



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:48 PM UTC

PDB ID : 7ZLM / pdb_00007zlm
Title : Crystal structure of SOCS2:ElonginB:ElonginC in complex with compound MN551
Authors : Ramachandran, S.; Ciulli, A.; Makukhin, N.
Deposited on : 2022-04-15
Resolution : 1.79 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

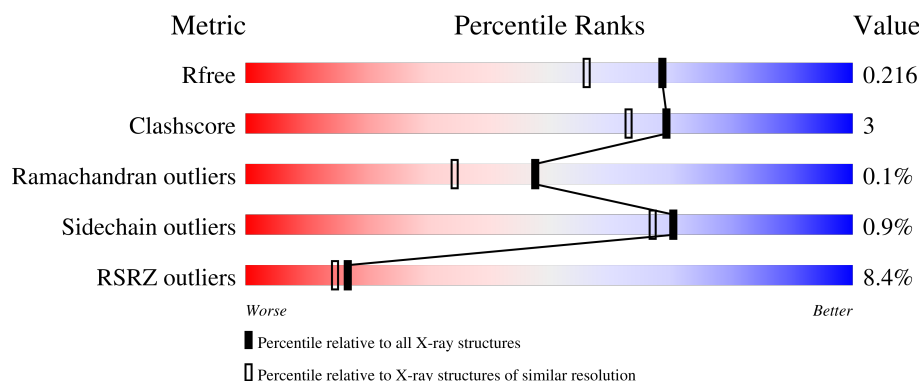
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

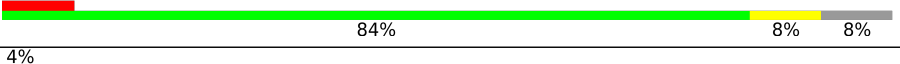
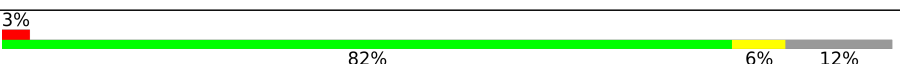
The reported resolution of this entry is 1.79 Å.

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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	169	
1	D	169	
1	G	169	
1	J	169	
2	B	118	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	118	
2	H	118	
2	K	118	
3	C	97	
3	F	97	
3	I	97	
3	L	97	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11856 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 Suppressor of cytokine signaling 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	S	0	3	0
			1266	813	213	232	8			
1	D	156	Total	C	N	O	S	0	1	0
			1237	797	205	228	7			
1	G	155	Total	C	N	O	S	0	0	0
			1225	788	203	227	7			
1	J	155	Total	C	N	O	S	0	0	0
			1228	790	207	224	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	SER	-	expression tag	UNP O14508
A	31	MET	-	expression tag	UNP O14508
D	30	SER	-	expression tag	UNP O14508
D	31	MET	-	expression tag	UNP O14508
G	30	SER	-	expression tag	UNP O14508
G	31	MET	-	expression tag	UNP O14508
J	30	SER	-	expression tag	UNP O14508
J	31	MET	-	expression tag	UNP O14508

- Molecule 2 is a protein called Elongin-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	104	Total	C	N	O	S	0	0	0
			810	511	135	159	5			
2	E	104	Total	C	N	O	S	0	0	0
			803	512	137	150	4			
2	H	101	Total	C	N	O	S	0	0	0
			749	475	127	143	4			
2	K	104	Total	C	N	O	S	0	1	0
			818	516	140	158	4			

- | Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|---------|-------|
| 3 | C | 85 | Total
671 | C
433 | N
107 | O
125 | S
6 | 0 | 0 | 0 |
| 3 | F | 84 | Total
658 | C
427 | N
105 | O
120 | S
6 | 0 | 0 | 0 |
| 3 | I | 85 | Total
653 | C
427 | N
100 | O
120 | S
6 | 0 | 0 | 0 |
| 3 | L | 86 | Total
667 | C
433 | N
107 | O
121 | S
6 | 0 | 0 | 0 |

Chain	Residue	Modelled	Actual	Comment	Reference
C	16	MET	-	initiating methionine	UNP Q15369
F	16	MET	-	initiating methionine	UNP Q15369
I	16	MET	-	initiating methionine	UNP Q15369
L	16	MET	-	initiating methionine	UNP Q15369

-
- The chemical structure is a complex molecule with several functional groups and labels. It features a central benzene ring (CZ) with substituents OBK, OH, OH, and OH. A phosphate group (P) is attached to the ring, with labels OBJ, OBI, and OH. The ring is also labeled with CE1, CE2, CD1, and CD2. A side chain (OG) is attached to the ring, leading to a chiral center (CB) with a wedge bond to a carbonyl group (C=O). The chiral center is labeled with CASI and N. The carbonyl group is attached to a nitrogen atom (N) which is part of a side chain (CAO) leading to a benzene ring (CAP). The benzene ring (CAP) has substituents CAQ, CAZ, CAT, and CAS. A side chain (CAV) is attached to the benzene ring, leading to a carbonyl group (C=O) and a chlorine atom (CL1). The side chain (CAV) is labeled with GAY and CAW. Another side chain (CAA) is attached to the benzene ring, leading to a carbonyl group (C=O) and a nitrogen atom (N). The side chain (CAA) is labeled with OAA and CAB. The nitrogen atom (N) is part of a side chain (CAC) leading to a benzene ring (CAF). The benzene ring (CAF) has substituents CAE, CAD, CAJ, and CAI. A side chain (CAH) is attached to the benzene ring, leading to a fluorine atom (F).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total 38	C 26	F 1	N 3	O 7	P 1	0	0
4	D	1	Total 38	C 26	F 1	N 3	O 7	P 1	0	0



WORLD WIDE
PDB
PROTEIN DATA BANK

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	G	1	Total	C	F	N	O	P	0	0
			38	26	1	3	7	1		
4	J	1	Total	C	F	N	O	P	0	0
			38	26	1	3	7	1		

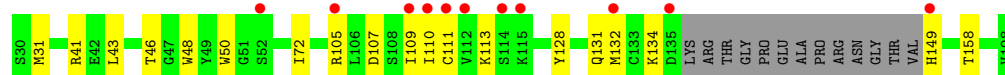
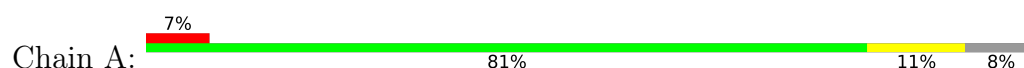
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	110	Total	O	0	0
			110	110		
5	B	104	Total	O	0	0
			104	104		
5	C	64	Total	O	0	0
			64	64		
5	D	84	Total	O	0	0
			84	84		
5	E	80	Total	O	0	0
			80	80		
5	F	62	Total	O	0	0
			62	62		
5	G	104	Total	O	0	0
			104	104		
5	H	31	Total	O	0	0
			31	31		
5	I	21	Total	O	0	0
			21	21		
5	J	100	Total	O	0	0
			100	100		
5	K	94	Total	O	0	0
			94	94		
5	L	65	Total	O	0	0
			65	65		

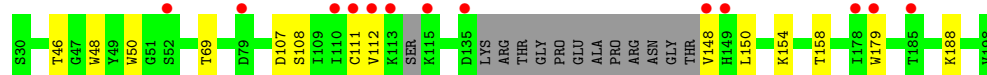
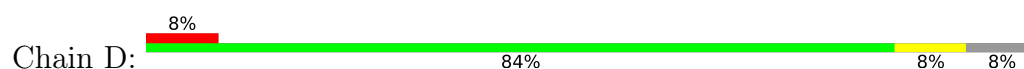
3 Residue-property plots [i](#)

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.

