



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:16 PM UTC

PDB ID : 5QSW / pdb_00005qsw
Title : PanDDA analysis group deposition – Crystal Structure of human STAG1 in complex with Z2856434884
Authors : Newman, J.A.; Katis, V.L.; Gavard, A.E.; von Delft, F.; Arrowsmith, C.H.; Edwards, A.; Bountra, C.; Gileadi, O.
Deposited on : 2019-05-25
Resolution : 3.03 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

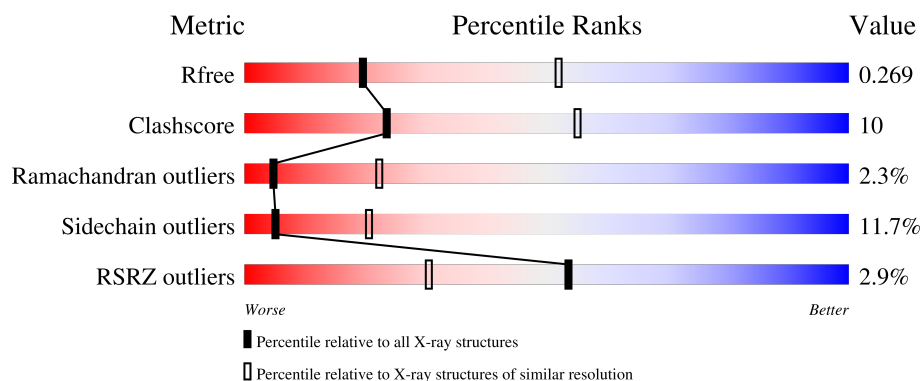
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.03 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	3685 (3.08-3.00)
Clashscore	190562	4007 (3.08-3.00)
Ramachandran outliers	187476	3834 (3.08-3.00)
Sidechain outliers	187428	3836 (3.08-3.00)
RSRZ outliers	180081	3684 (3.08-3.00)

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	339	4% 65% 20% • 12%
1	B	339	4% 65% 21% • 12%
1	C	339	• 61% 27% • • 7%
1	D	339	2% 61% 25% 5% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10266 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.

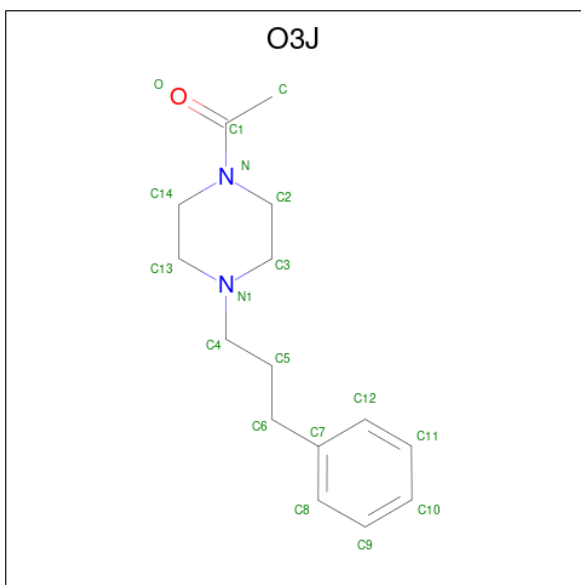
- Molecule 1 is a protein called Cohesin subunit SA-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	315	Total	C	N	O	S	0	0	0
			2591	1647	448	475	21			
1	A	297	Total	C	N	O	S	0	0	0
			2433	1550	417	446	20			
1	B	298	Total	C	N	O	S	0	0	0
			2452	1566	418	448	20			
1	D	311	Total	C	N	O	S	0	0	0
			2561	1627	439	475	20			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	82	SER	-	expression tag	UNP Q8WVM7
C	83	MET	-	expression tag	UNP Q8WVM7
C	84	GLY	-	expression tag	UNP Q8WVM7
C	85	GLY	-	expression tag	UNP Q8WVM7
A	82	SER	-	expression tag	UNP Q8WVM7
A	83	MET	-	expression tag	UNP Q8WVM7
A	84	GLY	-	expression tag	UNP Q8WVM7
A	85	GLY	-	expression tag	UNP Q8WVM7
B	82	SER	-	expression tag	UNP Q8WVM7
B	83	MET	-	expression tag	UNP Q8WVM7
B	84	GLY	-	expression tag	UNP Q8WVM7
B	85	GLY	-	expression tag	UNP Q8WVM7
D	82	SER	-	expression tag	UNP Q8WVM7
D	83	MET	-	expression tag	UNP Q8WVM7
D	84	GLY	-	expression tag	UNP Q8WVM7
D	85	GLY	-	expression tag	UNP Q8WVM7

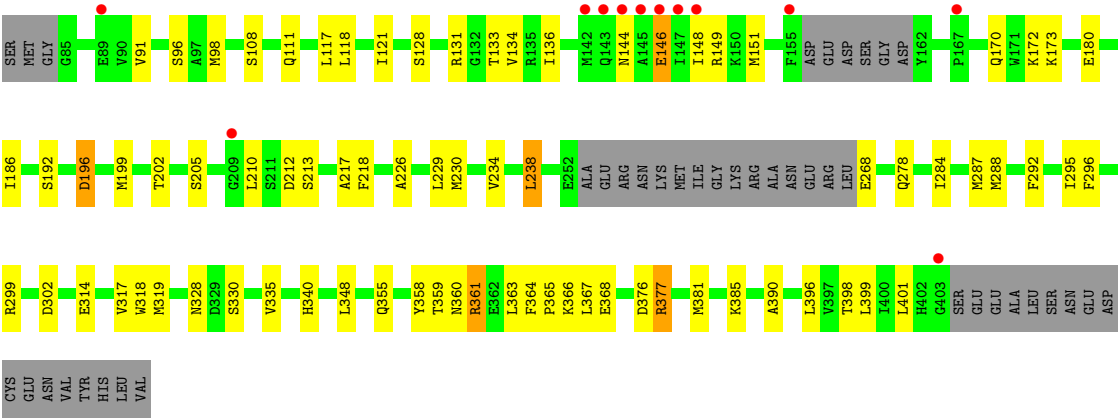
- Molecule 2 is 1-[4-(3-phenylpropyl)piperazin-1-yl]ethan-1-one (CCD ID: O3J) (formula: C₁₅H₂₂N₂O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			18	15	2	1		
2	A	1	Total	C	N	O	0	0
			18	15	2	1		
2	B	1	Total	C	N	O	0	0
			18	15	2	1		
2	D	1	Total	C	N	O	0	0
			18	15	2	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	40	Total	O	0	0
			40	40		
3	A	38	Total	O	0	0
			38	38		
3	B	26	Total	O	0	0
			26	26		
3	D	53	Total	O	0	0
			53	53		



