Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 08:08 am BST

PDB ID	:	5QSV
Title	:	PanDDA analysis group deposition – Crystal Structure of human STAG1 in complex with Z2856434783
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	:	2.76 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 following versions of software and data (see references ⓘ) were used in the production of this report:

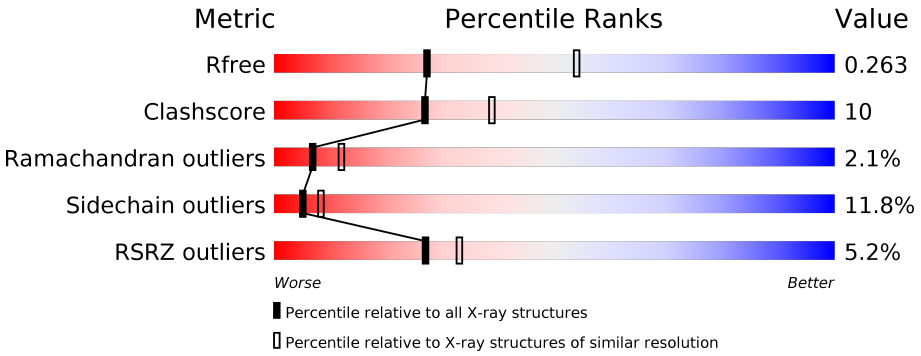
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.76 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 >=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 <=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	8% 61% 23% 12%
1	B	339	5% 64% 21% 12%
1	C	339	% 65% 24% 7%
1	D	339	4% 63% 23% 5% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10211 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.

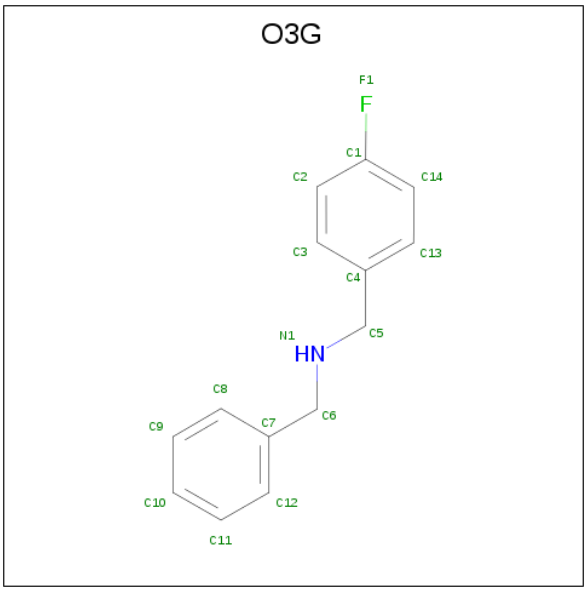
- Molecule 1 is a protein called Cohesin subunit SA-1.

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 N-benzyl-1-(4-fluorophenyl)methanamine (three-letter code: O3G) (formula: $C_{14}H_{14}FN$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C F N 16 14 1 1	0	0

- Molecule 3 is water.

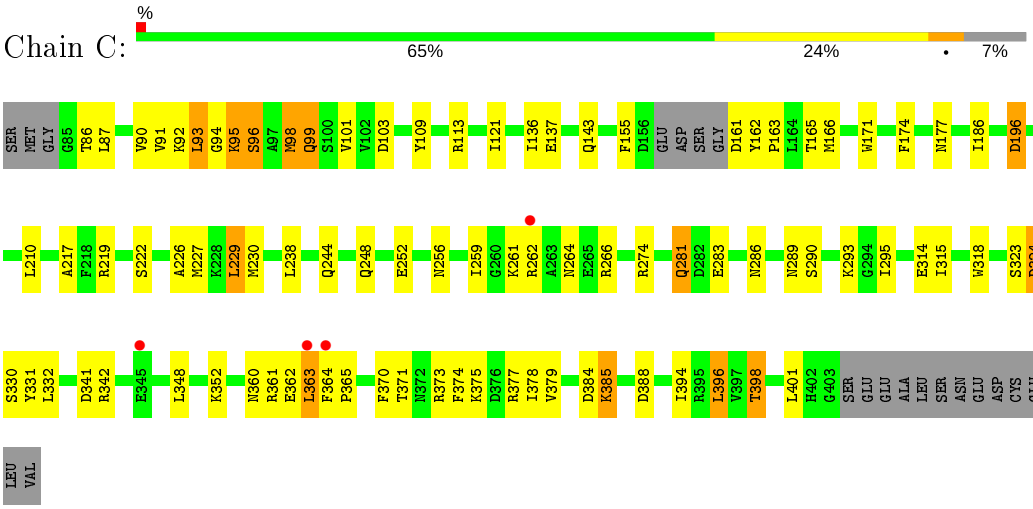
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	42	Total O 42 42	0	0
3	A	37	Total O 37 37	0	0
3	B	26	Total O 26 26	0	0
3	D	53	Total O 53 53	0	0