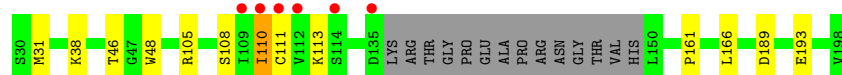
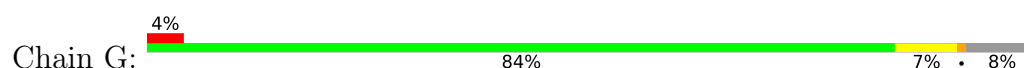
- Molecule 1: Suppressor of cytokine signaling 2



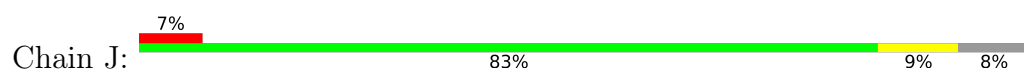
- Molecule 1: Suppressor of cytokine signaling 2



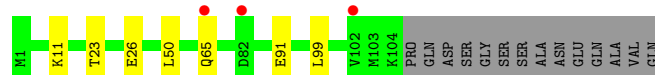
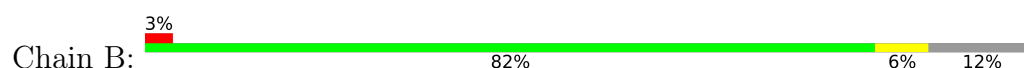
- Molecule 1: Suppressor of cytokine signaling 2



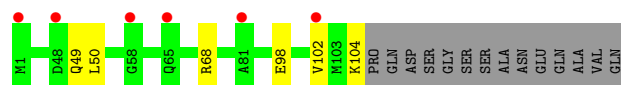
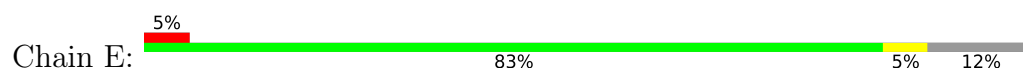
- Molecule 1: Suppressor of cytokine signaling 2



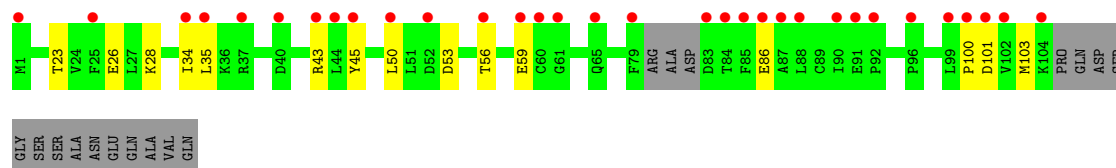
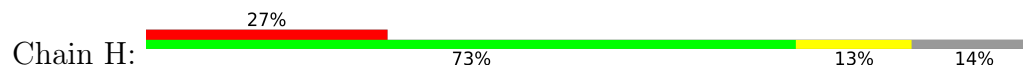
- Molecule 2: Elongin-B



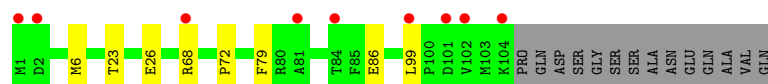
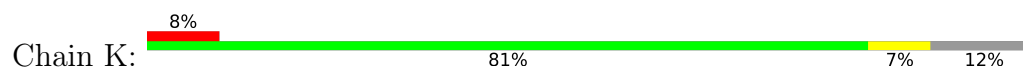
- Molecule 2: Elongin-B



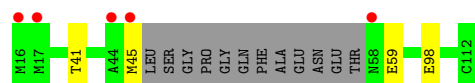
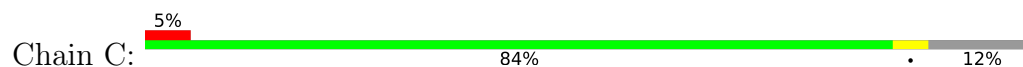
- Molecule 2: Elongin-B



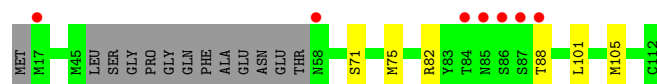
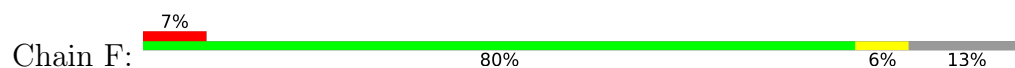
- Molecule 2: Elongin-B



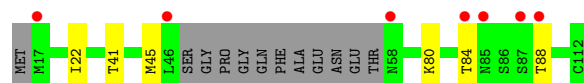
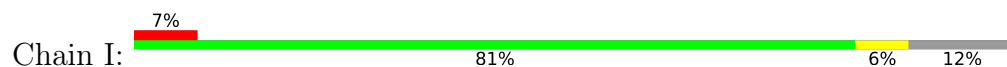
- Molecule 3: Elongin-C



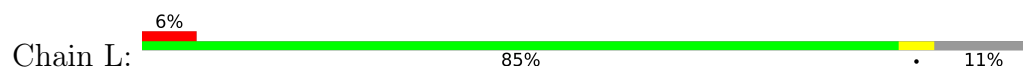
- Molecule 3: Elongin-C

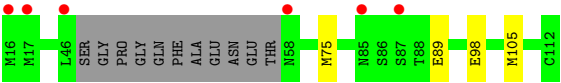


- Molecule 3: Elongin-C



- Molecule 3: Elongin-C





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.78Å 172.88Å 185.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	78.37 – 1.79 78.37 – 1.79	Depositor EDS
% Data completeness (in resolution range)	99.2 (78.37-1.79) 99.6 (78.37-1.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 1.78Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.189 , 0.217 0.189 , 0.216	Depositor DCC
R_{free} test set	8989 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11856	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.37	0/1293	0.53	0/1747
1	D	0.29	0/1265	0.49	0/1715
1	G	0.33	0/1251	0.49	0/1692
1	J	0.33	0/1255	0.51	0/1698
2	B	0.32	0/826	0.56	0/1120
2	E	0.26	0/819	0.50	0/1108
2	H	0.20	0/762	0.43	0/1035
2	K	0.32	0/834	0.59	0/1131
3	C	0.37	0/685	0.56	0/925
3	F	0.28	0/672	0.48	0/908
3	I	0.21	0/667	0.39	0/904
3	L	0.32	0/681	0.53	1/921 (0.1%)
All	All	0.31	0/11010	0.51	1/14904 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	75	MET	N-CA-CB	-5.25	102.39	110.12