● Molecule 1: Cohesin subunit SA-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	66.49Å 72.41Å 118.52Å 94.89° 98.60° 115.59°	Depositor
Resolution (Å)	115.52 – 3.03 115.52 – 3.03	Depositor EDS
% Data completeness (in resolution range)	98.1 (115.52-3.03) 98.1 (115.52-3.03)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.187 , 0.267 0.201 , 0.269	Depositor DCC
R_{free} test set	1876 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	89.0	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 68.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10266	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.74% 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: O3J

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	1.04	0/2470	1.57	3/3319 (0.1%)
1	B	1.03	0/2493	1.57	0/3353
1	C	1.02	1/2633 (0.0%)	1.56	4/3539 (0.1%)
1	D	0.99	0/2603	1.54	2/3501 (0.1%)
All	All	1.02	1/10199 (0.0%)	1.56	9/13712 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	162	TYR	N-CA	5.06	1.49	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	196	ASP	CA-CB-CG	7.37	119.97	112.60
1	A	196	ASP	CB-CA-C	6.69	118.03	109.80
1	C	196	ASP	CA-CB-CG	6.59	119.19	112.60
1	D	389	VAL	N-CA-C	-6.30	104.37	110.42
1	C	196	ASP	CB-CA-C	6.18	119.66	109.70
1	A	388	ASP	CA-CB-CG	5.58	118.18	112.60
1	C	383	LEU	CA-C-N	5.38	127.80	120.54
1	C	383	LEU	C-N-CA	5.38	127.80	120.54
1	D	358	TYR	CA-C-O	-5.14	115.10	120.55

There are no chirality outliers.

There are no planarity outliers.

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	2433	0	2457	35	0
1	B	2452	0	2469	48	0
1	C	2591	0	2613	63	0
1	D	2561	0	2568	63	0
2	A	18	0	0	0	0
2	B	18	0	0	4	0
2	C	18	0	0	4	0
2	D	18	0	0	3	0
3	A	38	0	0	7	0
3	B	26	0	0	1	0
3	C	40	0	0	2	0
3	D	53	0	0	8	0
All	All	10266	0	10107	206	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 10.