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.

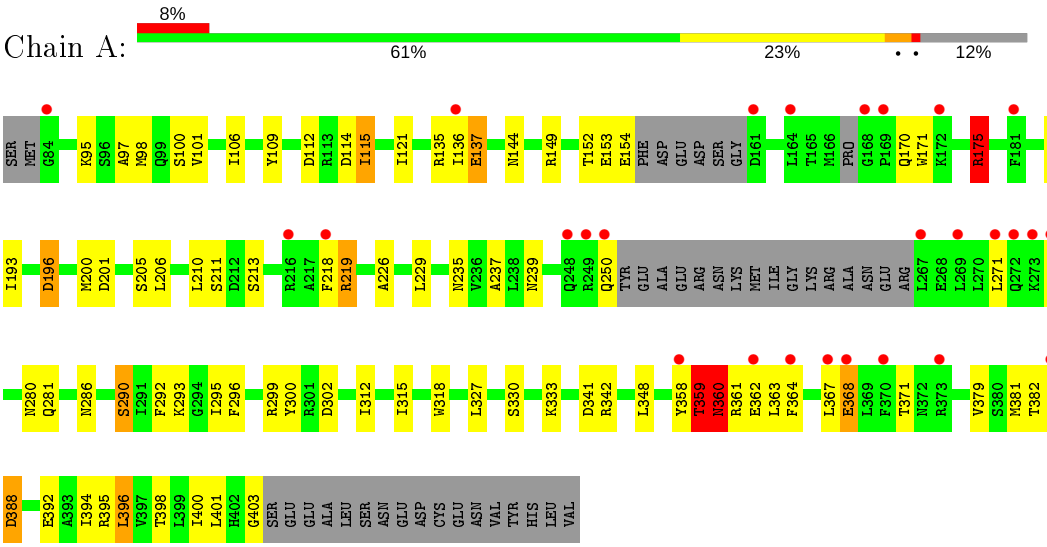
- Molecule 1: Cohesin subunit SA-1

Chain C:



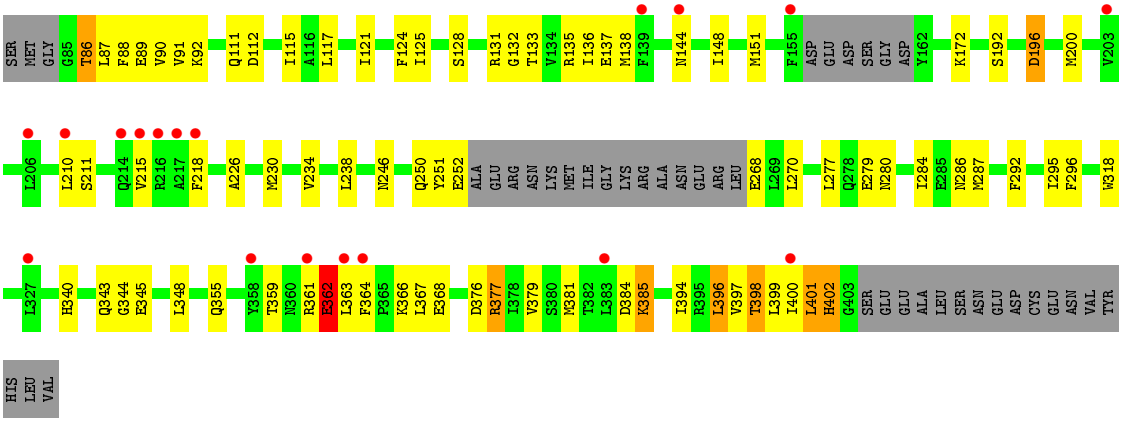
- Molecule 1: Cohesin subunit SA-1

Chain A:



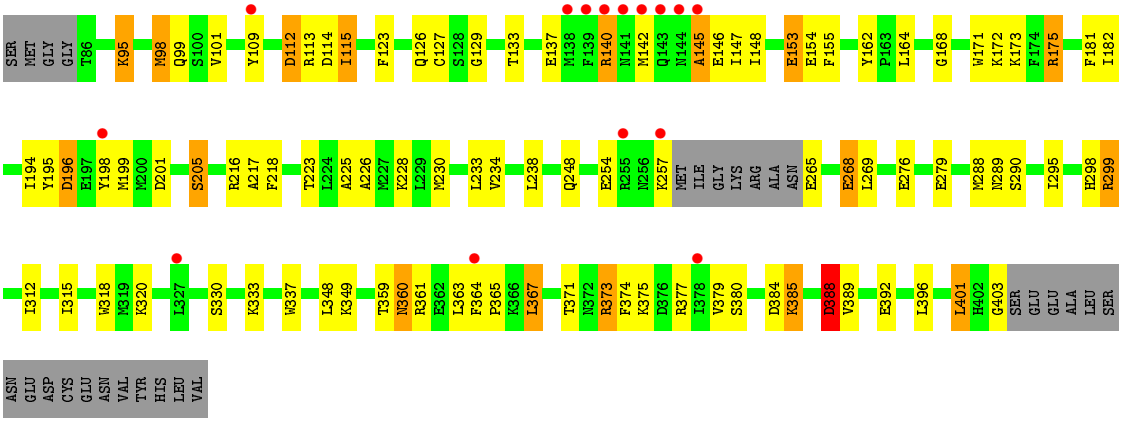
- Molecule 1: Cohesin subunit SA-1

Chain B:



- Molecule 1: Cohesin subunit SA-1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	66.44Å 71.75Å 118.78Å 95.13° 99.21° 115.27°	Depositor
Resolution (Å)	58.68 – 2.76 58.61 – 2.76	Depositor EDS
% Data completeness (in resolution range)	97.3 (58.68-2.76) 97.3 (58.61-2.76)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.198 , 0.264 0.208 , 0.263	Depositor DCC
R_{free} test set	2393 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	88.5	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 68.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10211	wwPDB-VP
Average B, all atoms (Å^2)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.80% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: O3G

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	0.72	0/2470	0.85	1/3319 (0.0%)
1	B	0.71	0/2493	0.84	0/3353
1	C	0.68	0/2633	0.85	1/3539 (0.0%)
1	D	0.68	0/2603	0.86	0/3501
All	All	0.70	0/10199	0.85	2/13712 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	175	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	C	196	ASP	CB-CA-C	6.40	123.20	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	359	THR	Peptide
1	D	168	GLY	Peptide

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	58	0
1	B	2452	0	2471	56	1
1	C	2591	0	2613	47	0
1	D	2561	0	2568	57	1
2	D	16	0	0	0	0
3	A	37	0	0	6	0
3	B	26	0	0	5	0
3	C	42	0	0	4	0
3	D	53	0	0	4	0
All	All	10211	0	10109	206	1

