



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 08:07 am BST

PDB ID : 5QSW  
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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

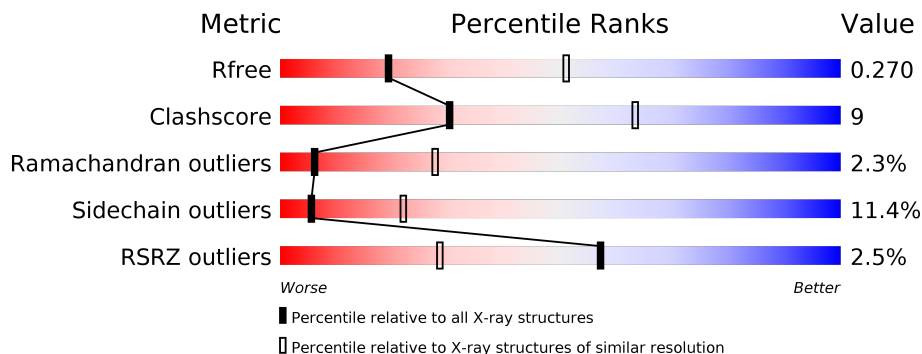
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.03 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))
$R_{free}$	130704	2752 (3.08-3.00)
Clashscore	141614	3096 (3.08-3.00)
Ramachandran outliers	138981	2986 (3.08-3.00)
Sidechain outliers	138945	2988 (3.08-3.00)
RSRZ outliers	127900	2636 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 67%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 50px;">5%      67%      18%      •      12%</p>
1	B	339	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 66%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 20%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 50px;">%      66%      20%      •      12%</p>
1	C	339	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 62%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 27%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 50px;">2%      62%      27%      • •      7%</p>
1	D	339	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 65%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 21%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 50px;">%      65%      21%      5%      8%</p>

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	O3J	A	501	-	-	-	X
2	O3J	C	501	-	-	-	X

## 2 Entry composition i

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.

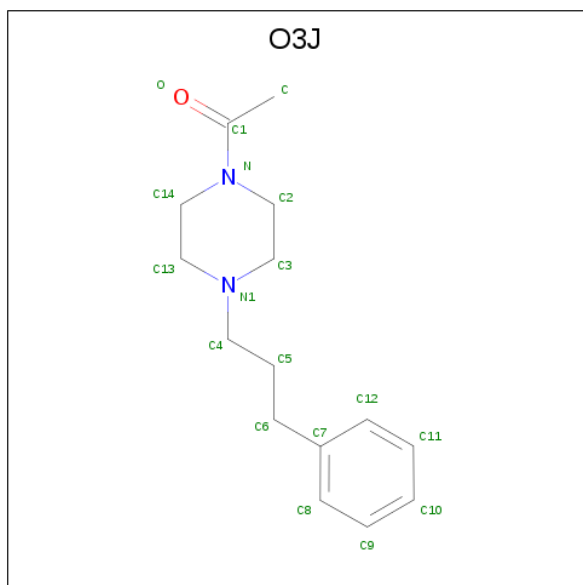
- Molecule 1 is a protein called Cohesin subunit SA-1.

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

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 (three-letter code: O3J) (formula: C<sub>15</sub>H<sub>22</sub>N<sub>2</sub>O) (labeled as "Ligand of Interest" by author).



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

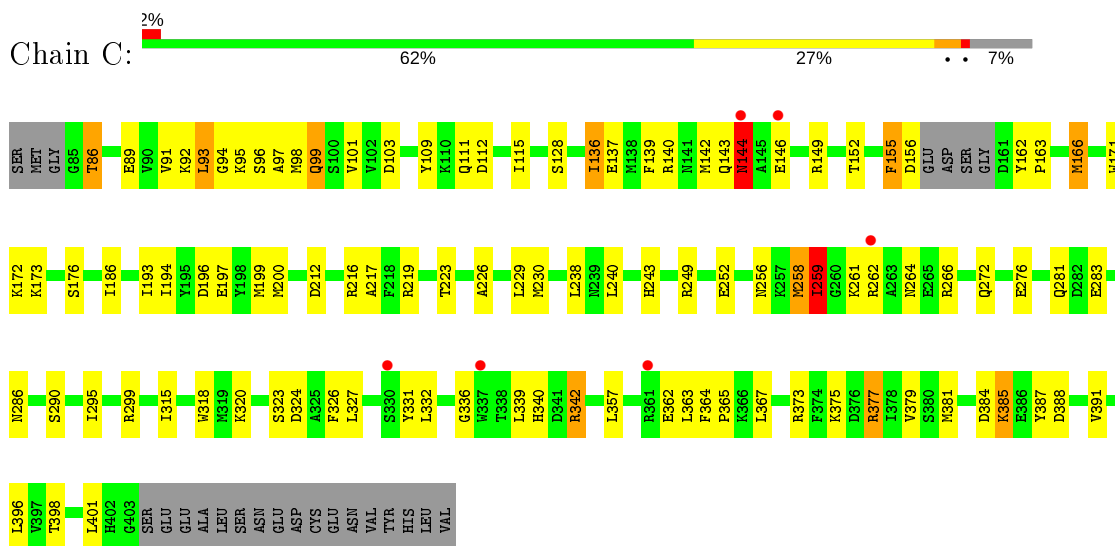
- Molecule 3 is water.