All (206) 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:C:95:LYS:HE3	1:C:103:ASP:OD2	1.47	1.13
1:D:98:MET:SD	3:D:641:HOH:O	2.14	1.03
1:C:95:LYS:CE	1:C:103:ASP:OD2	2.09	1.00
1:C:91:VAL:HG22	1:A:98:MET:HE1	1.50	0.91
1:D:144:ASN:OD1	2:D:501:O3J:C13	2.27	0.82
1:B:146:GLU:HG3	1:B:149:ARG:NH2	1.95	0.81
1:D:112:ASP:HB3	1:D:115:ILE:HD12	1.64	0.79
1:A:361:ARG:O	3:A:601:HOH:O	1.98	0.79
1:B:98:MET:HE1	1:B:180:GLU:HB3	1.65	0.78
1:A:146:GLU:OE2	3:A:602:HOH:O	1.99	0.78
1:B:146:GLU:CG	1:B:149:ARG:NH2	2.47	0.76
1:C:197:GLU:N	3:C:601:HOH:O	2.16	0.76
1:C:384:ASP:O	1:C:385:LYS:HB2	1.86	0.76
1:B:144:ASN:OD1	2:B:501:O3J:C13	2.35	0.75
1:D:265:GLU:N	3:D:601:HOH:O	2.18	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:LEU:HD22	1:B:218:PHE:CD1	2.23	0.73
1:B:299:ARG:NH1	1:B:302:ASP:OD2	2.25	0.70
1:D:333:LYS:HD2	1:D:337:TRP:CH2	2.26	0.69
1:C:340:HIS:CE1	1:C:377:ARG:HG3	2.28	0.69
1:D:226:ALA:HB2	1:D:295:ILE:HD13	1.73	0.69
1:C:139:PHE:O	2:C:501:O3J:C2	2.42	0.68
1:B:340:HIS:CE1	1:B:377:ARG:HG3	2.28	0.68
1:B:284:ILE:HA	1:B:287:MET:HE3	1.79	0.65
1:B:118:LEU:HD11	1:B:134:VAL:O	1.98	0.64
1:C:95:LYS:HE2	1:C:103:ASP:OD2	1.97	0.64
1:D:226:ALA:CB	1:D:295:ILE:HD13	2.28	0.63
2:B:501:O3J:C4	2:B:501:O3J:C8	2.77	0.63
1:D:146:GLU:O	1:D:149:ARG:HB3	1.99	0.63
1:C:284:ILE:HG22	1:C:288:MET:HE2	1.81	0.63
1:D:153:GLU:O	1:D:155:PHE:N	2.31	0.63
1:C:97:ALA:HB1	1:A:90:VAL:HG13	1.81	0.62
1:B:98:MET:HG3	3:D:614:HOH:O	2.00	0.62
1:B:91:VAL:HA	1:D:98:MET:HE1	1.82	0.61
1:A:284:ILE:HG22	1:A:288:MET:HE2	1.81	0.60
1:B:230:MET:HG2	1:B:318:TRP:CZ2	2.36	0.60
1:C:162:TYR:OH	1:C:216:ARG:NH1	2.35	0.60
1:C:143:GLN:OE1	1:C:144:ASN:ND2	2.36	0.59
1:C:240:LEU:HB2	1:C:281:GLN:HE21	1.66	0.59
1:D:306:GLU:HB2	3:D:637:HOH:O	2.02	0.59
1:B:146:GLU:O	1:B:149:ARG:N	2.35	0.59
1:A:98:MET:HE2	1:A:181:PHE:HB2	1.85	0.59
2:C:501:O3J:C4	2:C:501:O3J:C12	2.77	0.58
1:A:388:ASP:HB3	3:A:622:HOH:O	2.03	0.58
1:D:234:VAL:HA	1:D:288:MET:CE	2.33	0.58
1:C:230:MET:HG2	1:C:318:TRP:CE2	2.39	0.58
1:D:230:MET:HG2	1:D:318:TRP:CZ2	2.39	0.58
1:B:196:ASP:OD1	1:B:196:ASP:C	2.48	0.57
1:C:375:LYS:O	1:C:379:VAL:HB	2.04	0.57
1:A:112:ASP:HB3	1:A:115:ILE:CD1	2.34	0.57
1:C:86:THR:HG22	1:C:89:GLU:H	1.69	0.57
1:A:240:LEU:O	1:A:244:GLN:HB2	2.05	0.57
1:B:234:VAL:HA	1:B:288:MET:HE1	1.88	0.56
1:D:157:GLU:N	3:D:605:HOH:O	2.34	0.56
1:C:336:GLY:HA2	1:C:339:LEU:HD12	1.87	0.56
1:B:91:VAL:HG22	1:D:98:MET:CE	2.36	0.56
1:A:227:MET:HB3	1:A:314:GLU:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:342:ARG:H	1:C:342:ARG:CD	2.19	0.56
1:B:117:LEU:O	1:B:121:ILE:HG12	2.06	0.56
1:B:319:MET:HE1	1:B:335:VAL:HG21	1.86	0.55
1:B:146:GLU:HG2	1:B:149:ARG:NH2	2.21	0.55
1:B:360:ASN:C	1:B:361:ARG:O	2.48	0.55
1:C:144:ASN:HB3	2:C:501:O3J:C9	2.36	0.54
1:A:384:ASP:O	1:A:385:LYS:CB	2.56	0.54
1:B:144:ASN:OD1	2:B:501:O3J:C14	2.56	0.54
1:C:226:ALA:CB	1:C:295:ILE:HD13	2.38	0.53
1:D:147:ILE:O	1:D:150:LYS:N	2.41	0.53
1:D:200:MET:HE2	1:D:233:LEU:HD21	1.90	0.53
1:D:109:TYR:CZ	1:D:113:ARG:HG2	2.43	0.53
1:D:249:ARG:NE	1:D:249:ARG:HA	2.23	0.53
1:B:96:SER:HB3	3:B:617:HOH:O	2.07	0.53
1:D:165:THR:O	1:D:166:MET:C	2.51	0.53
1:D:142:MET:HE2	1:D:147:ILE:HG12	1.91	0.53
1:D:384:ASP:O	1:D:385:LYS:CB	2.57	0.52
1:C:240:LEU:HB2	1:C:281:GLN:NE2	2.23	0.52
1:A:121:ILE:HD12	1:A:206:LEU:HD22	1.91	0.52
1:B:360:ASN:ND2	1:B:363:LEU:HD13	2.25	0.52
1:A:296:PHE:CZ	1:A:315:ILE:HD12	2.46	0.51
1:B:234:VAL:HG22	1:B:288:MET:HE2	1.92	0.51
1:C:342:ARG:H	1:C:342:ARG:HD2	1.75	0.51
1:B:230:MET:O	1:B:234:VAL:HG23	2.10	0.51
1:D:299:ARG:NH1	1:D:302:ASP:OD2	2.44	0.51
1:C:340:HIS:NE2	1:C:377:ARG:HG3	2.26	0.51
1:C:351:LEU:HD11	1:C:381:MET:HE2	1.92	0.51
1:C:323:SER:O	1:C:327:LEU:HB3	2.11	0.50
1:D:146:GLU:O	1:D:149:ARG:N	2.43	0.50
1:C:384:ASP:O	1:C:385:LYS:CB	2.59	0.50
1:B:292:PHE:CE1	1:B:296:PHE:CD1	2.99	0.50
1:C:258:MET:O	1:C:259:ILE:O	2.28	0.50
1:B:284:ILE:HD13	1:B:287:MET:CE	2.42	0.49
1:D:248:GLN:HA	1:D:248:GLN:OE1	2.12	0.49
1:B:381:MET:O	1:B:390:ALA:HA	2.12	0.49
1:C:315:ILE:HA	1:C:318:TRP:CE3	2.47	0.49
1:D:107:GLU:CG	3:D:638:HOH:O	2.60	0.49
1:D:371:THR:O	1:D:375:LYS:HB2	2.12	0.49
1:D:98:MET:HE2	1:D:181:PHE:HB2	1.95	0.49
1:A:112:ASP:HB3	1:A:115:ILE:HD12	1.94	0.48
1:D:97:ALA:O	1:D:101:VAL:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:213:SER:O	1:D:219:ARG:HD3	2.14	0.48
1:C:194:ILE:HD11	1:C:200:MET:SD	2.53	0.48
1:D:340:HIS:ND1	1:D:377:ARG:HG3	2.28	0.48
1:C:162:TYR:CD1	1:C:217:ALA:HA	2.49	0.48
1:C:240:LEU:CB	1:C:281:GLN:HE21	2.27	0.48
1:C:155:PHE:O	1:C:156:ASP:C	2.56	0.48
1:B:359:THR:HA	1:B:399:LEU:HD22	1.96	0.48
1:B:234:VAL:HA	1:B:288:MET:CE	2.44	0.47
