



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 11:51 AM UTC

PDB ID : 9UJI / pdb_00009uji
Title : Crystal structure of the BTB domain mouse Keap1 in complex with CDDO-Im
Authors : Iso, T.; Suzuki, T.; Takagi, K.; Mizushima, T.; Yamamoto, M.
Deposited on : 2025-04-17
Resolution : 2.44 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

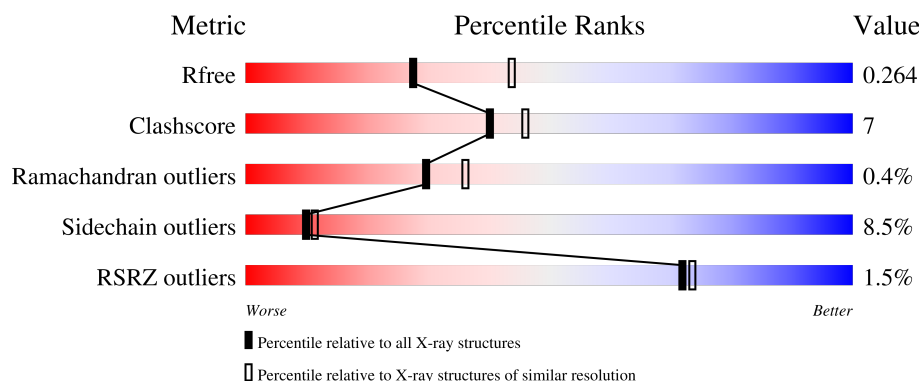
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.44 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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	130	
1	B	130	
1	C	130	
1	D	130	
1	E	130	

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Mol	Chain	Length	Quality of chain
1	F	130	<div><div></div><div>2%</div><div>85%</div><div>10%</div><div>5%</div><div></div></div>
1	G	130	<div><div></div><div>%</div><div>82%</div><div>14%</div><div>...</div><div></div></div>
1	H	130	<div><div></div><div>5%</div><div>84%</div><div>15%</div><div></div><div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8360 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.

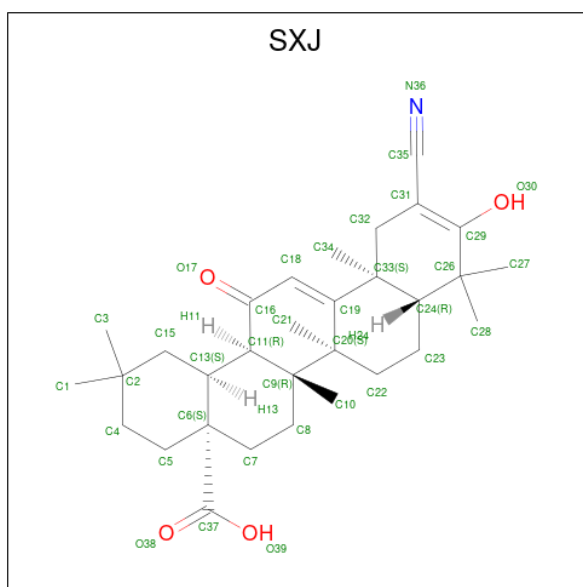
- Molecule 1 is a protein called Kelch-like ECH-associated protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	129	Total	C	N	O	S	0	0	0
			1010	642	170	188	10			
1	B	130	Total	C	N	O	S	0	0	0
			1018	648	171	189	10			
1	C	129	Total	C	N	O	S	0	0	0
			1010	642	170	188	10			
1	D	130	Total	C	N	O	S	0	0	0
			1018	648	171	189	10			
1	E	127	Total	C	N	O	S	0	0	0
			992	632	166	184	10			
1	F	129	Total	C	N	O	S	0	0	0
			1006	639	169	188	10			
1	G	129	Total	C	N	O	S	0	0	0
			1010	642	170	188	10			
1	H	130	Total	C	N	O	S	0	0	0
			1014	645	170	189	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	172	ALA	SER	engineered mutation	UNP Q9Z2X8
B	172	ALA	SER	engineered mutation	UNP Q9Z2X8
C	172	ALA	SER	engineered mutation	UNP Q9Z2X8
D	172	ALA	SER	engineered mutation	UNP Q9Z2X8
E	172	ALA	SER	engineered mutation	UNP Q9Z2X8
F	172	ALA	SER	engineered mutation	UNP Q9Z2X8
G	172	ALA	SER	engineered mutation	UNP Q9Z2X8
H	172	ALA	SER	engineered mutation	UNP Q9Z2X8

- Molecule 2 is (13alpha,18alpha)-2-cyano-3-hydroxy-12-oxooleana-2,9(11)-dien-28-oic acid (CCD ID: SXJ) (formula: C₃₁H₄₃NO₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			35	31	1	3		
2	B	1	Total	C	N	O	0	0
			35	31	1	3		
2	C	1	Total	C	N	O	0	0
			35	31	1	3		
2	D	1	Total	C	N	O	0	0
			35	31	1	3		
2	E	1	Total	C	N	O	0	0
			35	31	1	3		
2	F	1	Total	C	N	O	0	0
			35	31	1	3		
2	G	1	Total	C	N	O	0	0
			35	31	1	3		
2	H	1	Total	C	N	O	0	0
			35	31	1	3		


- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

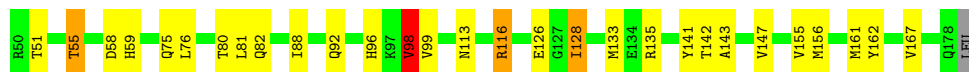
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		

3 Residue-property plots [i](#)


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

- Molecule 1: Kelch-like ECH-associated protein 1

Chain A: 




- Molecule 1: Kelch-like ECH-associated protein 1

Chain B: 




- Molecule 1: Kelch-like ECH-associated protein 1

Chain C: 




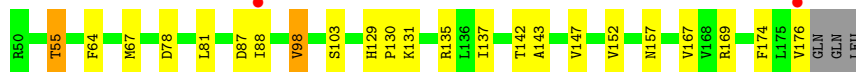
- Molecule 1: Kelch-like ECH-associated protein 1

Chain D: 




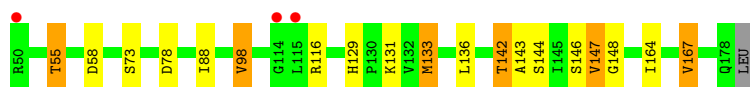
- Molecule 1: Kelch-like ECH-associated protein 1

Chain E: 




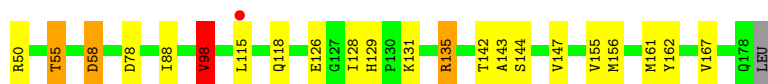
- Molecule 1: Kelch-like ECH-associated protein 1

Chain F:  2% 85% 10% 5% .




• Molecule 1: Kelch-like ECH-associated protein 1

Chain G:  % 82% 14% ...



• Molecule 1: Kelch-like ECH-associated protein 1

Chain H:  5% 84% 15% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.55Å 79.46Å 110.88Å 90.00° 94.60° 90.00°	Depositor
Resolution (Å)	42.52 – 2.44 42.52 – 2.44	Depositor EDS
% Data completeness (in resolution range)	97.8 (42.52-2.44) 97.8 (42.52-2.44)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.206 , 0.256 0.209 , 0.264	Depositor DCC
R_{free} test set	2345 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	68.0	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 27.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8360	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% 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: SXJ, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.67	0/1027	1.25	6/1386 (0.4%)
1	B	0.64	0/1035	1.16	4/1397 (0.3%)
1	C	0.62	0/1027	1.20	1/1386 (0.1%)
1	D	0.65	0/1035	1.21	7/1397 (0.5%)
1	E	0.64	0/1009	1.21	4/1362 (0.3%)
1	F	0.63	0/1023	1.24	4/1382 (0.3%)
1	G	0.59	0/1027	1.22	4/1386 (0.3%)
1	H	0.57	0/1031	1.16	3/1393 (0.2%)
All	All	0.63	0/8214	1.21	33/11089 (0.3%)

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	B	0	1
1	D	0	1
1	G	0	1
All	All	0	3

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	VAL	N-CA-CB	10.30	123.34	110.47
1	F	98	VAL	N-CA-CB	9.61	121.18	110.51
1	B	98	VAL	N-CA-CB	7.85	121.22	110.54
1	D	98	VAL	N-CA-CB	7.79	121.14	110.54
1	E	98	VAL	N-CA-CB	7.29	120.45	110.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	98	VAL	CB-CA-C	-6.91	102.81	112.14
1	A	98	VAL	CB-CA-C	-6.69	103.28	112.04
1	H	98	VAL	N-CA-CB	6.68	118.82	110.47
1	C	98	VAL	N-CA-CB	6.65	119.59	110.54
1	E	78	ASP	CA-CB-CG	6.58	119.18	112.60
1	G	98	VAL	N-CA-CB	6.53	119.42	110.54
1	F	78	ASP	CA-CB-CG	6.43	119.03	112.60
1	F	142	THR	CA-CB-OG1	-6.35	100.08	109.60
1	D	154	HIS	CA-CB-CG	-6.34	107.45	113.80
1	B	58	ASP	CA-CB-CG	6.07	118.67	112.60
1	H	98	VAL	CB-CA-C	-6.03	104.15	112.04
1	D	51	THR	CA-CB-OG1	-6.00	100.60	109.60
1	D	178	GLN	CB-CA-C	-5.98	100.61	110.72
1	D	111	PHE	CA-CB-CG	5.95	119.75	113.80
1	A	80	THR	CA-CB-OG1	-5.74	100.98	109.60
1	B	98	VAL	CB-CA-C	-5.67	104.48	112.14
1	G	135	ARG	CA-CB-CG	-5.63	102.83	114.10
1	A	82	GLN	N-CA-CB	-5.54	101.27	110.47
1	D	98	VAL	CB-CA-C	-5.39	104.87	112.14
1	G	58	ASP	CA-CB-CG	5.38	117.97	112.60
1	G	78	ASP	CA-CB-CG	5.36	117.96	112.60
1	B	117	GLU	CB-CA-C	5.30	118.53	109.72
1	F	98	VAL	CB-CA-C	-5.22	105.20	111.88
1	D	88	ILE	CB-CA-C	5.22	114.44	109.33
1	A	99	VAL	N-CA-CB	5.20	117.23	110.57
1	E	87	ASP	CA-CB-CG	5.19	117.79	112.60
1	H	154	HIS	CA-CB-CG	-5.09	108.71	113.80
1	A	59	HIS	CB-CA-C	-5.04	102.74	110.81

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	117	GLU	Peptide
1	D	50	ARG	Sidechain
1	G	135	ARG	Sidechain

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	1010	0	1010	19	0
1	B	1018	0	1021	12	0
1	C	1010	0	1010	16	0
1	D	1018	0	1021	14	0
1	E	992	0	994	14	0
1	F	1006	0	999	8	0
1	G	1010	0	1010	11	0
1	H	1014	0	1010	10	0
2	A	35	0	40	2	0
2	B	35	0	40	4	0
2	C	35	0	40	5	0
2	D	35	0	41	5	0
2	E	35	0	40	4	0
2	F	35	0	40	4	0
2	G	35	0	40	5	0
2	H	35	0	40	4	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
All	All	8360	0	8396	110	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 7.