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

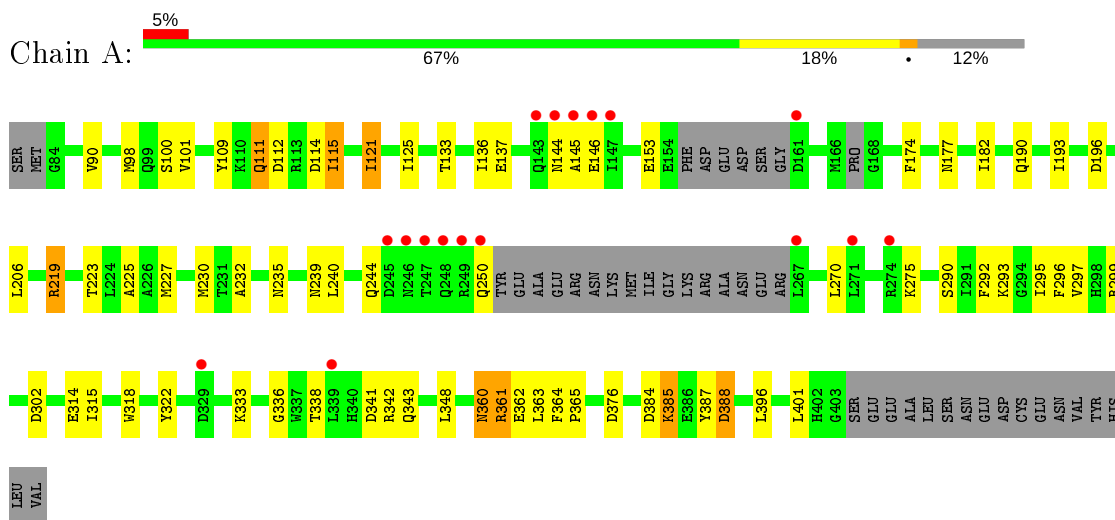
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Cohesin subunit SA-1

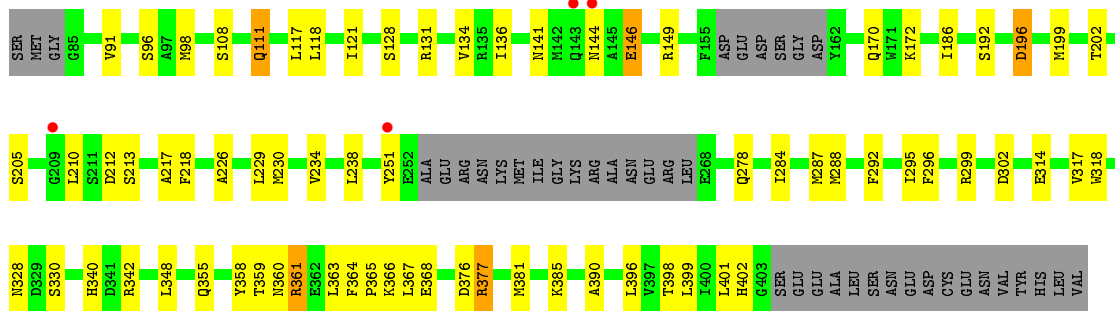


- Molecule 1: Cohesin subunit SA-1

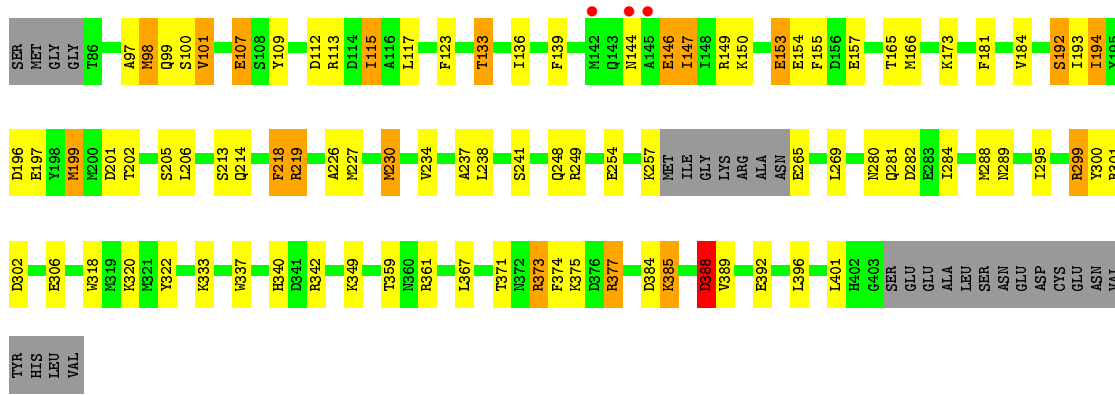


- Molecule 1: Cohesin subunit SA-1





● Molecule 1: Cohesin subunit SA-1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.52 (at 3.01Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.187 , 0.267 0.202 , 0.270	Depositor DCC
$R_{free}$ test set	1844 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	89.0	Xtrriage
Anisotropy	0.039	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 67.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10266	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	98.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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	0.71	0/2470	0.85	0/3319
1	B	0.70	0/2493	0.84	0/3353
1	C	0.69	0/2633	0.84	0/3539
1	D	0.68	0/2603	0.86	0/3501
All	All	0.69	0/10199	0.85	0/13712

There are no bond length outliers.