1:B:128:SER:O	1:B:217:ALA:HB1	2.14	0.47
1:D:99:GLN:HA	1:D:184:VAL:HG11	1.96	0.47
1:D:237:ALA:HB1	1:D:281:GLN:HE22	1.79	0.47
1:B:226:ALA:CB	1:B:295:ILE:HD13	2.45	0.47
1:B:146:GLU:HG2	1:B:149:ARG:HH22	1.79	0.47
1:B:314:GLU:O	1:B:317:VAL:HB	2.15	0.47
1:D:388:ASP:O	1:D:392:GLU:HG2	2.14	0.47
1:C:86:THR:HG21	3:A:626:HOH:O	2.15	0.47
1:B:363:LEU:O	1:B:367:LEU:HD22	2.13	0.47
1:D:146:GLU:O	1:D:149:ARG:CB	2.63	0.47
1:A:338:THR:O	1:A:341:ASP:HB2	2.14	0.47
1:A:121:ILE:O	1:A:125:ILE:HG12	2.14	0.47
1:B:146:GLU:O	1:B:149:ARG:HB3	2.14	0.47
1:C:112:ASP:HB3	1:C:115:ILE:HG12	1.97	0.46
1:A:98:MET:HA	1:A:98:MET:HE3	1.98	0.46
1:D:192:SER:OG	1:D:193:ILE:N	2.35	0.46
1:C:93:LEU:O	1:C:95:LYS:N	2.44	0.46
1:A:219:ARG:O	1:A:223:THR:OG1	2.24	0.46
1:D:388:ASP:OD2	1:D:389:VAL:N	2.48	0.46
1:C:223:THR:OG1	1:C:299:ARG:HG3	2.16	0.46
1:A:174:PHE:O	1:A:177:ASN:N	2.48	0.46
1:A:200:MET:HE3	1:A:200:MET:HA	1.96	0.46
1:B:91:VAL:HG21	1:D:123:PHE:CE1	2.51	0.46
1:D:373:ARG:HG2	1:D:374:PHE:CE2	2.51	0.46
1:A:190:GLN:HE22	1:A:239:ASN:ND2	2.13	0.46
1:C:364:PHE:HB3	1:C:365:PRO:HD3	1.98	0.46
1:B:328:ASN:OD1	1:B:330:SER:OG	2.34	0.45
1:D:234:VAL:HA	1:D:288:MET:HE2	1.97	0.45
1:D:384:ASP:O	1:D:385:LYS:HB3	2.14	0.45
1:C:326:PHE:HA	1:C:331:TYR:HD2	1.82	0.45
1:D:388:ASP:OD2	1:D:388:ASP:C	2.58	0.45
1:A:315:ILE:HA	1:A:318:TRP:CE3	2.51	0.45
1:C:98:MET:O	1:C:101:VAL:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:MET:HG2	1:A:318:TRP:CZ2	2.52	0.45
1:C:381:MET:O	1:C:384:ASP:HB2	2.17	0.45
1:C:96:SER:H	1:C:99:GLN:HG3	1.81	0.44
1:C:312:ILE:O	1:C:313:GLU:C	2.59	0.44
1:A:190:GLN:HE22	1:A:239:ASN:HD22	1.66	0.44
1:C:143:GLN:O	1:C:146:GLU:N	2.48	0.44
1:B:202:THR:HG23	2:B:501:O3J:C6	2.47	0.44
1:C:240:LEU:CB	1:C:281:GLN:NE2	2.81	0.44
1:D:234:VAL:HA	1:D:288:MET:HE1	1.98	0.44
1:A:109:TYR:CE2	1:A:193:ILE:HG23	2.53	0.44
1:A:299:ARG:O	1:A:302:ASP:HB2	2.18	0.44
1:A:145:ALA:HB3	3:A:623:HOH:O	2.18	0.43
1:C:327:LEU:CD1	1:C:332:LEU:HD11	2.48	0.43
1:D:227:MET:O	1:D:230:MET:HB3	2.19	0.43
1:A:232:ALA:HA	3:A:636:HOH:O	2.18	0.43
1:D:98:MET:HG3	1:D:181:PHE:HA	2.01	0.43
1:D:136:ILE:O	1:D:139:PHE:HB3	2.17	0.43
1:D:238:LEU:HD12	1:D:238:LEU:HA	1.83	0.43
1:B:238:LEU:HD12	1:B:238:LEU:HA	1.90	0.43
1:C:162:TYR:CE1	1:C:217:ALA:HA	2.54	0.43
1:C:357:LEU:HB3	1:C:367:LEU:HD11	2.01	0.43
1:D:200:MET:HE1	1:D:229:LEU:HD11	2.01	0.42
1:C:163:PRO:HB3	1:C:171:TRP:CZ3	2.54	0.42
1:A:354:LEU:O	1:A:355:GLN:C	2.62	0.42
1:D:196:ASP:OD1	1:D:196:ASP:C	2.62	0.42
1:B:230:MET:HG2	1:B:318:TRP:CH2	2.54	0.42
1:D:202:THR:HG23	2:D:501:O3J:C6	2.50	0.42
1:C:149:ARG:O	1:C:152:THR:HB	2.20	0.42
1:D:194:ILE:HD12	1:D:284:ILE:HD11	2.00	0.42
1:D:351:LEU:HD11	1:D:381:MET:HE2	2.02	0.42
1:D:300:TYR:CZ	1:D:301:ARG:HG3	2.54	0.42
1:C:136:ILE:O	1:C:140:ARG:HG3	2.20	0.42
1:A:364:PHE:N	1:A:365:PRO:HD2	2.34	0.42
1:B:358:TYR:CE2	1:B:367:LEU:HG	2.54	0.42
1:C:226:ALA:HB2	1:C:295:ILE:HD13	2.01	0.42
1:D:342:ARG:NH1	3:D:604:HOH:O	2.29	0.42
1:C:144:ASN:HB3	2:C:501:O3J:C8	2.49	0.42
1:C:387:TYR:O	1:C:391:VAL:HG23	2.20	0.42
1:A:182:ILE:CD1	1:A:225:ALA:HA	2.50	0.41
1:C:243:HIS:HB3	3:C:639:HOH:O	2.19	0.41
1:A:270:LEU:HD23	1:A:270:LEU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:ILE:O	1:A:299:ARG:HG2	2.20	0.41
1:D:117:LEU:HD21	1:D:199:MET:HA	2.02	0.41
1:D:206:LEU:HA	2:D:501:O3J:C9	2.51	0.41
1:C:272:GLN:HA	1:C:272:GLN:OE1	2.20	0.41
1:C:92:LYS:O	1:C:93:LEU:HB2	2.21	0.41
1:C:340:HIS:NE2	1:C:377:ARG:CG	2.83	0.41
1:A:361:ARG:HG3	3:A:612:HOH:O	2.20	0.41
1:B:148:ILE:HA	1:B:151:MET:HE3	2.00	0.41
1:B:186:ILE:HD11	1:B:229:LEU:CD1	2.51	0.41
1:B:365:PRO:O	1:B:368:GLU:CG	2.68	0.41
1:D:218:PHE:HD1	1:D:218:PHE:HA	1.81	0.41
1:C:196:ASP:OD1	1:C:196:ASP:C	2.63	0.41
1:B:226:ALA:HB2	1:B:295:ILE:HD13	2.03	0.41
1:C:109:TYR:CE2	1:C:193:ILE:HG23	2.56	0.41
1:C:142:MET:HE3	1:C:146:GLU:HG2	2.03	0.41
1:B:360:ASN:O	1:B:361:ARG:O	2.39	0.41
1:D:133:THR:HB	3:D:602:HOH:O	2.20	0.41
1:C:86:THR:HG22	1:C:89:GLU:N	2.33	0.41
1:C:162:TYR:CD1	1:C:217:ALA:HB2	2.56	0.40
1:D:195:TYR:C	1:D:196:ASP:O	2.62	0.40
1:D:201:ASP:O	1:D:205:SER:HB2	2.20	0.40
1:B:355:GLN:O	1:B:359:THR:HG23	2.21	0.40
1:D:153:GLU:C	1:D:155:PHE:H	2.27	0.40
1:D:234:VAL:CA	1:D:288:MET:HE2	2.51	0.40
1:C:166:MET:HG2	1:C:171:TRP:CD1	2.57	0.40
1:A:292:PHE:O	1:A:297:VAL:HG13	2.22	0.40
1:D:147:ILE:O	1:D:148:ILE:C	2.65	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	289/339 (85%)	255 (88%)	26 (9%)	8 (3%)	4	18
1	B	292/339 (86%)	265 (91%)	23 (8%)	4 (1%)	9	33
1	C	311/339 (92%)	289 (93%)	15 (5%)	7 (2%)	5	22
1	D	307/339 (91%)	280 (91%)	19 (6%)	8 (3%)	4	20
All	All	1199/1356 (88%)	1089 (91%)	83 (7%)	27 (2%)	5	22