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	1.45	1.17
1:A:361:ARG:O	3:A:501:HOH:O	1.82	0.95
1:B:394:ILE:O	1:B:398:THR:HG22	1.66	0.94
1:D:98:MET:SD	3:D:638:HOH:O	2.24	0.93
1:D:216:ARG:HD3	3:D:639:HOH:O	1.70	0.91
1:C:95:LYS:CE	1:C:103:ASP:OD2	2.20	0.90
1:D:114:ASP:OD2	1:D:140:ARG:NH2	2.15	0.79
1:B:230:MET:HG2	1:B:318:TRP:CZ2	2.21	0.76
1:A:135:ARG:NH1	1:A:137:GLU:OE2	2.18	0.76
1:B:86:THR:HG22	1:B:89:GLU:H	1.53	0.74
1:D:153:GLU:O	1:D:155:PHE:N	2.21	0.74
1:A:153:GLU:O	1:A:154:GLU:HG3	1.88	0.72
1:C:289:ASN:ND2	3:C:501:HOH:O	2.15	0.71
1:B:246:ASN:O	1:B:250:GLN:HG3	1.92	0.69
1:C:226:ALA:HB2	1:C:295:ILE:HD13	1.77	0.67
1:B:91:VAL:HG22	1:D:98:MET:CE	2.25	0.66
1:C:226:ALA:CB	1:C:295:ILE:HD13	2.24	0.66
1:A:388:ASP:O	1:A:392:GLU:HG2	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:MET:HE3	1:A:98:MET:HA	1.80	0.63
1:B:117:LEU:O	1:B:121:ILE:HG12	1.98	0.62
1:D:333:LYS:HD2	1:D:337:TRP:CH2	2.34	0.61
1:B:394:ILE:O	1:B:398:THR:CG2	2.46	0.61
1:D:164:LEU:HD22	1:D:175:ARG:HG3	1.82	0.60
1:D:315:ILE:HA	1:D:318:TRP:CE3	2.36	0.60
1:B:200:MET:HG3	1:B:287:MET:SD	2.42	0.60
1:C:384:ASP:O	1:C:385:LYS:HB2	2.02	0.60
1:C:96:SER:HB3	1:C:99:GLN:HG3	1.84	0.60
1:A:226:ALA:HB2	1:A:295:ILE:HD13	1.83	0.59
1:B:340:HIS:CE1	1:B:377:ARG:HG3	2.37	0.59
1:D:164:LEU:CD2	1:D:175:ARG:HG3	2.32	0.59
1:A:394:ILE:HD12	1:B:401:LEU:HD12	1.85	0.59
1:A:296:PHE:CZ	1:A:315:ILE:HD12	2.39	0.58
1:B:279:GLU:HB3	3:B:526:HOH:O	2.02	0.58
1:B:112:ASP:HB3	1:B:115:ILE:HG12	1.85	0.58
1:A:388:ASP:HB3	3:A:533:HOH:O	2.02	0.58
1:A:200:MET:HE1	1:A:229:LEU:HD11	1.85	0.58
1:A:237:ALA:HB1	1:A:281:GLN:HE22	1.69	0.58
1:D:109:TYR:CZ	1:D:113:ARG:HG2	2.38	0.58
1:B:384:ASP:O	1:B:385:LYS:HB2	2.04	0.57
1:D:145:ALA:O	1:D:148:ILE:N	2.35	0.57
1:A:392:GLU:OE1	1:A:395:ARG:NH1	2.37	0.57
1:D:384:ASP:O	1:D:385:LYS:HB3	2.04	0.57
1:C:101:VAL:HG23	3:C:518:HOH:O	2.05	0.57
1:D:248:GLN:HA	1:D:248:GLN:OE1	2.06	0.56
1:D:298:HIS:HD2	3:D:651:HOH:O	1.88	0.55
1:A:112:ASP:HB3	1:A:115:ILE:CD1	2.36	0.55
1:C:394:ILE:O	1:C:398:THR:HG22	2.07	0.55
1:C:341:ASP:OD1	3:C:502:HOH:O	2.18	0.55
1:D:230:MET:HG2	1:D:318:TRP:CE2	2.41	0.55
1:D:312:ILE:O	1:D:315:ILE:HG22	2.06	0.55
1:D:373:ARG:HG2	1:D:374:PHE:CE2	2.41	0.55
1:D:384:ASP:O	1:D:385:LYS:CB	2.54	0.55