There are no bond angle outliers.

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	2433	0	2457	32	0
1	B	2452	0	2469	45	0
1	C	2591	0	2613	60	0
1	D	2561	0	2568	55	0
2	A	18	0	0	1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	187	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 9.

All (187) 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:A:144:ASN:OD1	2:A:501:O3J:C13	2.01	1.08
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: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: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
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:B:340:HIS:CE1	1:B:377:ARG:HG3	2.28	0.68
1:C:139:PHE:O	2:C:501:O3J:C2	2.42	0.68
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: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:230:MET:HG2	1:B:318:TRP:CZ2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:VAL:HG13	1:D:98:MET:HE2	1.83	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
2:C:501:O3J:C12	2:C:501:O3J:C4	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: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: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
1:B:117:LEU:O	1:B:121:ILE:HG12	2.06	0.56
1:C:342:ARG:H	1:C:342:ARG:CD	2.19	0.56
1:B:146:GLU:HG2	1:B:149:ARG:NH2	2.21	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:109:TYR:CZ	1:D:113:ARG:HG2	2.43	0.53
1:D:249:ARG:HA	1:D:249:ARG:NE	2.23	0.53
1:B:96:SER:HB3	3:B:617:HOH:O	2.07	0.53
1:B:196:ASP:C	1:B:196:ASP:OD1	2.48	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:B:360:ASN:C	1:B:361:ARG:O	2.48	0.52
1:A:296:PHE:CZ	1:A:315:ILE:HD12	2.46	0.51
1:C:91:VAL:HG22	1:A:98:MET:CE	2.41	0.51
1:C:342:ARG:HD2	1:C:342:ARG:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:340:HIS:NE2	1:C:377:ARG:HG3	2.26	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: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
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:D:165:THR:O	1:D:166:MET:C	2.51	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: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:D:384:ASP:O	1:D:385:LYS:HB3	2.14	0.47
1:B:128:SER:O	1:B:217:ALA:HB1	2.14	0.47
1:B:234:VAL:HA	1:B:288:MET:HE1	1.96	0.47
1:D:237:ALA:HB1	1:D:281:GLN:HE22	1.79	0.47
1:D:99:GLN:HA	1:D:184:VAL:HG11	1.96	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:D:388:ASP:O	1:D:392:GLU:HG2	2.14	0.47
1:B:314:GLU:O	1:B:317:VAL:HB	2.15	0.47
1:B:363:LEU:O	1:B:367:LEU:HD22	2.13	0.47
1:C:86:THR:HG21	3:A:626:HOH:O	2.15	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:D:192:SER:OG	1:D:193:ILE:N	2.35	0.46
1:A:219:ARG:O	1:A:223:THR:OG1	2.24	0.46
1:C:93:LEU:O	1:C:95:LYS:N	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:388:ASP:OD2	1:D:389:VAL:N	2.48	0.46
1:A:174:PHE:O	1:A:177:ASN:N	2.48	0.46
1:C:223:THR:OG1	1:C:299:ARG:HG3	2.16	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:C:326:PHE:HA	1:C:331:TYR:HD2	1.82	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
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:A:190:GLN:HE22	1:A:239:ASN:HD22	1.66	0.44
1:C:91:VAL:HG22	1:A:98:MET:HE1	1.99	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:B:91:VAL:HA	1:D:98:MET:HE1	1.99	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:136:ILE:O	1:D:139:PHE:HB3	2.17	0.43
1:D:98:MET:HG3	1:D:181:PHE:HA	2.01	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:155:PHE:O	1:C:156:ASP:C	2.56	0.43
1:B:284:ILE:HA	1:B:287:MET:CE	2.49	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:C:163:PRO:HB3	1:C:171:TRP:CZ3	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:300:TYR:CZ	1:D:301:ARG:HG3	2.54	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:136:ILE:O	1:C:140:ARG:HG3	2.20	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:387:TYR:O	1:C:391:VAL:HG23	2.20	0.42
1:C:144:ASN:HB3	2:C:501:O3J:C8	2.49	0.42
1:A:182:ILE:CD1	1:A:225:ALA:HA	2.50	0.41
1:A:270:LEU:HD23	1:A:270:LEU:N	2.35	0.41
1:C:243:HIS:HB3	3:C:639:HOH:O	2.19	0.41
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:OE1	1:C:272:GLN:HA	2.20	0.41
1:C:92:LYS:O	1:C:93:LEU:HB2	2.21	0.41
1:A:361:ARG:HG3	3:A:612:HOH:O	2.20	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:C:340:HIS:NE2	1:C:377:ARG:CG	2.83	0.41
1:D:218:PHE:HA	1:D:218:PHE:HD1	1.81	0.41
1:B:226:ALA:HB2	1:B:295:ILE:HD13	2.03	0.41
1:B:360:ASN:O	1:B:361:ARG:O	2.39	0.41
1:C:109:TYR:CE2	1:C:193:ILE:HG23	2.56	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:D:388:ASP:C	1:D:388:ASP:OD2	2.58	0.41
1:C:162:TYR:CD1	1:C:217:ALA:HB2	2.56	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:C:142:MET:HE3	1:C:146:GLU:HG2	2.03	0.40
1:D:234:VAL:CA	1:D:288:MET:HE2	2.51	0.40
1:A:292:PHE:O	1:A:297:VAL:HG13	2.22	0.40
1:C:166:MET:HG2	1:C:171:TRP:CD1	2.57	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%)	5	23
1	B	292/339 (86%)	265 (91%)	23 (8%)	4 (1%)	11	40
1	C	311/339 (92%)	289 (93%)	15 (5%)	7 (2%)	6	27
1	D	307/339 (91%)	280 (91%)	19 (6%)	8 (3%)	5	24
All	All	1199/1356 (88%)	1089 (91%)	83 (7%)	27 (2%)	6	27