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	93	LEU
1	C	144	ASN
1	B	361	ARG
1	B	385	LYS
1	D	153	GLU
1	D	154	GLU
1	C	259	ILE
1	C	385	LYS
1	A	360	ASN
1	A	385	LYS
1	A	387	TYR
1	A	388	ASP
1	B	108	SER
1	B	111	GLN
1	D	385	LYS
1	C	94	GLY
1	C	362	GLU
1	A	111	GLN
1	A	153	GLU
1	D	280	ASN
1	D	388	ASP
1	C	258	MET
1	A	361	ARG
1	D	192	SER
1	D	146	GLU
1	A	336	GLY
1	D	147	ILE

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	269/306 (88%)	240 (89%)	29 (11%)	6	24
1	B	271/306 (89%)	247 (91%)	24 (9%)	9	32
1	C	285/306 (93%)	243 (85%)	42 (15%)	3	13
1	D	283/306 (92%)	248 (88%)	35 (12%)	4	18
All	All	1108/1224 (90%)	978 (88%)	130 (12%)	5	20

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	86	THR
1	C	98	MET
1	C	99	GLN
1	C	111	GLN
1	C	113	ARG
1	C	128	SER
1	C	136	ILE
1	C	137	GLU
1	C	144	ASN
1	C	155	PHE
1	C	166	MET
1	C	172	LYS
1	C	173	LYS
1	C	176	SER
1	C	186	ILE
1	C	196	ASP
1	C	212	ASP
1	C	219	ARG
1	C	229	LEU
1	C	238	LEU
1	C	249	ARG
1	C	252	GLU
1	C	256	ASN
1	C	259	ILE
1	C	261	LYS
1	C	262	ARG
1	C	264	ASN
1	C	266	ARG

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Mol	Chain	Res	Type
1	C	276	GLU
1	C	281	GLN
1	C	283	GLU
1	C	286	ASN
1	C	290	SER
1	C	324	ASP
1	C	342	ARG
1	C	363	LEU
1	C	377	ARG
1	C	379	VAL
1	C	388	ASP
1	C	396	LEU
1	C	398	THR
1	C	401	LEU
1	A	100	SER
1	A	101	VAL
1	A	115	ILE
1	A	121	ILE
1	A	133	THR
1	A	136	ILE
1	A	137	GLU
1	A	154	GLU
1	A	196	ASP
1	A	219	ARG
1	A	235	ASN
1	A	250	GLN
1	A	268	GLU
1	A	270	LEU
1	A	275	LYS
1	A	290	SER
1	A	293	LYS
1	A	333	LYS
1	A	342	ARG
1	A	343	GLN
1	A	348	LEU
1	A	360	ASN
1	A	362	GLU
1	A	363	LEU
1	A	367	LEU
1	A	376	ASP
1	A	379	VAL
1	A	396	LEU

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Mol	Chain	Res	Type
1	A	401	LEU
1	B	131	ARG
1	B	133	THR
1	B	136	ILE
1	B	146	GLU
1	B	170	GLN
1	B	172	LYS
1	B	173	LYS
1	B	192	SER
1	B	196	ASP
1	B	199	MET
1	B	205	SER
1	B	212	ASP
1	B	213	SER
1	B	238	LEU
1	B	268	GLU
1	B	278	GLN
1	B	348	LEU
1	B	364	PHE
1	B	366	LYS
1	B	376	ASP
1	B	377	ARG
1	B	396	LEU
1	B	398	THR
1	B	401	LEU
1	D	95	LYS
1	D	98	MET
1	D	100	SER
1	D	101	VAL
1	D	107	GLU
1	D	115	ILE
1	D	133	THR
1	D	135	ARG
1	D	137	GLU
1	D	143	GLN
1	D	163	PRO
1	D	173	LYS
1	D	194	ILE
1	D	196	ASP
1	D	197	GLU
1	D	214	GLN
1	D	218	PHE

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Mol	Chain	Res	Type
1	D	219	ARG
1	D	238	LEU
1	D	241	SER
1	D	254	GLU
1	D	257	LYS
1	D	269	LEU
1	D	289	ASN
1	D	320	LYS
1	D	342	ARG
1	D	349	LYS
1	D	359	THR
1	D	361	ARG
1	D	362	GLU
1	D	367	LEU
1	D	373	ARG
1	D	388	ASP
1	D	396	LEU
1	D	401	LEU

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

Mol	Chain	Res	Type
1	C	99	GLN
1	C	144	ASN
1	C	235	ASN
1	C	256	ASN
1	C	264	ASN
1	C	289	ASN
1	A	126	GLN
1	A	190	GLN
1	A	250	GLN
1	A	281	GLN
1	A	286	ASN
1	A	340	HIS
1	A	360	ASN
1	B	170	GLN
1	B	278	GLN
1	B	340	HIS
1	D	99	GLN
1	D	126	GLN
1	D	143	GLN
1	D	214	GLN

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Mol	Chain	Res	Type
1	D	220	HIS
1	D	360	ASN

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 ⓘ

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	$\# Z > 2$
2	O3J	D	501	-	19,19,19	1.13	1 (5%)	24,24,24	1.02	1 (4%)
2	O3J	A	501	-	19,19,19	0.81	0	24,24,24	1.18	2 (8%)
2	O3J	C	501	-	19,19,19	1.15	1 (5%)	24,24,24	1.43	4 (16%)
2	O3J	B	501	-	19,19,19	1.18	1 (5%)	24,24,24	1.36	4 (16%)

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	O3J	D	501	-	-	4/10/20/20	1/2/2/2
2	O3J	A	501	-	-	6/10/20/20	0/2/2/2
2	O3J	C	501	-	-	5/10/20/20	1/2/2/2
2	O3J	B	501	-	-	3/10/20/20	1/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	O3J	C13-N1	2.50	1.53	1.46
2	D	501	O3J	C2-N	-2.39	1.42	1.47
2	B	501	O3J	C3-C2	2.12	1.59	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	O3J	C5-C4-N1	-3.67	103.63	113.93
2	C	501	O3J	C3-N1-C13	3.38	116.12	108.84
2	C	501	O3J	C4-N1-C3	-3.25	102.58	111.24
2	D	501	O3J	C5-C4-N1	-3.01	105.48	113.93
2	B	501	O3J	C5-C4-N1	-2.61	106.60	113.93
2	A	501	O3J	C2-C3-N1	-2.56	105.48	110.65
2	C	501	O3J	C4-C5-C6	-2.46	106.60	113.05
2	B	501	O3J	C12-C7-C8	2.39	121.78	118.23
2	C	501	O3J	C2-C3-N1	-2.22	106.18	110.65
2	B	501	O3J	C4-C5-C6	-2.07	107.61	113.05
2	B	501	O3J	C3-N1-C13	2.02	113.19	108.84