1:C:162:TYR:CE2	1:C:165:THR:HG23	2.42	0.54
1:B:144:ASN:O	1:B:148:ILE:HD12	2.07	0.54
1:C:244:GLN:OE1	1:C:281:GLN:OE1	2.24	0.54
1:D:388:ASP:OD2	1:D:389:VAL:N	2.41	0.54
1:B:284:ILE:HA	1:B:287:MET:CE	2.38	0.54
1:C:315:ILE:HA	1:C:318:TRP:CE3	2.43	0.54
1:C:360:ASN:ND2	1:C:363:LEU:HG	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:THR:O	1:A:360:ASN:HB2	2.09	0.53
1:B:132:GLY:HA2	3:B:525:HOH:O	2.09	0.53
1:C:230:MET:HG2	1:C:318:TRP:CE2	2.44	0.53
1:A:106:ILE:HD11	1:A:188:GLN:HB2	1.90	0.52
1:A:226:ALA:CB	1:A:295:ILE:HD13	2.39	0.52
1:B:377:ARG:HD3	1:B:377:ARG:O	2.09	0.52
1:D:371:THR:O	1:D:375:LYS:HB2	2.09	0.52
1:D:388:ASP:O	1:D:392:GLU:HG2	2.10	0.52
1:B:226:ALA:HB2	1:B:295:ILE:HD13	1.92	0.52
1:A:396:LEU:HD22	1:A:400:ILE:HD11	1.91	0.52
1:A:396:LEU:HD22	1:A:400:ILE:CD1	2.40	0.52
1:D:98:MET:HB2	3:D:604:HOH:O	2.10	0.52
1:A:299:ARG:NH1	1:A:302:ASP:OD2	2.42	0.51
1:D:162:TYR:CD1	1:D:217:ALA:HB2	2.46	0.51
1:C:162:TYR:CD1	1:C:217:ALA:HB2	2.45	0.51
1:C:352:LYS:HA	1:C:352:LYS:HE2	1.92	0.51
1:B:135:ARG:NH1	3:B:501:HOH:O	2.44	0.51
1:A:286:ASN:O	1:A:290:SER:OG	2.29	0.51
1:A:201:ASP:O	1:A:205:SER:OG	2.18	0.50
1:D:276:GLU:O	1:D:279:GLU:HB2	2.11	0.50
1:B:91:VAL:HG13	1:D:98:MET:HE2	1.94	0.50
1:A:295:ILE:O	1:A:299:ARG:HG2	2.12	0.50
1:A:106:ILE:CD1	1:A:188:GLN:HB2	2.41	0.50
1:D:123:PHE:CE1	1:D:127:CYS:SG	3.05	0.50
1:B:234:VAL:O	1:B:238:LEU:HB2	2.13	0.49
1:A:109:TYR:CE2	1:A:193:ILE:HG23	2.48	0.49
1:B:91:VAL:HG22	1:D:98:MET:HE1	1.92	0.49
1:A:121:ILE:HD12	1:A:206:LEU:HD22	1.94	0.49
1:B:125:ILE:HG21	1:B:132:GLY:HA3	1.94	0.49
1:A:153:GLU:O	1:A:154:GLU:CG	2.58	0.49
1:D:234:VAL:HA	1:D:288:MET:CE	2.43	0.49
1:A:97:ALA:O	1:A:101:VAL:CG1	2.61	0.48
1:B:215:VAL:HB	1:B:218:PHE:HD2	1.78	0.48
1:A:210:LEU:HD22	1:A:218:PHE:CD1	2.47	0.48
1:B:210:LEU:HD22	1:B:218:PHE:CD1	2.48	0.48
1:C:324:ASP:OD2	1:C:324:ASP:N	2.45	0.48
1:C:378:ILE:HG23	1:C:396:LEU:HD13	1.95	0.48
1:C:162:TYR:CD1	1:C:217:ALA:HA	2.48	0.48
1:B:292:PHE:CE1	1:B:296:PHE:CD1	3.01	0.48
1:D:234:VAL:N	1:D:288:MET:HE2	2.28	0.48
1:D:360:ASN:HD22	1:D:360:ASN:C	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:GLY:O	1:B:133:THR:HG23	2.13	0.47
1:C:91:VAL:HG22	1:A:98:MET:CE	2.44	0.47
1:B:344:GLY:N	3:B:503:HOH:O	2.47	0.47