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

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Mol	Chain	Res	Type
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 [i](#)

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%)	242 (90%)	27 (10%)	7 27
1	B	271/306 (89%)	246 (91%)	25 (9%)	9 31
1	C	285/306 (93%)	244 (86%)	41 (14%)	3 14
1	D	283/306 (92%)	250 (88%)	33 (12%)	5 21
All	All	1108/1224 (90%)	982 (89%)	126 (11%)	5 22

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	86	THR
1	C	99	GLN
1	C	111	GLN
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	199	MET
1	C	212	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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
1	C	276	GLU
1	C	283	GLU
1	C	286	ASN
1	C	290	SER
1	C	320	LYS
1	C	324	ASP
1	C	342	ARG
1	C	363	LEU
1	C	373	ARG
1	C	377	ARG
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	111	GLN
1	A	114	ASP
1	A	115	ILE
1	A	121	ILE
1	A	133	THR
1	A	136	ILE
1	A	137	GLU
1	A	196	ASP
1	A	219	ARG
1	A	235	ASN
1	A	250	GLN
1	A	275	LYS
1	A	290	SER
1	A	293	LYS
1	A	322	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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	376	ASP
1	A	396	LEU
1	A	401	LEU
1	B	111	GLN
1	B	131	ARG
1	B	136	ILE
1	B	141	ASN
1	B	146	GLU
1	B	170	GLN
1	B	172	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	251	TYR
1	B	278	GLN
1	B	342	ARG
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	B	402	HIS
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	173	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	194	ILE
1	D	196	ASP
1	D	197	GLU
1	D	199	MET
1	D	214	GLN
1	D	218	PHE
1	D	219	ARG
1	D	230	MET
1	D	241	SER
1	D	254	GLU
1	D	257	LYS
1	D	269	LEU
1	D	282	ASP
1	D	289	ASN
1	D	299	ARG
1	D	320	LYS
1	D	322	TYR
1	D	349	LYS
1	D	359	THR
1	D	361	ARG
1	D	367	LEU
1	D	373	ARG
1	D	377	ARG
1	D	388	ASP
1	D	396	LEU
1	D	401	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	99	GLN
1	C	235	ASN
1	C	256	ASN
1	C	264	ASN
1	C	281	GLN
1	C	289	ASN
1	A	190	GLN
1	A	250	GLN
1	A	281	GLN
1	B	235	ASN
1	B	278	GLN
1	B	360	ASN

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Mol	Chain	Res	Type
1	D	99	GLN
1	D	143	GLN
1	D	214	GLN
1	D	244	GLN
1	D	360	ASN

### 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 carbohydrates 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	$\# Z  > 2$
2	O3J	A	501	-	19,19,19	0.78	0	24,24,24	1.24	2 (8%)
2	O3J	B	501	-	19,19,19	1.12	1 (5%)	24,24,24	1.35	3 (12%)
2	O3J	C	501	-	19,19,19	1.09	1 (5%)	24,24,24	1.41	4 (16%)
2	O3J	D	501	-	19,19,19	1.08	1 (5%)	24,24,24	1.06	1 (4%)

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	A	501	-	-	5/10/20/20	0/2/2/2
2	O3J	B	501	-	-	3/10/20/20	1/2/2/2
2	O3J	C	501	-	-	4/10/20/20	1/2/2/2
2	O3J	D	501	-	-	4/10/20/20	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	2.43	1.53	1.46
2	D	501	O3J	C2-N	-2.40	1.42	1.47
2	B	501	O3J	C3-C2	2.05	1.59	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	O3J	C5-C4-N1	-4.05	103.63	113.84
2	C	501	O3J	C4-N1-C3	-3.39	102.58	111.23
2	D	501	O3J	C5-C4-N1	-3.31	105.48	113.84
2	C	501	O3J	C3-N1-C13	3.24	116.12	108.83
2	B	501	O3J	C5-C4-N1	-2.87	106.60	113.84
2	A	501	O3J	C2-C3-N1	-2.51	105.48	110.64
2	C	501	O3J	C4-C5-C6	-2.41	106.60	113.20
2	B	501	O3J	C12-C7-C8	2.30	121.78	118.17
2	C	501	O3J	C2-C3-N1	-2.18	106.18	110.64
2	B	501	O3J	C4-C5-C6	-2.04	107.61	113.20

There are no chirality outliers.