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	O3J	C5-C4-N1-C13
2	C	501	O3J	N1-C4-C5-C6
2	A	501	O3J	C5-C4-N1-C13
2	A	501	O3J	C5-C4-N1-C3
2	D	501	O3J	N1-C4-C5-C6
2	A	501	O3J	N1-C4-C5-C6
2	B	501	O3J	N1-C4-C5-C6
2	A	501	O3J	C5-C6-C7-C8
2	D	501	O3J	C5-C6-C7-C12
2	D	501	O3J	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
2	C	501	O3J	C5-C6-C7-C8
2	A	501	O3J	C5-C6-C7-C12
2	D	501	O3J	C5-C4-N1-C13
2	C	501	O3J	C5-C6-C7-C12
2	B	501	O3J	C5-C6-C7-C8
2	B	501	O3J	C5-C6-C7-C12
2	C	501	O3J	C4-C5-C6-C7
2	A	501	O3J	C4-C5-C6-C7

All (3) ring outliers are listed below:

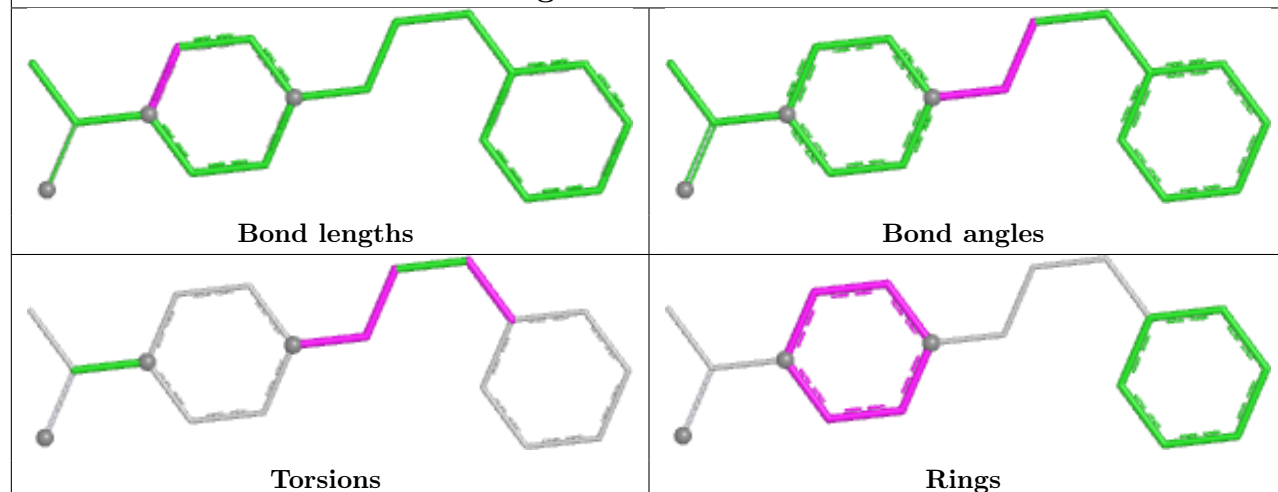
Mol	Chain	Res	Type	Atoms
2	C	501	O3J	C13-C14-C2-C3-N-N1
2	D	501	O3J	C13-C14-C2-C3-N-N1
2	B	501	O3J	C13-C14-C2-C3-N-N1

3 monomers are involved in 11 short contacts:

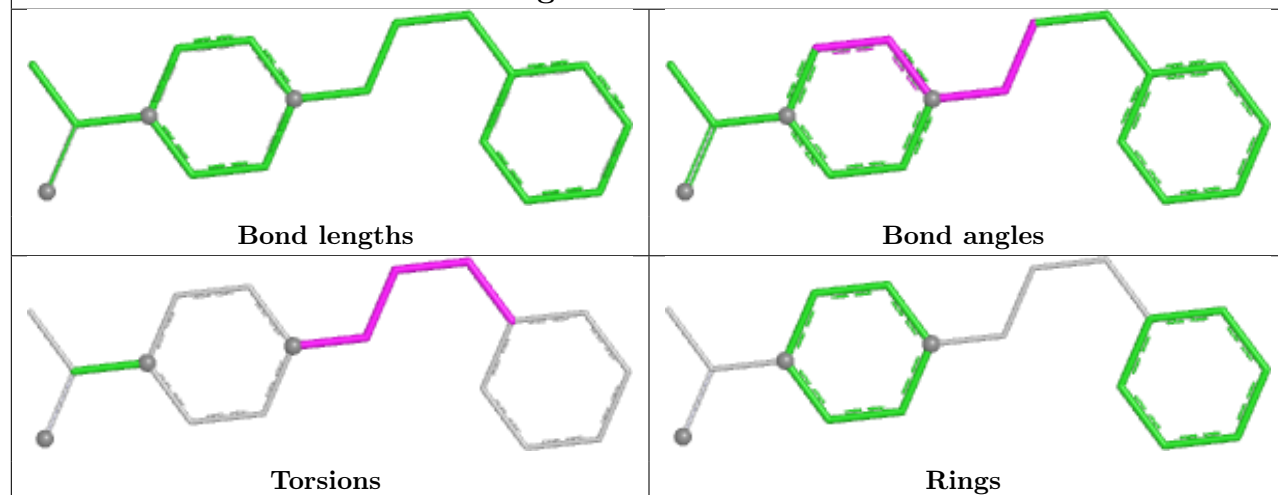
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	O3J	3	0
2	C	501	O3J	4	0
2	B	501	O3J	4	0

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.