1:C:91:VAL:HG22	1:A:98:MET:HE2	1.96	0.47
1:D:182:ILE:CD1	1:D:225:ALA:HA	2.45	0.47
1:A:149:ARG:O	1:A:152:THR:HB	2.14	0.47
1:B:91:VAL:HA	1:D:98:MET:HE1	1.96	0.47
1:B:359:THR:HA	1:B:399:LEU:HD22	1.97	0.47
1:B:250:GLN:HB3	1:B:270:LEU:HD11	1.96	0.47
1:C:371:THR:O	1:C:375:LYS:HB3	2.15	0.47
1:B:246:ASN:O	1:B:250:GLN:CG	2.61	0.47
1:B:284:ILE:HA	1:B:287:MET:HE3	1.97	0.46
1:D:265:GLU:O	1:D:268:GLU:HG2	2.16	0.46
1:A:384:ASP:O	1:A:385:LYS:CB	2.63	0.46
1:C:174:PHE:HB2	3:A:512:HOH:O	2.15	0.46
1:D:145:ALA:O	1:D:147:ILE:N	2.49	0.46
1:D:112:ASP:HB3	1:D:115:ILE:HD12	1.96	0.46
1:D:195:TYR:C	1:D:196:ASP:O	2.53	0.46
1:B:125:ILE:HG23	1:B:151:MET:SD	2.56	0.46
1:D:95:LYS:HD2	1:D:99:GLN:HG2	1.97	0.46
1:A:277:LEU:O	1:A:280:ASN:HB2	2.16	0.46
1:C:326:PHE:HA	1:C:331:TYR:CD2	2.51	0.45
1:C:326:PHE:HA	1:C:331:TYR:HD2	1.82	0.45
1:A:196:ASP:C	1:A:196:ASP:OD1	2.54	0.45
1:B:355:GLN:O	1:B:359:THR:HG23	2.17	0.45
1:D:388:ASP:OD2	1:D:388:ASP:C	2.55	0.45
1:B:124:PHE:O	1:B:128:SER:OG	2.27	0.45
1:C:121:ILE:HG12	1:C:206:LEU:HD22	1.98	0.45
1:C:143:GLN:HE21	1:C:143:GLN:HA	1.82	0.45
1:C:163:PRO:HB3	1:C:171:TRP:CZ3	2.51	0.45
1:C:93:LEU:HG	1:C:93:LEU:O	2.17	0.45
1:C:92:LYS:HE3	1:A:171:TRP:CH2	2.52	0.45
1:A:190:GLN:HE22	1:A:239:ASN:HD22	1.65	0.45
1:D:98:MET:HG3	1:D:181:PHE:HA	1.99	0.45
1:A:327:LEU:HD23	1:A:363:LEU:HG	1.99	0.44
1:A:383:LEU:HD12	1:B:379:VAL:CG1	2.47	0.44
1:C:327:LEU:CD1	1:C:332:LEU:HD11	2.48	0.44
1:D:230:MET:HG2	1:D:318:TRP:CZ2	2.53	0.44
1:A:381:MET:O	1:A:384:ASP:HB2	2.18	0.44
1:B:230:MET:HG2	1:B:318:TRP:CH2	2.52	0.44
1:B:284:ILE:HD13	1:B:287:MET:CE	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:ILE:HA	1:A:318:TRP:CE3	2.53	0.44
1:B:277:LEU:O	1:B:280:ASN:HB2	2.18	0.44
1:A:388:ASP:CB	3:A:533:HOH:O	2.62	0.44
1:A:98:MET:HA	1:A:101:VAL:HG13	2.00	0.44
1:D:137:GLU:HA	1:D:140:ARG:HB2	1.99	0.44
1:C:227:MET:HB3	1:C:314:GLU:HG2	1.99	0.43
1:D:363:LEU:O	1:D:367:LEU:HD22	2.17	0.43
1:A:98:MET:CE	1:A:98:MET:HA	2.46	0.43
1:D:238:LEU:HA	1:D:238:LEU:HD12	1.81	0.43
1:A:213:SER:O	1:A:219:ARG:HD3	2.18	0.43
1:C:98:MET:CE	1:C:177:ASN:O	2.66	0.43
1:C:200:MET:HE1	1:C:229:LEU:HD21	2.00	0.43
1:B:92:LYS:HD2	1:D:171:TRP:CH2	2.53	0.43
1:D:201:ASP:O	1:D:205:SER:HB2	2.18	0.43