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1266	0	1264	12	0
1	D	1237	0	1200	8	0
1	G	1225	0	1221	10	0
1	J	1228	0	1221	10	0
2	B	810	0	791	5	0
2	E	803	0	803	4	0
2	H	749	0	726	8	0
2	K	818	0	804	4	0
3	C	671	0	659	3	0
3	F	658	0	646	4	0
3	I	653	0	632	6	0
3	L	667	0	647	3	0
4	A	38	0	0	1	0
4	D	38	0	0	1	0
4	G	38	0	0	0	0
4	J	38	0	0	0	0
5	A	110	0	0	1	0
5	B	104	0	0	1	0
5	C	64	0	0	0	0
5	D	84	0	0	0	0
5	E	80	0	0	2	0
5	F	62	0	0	0	0
5	G	104	0	0	1	0
5	H	31	0	0	0	0
5	I	21	0	0	0	0
5	J	100	0	0	2	0
5	K	94	0	0	0	0
5	L	65	0	0	1	0
All	All	11856	0	10614	75	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 3.

All (75) 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:J:45:GLN:NE2	5:J:301:HOH:O	2.28	0.67
2:H:56:THR:HG23	2:H:59:GLU:H	1.60	0.66
2:H:34:ILE:HG22	2:H:35:LEU:HD23	1.78	0.66
2:K:23:THR:OG1	2:K:26:GLU:HG3	1.98	0.64
3:I:80:LYS:NZ	3:I:84:THR:HG21	2.13	0.63
2:H:43:ARG:NH2	2:H:86:GLU:O	2.32	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:105:ARG:NH2	1:G:113:LYS:HE2	2.16	0.60
1:G:161:PRO:HG2	1:G:166:LEU:HD21	1.82	0.60
1:J:72:ILE:HD11	1:J:126:ILE:HD11	1.83	0.60
2:B:65:GLN:NE2	5:B:202:HOH:O	2.32	0.59
1:A:149:HIS:NE2	5:A:301:HOH:O	2.32	0.57
2:H:28:LYS:NZ	2:H:53:ASP:OD1	2.37	0.57
2:E:68:ARG:NH1	5:E:201:HOH:O	2.37	0.57
1:J:48:TRP:HZ3	1:J:72:ILE:HG13	1.69	0.57
1:A:43:LEU:HD11	1:A:72[A]:ILE:HG21	1.87	0.56
3:I:41:THR:HG22	3:I:45:MET:HE3	1.87	0.56
2:B:99:LEU:HG	3:C:98:GLU:HG3	1.87	0.56
3:I:80:LYS:HZ2	3:I:84:THR:HG21	1.70	0.55
1:A:105:ARG:NH2	1:A:113:LYS:HE2	2.23	0.54
1:G:189:ASP:O	1:G:193:GLU:HG3	2.08	0.52
1:G:108:SER:CB	1:G:113:LYS:HG3	2.39	0.52
1:G:105:ARG:HH22	1:G:113:LYS:HE2	1.73	0.52
2:H:43:ARG:NH1	2:H:45:TYR:OH	2.44	0.51
1:J:50:TRP:CE2	1:J:158:THR:HG22	2.45	0.51
3:I:80:LYS:O	3:I:84:THR:HG23	2.11	0.51
1:A:105:ARG:HH22	1:A:113:LYS:HE2	1.76	0.51
1:D:111:CYS:SG	4:D:201:JIH:CAW	3.00	0.50
2:E:49:GLN:NE2	2:E:50:LEU:O	2.45	0.50
1:G:31:MET:HA	1:G:31:MET:HE2	1.94	0.49
1:G:46:THR:HB	1:G:48:TRP:CE2	2.48	0.49
1:D:107:ASP:O	1:D:111:CYS:HB3	2.12	0.48
1:G:108:SER:HB2	1:G:113:LYS:HG3	1.95	0.48
2:H:45:TYR:CZ	2:H:50:LEU:HD23	2.47	0.48
3:L:89:GLU:OE1	5:L:201:HOH:O	2.20	0.48
1:A:107:ASP:OD1	1:A:109:ILE:HG22	2.12	0.48
1:D:46:THR:HB	1:D:48:TRP:CE2	2.48	0.48
2:K:99:LEU:HD13	3:L:98:GLU:HA	1.96	0.48
1:G:38:LYS:HE3	1:G:38:LYS:HB2	1.50	0.48
1:D:50:TRP:CE2	1:D:158:THR:HG22	2.49	0.47
1:J:178:ILE:HG12	1:J:195:LYS:NZ	2.30	0.47
2:H:100:PRO:HD2	2:H:103:MET:HG3	1.95	0.47
1:A:110:ILE:HG21	4:A:201:JIH:CAZ	2.46	0.46
1:D:179[A]:TRP:HA	1:D:188:LYS:HD3	1.96	0.46
2:K:6:MET:HG3	2:K:72:PRO:HG2	1.97	0.46
1:J:31:MET:HA	1:J:31:MET:HE2	1.98	0.46
3:I:41:THR:O	3:I:45:MET:HG3	2.16	0.46
2:K:79:PHE:O	2:K:86:GLU:HG2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:46:THR:HB	1:J:48:TRP:CE2	2.51	0.45
2:H:23:THR:OG1	2:H:26:GLU:HG3	2.17	0.45
1:D:50:TRP:CD2	1:D:158:THR:HG22	2.52	0.45
3:F:82:ARG:HH22	3:F:88:THR:HG21	1.80	0.45
1:J:50:TRP:CD2	1:J:158:THR:HG22	2.52	0.45
2:B:23:THR:OG1	2:B:26:GLU:HG3	2.16	0.44
2:E:102:VAL:HG22	5:E:257:HOH:O	2.18	0.44
2:B:11:LYS:HE3	2:B:91:GLU:OE1	2.18	0.43
1:A:41:ARG:HH11	1:A:41:ARG:HG3	1.83	0.43
1:A:131:GLN:OE1	1:A:134:LYS:HE2	2.18	0.43
3:C:41:THR:O	3:C:45:MET:HG3	2.19	0.43
3:F:105:MET:HB3	3:F:105:MET:HE2	1.73	0.43
3:F:71:SER:O	3:F:75:MET:HG3	2.19	0.43
3:I:22:ILE:N	3:I:22:ILE:HD12	2.34	0.43
1:A:31[B]:MET:HB3	1:A:31[B]:MET:HE2	1.86	0.43
1:A:50:TRP:CD2	1:A:158:THR:HG22	2.54	0.42
2:E:98:GLU:OE2	2:E:104:LYS:NZ	2.44	0.42
1:A:128:TYR:O	1:A:132:MET:HG2	2.18	0.42
1:G:110:ILE:HA	5:G:384:HOH:O	2.19	0.42
1:J:117:LYS:HD3	1:J:128:TYR:CZ	2.53	0.42
1:A:46:THR:HB	1:A:48:TRP:CE2	2.54	0.42
3:F:101:LEU:O	3:F:105:MET:HG3	2.19	0.42
1:D:69:THR:HA	1:D:154:LYS:O	2.20	0.41
3:C:41:THR:HG22	3:C:45:MET:HE3	2.03	0.41
1:D:148:VAL:C	1:D:150:LEU:H	2.28	0.41
1:J:106:LEU:HB2	1:J:116:LEU:HD13	2.03	0.41
5:J:393:HOH:O	3:L:105:MET:HE1	2.21	0.41
2:B:65:GLN:H	2:B:65:GLN:CD	2.29	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	155/169 (92%)	151 (97%)	4 (3%)	0	100	100
1	D	151/169 (89%)	143 (95%)	7 (5%)	1 (1%)	18	8
1	G	151/169 (89%)	148 (98%)	3 (2%)	0	100	100
1	J	151/169 (89%)	146 (97%)	5 (3%)	0	100	100
2	B	102/118 (86%)	98 (96%)	4 (4%)	0	100	100
2	E	102/118 (86%)	98 (96%)	4 (4%)	0	100	100
2	H	97/118 (82%)	93 (96%)	4 (4%)	0	100	100
2	K	103/118 (87%)	100 (97%)	3 (3%)	0	100	100
3	C	81/97 (84%)	80 (99%)	1 (1%)	0	100	100
3	F	80/97 (82%)	78 (98%)	2 (2%)	0	100	100
3	I	81/97 (84%)	81 (100%)	0	0	100	100
3	L	82/97 (84%)	81 (99%)	1 (1%)	0	100	100
All	All	1336/1536 (87%)	1297 (97%)	38 (3%)	1 (0%)	48	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	112	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	137/149 (92%)	136 (99%)	1 (1%)	76	73
1	D	129/149 (87%)	128 (99%)	1 (1%)	73	70
1	G	132/149 (89%)	130 (98%)	2 (2%)	57	49
1	J	131/149 (88%)	130 (99%)	1 (1%)	73	70
2	B	89/103 (86%)	88 (99%)	1 (1%)	65	60
2	E	86/103 (84%)	86 (100%)	0	100	100
2	H	78/103 (76%)	77 (99%)	1 (1%)	61	54