All (110) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:MET:HE3	1:C:156:MET:HE3	1.68	0.75
2:D:201:SXJ:H10B	2:D:201:SXJ:H15	1.70	0.73
2:C:201:SXJ:H28A	2:C:201:SXJ:H34	1.70	0.73
1:A:147:VAL:HG11	1:A:155:VAL:HG21	1.70	0.72
2:B:201:SXJ:H34	2:B:201:SXJ:H28A	1.72	0.71
2:E:201:SXJ:H28A	2:E:201:SXJ:H34	1.72	0.70
1:A:128:ILE:CD1	1:A:162:TYR:HE2	2.05	0.68
1:F:129:HIS:HD2	1:F:131:LYS:H	1.41	0.68
1:C:128:ILE:CD1	1:C:162:TYR:HE2	2.09	0.65
1:A:156:MET:HE3	1:C:156:MET:CE	2.27	0.65
1:B:156:MET:SD	1:G:156:MET:HE1	2.37	0.65
1:E:142:THR:O	1:E:143:ALA:HB3	1.96	0.64
2:A:201:SXJ:H34	2:A:201:SXJ:H28A	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:VAL:HG11	1:D:96:HIS:CD2	2.34	0.63
1:E:129:HIS:HD2	1:E:131:LYS:H	1.46	0.63
1:A:135:ARG:HD3	1:A:147:VAL:HG12	1.81	0.62
2:A:201:SXJ:H10B	2:A:201:SXJ:H15	1.81	0.62
1:D:142:THR:O	1:D:143:ALA:HB3	2.00	0.61
2:G:201:SXJ:H28A	2:G:201:SXJ:H34	1.85	0.59
1:E:143:ALA:O	1:F:55:THR:HA	2.03	0.59
1:G:147:VAL:HG11	1:G:155:VAL:HG21	1.84	0.59
1:A:98:VAL:HG11	1:B:96:HIS:CD2	2.40	0.57
1:G:142:THR:O	1:G:143:ALA:HB3	2.05	0.57
2:F:201:SXJ:H10B	2:F:201:SXJ:H15	1.86	0.56
2:C:201:SXJ:C18	2:C:201:SXJ:H10	2.34	0.56
2:E:201:SXJ:H10B	2:E:201:SXJ:H15	1.88	0.56
1:B:148:GLY:HA3	2:B:201:SXJ:N36	2.20	0.56
1:E:55:THR:HB	1:F:144:SER:OG	2.06	0.55
1:B:129:HIS:HD2	1:B:131:LYS:H	1.56	0.54
2:G:201:SXJ:C18	2:G:201:SXJ:H10	2.37	0.54
1:H:148:GLY:HA3	2:H:201:SXJ:N36	2.22	0.54
1:B:142:THR:O	1:B:143:ALA:HB3	2.08	0.54
1:C:55:THR:HA	1:D:143:ALA:O	2.07	0.54
1:A:128:ILE:HD13	1:A:162:TYR:HE2	1.73	0.54
2:B:201:SXJ:H15	2:B:201:SXJ:H10B	1.89	0.53
2:B:201:SXJ:H28A	2:B:201:SXJ:C34	2.39	0.53
1:A:98:VAL:CG1	1:B:96:HIS:CD2	2.92	0.53
1:D:163:GLN:HE21	1:E:169:ARG:HH21	1.57	0.52
1:C:144:SER:OG	1:D:55:THR:HB	2.11	0.51
1:G:55:THR:HB	1:H:144:SER:OG	2.10	0.51
2:D:201:SXJ:H28A	2:D:201:SXJ:H34	1.93	0.51
2:C:201:SXJ:H28A	2:C:201:SXJ:C34	2.41	0.50
1:D:81:LEU:HD12	1:D:137:ILE:HD11	1.94	0.50
2:H:201:SXJ:C18	2:H:201:SXJ:H10	2.42	0.49
1:C:98:VAL:CG1	1:D:96:HIS:CD2	2.95	0.49
1:E:142:THR:O	1:E:143:ALA:CB	2.58	0.49
1:F:164:ILE:HG22	1:F:167:VAL:HG13	1.93	0.49
1:G:144:SER:OG	1:H:55:THR:HB	2.12	0.49
1:B:156:MET:CE	1:G:156:MET:HE1	2.43	0.49
1:G:129:HIS:CG	2:G:201:SXJ:H21B	2.47	0.49
1:A:55:THR:HB	1:B:144:SER:OG	2.13	0.49
1:F:147:VAL:HG22	1:F:148:GLY:O	2.12	0.48
1:A:55:THR:HA	1:B:143:ALA:O	2.13	0.48
1:C:128:ILE:HD11	1:C:161:MET:SD	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:201:SXJ:H10B	2:E:201:SXJ:C15	2.42	0.48
1:E:176:VAL:HG12	1:E:176:VAL:O	2.14	0.48
1:G:98:VAL:HG11	1:H:96:HIS:CD2	2.48	0.48
2:G:201:SXJ:H10B	2:G:201:SXJ:H15	1.95	0.48
1:G:128:ILE:HD11	1:G:161:MET:SD	2.54	0.48
1:C:55:THR:HB	1:D:144:SER:OG	2.14	0.47
1:C:142:THR:O	1:C:143:ALA:HB3	2.15	0.47
1:D:64:PHE:HA	1:D:67:MET:HE2	1.95	0.47
1:H:71:ARG:HD3	1:H:141:TYR:CE1	2.50	0.47
1:D:147:VAL:HG11	1:D:155:VAL:HG21	1.96	0.47
1:G:129:HIS:HD2	1:G:131:LYS:H	1.62	0.46
2:H:201:SXJ:H34	2:H:201:SXJ:H28A	1.98	0.46
1:F:148:GLY:HA3	2:F:201:SXJ:N36	2.31	0.46
2:D:201:SXJ:H11	2:D:201:SXJ:O38	2.16	0.46
1:A:75:GLN:O	1:A:76:LEU:HB2	2.16	0.45
1:A:96:HIS:CD2	1:B:98:VAL:HG11	2.52	0.45
1:E:135:ARG:HH11	1:E:135:ARG:HG3	1.81	0.45
2:F:201:SXJ:H28A	2:F:201:SXJ:H34	1.98	0.45
1:A:81:LEU:O	1:A:92:GLN:HA	2.17	0.45
1:A:128:ILE:HD11	1:A:162:TYR:HE2	1.81	0.45
2:C:201:SXJ:H15A	2:C:201:SXJ:O17	2.17	0.45
1:A:156:MET:CE	1:C:156:MET:HE3	2.43	0.45
1:C:64:PHE:HA	1:C:67:MET:HE2	2.00	0.44
1:C:128:ILE:HD11	1:C:161:MET:CE	2.47	0.44
1:H:142:THR:O	1:H:143:ALA:HB3	2.18	0.44
2:H:201:SXJ:H10B	2:H:201:SXJ:H15	2.00	0.44
1:A:142:THR:O	1:A:143:ALA:HB3	2.16	0.44
1:E:129:HIS:CD2	1:E:131:LYS:H	2.31	0.44
1:E:81:LEU:HD12	1:E:137:ILE:HD11	2.00	0.44
1:A:96:HIS:ND1	1:A:141:TYR:OH	2.42	0.44
1:D:172:ALA:HB1	1:E:157:ASN:HD22	1.82	0.44
1:F:142:THR:O	1:F:143:ALA:HB3	2.18	0.44
1:A:128:ILE:CD1	1:A:162:TYR:CE2	2.94	0.43
1:G:128:ILE:CD1	1:G:162:TYR:HE2	2.31	0.43
2:E:201:SXJ:H28A	2:E:201:SXJ:C34	2.44	0.43
2:D:201:SXJ:H10B	2:D:201:SXJ:C15	2.42	0.43
1:E:129:HIS:CD2	1:E:130:PRO:HD2	2.53	0.43
1:H:128:ILE:CD1	1:H:162:TYR:HE2	2.32	0.42
2:G:201:SXJ:H28A	2:G:201:SXJ:C34	2.47	0.42
1:H:57:GLU:HA	1:H:57:GLU:OE1	2.19	0.42
1:C:128:ILE:HD13	1:C:162:TYR:HE2	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:164:ILE:HG22	1:D:167:VAL:HG13	2.02	0.42
1:D:164:ILE:O	1:D:168:VAL:HG23	2.20	0.42
1:F:133:MET:CE	1:F:136:LEU:HD12	2.49	0.42
1:E:152:VAL:HG21	1:E:174:PHE:CE2	2.55	0.41
1:A:96:HIS:CD2	1:B:98:VAL:CG1	3.03	0.41
1:C:84:LYS:HD2	1:C:90:ALA:HB2	2.03	0.41
1:D:129:HIS:HD2	1:D:131:LYS:H	1.69	0.41
1:H:96:HIS:ND1	1:H:141:TYR:OH	2.48	0.41
2:F:201:SXJ:O17	2:F:201:SXJ:H15A	2.20	0.41
2:D:201:SXJ:C18	2:D:201:SXJ:H10	2.50	0.41
1:H:74:GLN:OE1	1:H:94:MET:SD	2.79	0.41
2:C:201:SXJ:H10B	2:C:201:SXJ:H15	2.03	0.41
1:C:164:ILE:HG22	1:C:167:VAL:HG13	2.03	0.40
1:B:84:LYS:HD2	1:B:90:ALA:HB2	2.04	0.40
1:E:64:PHE:HA	1:E:67:MET:HE2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	127/130 (98%)	124 (98%)	2 (2%)	1 (1%)	16	18
1	B	128/130 (98%)	125 (98%)	2 (2%)	1 (1%)	16	18
1	C	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
1	D	128/130 (98%)	123 (96%)	3 (2%)	2 (2%)	7	6
1	E	125/130 (96%)	123 (98%)	2 (2%)	0	100	100
1	F	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
1	G	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
1	H	128/130 (98%)	124 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1017/1040 (98%)	988 (97%)	25 (2%)	4 (0%)	30	36