1:A:312:ILE:O	1:A:315:ILE:HG22	2.19	0.43
1:A:358:TYR:O	1:A:360:ASN:N	2.51	0.43
1:A:364:PHE:CE1	1:A:403:GLY:HA3	2.53	0.43
1:A:395:ARG:O	1:A:398:THR:OG1	2.35	0.43
1:C:109:TYR:CZ	1:C:113:ARG:HG2	2.54	0.43
1:D:364:PHE:N	1:D:365:PRO:CD	2.81	0.43
1:D:401:LEU:HA	1:D:401:LEU:HD23	1.86	0.43
1:B:343:GLN:NE2	1:B:343:GLN:HA	2.34	0.42
1:B:86:THR:O	1:B:90:VAL:HG23	2.19	0.42
1:C:384:ASP:O	1:C:385:LYS:CB	2.67	0.42
1:C:87:LEU:O	1:C:91:VAL:HG23	2.20	0.42
1:A:292:PHE:O	1:A:296:PHE:HB3	2.19	0.42
1:A:97:ALA:HB3	3:A:510:HOH:O	2.19	0.42
1:D:153:GLU:C	1:D:155:PHE:H	2.19	0.42
1:D:226:ALA:CB	1:D:295:ILE:HD13	2.50	0.42
1:C:92:LYS:O	1:C:93:LEU:HB2	2.20	0.42
1:D:234:VAL:HA	1:D:288:MET:HE1	2.01	0.42
1:B:361:ARG:O	1:B:362:GLU:CB	2.67	0.42
1:C:210:LEU:HB2	1:C:222:SER:HB3	2.02	0.42
1:D:228:LYS:HD3	1:D:228:LYS:HA	1.89	0.42
1:D:364:PHE:CE2	1:D:403:GLY:HA3	2.55	0.42
1:A:299:ARG:O	1:A:302:ASP:HB2	2.20	0.42
1:C:90:VAL:HG11	1:A:101:VAL:HB	2.02	0.42
1:A:360:ASN:HD22	1:A:360:ASN:HA	1.73	0.41
1:B:86:THR:CG2	1:B:88:PHE:HB3	2.49	0.41
1:C:162:TYR:CD1	1:C:217:ALA:CB	3.03	0.41
1:C:274:ARG:HG3	3:C:512:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ARG:HH11	1:A:175:ARG:HG3	1.85	0.41
1:B:196:ASP:C	1:B:196:ASP:OD1	2.59	0.41
1:B:396:LEU:HD22	1:B:400:ILE:CD1	2.50	0.41
1:D:330:SER:O	1:D:333:LYS:HE3	2.20	0.41
1:B:381:MET:O	1:B:384:ASP:HB2	2.20	0.41
1:B:210:LEU:HD22	1:B:218:PHE:HD1	1.86	0.41
1:A:97:ALA:O	1:A:101:VAL:HG12	2.20	0.41
1:B:343:GLN:NE2	1:B:343:GLN:CA	2.83	0.41
1:D:230:MET:O	1:D:233:LEU:N	2.53	0.41
1:B:121:ILE:HG22	1:B:125:ILE:HD11	2.02	0.41
1:B:86:THR:HG22	1:B:89:GLU:N	2.28	0.41
1:A:360:ASN:C	3:A:501:HOH:O	2.59	0.41
1:D:126:GLN:O	1:D:129:GLY:N	2.44	0.41
1:D:223:THR:OG1	1:D:299:ARG:HG3	2.20	0.41
1:B:363:LEU:O	1:B:367:LEU:HD22	2.20	0.41
1:A:382:THR:HB	1:B:397:VAL:HG11	2.02	0.41
1:B:87:LEU:O	1:B:91:VAL:HG23	2.21	0.41
1:C:93:LEU:O	1:C:95:LYS:N	2.41	0.41
1:C:370:PHE:CE1	1:C:374:PHE:CD2	3.08	0.40
1:C:248:GLN:OE1	1:C:274:ARG:HD2	2.21	0.40
1:C:364:PHE:HB3	1:C:365:PRO:HD3	2.03	0.40
1:A:170:GLN:CG	1:A:171:TRP:CD1	3.05	0.40
1:B:343:GLN:HB3	3:B:503:HOH:O	2.21	0.40
1:D:226:ALA:HB2	1:D:295:ILE:HD13	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:ASN:OD1	1:D:373:ARG:NH2[1_665]	2.10	0.10