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	K	89/103 (86%)	87 (98%)	2 (2%)	45	34
3	C	74/86 (86%)	73 (99%)	1 (1%)	59	52
3	F	71/86 (83%)	71 (100%)	0	100	100
3	I	69/86 (80%)	68 (99%)	1 (1%)	59	52
3	L	70/86 (81%)	70 (100%)	0	100	100
All	All	1155/1352 (85%)	1144 (99%)	11 (1%)	70	64

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	CYS
2	B	50	LEU
3	C	59	GLU
1	D	108	SER
1	G	110	ILE
1	G	111	CYS
2	H	101	ASP
3	I	88	THR
1	J	110	ILE
2	K	68[A]	ARG
2	K	68[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	GLN
1	A	197	GLN
2	B	49	GLN
1	D	45	GLN
1	D	149	HIS
3	I	35	HIS
3	I	61	ASN
3	I	108	ASN
1	J	32	GLN
1	J	197	GLN

5.3.3 RNA ⓘ

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](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	JIH	G	201	1	40,40,41	1.16	3 (7%)	55,55,56	1.28	6 (10%)
4	JIH	D	201	-	40,40,41	1.28	3 (7%)	55,55,56	1.37	6 (10%)
4	JIH	J	201	1	40,40,41	1.07	4 (10%)	55,55,56	1.16	4 (7%)
4	JIH	A	201	1	40,40,41	0.98	3 (7%)	55,55,56	1.15	1 (1%)

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
4	JIH	G	201	1	-	0/30/30/32	0/3/3/3
4	JIH	D	201	-	-	0/30/30/32	0/3/3/3
4	JIH	J	201	1	-	0/30/30/32	0/3/3/3
4	JIH	A	201	1	-	1/30/30/32	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	201	JIH	CAT-NAU	-4.85	1.31	1.41
4	G	201	JIH	PBH-OBJ	3.74	1.62	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	201	JIH	PBH-OBJ	3.11	1.60	1.50
4	J	201	JIH	CAT-NAU	-3.03	1.35	1.41
4	G	201	JIH	CAT-NAU	-2.91	1.35	1.41
4	A	201	JIH	CAT-NAU	-2.90	1.35	1.41
4	J	201	JIH	PBH-OH	2.89	1.65	1.59
4	D	201	JIH	PBH-OBJ	2.59	1.58	1.50
4	J	201	JIH	PBH-OBJ	2.31	1.57	1.50
4	G	201	JIH	PBH-OH	2.20	1.63	1.59
4	D	201	JIH	CAV-NAU	-2.18	1.32	1.36
4	A	201	JIH	PBH-OH	2.11	1.63	1.59
4	J	201	JIH	CAW-CAV	2.07	1.54	1.50

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	201	JIH	CAW-CAV-NAU	-4.62	108.00	114.95
4	D	201	JIH	OAY-CAV-NAU	3.23	127.48	123.06
4	G	201	JIH	OBK-PBH-OBI	2.92	118.75	107.80
4	A	201	JIH	OAY-CAV-NAU	2.85	126.96	123.06
4	G	201	JIH	CAO-CAP-CAZ	-2.67	114.92	120.63
4	G	201	JIH	CAS-CAT-NAU	2.52	128.88	120.41
4	D	201	JIH	CAZ-CAT-NAU	-2.45	112.17	120.13
4	J	201	JIH	OAY-CAV-NAU	2.44	126.41	123.06
4	J	201	JIH	CAS-CAT-NAU	2.42	128.53	120.41
4	J	201	JIH	CAT-CAZ-CAP	2.34	123.89	120.87
4	G	201	JIH	CAR-CAQ-CAP	-2.33	117.34	120.61
4	G	201	JIH	OAY-CAV-NAU	2.31	126.22	123.06
4	G	201	JIH	CAE-CAF-CAG	2.17	120.61	118.38
4	D	201	JIH	CAO-CAP-CAZ	-2.08	116.18	120.63
4	J	201	JIH	CAR-CAQ-CAP	-2.07	117.70	120.61
4	D	201	JIH	CAC-CAD-CAE	-2.04	117.88	120.89
4	D	201	JIH	CG-CB-CA	-2.01	108.02	113.36

There are no chirality outliers.