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116	ARG
1	D	115	LEU
1	B	143	ALA
1	D	114	GLY

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	112/113 (99%)	100 (89%)	12 (11%)	6	6
1	B	113/113 (100%)	103 (91%)	10 (9%)	9	10
1	C	112/113 (99%)	99 (88%)	13 (12%)	5	5
1	D	113/113 (100%)	105 (93%)	8 (7%)	13	16
1	E	110/113 (97%)	104 (94%)	6 (6%)	19	26
1	F	111/113 (98%)	101 (91%)	10 (9%)	9	10
1	G	112/113 (99%)	103 (92%)	9 (8%)	11	13
1	H	112/113 (99%)	104 (93%)	8 (7%)	13	16
All	All	895/904 (99%)	819 (92%)	76 (8%)	10	11

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	THR
1	A	55	THR
1	A	58	ASP
1	A	88	ILE
1	A	98	VAL
1	A	113	ASN

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Mol	Chain	Res	Type
1	A	116	ARG
1	A	126	GLU
1	A	128	ILE
1	A	133	MET
1	A	161	MET
1	A	167	VAL
1	B	55	THR
1	B	86	GLU
1	B	98	VAL
1	B	113	ASN
1	B	115	LEU
1	B	118	GLN
1	B	120	MET
1	B	161	MET
1	B	167	VAL
1	B	176	VAL
1	C	50	ARG
1	C	55	THR
1	C	58	ASP
1	C	86	GLU
1	C	88	ILE
1	C	98	VAL
1	C	115	LEU
1	C	124	SER
1	C	133	MET
1	C	147	VAL
1	C	161	MET
1	C	167	VAL
1	C	169	ARG
1	D	50	ARG
1	D	55	THR
1	D	88	ILE
1	D	98	VAL
1	D	115	LEU
1	D	118	GLN
1	D	135	ARG
1	D	167	VAL
1	E	55	THR
1	E	88	ILE
1	E	98	VAL
1	E	103	SER
1	E	147	VAL

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Mol	Chain	Res	Type
1	E	167	VAL
1	F	55	THR
1	F	58	ASP
1	F	73	SER
1	F	88	ILE
1	F	98	VAL
1	F	116	ARG
1	F	133	MET
1	F	146	SER
1	F	147	VAL
1	F	167	VAL
1	G	50	ARG
1	G	55	THR
1	G	58	ASP
1	G	88	ILE
1	G	98	VAL
1	G	115	LEU
1	G	118	GLN
1	G	126	GLU
1	G	167	VAL
1	H	55	THR
1	H	88	ILE
1	H	98	VAL
1	H	118	GLN
1	H	124	SER
1	H	133	MET
1	H	167	VAL
1	H	176	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	ASN
1	A	129	HIS
1	A	157	ASN
1	A	177	GLN
1	A	178	GLN
1	B	75	GLN
1	B	113	ASN
1	B	118	GLN
1	C	118	GLN
1	C	178	GLN

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Mol	Chain	Res	Type
1	D	129	HIS
1	D	157	ASN
1	D	163	GLN
1	E	113	ASN
1	E	118	GLN
1	E	129	HIS
1	E	157	ASN
1	F	118	GLN
1	F	129	HIS
1	F	177	GLN
1	G	118	GLN
1	H	74	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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
2	SXJ	C	201	1	37,39,40	2.57	5 (13%)	51,68,70	1.66	10 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SXJ	A	201	1	37,39,40	2.69	4 (10%)	51,68,70	4.06	22 (43%)
2	SXJ	D	201	1	37,39,40	2.75	4 (10%)	51,68,70	1.92	17 (33%)
2	SXJ	G	201	1	37,39,40	2.81	4 (10%)	51,68,70	1.55	11 (21%)
2	SXJ	B	201	1	37,39,40	2.86	4 (10%)	51,68,70	1.77	10 (19%)
2	SXJ	F	201	1	37,39,40	2.62	5 (13%)	51,68,70	1.61	13 (25%)
2	SXJ	E	201	1	37,39,40	2.87	2 (5%)	51,68,70	2.13	16 (31%)
2	SXJ	H	201	1	37,39,40	2.68	2 (5%)	51,68,70	1.65	11 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SXJ	C	201	1	-	1/3/102/105	0/5/5/5
2	SXJ	A	201	1	-	1/3/102/105	0/5/5/5
2	SXJ	D	201	1	-	2/3/102/105	0/5/5/5
2	SXJ	G	201	1	-	1/3/102/105	0/5/5/5
2	SXJ	B	201	1	-	2/3/102/105	0/5/5/5
2	SXJ	F	201	1	-	2/3/102/105	0/5/5/5
2	SXJ	E	201	1	-	1/3/102/105	0/5/5/5
2	SXJ	H	201	1	-	2/3/102/105	0/5/5/5

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	201	SXJ	C35-C31	-16.50	1.25	1.43
2	B	201	SXJ	C35-C31	-16.36	1.25	1.43
2	G	201	SXJ	C35-C31	-15.94	1.26	1.43
2	H	201	SXJ	C35-C31	-15.30	1.26	1.43
2	D	201	SXJ	C35-C31	-15.24	1.26	1.43
2	A	201	SXJ	C35-C31	-14.95	1.27	1.43
2	F	201	SXJ	C35-C31	-14.35	1.27	1.43
2	C	201	SXJ	C35-C31	-13.69	1.28	1.43
2	A	201	SXJ	C18-C19	3.34	1.37	1.34
2	D	201	SXJ	C18-C16	3.23	1.52	1.46
2	C	201	SXJ	C33-C24	-2.99	1.52	1.56
2	F	201	SXJ	C18-C16	2.90	1.51	1.46
2	H	201	SXJ	C9-C20	-2.69	1.54	1.59
2	B	201	SXJ	C18-C19	2.63	1.37	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	201	SXJ	C9-C20	-2.60	1.55	1.59
2	B	201	SXJ	C9-C20	-2.59	1.55	1.59
2	A	201	SXJ	C4-C2	2.49	1.57	1.53
2	F	201	SXJ	C9-C20	-2.47	1.55	1.59
2	C	201	SXJ	C9-C20	-2.42	1.55	1.59
2	E	201	SXJ	C9-C20	-2.40	1.55	1.59
2	C	201	SXJ	C35-N36	2.40	1.19	1.14
2	B	201	SXJ	C18-C16	2.29	1.50	1.46
2	A	201	SXJ	C18-C16	2.28	1.50	1.46
2	G	201	SXJ	C26-C24	-2.24	1.53	1.56
2	F	201	SXJ	C7-C6	2.16	1.57	1.54
2	F	201	SXJ	C26-C24	2.13	1.59	1.56
2	D	201	SXJ	C18-C19	2.06	1.36	1.34
2	D	201	SXJ	C9-C20	-2.05	1.55	1.59
2	C	201	SXJ	C22-C20	-2.01	1.51	1.54
2	G	201	SXJ	C34-C33	-2.00	1.51	1.54

