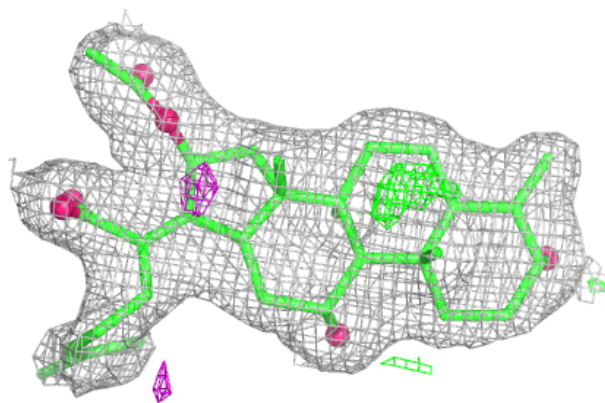
**Electron density around FUA C 701:**

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



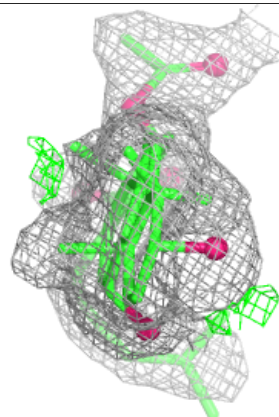
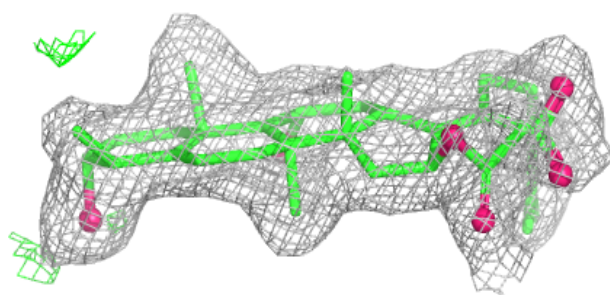
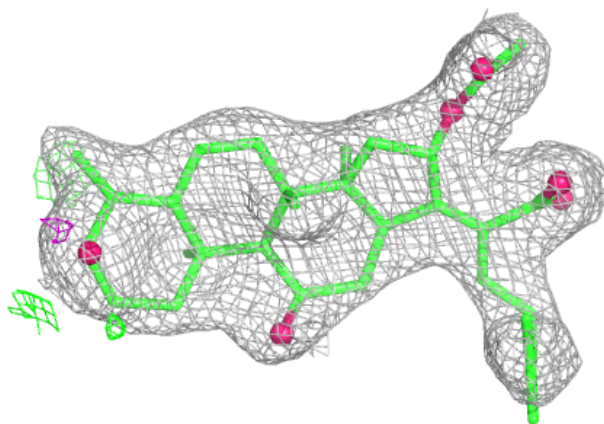
Electron density around FUA D 705:

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

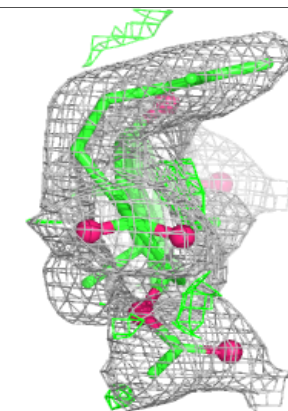
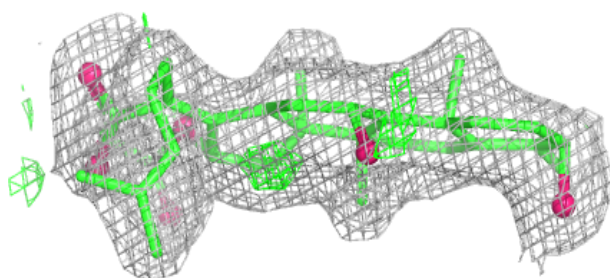
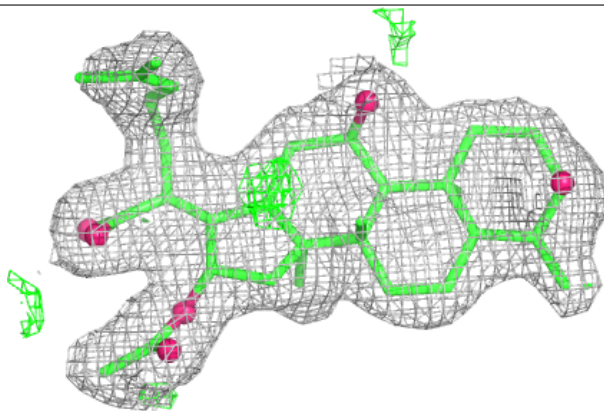


Electron density around FUA B 703:

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

**Electron density around FUA A 702:**

$2mF_o-DF_c$ (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.