All (16) 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	B	501	O3J	C5-C6-C7-C8
2	C	501	O3J	C5-C6-C7-C12
2	B	501	O3J	C5-C6-C7-C12

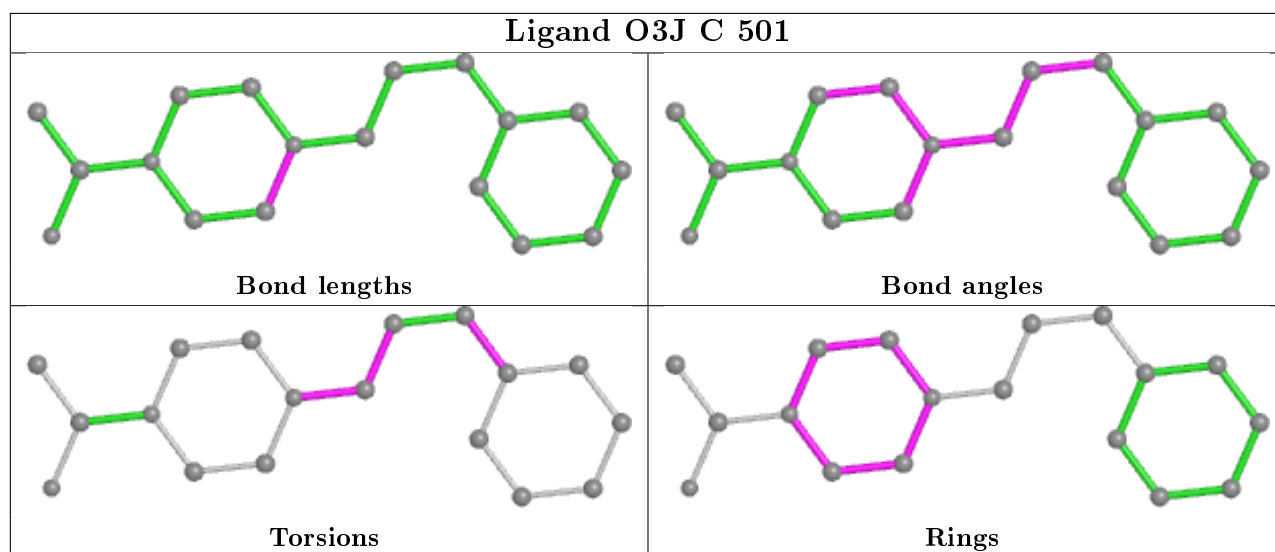
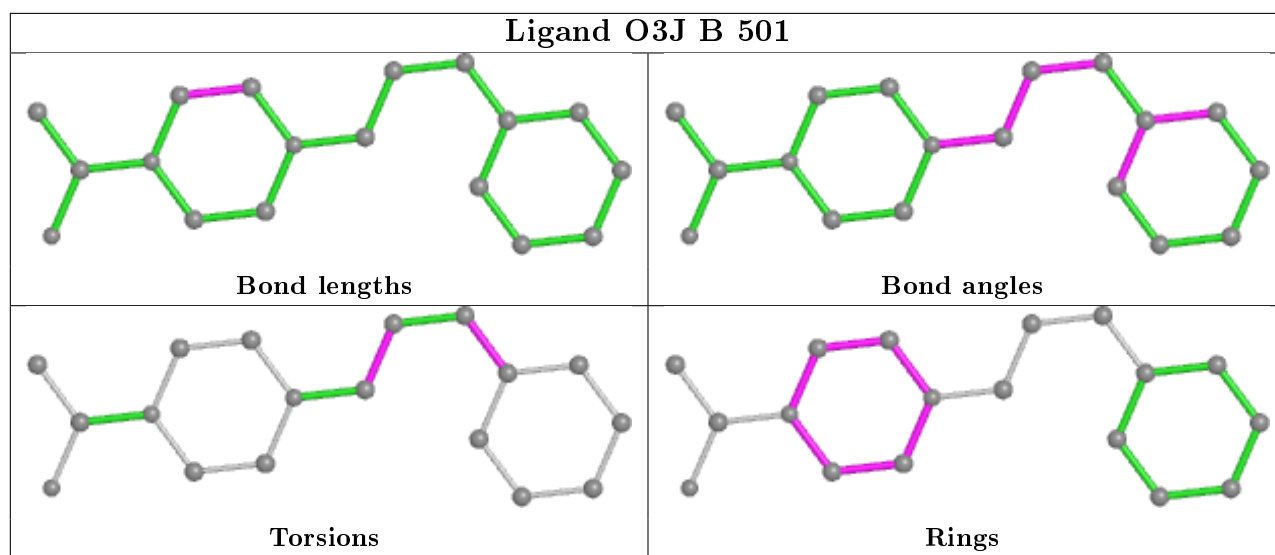
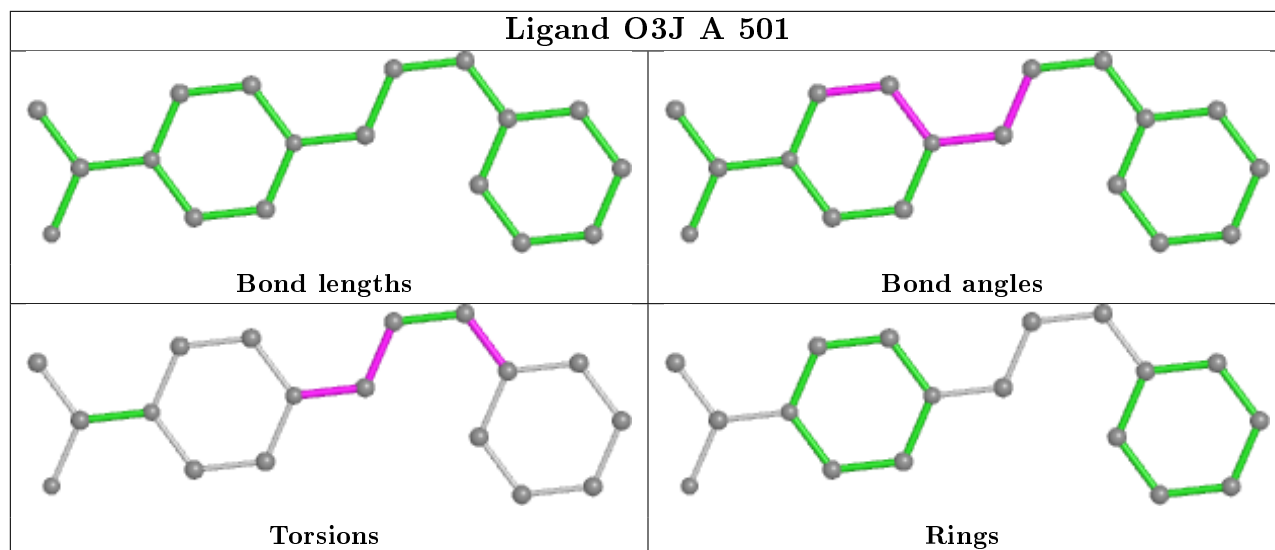
All (3) ring outliers are listed below:

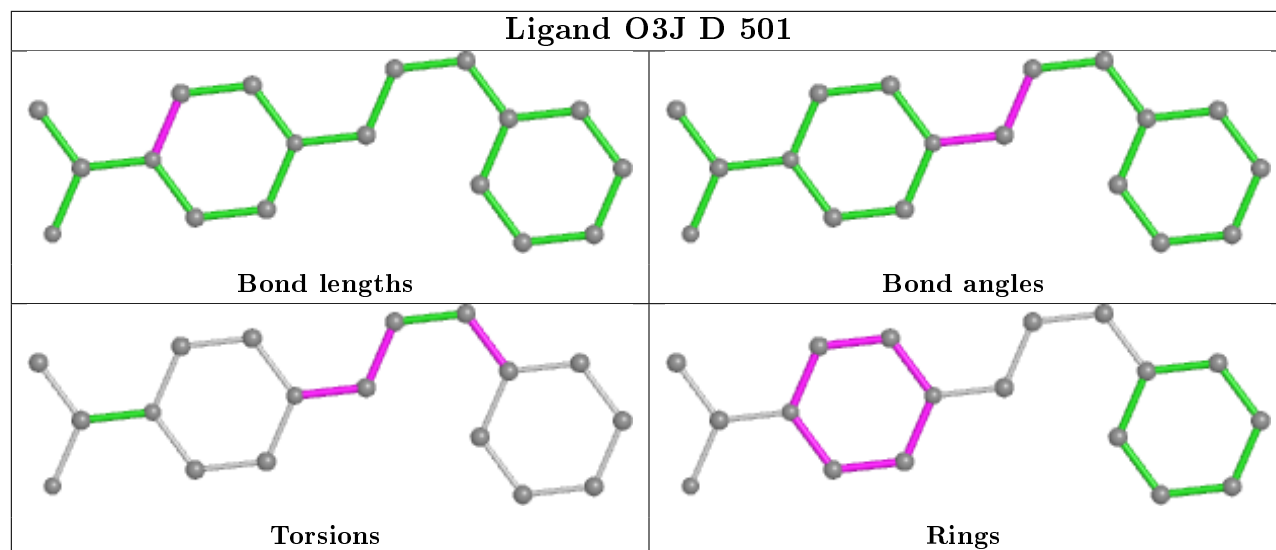
Mol	Chain	Res	Type	Atoms
2	C	501	O3J	C13-C14-C2-C3-N-N1
2	D	501	O3J	C13-C14-C2-C3-N-N1
2	B	501	O3J	C13-C14-C2-C3-N-N1

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	O3J	1	0
2	B	501	O3J	4	0
2	C	501	O3J	4	0
2	D	501	O3J	3	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.