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	SXJ	C4-C2-C15	-15.68	89.11	108.66
2	A	201	SXJ	C1-C2-C4	-11.79	93.06	110.04
2	A	201	SXJ	C3-C2-C15	10.83	127.65	109.86
2	A	201	SXJ	C3-C2-C4	-10.60	94.78	110.04
2	E	201	SXJ	C15-C13-C6	-8.51	104.10	111.24
2	D	201	SXJ	C15-C13-C6	-5.74	106.42	111.24
2	A	201	SXJ	C5-C4-C2	5.24	118.14	113.17
2	B	201	SXJ	O38-C37-C6	-5.07	115.36	126.36
2	C	201	SXJ	C15-C13-C6	4.77	115.25	111.24
2	B	201	SXJ	C34-C33-C32	-4.59	104.11	108.89
2	E	201	SXJ	C28-C26-C29	-4.53	103.19	108.66
2	B	201	SXJ	C15-C13-C6	-4.46	107.49	111.24
2	D	201	SXJ	O17-C16-C11	-4.43	115.32	121.39
2	H	201	SXJ	C35-C31-C29	-4.23	113.95	120.15
2	A	201	SXJ	C8-C9-C20	4.16	114.23	110.22
2	G	201	SXJ	C8-C9-C20	4.12	114.20	110.22
2	A	201	SXJ	C2-C15-C13	4.10	120.75	114.07
2	C	201	SXJ	C31-C35-N36	-4.05	170.67	177.08
2	A	201	SXJ	C13-C6-C37	4.01	115.15	109.13
2	A	201	SXJ	C1-C2-C15	3.97	116.39	109.86
2	E	201	SXJ	C3-C2-C15	3.88	116.23	109.86
2	H	201	SXJ	C15-C13-C6	-3.83	108.02	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	201	SXJ	C3-C2-C4	-3.66	104.77	110.04
2	H	201	SXJ	O38-C37-C6	-3.50	118.76	126.36
2	B	201	SXJ	C13-C6-C37	3.47	114.33	109.13
2	A	201	SXJ	C3-C2-C1	3.45	115.49	109.34
2	D	201	SXJ	C27-C26-C29	-3.42	104.53	108.66
2	H	201	SXJ	C8-C9-C20	3.40	113.51	110.22
2	F	201	SXJ	C21-C20-C9	-3.38	109.30	112.31
2	C	201	SXJ	C8-C9-C11	3.32	111.95	107.91
2	A	201	SXJ	C28-C26-C29	-3.31	104.67	108.66
2	D	201	SXJ	O38-C37-C6	-3.30	119.20	126.36
2	E	201	SXJ	C33-C19-C20	3.21	125.17	120.14
2	B	201	SXJ	C8-C9-C20	3.21	113.32	110.22
2	C	201	SXJ	C13-C6-C37	3.20	113.93	109.13
2	F	201	SXJ	C28-C26-C29	-3.19	104.81	108.66
2	F	201	SXJ	C21-C20-C19	-3.17	102.56	107.33
2	A	201	SXJ	C35-C31-C29	-3.07	115.64	120.15
2	H	201	SXJ	C27-C26-C29	-3.07	104.96	108.66
2	F	201	SXJ	C8-C9-C20	2.99	113.11	110.22
2	E	201	SXJ	O38-C37-C6	-2.94	119.97	126.36
2	A	201	SXJ	C10-C9-C20	-2.93	106.67	109.98
2	D	201	SXJ	C5-C6-C13	2.88	114.84	110.06
2	B	201	SXJ	C13-C11-C16	2.86	115.77	113.33
2	G	201	SXJ	C34-C33-C32	2.85	111.86	108.89
2	E	201	SXJ	C1-C2-C15	-2.85	105.18	109.86
2	C	201	SXJ	C33-C19-C20	2.84	124.59	120.14
2	C	201	SXJ	O17-C16-C18	-2.82	116.78	121.46
2	D	201	SXJ	C22-C23-C24	-2.80	105.64	111.05
2	D	201	SXJ	C11-C16-C18	2.77	122.25	116.87
2	F	201	SXJ	C10-C9-C20	-2.75	106.87	109.98
2	C	201	SXJ	C28-C26-C29	-2.74	105.35	108.66
2	E	201	SXJ	O17-C16-C18	-2.70	116.98	121.46
2	D	201	SXJ	C24-C33-C19	2.69	112.92	107.98
2	A	201	SXJ	C21-C20-C19	-2.67	103.30	107.33
2	F	201	SXJ	C9-C11-C16	-2.67	105.48	108.89
2	A	201	SXJ	C13-C11-C16	2.66	115.60	113.33
2	E	201	SXJ	C13-C6-C37	2.66	113.12	109.13
2	B	201	SXJ	C24-C33-C19	2.65	112.84	107.98
2	G	201	SXJ	C21-C20-C22	-2.63	103.50	107.78
2	B	201	SXJ	C21-C20-C19	-2.62	103.38	107.33
2	G	201	SXJ	C8-C9-C11	2.62	111.09	107.91
2	D	201	SXJ	C35-C31-C29	-2.60	116.34	120.15
2	A	201	SXJ	C15-C13-C6	-2.58	109.08	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	SXJ	C10-C9-C8	-2.55	103.64	107.83
2	D	201	SXJ	C9-C11-C16	-2.53	105.66	108.89
2	H	201	SXJ	C21-C20-C9	-2.52	110.06	112.31
2	E	201	SXJ	C33-C19-C18	-2.52	116.79	124.07
2	E	201	SXJ	C28-C26-C27	2.51	111.82	107.87
2	E	201	SXJ	C34-C33-C32	2.47	111.47	108.89
2	E	201	SXJ	C11-C16-C18	2.45	121.64	116.87
2	G	201	SXJ	C5-C6-C13	2.44	114.11	110.06
2	F	201	SXJ	C1-C2-C4	2.44	113.55	110.04
2	F	201	SXJ	C33-C19-C20	2.44	123.95	120.14
2	A	201	SXJ	C5-C6-C13	-2.42	106.04	110.06
2	G	201	SXJ	C33-C19-C18	-2.39	117.14	124.07
2	H	201	SXJ	C2-C15-C13	-2.38	110.19	114.07
2	G	201	SXJ	C1-C2-C15	2.38	113.78	109.86
2	B	201	SXJ	C3-C2-C1	2.37	113.56	109.34
2	F	201	SXJ	C11-C16-C18	2.36	121.45	116.87
2	H	201	SXJ	C11-C16-C18	2.35	121.44	116.87
2	H	201	SXJ	C13-C6-C37	2.34	112.64	109.13
2	D	201	SXJ	C3-C2-C1	-2.32	105.19	109.34
2	E	201	SXJ	C9-C11-C16	-2.30	105.95	108.89
2	D	201	SXJ	C20-C9-C11	2.29	109.74	107.96
2	H	201	SXJ	C33-C19-C20	2.28	123.71	120.14
2	E	201	SXJ	C1-C2-C4	2.27	113.31	110.04
2	B	201	SXJ	C21-C20-C9	-2.26	110.29	112.31
2	D	201	SXJ	C7-C6-C5	-2.26	106.90	110.95
2	C	201	SXJ	C33-C24-C26	-2.25	113.63	116.78
2	F	201	SXJ	C13-C11-C16	2.22	115.22	113.33
2	D	201	SXJ	C8-C9-C20	2.22	112.37	110.22
2	D	201	SXJ	C10-C9-C20	-2.22	107.47	109.98
2	F	201	SXJ	C28-C26-C24	2.22	118.14	111.67
2	A	201	SXJ	C33-C24-C26	-2.21	113.68	116.78
2	C	201	SXJ	C33-C19-C18	-2.19	117.72	124.07
2	G	201	SXJ	C33-C19-C20	2.19	123.57	120.14
2	A	201	SXJ	C28-C26-C24	2.18	118.03	111.67
2	F	201	SXJ	C15-C13-C6	-2.17	109.41	111.24
2	G	201	SXJ	C10-C9-C20	-2.16	107.54	109.98
2	D	201	SXJ	C8-C9-C11	-2.12	105.32	107.91
2	G	201	SXJ	C23-C22-C20	-2.12	109.76	112.86
2	A	201	SXJ	C22-C20-C19	2.12	115.72	112.53
2	E	201	SXJ	C33-C24-C26	-2.06	113.89	116.78
2	G	201	SXJ	C22-C23-C24	-2.06	107.06	111.05
2	C	201	SXJ	C7-C8-C9	-2.06	110.27	113.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	201	SXJ	O17-C16-C11	-2.05	118.57	121.39
2	F	201	SXJ	C5-C6-C13	2.03	113.43	110.06
2	D	201	SXJ	C1-C2-C4	-2.03	107.12	110.04
2	A	201	SXJ	O17-C16-C18	-2.02	118.11	121.46

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	201	SXJ	O38-C37-C6-C13
2	D	201	SXJ	O38-C37-C6-C13
2	F	201	SXJ	O38-C37-C6-C13
2	H	201	SXJ	O38-C37-C6-C13
2	B	201	SXJ	O38-C37-C6-C5
2	D	201	SXJ	O38-C37-C6-C5
2	F	201	SXJ	O38-C37-C6-C5
2	H	201	SXJ	O38-C37-C6-C5
2	A	201	SXJ	O38-C37-C6-C13
2	C	201	SXJ	O38-C37-C6-C13
2	E	201	SXJ	O38-C37-C6-C13
2	G	201	SXJ	O38-C37-C6-C13

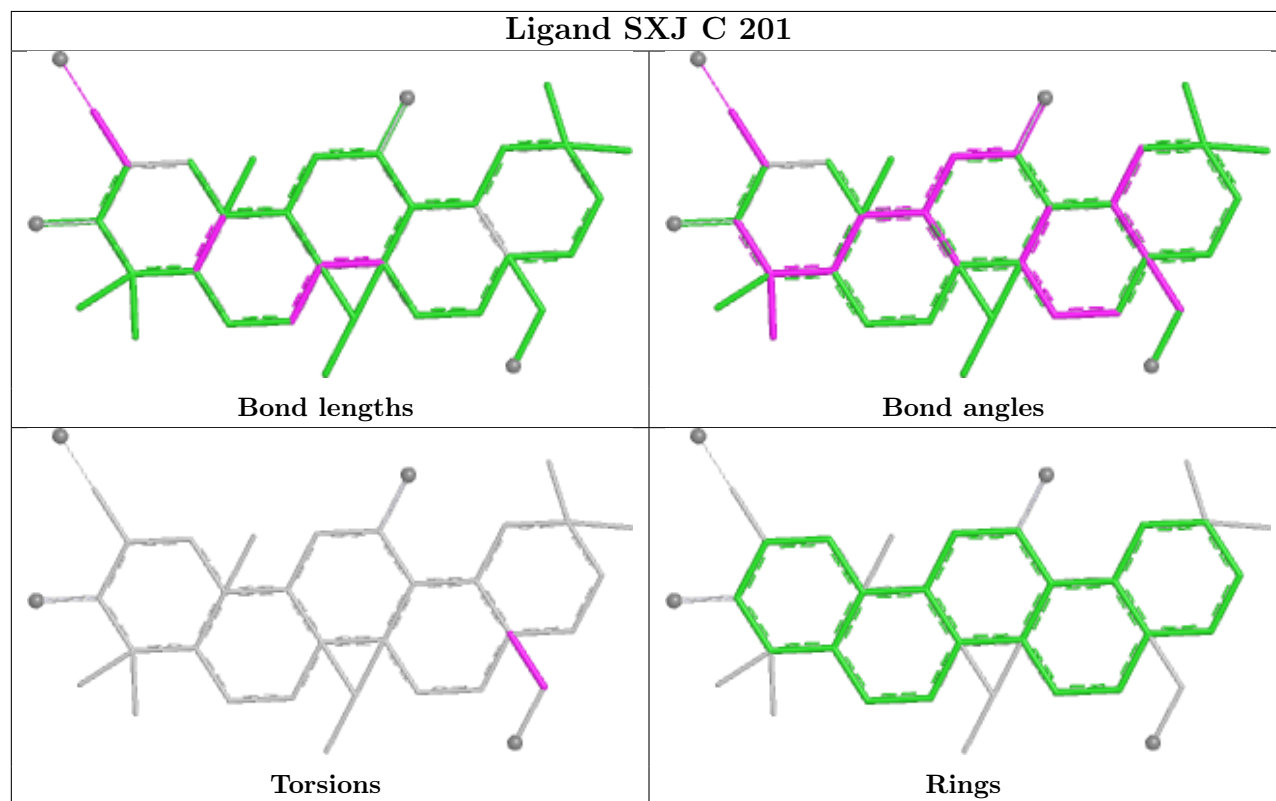
There are no ring outliers.