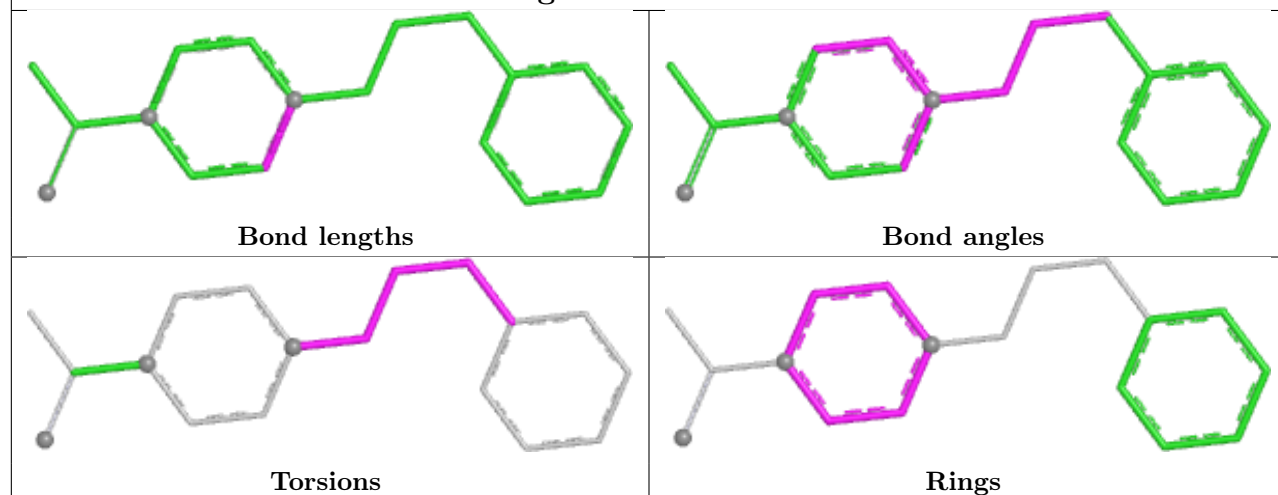
Ligand O3J D 501

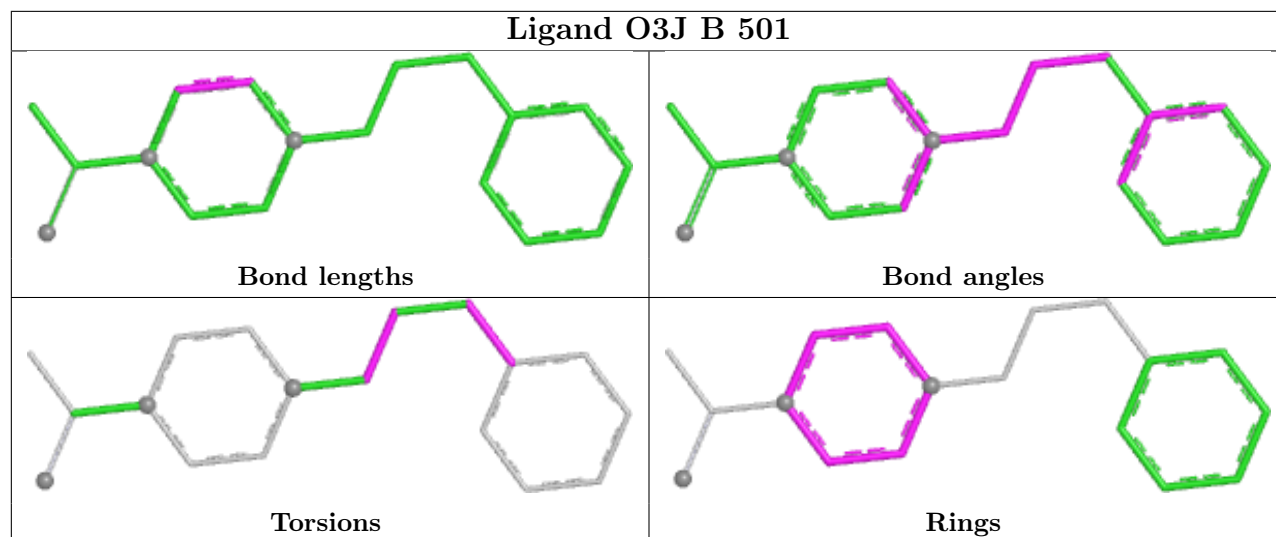


Ligand O3J A 501



Ligand O3J C 501





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	297/339 (87%)	0.19	12 (4%)	42 23	38, 101, 154, 208	6 (2%)
1	B	298/339 (87%)	-0.06	12 (4%)	42 23	46, 96, 143, 179	6 (2%)
1	C	315/339 (92%)	-0.21	4 (1%)	75 52	55, 90, 134, 179	2 (0%)
1	D	311/339 (91%)	-0.07	8 (2%)	57 33	45, 82, 133, 157	7 (2%)
All	All	1221/1356 (90%)	-0.04	36 (2%)	53 30	38, 92, 140, 208	21 (1%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	144	ASN	23.0
1	A	147	ILE	15.4
1	A	143	GLN	15.0
1	D	144	ASN	14.5
1	A	145	ALA	13.9
1	A	146	GLU	12.6
1	A	139	PHE	12.1
1	B	144	ASN	10.9
1	B	142	MET	10.4
1	D	147	ILE	10.0
1	D	145	ALA	9.5
1	B	147	ILE	9.1
1	D	143	GLN	8.7
1	C	143	GLN	8.2
1	D	142	MET	7.9
1	B	145	ALA	7.5
1	B	143	GLN	7.4
1	D	141	ASN	7.0
1	D	146	GLU	6.8
1	B	146	GLU	6.2
1	C	144	ASN	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	247	THR	4.6
1	C	146	GLU	2.9
1	A	248	GLN	2.8
1	B	155	PHE	2.7
1	A	339	LEU	2.7
1	A	269	LEU	2.5
1	B	89	GLU	2.4
1	D	403	GLY	2.3
1	A	164	LEU	2.2
1	A	148	ILE	2.1
1	B	148	ILE	2.1
1	C	149	ARG	2.1
1	B	403	GLY	2.1
1	B	167	PRO	2.1
1	B	209	GLY	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](#)