All (1) torsion outliers are listed below:

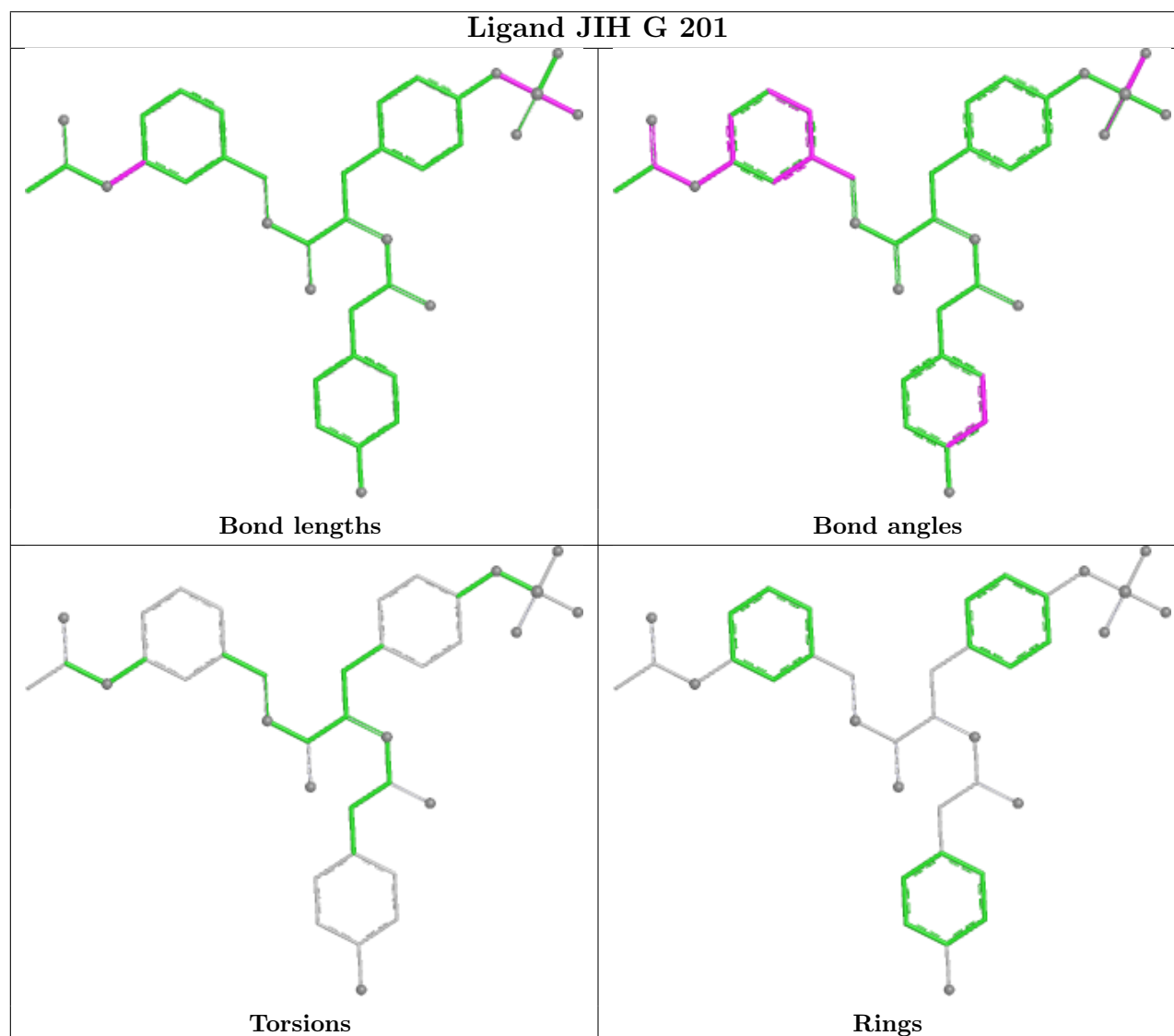
Mol	Chain	Res	Type	Atoms
4	A	201	JIH	N-CA-CB-CG

There are no ring outliers.

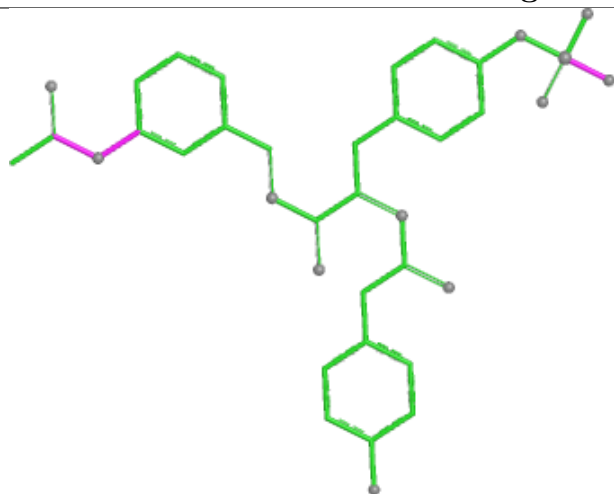
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	201	JIH	1	0
4	A	201	JIH	1	0

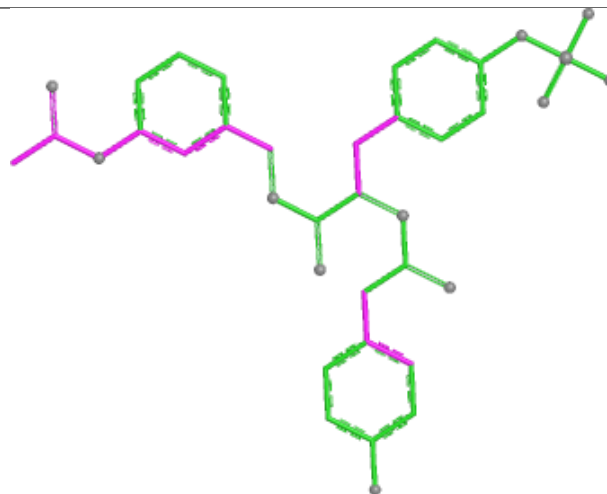
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.