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	297/339 (87%)	0.35	17 (5%) 23 8	62, 101, 154, 208	6 (2%)
1	B	298/339 (87%)	0.03	4 (1%) 77 51	59, 97, 143, 179	6 (2%)
1	C	315/339 (92%)	-0.03	6 (1%) 66 38	55, 90, 134, 179	2 (0%)
1	D	311/339 (91%)	0.00	3 (0%) 82 59	49, 83, 133, 157	7 (2%)
All	All	1221/1356 (90%)	0.09	30 (2%) 57 28	49, 93, 140, 208	21 (1%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	250	GLN	19.0
1	A	249	ARG	11.8
1	A	247	THR	9.2
1	A	248	GLN	7.9
1	A	144	ASN	4.4
1	C	262	ARG	4.3
1	A	246	ASN	4.3
1	A	145	ALA	3.6
1	A	271	LEU	3.5
1	B	143	GLN	3.4
1	C	337	TRP	3.2
1	A	143	GLN	3.1
1	B	144	ASN	2.9
1	A	146	GLU	2.8
1	C	330	SER	2.8
1	C	146	GLU	2.8
1	A	147	ILE	2.7
1	D	145	ALA	2.6
1	D	144	ASN	2.6
1	A	274	ARG	2.5
1	A	329	ASP	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	361	ARG	2.4
1	C	144	ASN	2.4
1	B	251	TYR	2.4
1	A	245	ASP	2.3
1	A	161	ASP	2.2
1	D	142	MET	2.1
1	B	209	GLY	2.1
1	A	267	LEU	2.0
1	A	339	LEU	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 carbohydrates in this entry.

## 6.4 Ligands [\(i\)](#)

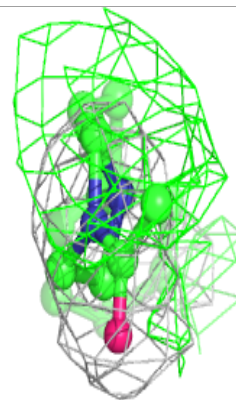
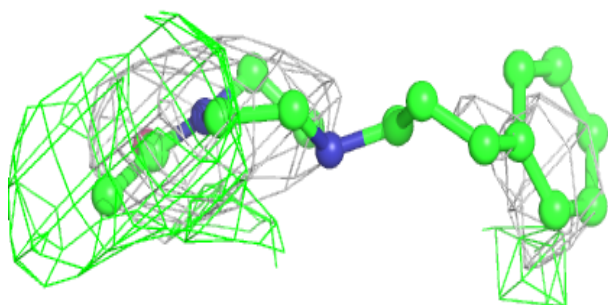
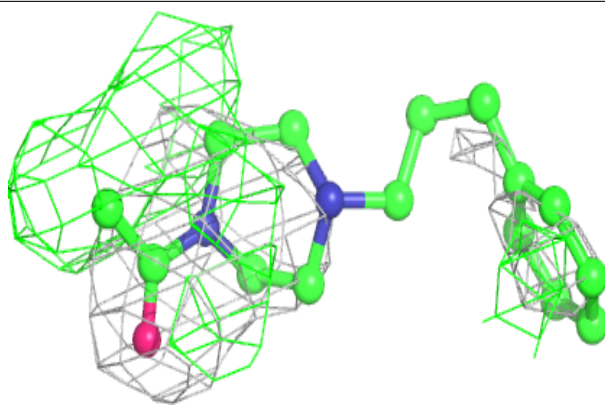
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	0.67	0.62	53,65,77,79	18
2	O3J	A	501	18/18	0.69	0.60	39,42,45,45	18
2	O3J	D	501	18/18	0.83	0.48	37,42,54,60	18
2	O3J	B	501	18/18	0.84	0.58	53,60,65,65	18