8 monomers are involved in 33 short contacts:

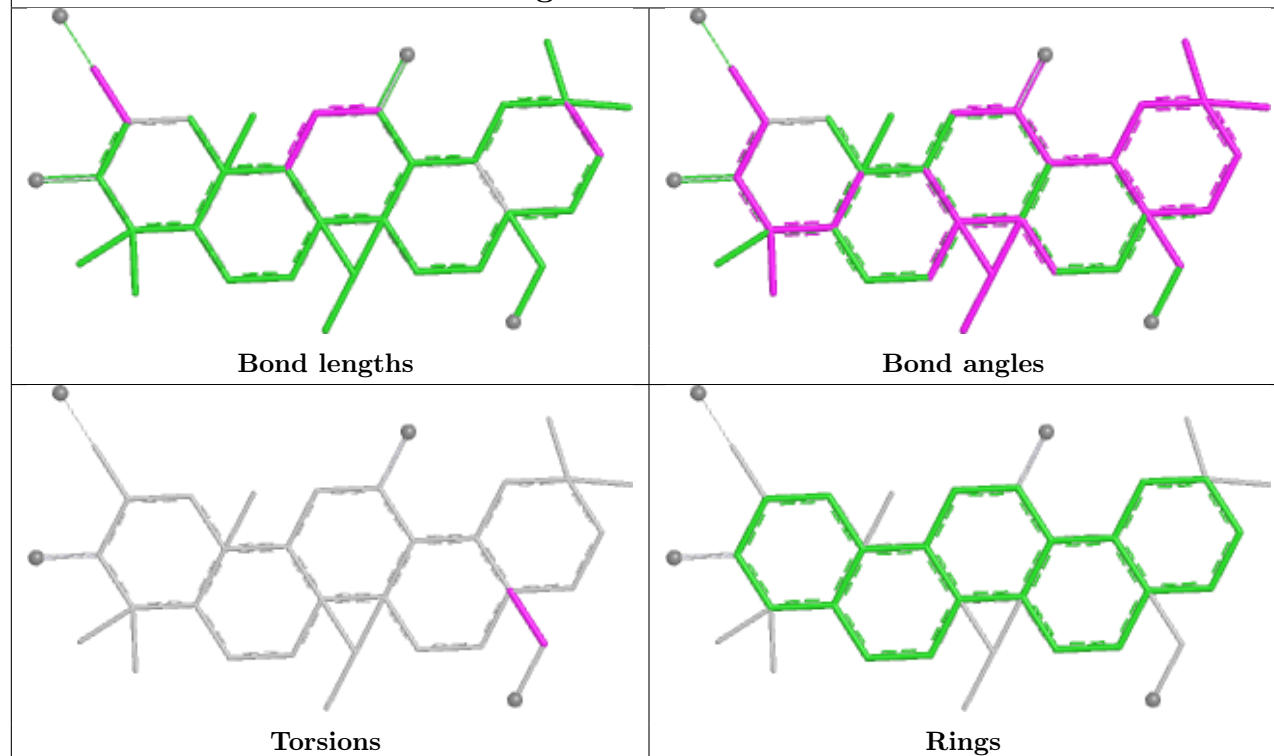
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	201	SXJ	5	0
2	A	201	SXJ	2	0
2	D	201	SXJ	5	0
2	G	201	SXJ	5	0
2	B	201	SXJ	4	0
2	F	201	SXJ	4	0
2	E	201	SXJ	4	0
2	H	201	SXJ	4	0

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

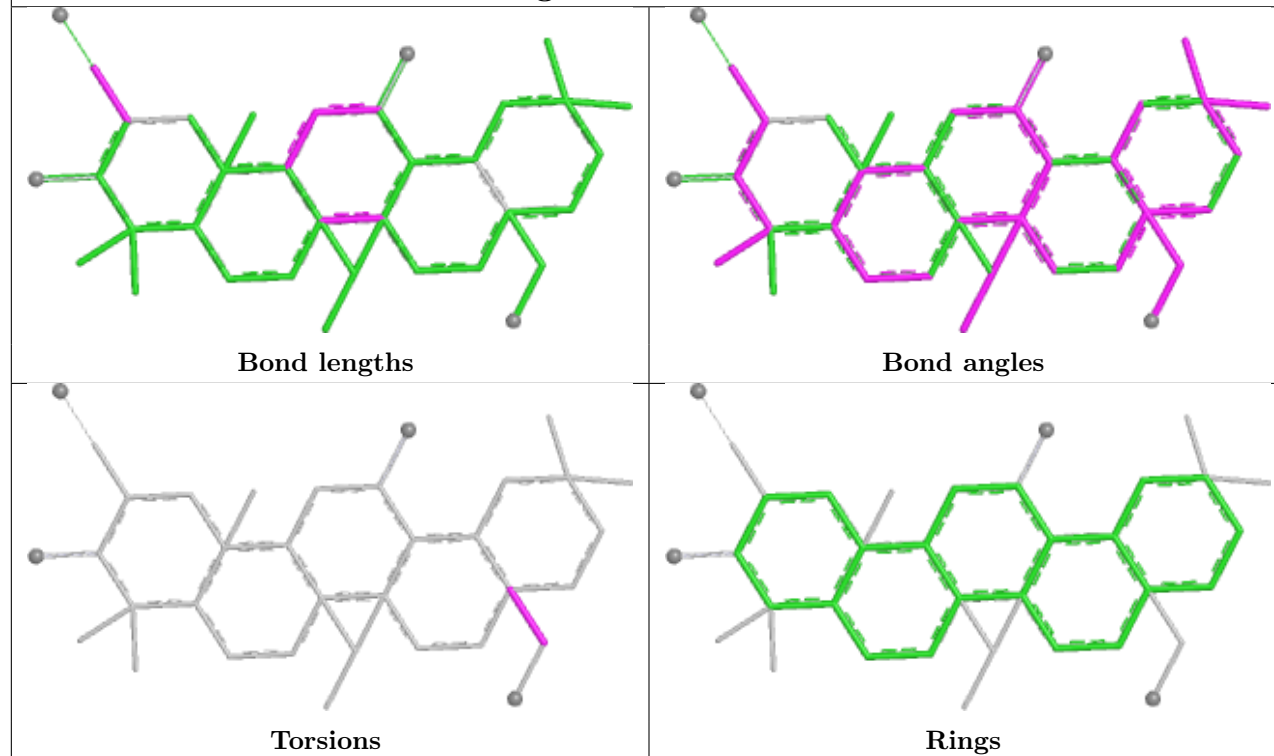
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