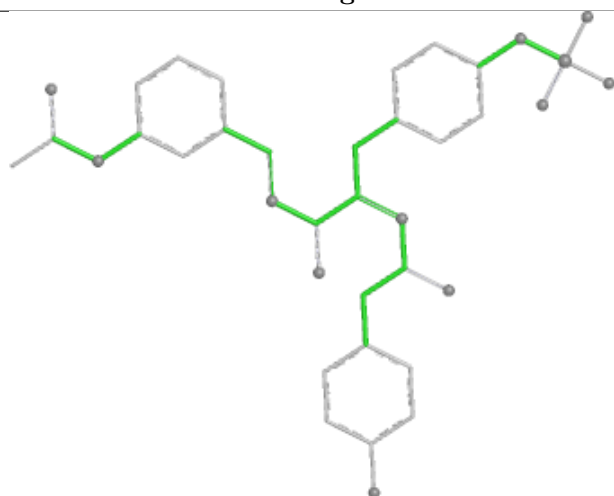
Ligand JIH D 201



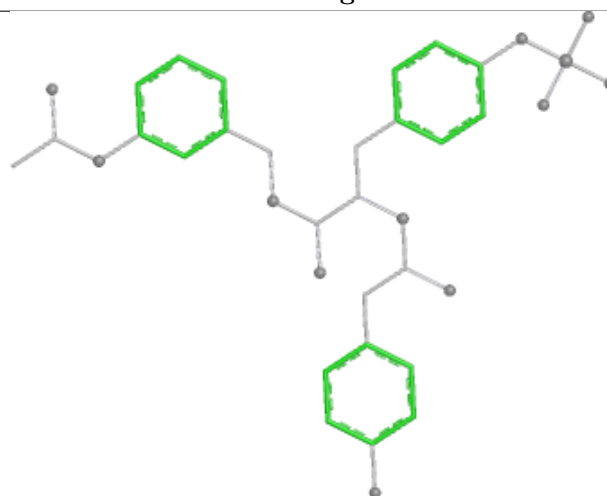
Bond lengths



Bond angles

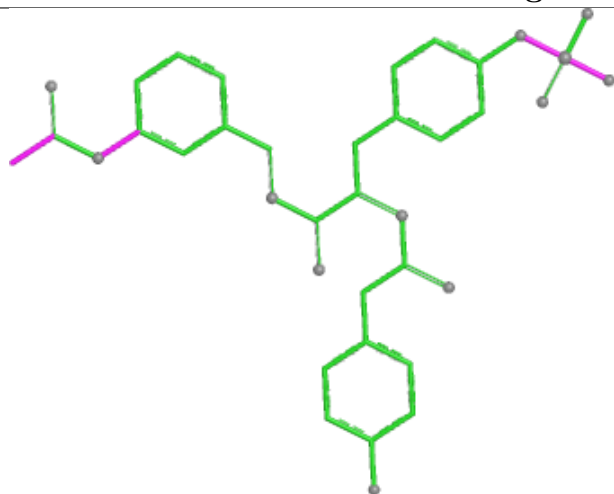


Torsions

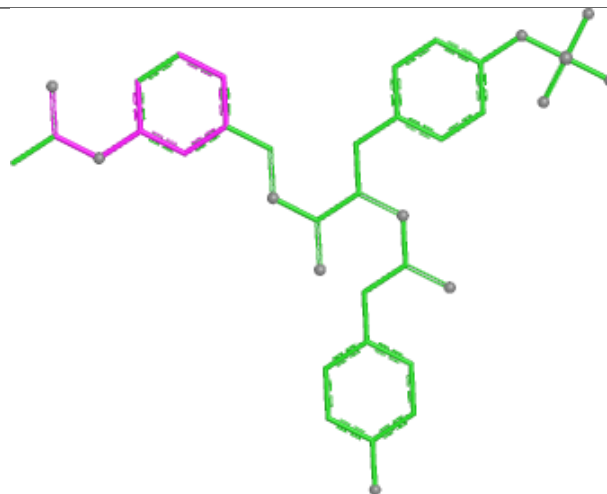


Rings

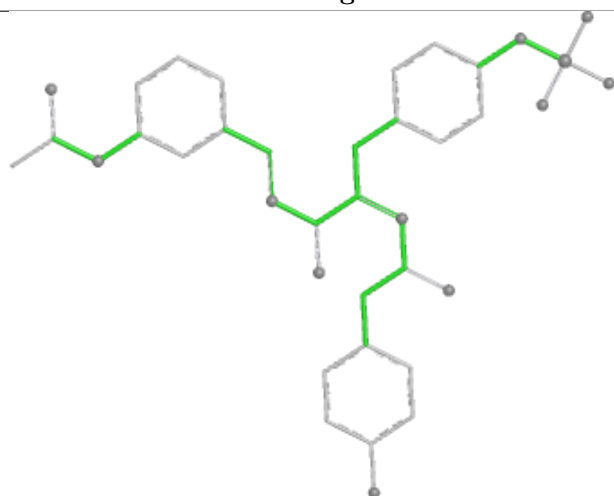
Ligand JIH J 201



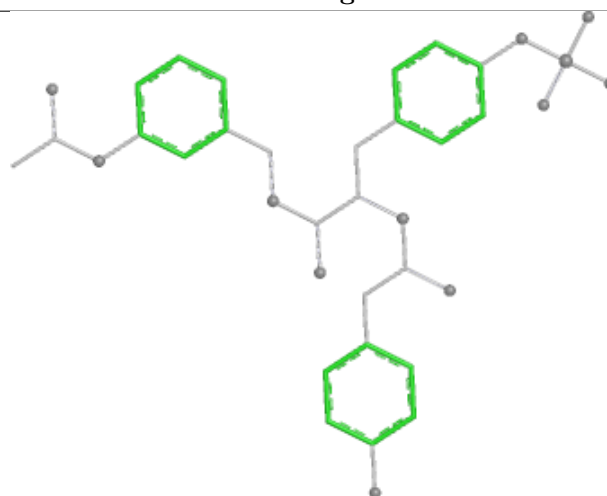
Bond lengths



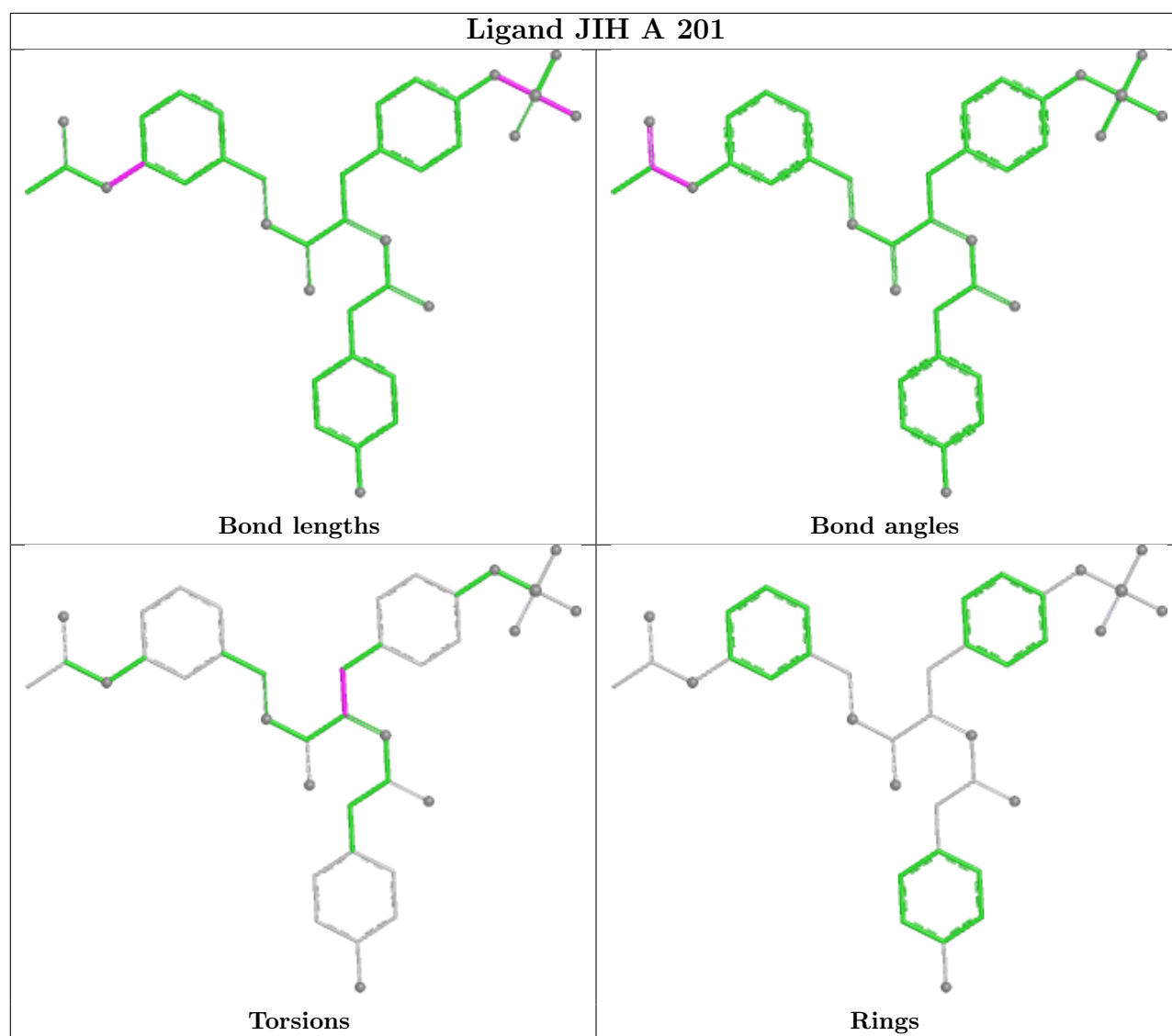
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	156/169 (92%)	0.13	11 (7%) 22 20	9, 26, 57, 80	3 (1%)
1	D	156/169 (92%)	0.55	13 (8%) 17 15	24, 34, 60, 88	1 (0%)
1	G	155/169 (91%)	0.21	6 (3%) 43 43	19, 30, 56, 83	0
1	J	155/169 (91%)	0.28	11 (7%) 22 20	20, 30, 58, 96	0
2	B	104/118 (88%)	0.10	3 (2%) 53 53	19, 32, 50, 66	0
2	E	104/118 (88%)	0.38	6 (5%) 29 27	24, 37, 59, 66	0
2	H	101/118 (85%)	1.48	32 (31%) 1 1	35, 62, 81, 98	0
2	K	104/118 (88%)	0.39	9 (8%) 16 14	14, 37, 58, 67	1 (0%)
3	C	85/97 (87%)	0.04	5 (5%) 28 27	19, 28, 58, 77	0
3	F	84/97 (86%)	0.38	7 (8%) 17 15	24, 37, 64, 75	0
3	I	85/97 (87%)	0.71	7 (8%) 17 15	30, 46, 71, 85	0
3	L	86/97 (88%)	0.31	6 (6%) 22 21	21, 33, 58, 72	0
All	All	1375/1536 (89%)	0.40	116 (8%) 17 15	9, 34, 66, 98	5 (0%)