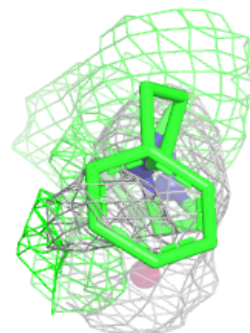
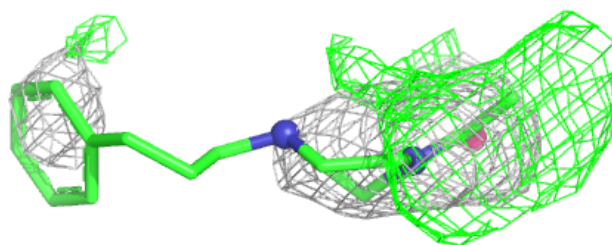
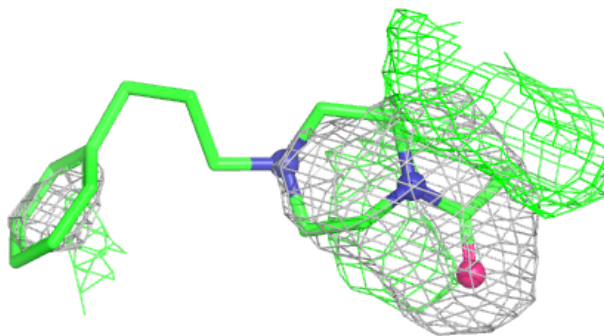
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	O3J	C	501	18/18	0.86	0.32	53,65,77,79	18
2	O3J	A	501	18/18	0.88	0.36	39,42,45,45	18
2	O3J	D	501	18/18	0.88	0.26	37,42,54,60	18
2	O3J	B	501	18/18	0.91	0.26	53,60,65,65	18

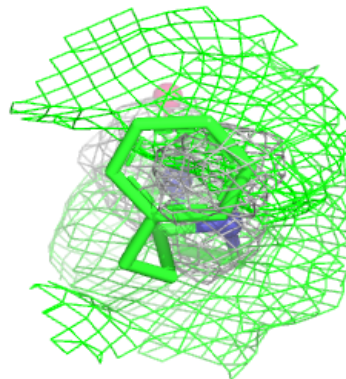
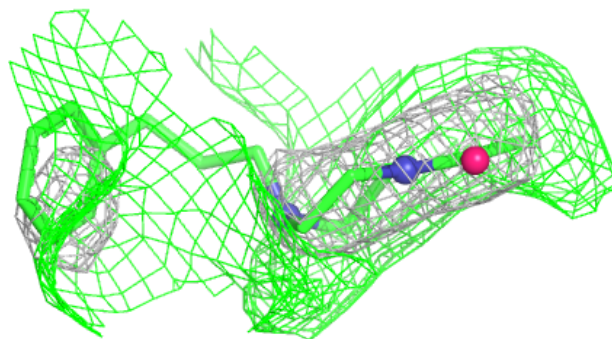
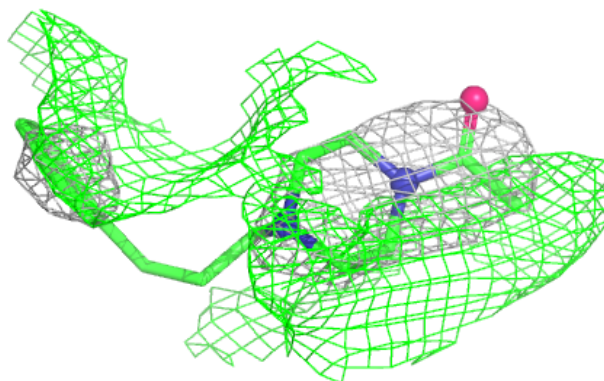
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around O3J C 501:

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

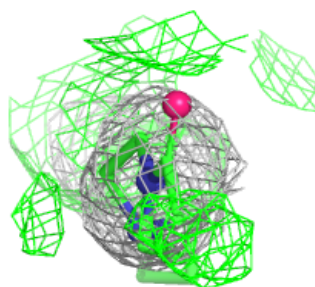
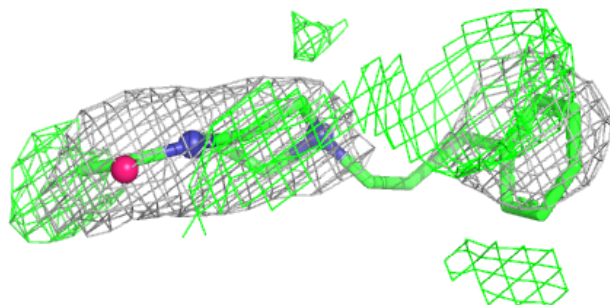
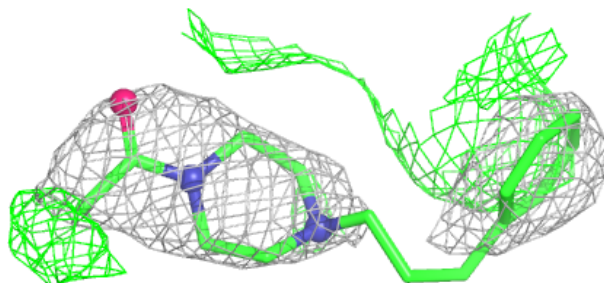
**Electron density around O3J A 501:**

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

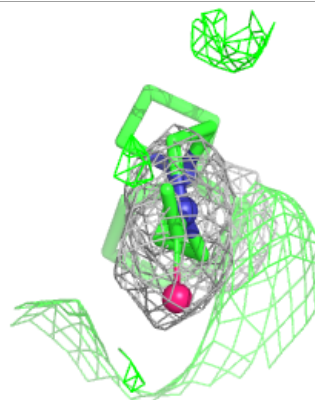
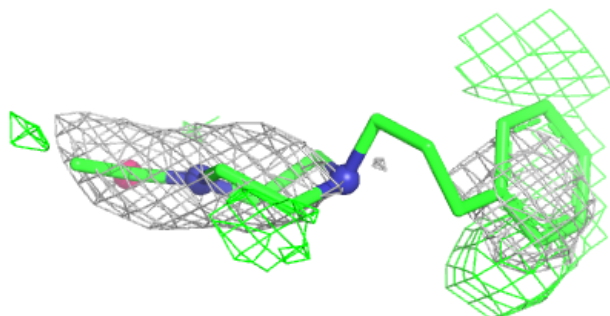
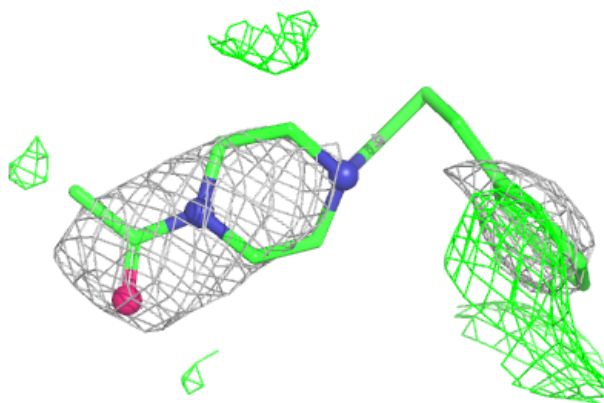


Electron density around O3J D 501:

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

**Electron density around O3J B 501:**

$2mF_o-DF_c$ (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.