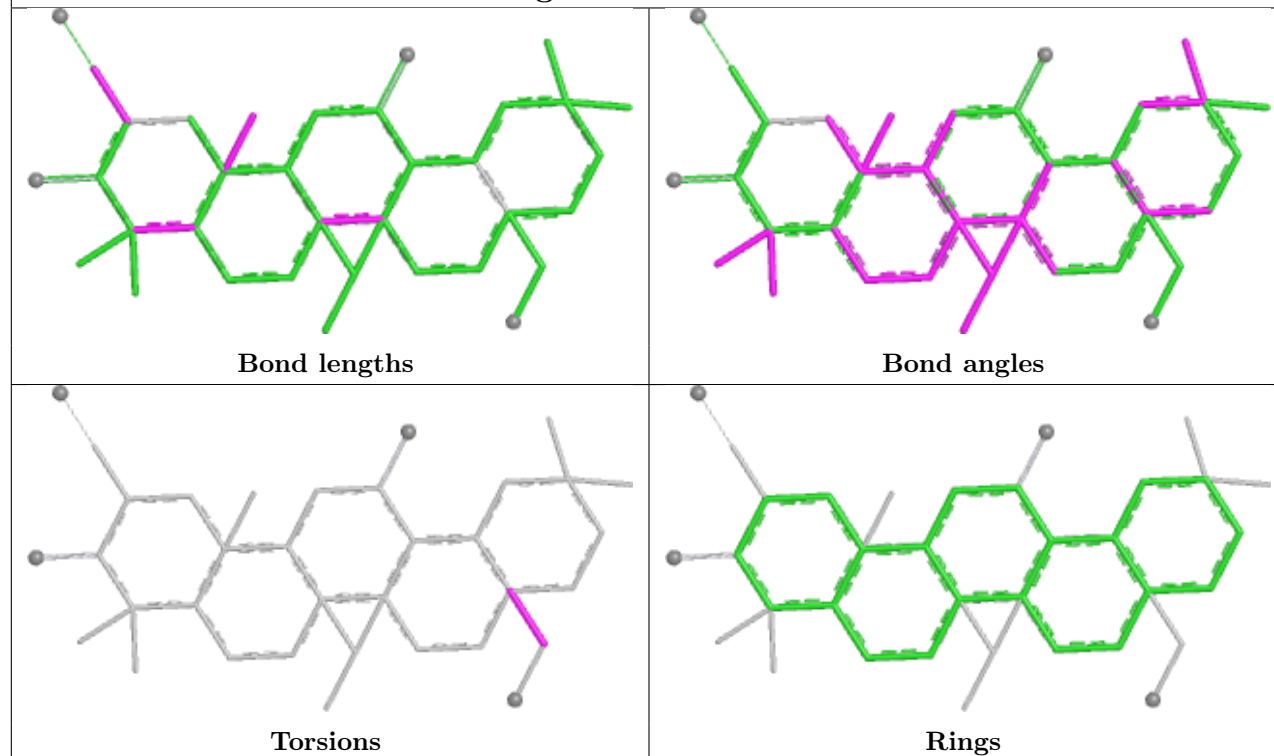
Ligand SXJ A 201



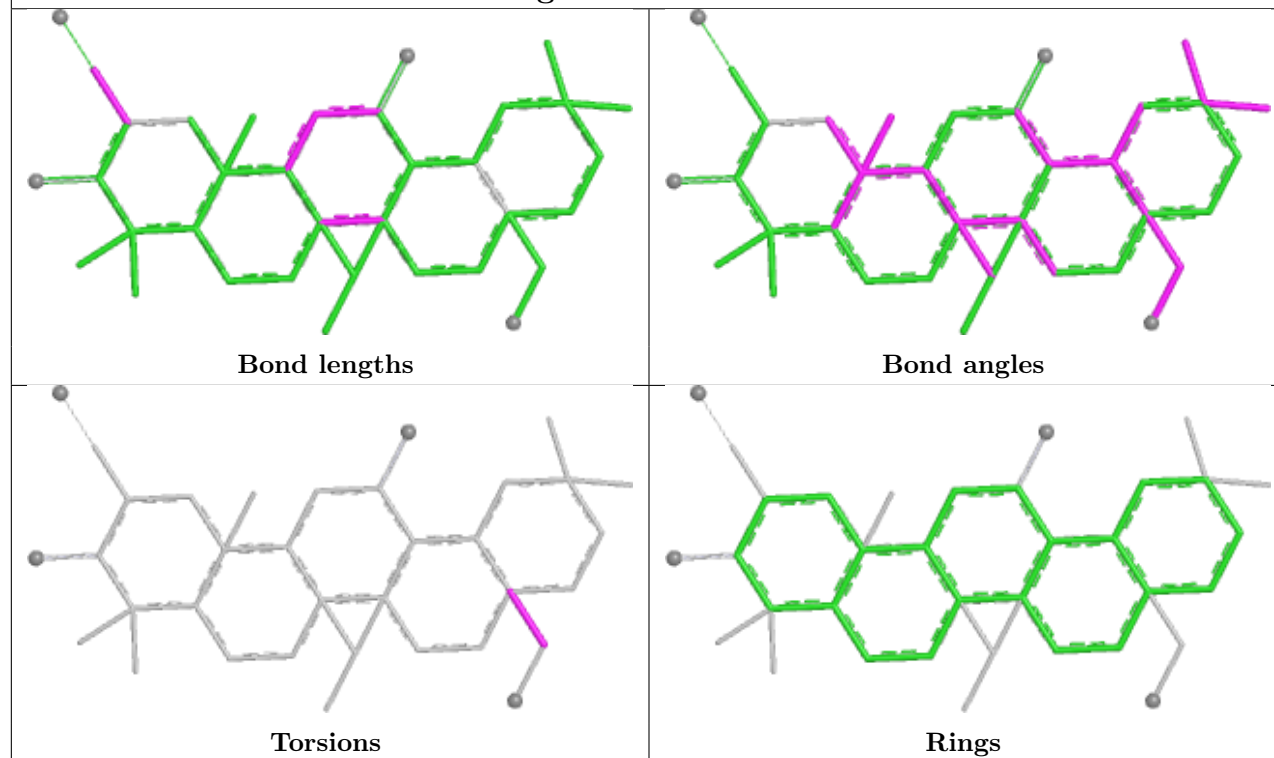
Ligand SXJ D 201



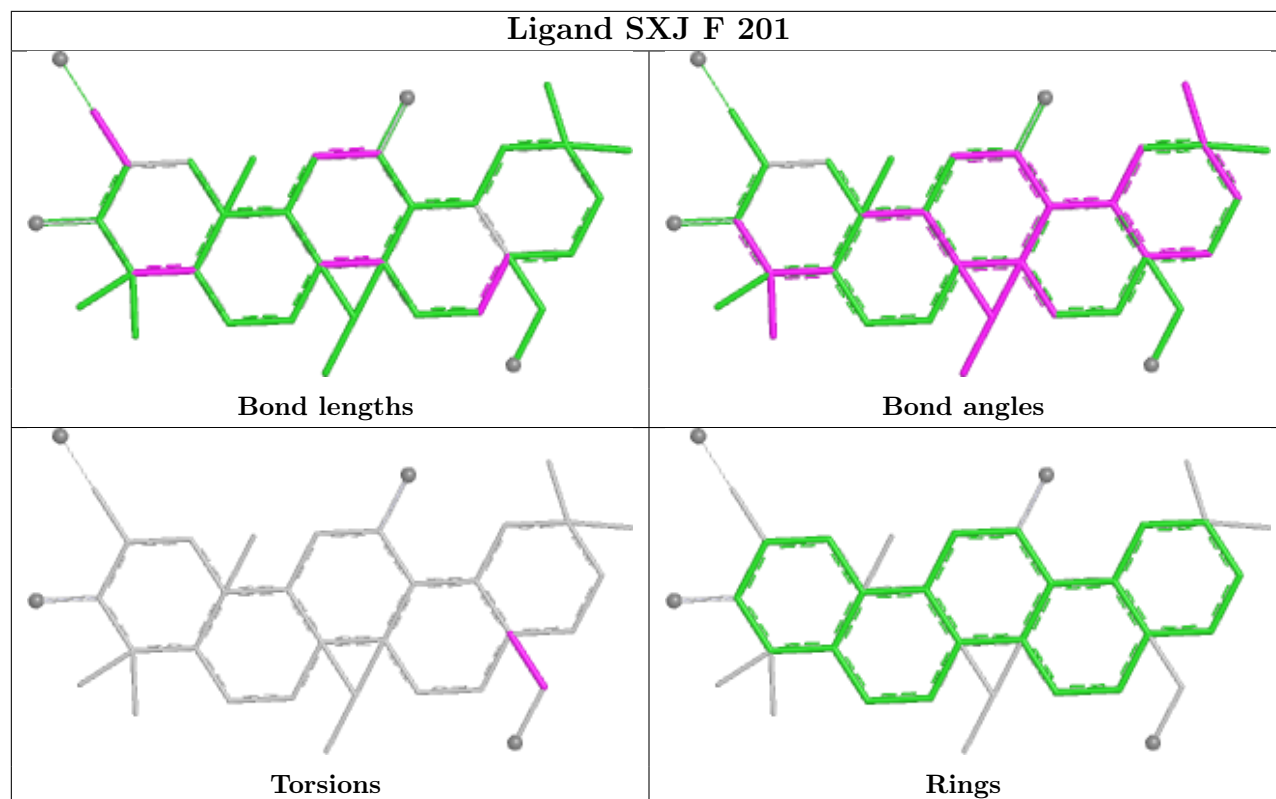
Ligand SXJ G 201



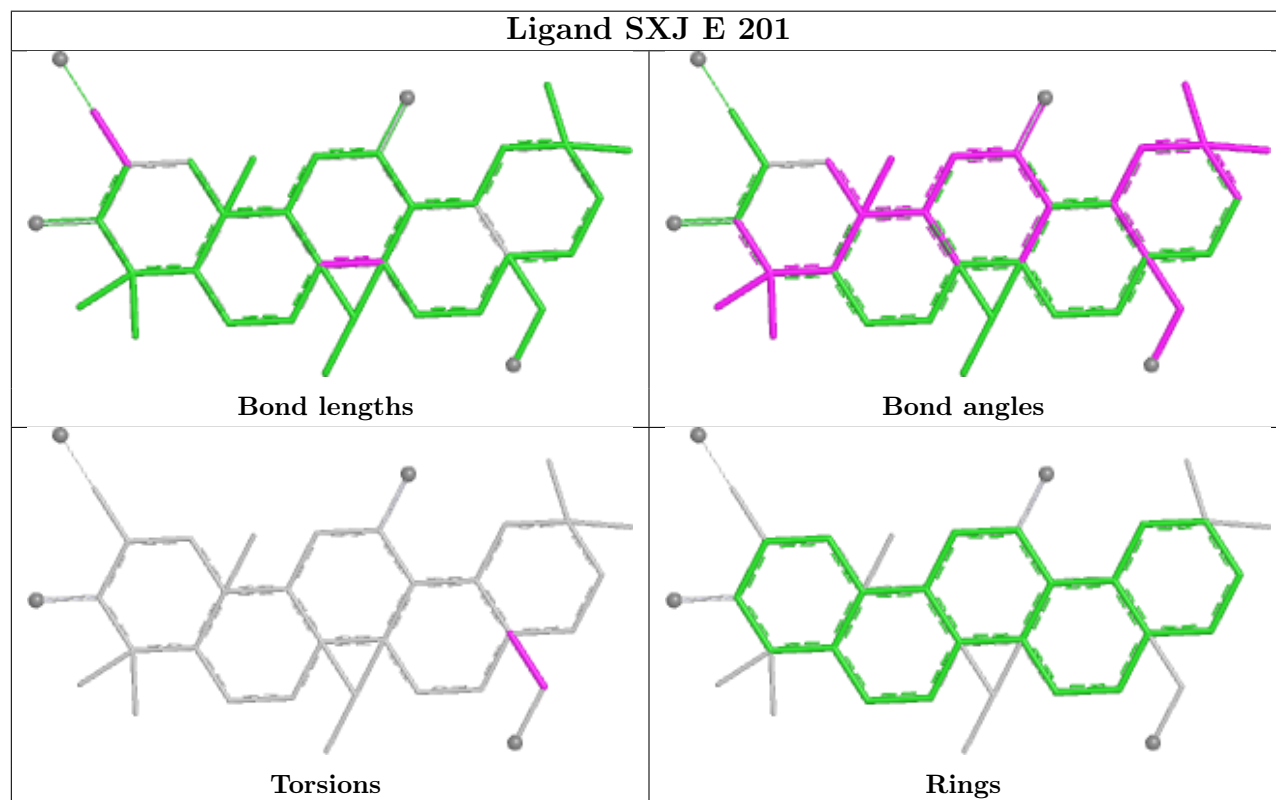
Ligand SXJ B 201

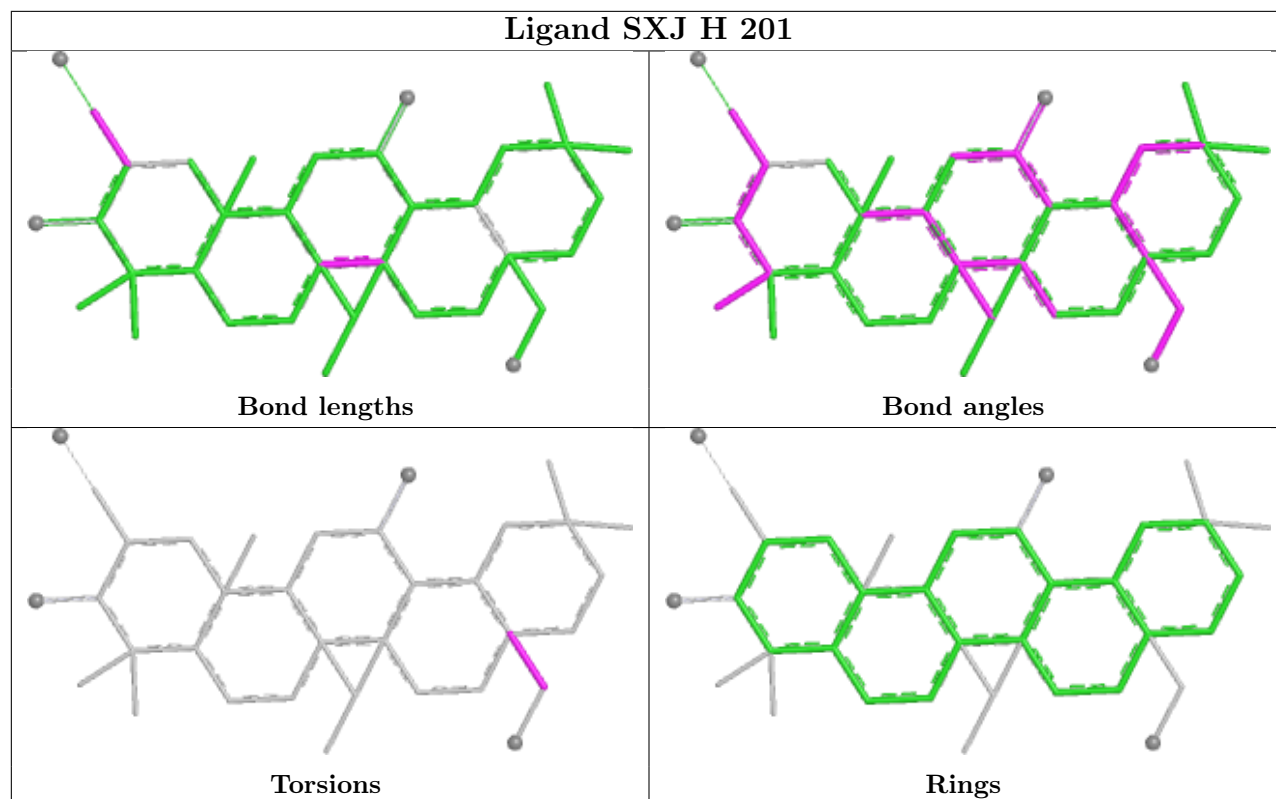


Ligand SXJ F 201



Ligand SXJ E 201





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	129/130 (99%)	-0.14	0 100 100	43, 59, 118, 145	0
1	B	130/130 (100%)	-0.14	1 (0%) 82 83	45, 65, 112, 157	0
1	C	129/130 (99%)	-0.01	1 (0%) 82 83	46, 66, 112, 145	0
1	D	130/130 (100%)	0.10	2 (1%) 72 73	50, 72, 133, 163	0
1	E	127/130 (97%)	0.16	2 (1%) 70 72	48, 67, 122, 157	0
1	F	129/130 (99%)	-0.01	3 (2%) 61 62	44, 64, 126, 154	0
1	G	129/130 (99%)	0.04	1 (0%) 82 83	53, 71, 130, 191	0
1	H	130/130 (100%)	0.30	6 (4%) 37 34	55, 80, 143, 181	0
All	All	1033/1040 (99%)	0.04	16 (1%) 72 73	43, 68, 127, 191	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	115	LEU	4.4
1	D	179	LEU	3.3
1	B	115	LEU	3.3
1	H	84	LYS	3.1
1	F	114	GLY	2.7