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	148	VAL	11.2
1	D	179[A]	TRP	9.4
1	A	110	ILE	7.6
1	G	110	ILE	7.4
1	G	111	CYS	6.8
1	A	112	VAL	6.2
1	J	112	VAL	5.7
1	G	112	VAL	5.4
2	K	1	MET	5.4
2	H	85	PHE	5.2
1	D	113	LYS	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	104	LYS	4.7
3	L	46	LEU	4.7
2	H	40	ASP	4.5
3	C	16	MET	4.3
1	D	149	HIS	4.3
1	D	115	LYS	4.3
3	I	88	THR	4.3
2	K	81	ALA	4.3
1	D	112	VAL	4.2
3	F	58	ASN	4.2
1	A	111	CYS	4.2
2	K	102	VAL	4.2
1	D	135	ASP	4.1
1	G	135	ASP	4.1
1	A	135	ASP	4.1
3	I	58	ASN	4.1
2	B	102	VAL	4.0
3	L	58	ASN	3.9
1	A	114	SER	3.8
1	D	111	CYS	3.8
1	A	149	HIS	3.8
3	L	16	MET	3.8
1	J	149	HIS	3.8
1	J	115	LYS	3.6
1	J	111	CYS	3.6
3	F	85	ASN	3.5
1	J	114	SER	3.5
2	H	84	THR	3.5
3	I	87	SER	3.5
2	H	83	ASP	3.4
3	C	45	MET	3.4
1	A	115	LYS	3.3
2	H	101	ASP	3.3
1	J	30	SER	3.2
2	H	102	VAL	3.2
3	I	17	MET	3.1
1	D	185	THR	3.1
2	H	87	ALA	3.1
2	H	79	PHE	3.1
2	B	65	GLN	3.0
1	J	110	ILE	2.9
2	H	25	PHE	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	F	88	THR	2.8
2	E	81	ALA	2.8
2	H	52	ASP	2.8
1	D	79	ASP	2.8
1	J	116	LEU	2.7
1	G	114	SER	2.7
3	F	17	MET	2.7
2	H	100	PRO	2.6
3	F	86	SER	2.6
2	E	1	MET	2.6
2	H	61	GLY	2.6
2	K	2	ASP	2.6
2	E	102	VAL	2.6
3	I	85	ASN	2.6
2	K	68[A]	ARG	2.6
1	G	109	ILE	2.5
2	H	91	GLU	2.5
3	L	17	MET	2.5
1	D	52	SER	2.5
2	H	65	GLN	2.4
3	C	44	ALA	2.4
2	H	90	ILE	2.4
2	K	84	THR	2.4
3	C	58	ASN	2.4
2	E	48	ASP	2.4
3	C	17	MET	2.4
2	K	99	LEU	2.4
1	J	109	ILE	2.4
2	H	99	LEU	2.4
1	D	110	ILE	2.4
3	L	85	ASN	2.3
3	L	87	SER	2.3
2	H	86	GLU	2.3
2	K	104	LYS	2.3
2	H	60	CYS	2.3
2	H	88	LEU	2.3
3	I	46	LEU	2.3
1	D	178	ILE	2.3
2	H	1	MET	2.3
3	I	84	THR	2.2
2	H	45	TYR	2.2
1	A	109	ILE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	59	GLU	2.2
2	H	37	ARG	2.2
3	F	84	THR	2.2
3	F	87	SER	2.2
2	K	101	ASP	2.2
2	E	58	GLY	2.2
1	J	134	LYS	2.2
1	A	105	ARG	2.2
2	H	56	THR	2.2
2	H	92	PRO	2.2
1	A	52	SER	2.1
2	H	44	LEU	2.1
2	H	50	LEU	2.1
2	E	65	GLN	2.1
2	H	34	ILE	2.1
1	J	31	MET	2.1
2	B	82	ASP	2.1
2	H	43	ARG	2.1
2	H	96	PRO	2.1
2	H	35	LEU	2.0
1	A	132	MET	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($\text{\AA}^2$)	Q<0.9
4	JIH	A	201	38/39	0.97	0.08	18,25,50,56	0
4	JIH	G	201	38/39	0.97	0.07	18,24,45,65	0

Continued on next page...