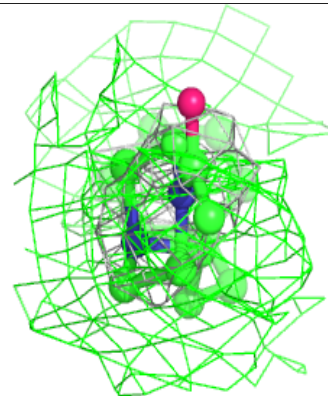
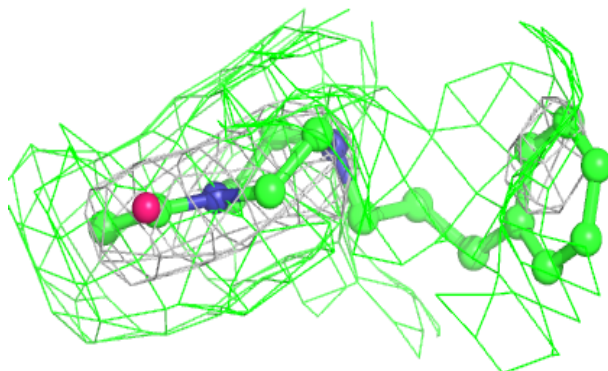
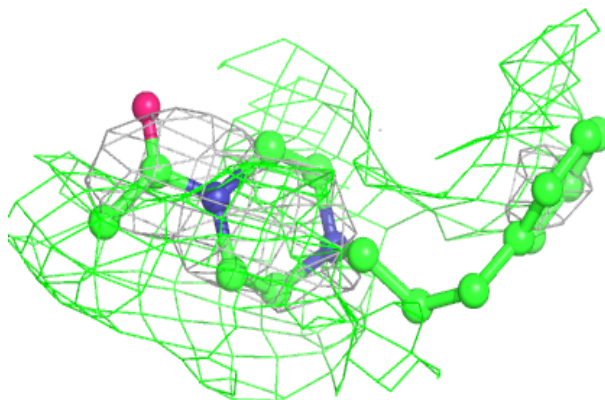
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

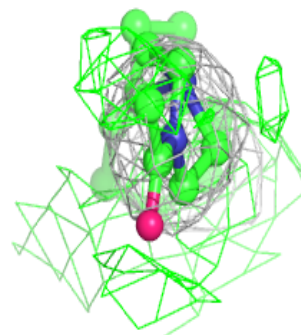
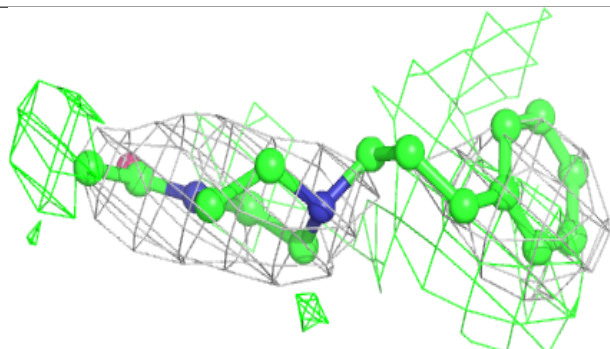
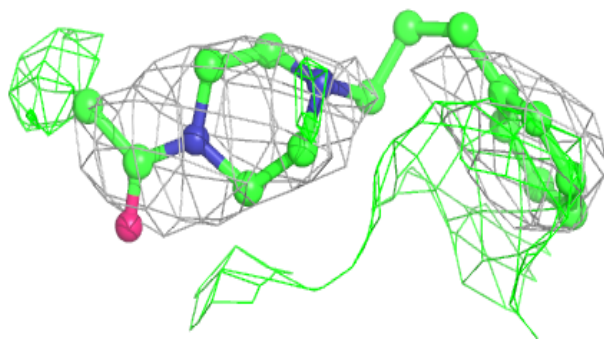
**Electron density around O3J A 501:**

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

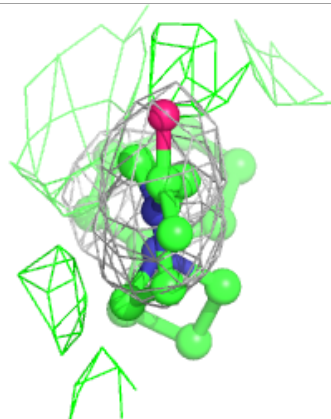
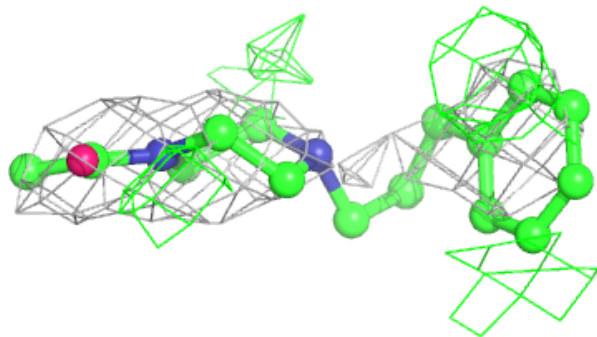
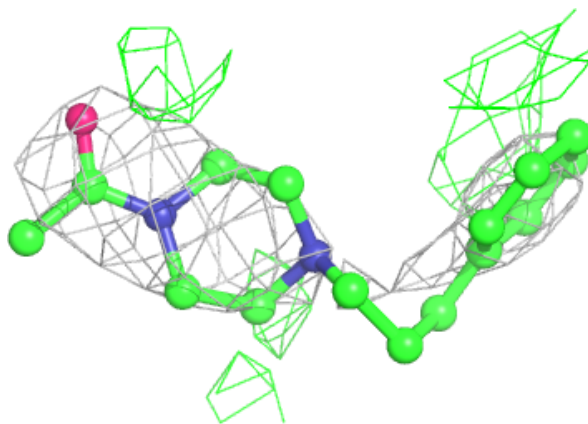


**Electron density around O3J D 501:**

$2mF_o-DF_c$  (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.