1	C	88	ILE	2.6
1	H	88	ILE	2.4
1	H	119	GLY	2.3
1	F	115	LEU	2.2
1	E	88	ILE	2.2
1	H	117	GLU	2.2
1	H	116	ARG	2.1
1	E	176	VAL	2.1
1	D	115	LEU	2.1
1	F	50	ARG	2.0
1	H	90	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

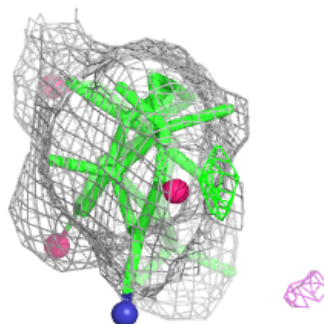
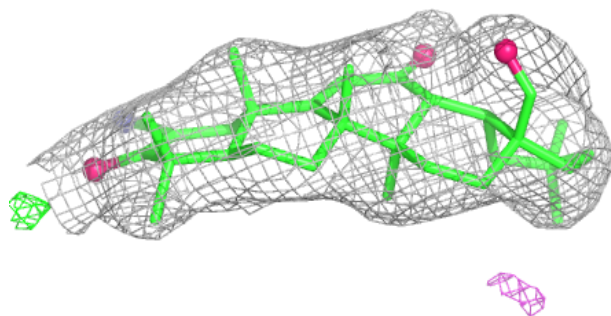
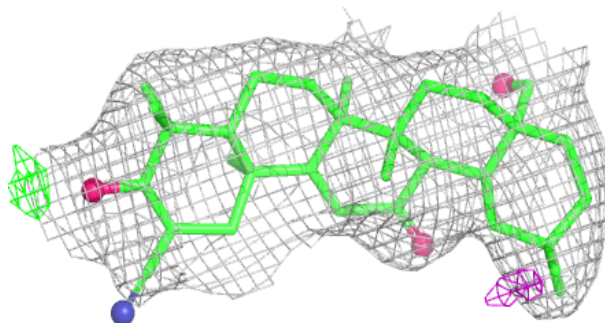
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CA	C	202	1/1	0.91	0.10	93,93,93,93	0
2	SXJ	D	201	35/36	0.93	0.09	65,76,85,88	0
2	SXJ	E	201	35/36	0.93	0.09	55,70,80,91	0
2	SXJ	C	201	35/36	0.93	0.08	56,67,72,77	0
2	SXJ	F	201	35/36	0.94	0.07	51,61,71,74	0
2	SXJ	H	201	35/36	0.94	0.09	82,96,119,129	0
3	CA	A	202	1/1	0.94	0.09	90,90,90,90	0
2	SXJ	A	201	35/36	0.94	0.08	65,77,95,95	0
2	SXJ	G	201	35/36	0.95	0.08	58,67,80,83	0
2	SXJ	B	201	35/36	0.96	0.07	70,81,99,103	0

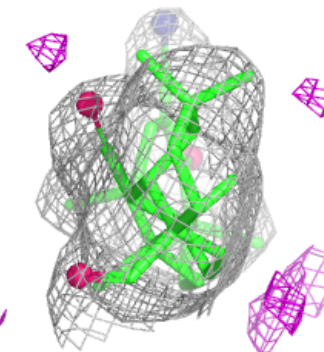
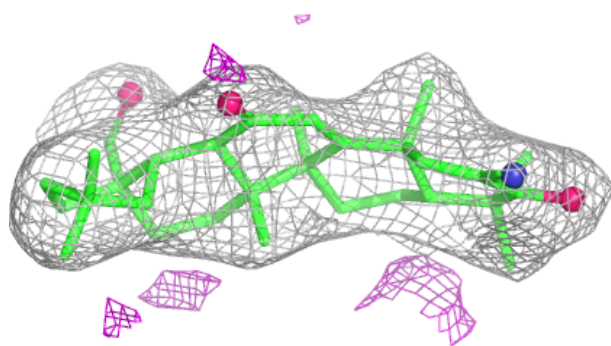
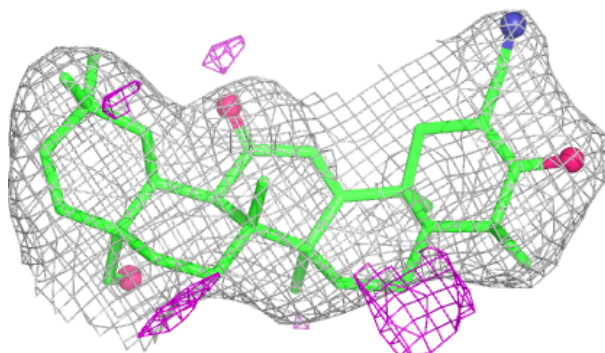
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SXJ D 201:

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

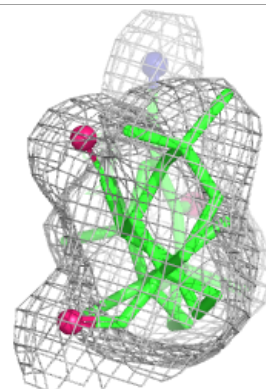
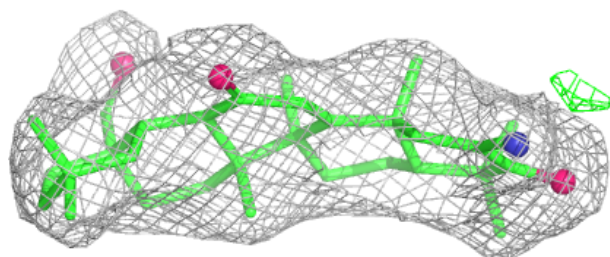
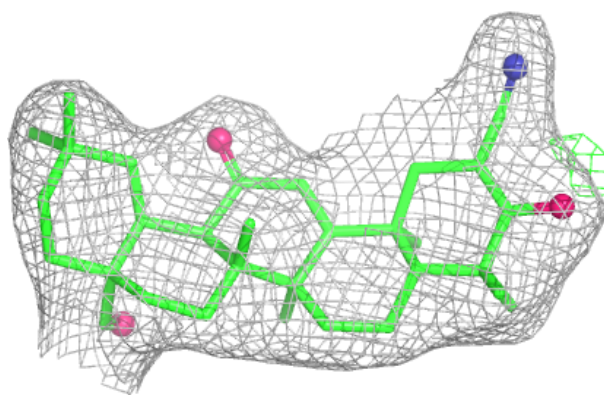
**Electron density around SXJ E 201:**

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

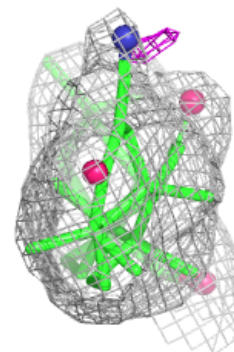
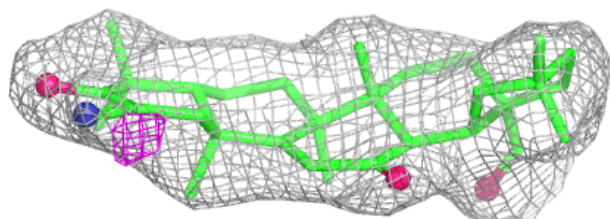
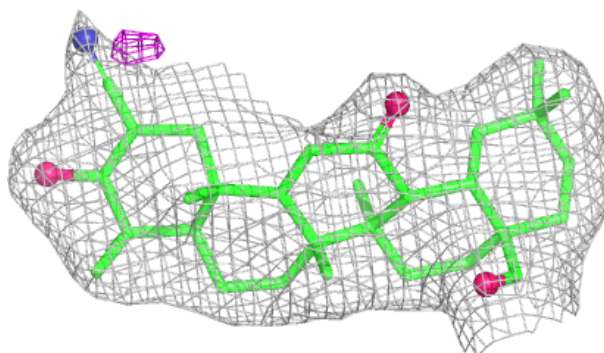


Electron density around SXJ C 201:

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

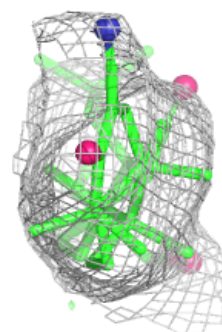
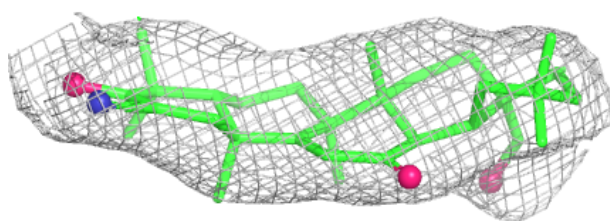
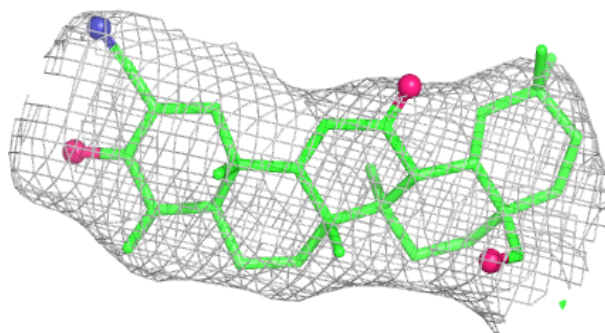
**Electron density around SXJ F 201:**

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

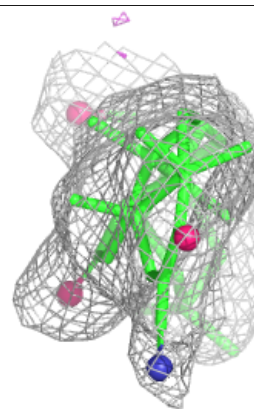
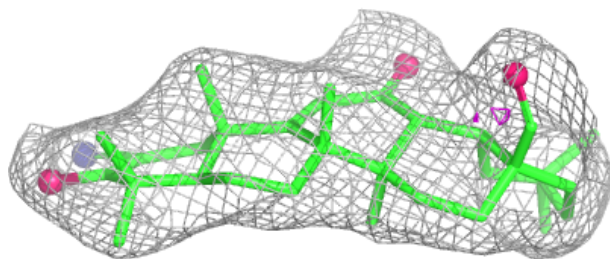
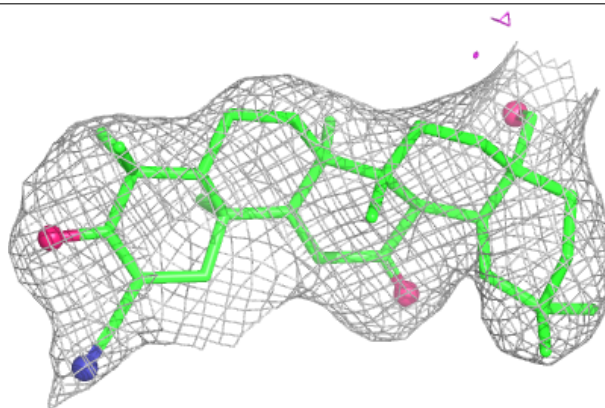


Electron density around SXJ H 201:

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

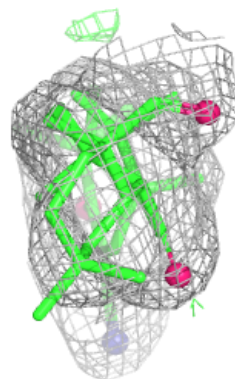
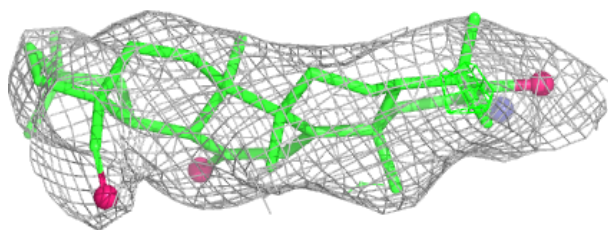
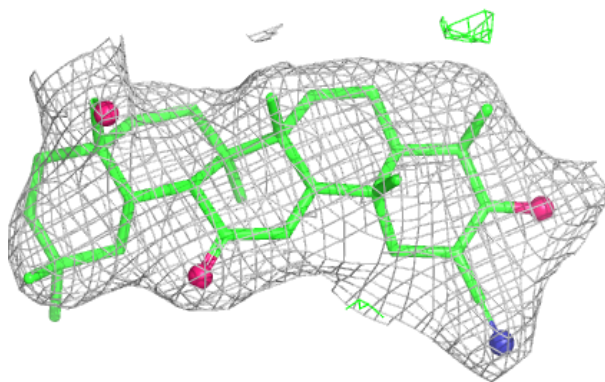
**Electron density around SXJ A 201:**

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

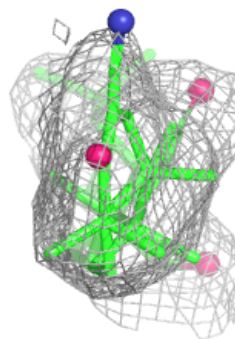
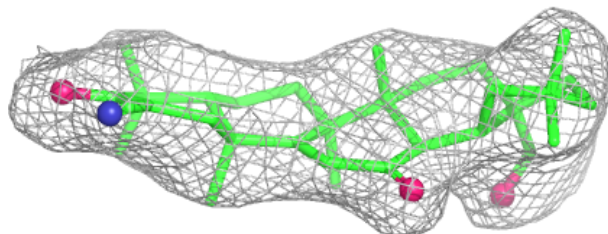
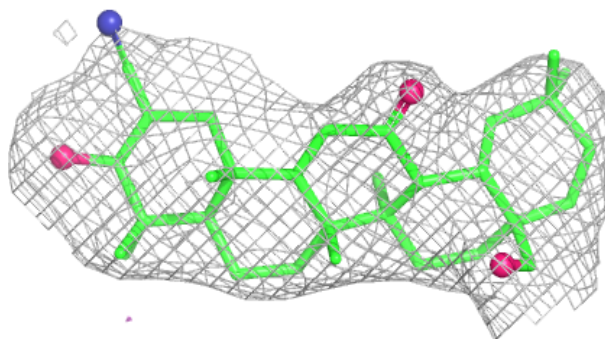


Electron density around SXJ G 201:

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

**Electron density around SXJ B 201:**

$2mF_o-DF_c$ (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.