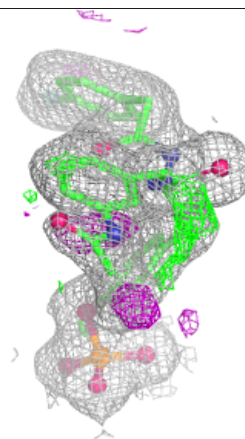
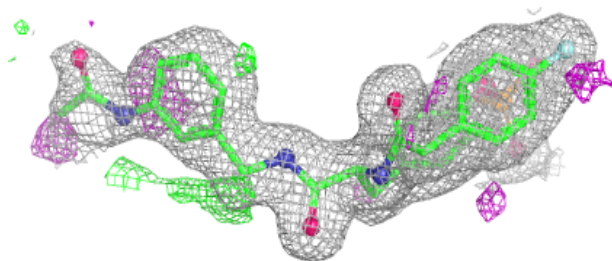
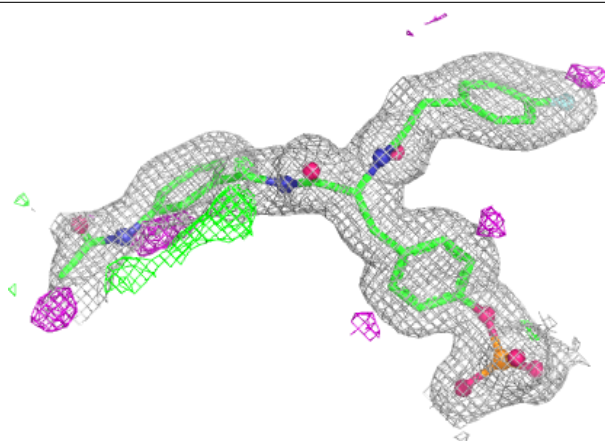
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	JIH	J	201	38/39	0.97	0.08	21,29,46,56	0
4	JIH	D	201	38/39	0.98	0.06	21,25,43,59	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.

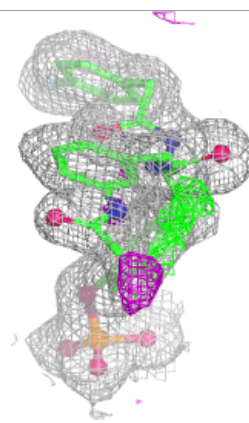
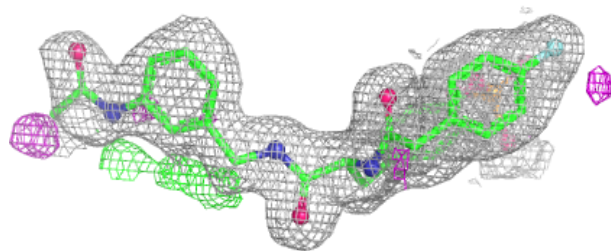
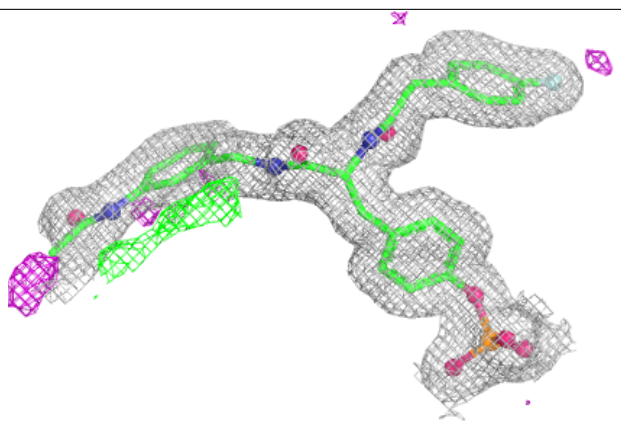
Electron density around JIH A 201:

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

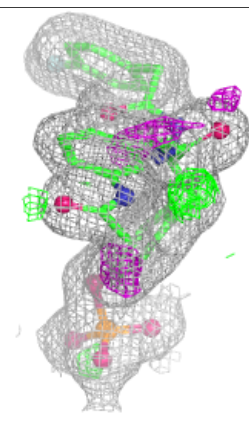
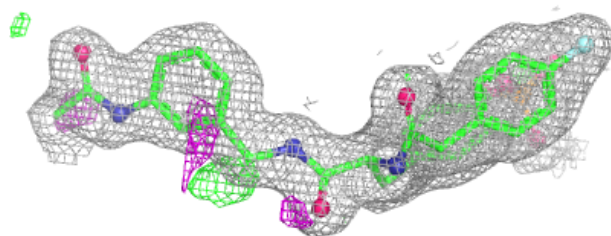
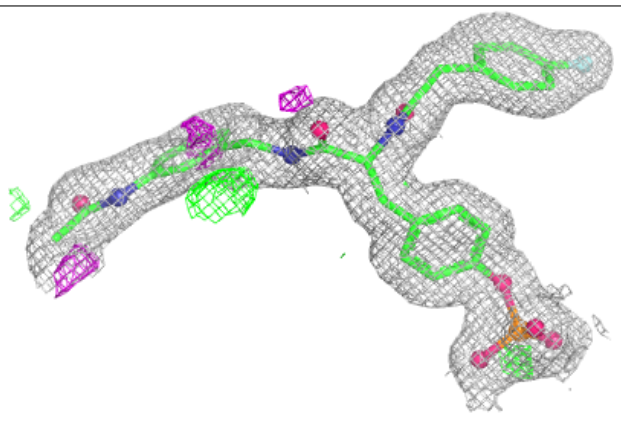


Electron density around JIH G 201:

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

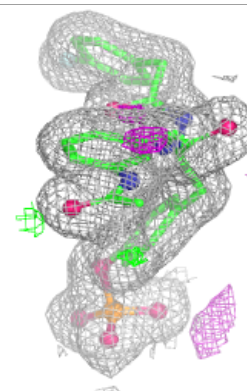
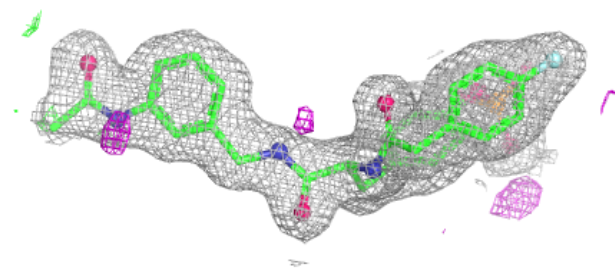
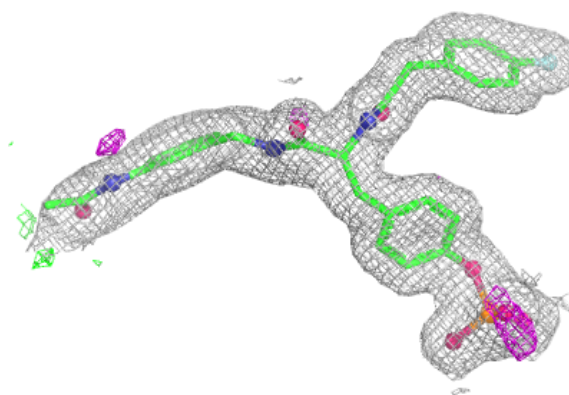
**Electron density around JIH J 201:**

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



Electron density around JIH 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.