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%)	249 (86%)	34 (12%)	6 (2%)	7	12
1	B	292/339 (86%)	254 (87%)	32 (11%)	6 (2%)	7	12
1	C	311/339 (92%)	285 (92%)	20 (6%)	6 (2%)	8	14
1	D	307/339 (91%)	274 (89%)	26 (8%)	7 (2%)	6	10
All	All	1199/1356 (88%)	1062 (89%)	112 (9%)	25 (2%)	7	12

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	93	LEU
1	A	360	ASN
1	B	385	LYS
1	D	146	GLU
1	D	154	GLU
1	C	94	GLY
1	C	259	ILE
1	C	385	LYS
1	A	359	THR
1	A	385	LYS
1	A	388	ASP
1	B	345	GLU
1	B	362	GLU
1	B	368	GLU
1	D	145	ALA
1	D	153	GLU
1	D	385	LYS
1	D	388	ASP
1	A	341	ASP
1	C	362	GLU
1	B	402	HIS
1	C	361	ARG
1	A	368	GLU
1	B	111	GLN
1	D	112	ASP

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%)	238 (88%)	31 (12%)	5 9
1	B	271/306 (89%)	249 (92%)	22 (8%)	11 21
1	C	285/306 (93%)	244 (86%)	41 (14%)	3 4
1	D	283/306 (92%)	246 (87%)	37 (13%)	4 6
All	All	1108/1224 (90%)	977 (88%)	131 (12%)	5 8

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	86	THR
1	C	95	LYS
1	C	96	SER
1	C	98	MET
1	C	99	GLN
1	C	136	ILE
1	C	137	GLU
1	C	155	PHE
1	C	161	ASP
1	C	166	MET
1	C	186	ILE
1	C	196	ASP
1	C	199	MET
1	C	219	ARG
1	C	229	LEU
1	C	238	LEU
1	C	252	GLU
1	C	256	ASN
1	C	261	LYS
1	C	262	ARG
1	C	264	ASN
1	C	266	ARG
1	C	281	GLN
1	C	283	GLU
1	C	286	ASN
1	C	290	SER
1	C	293	LYS
1	C	323	SER
1	C	324	ASP
1	C	327	LEU

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Mol	Chain	Res	Type
1	C	330	SER
1	C	342	ARG
1	C	348	LEU
1	C	363	LEU
1	C	373	ARG
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	95	LYS
1	A	100	SER
1	A	114	ASP
1	A	115	ILE
1	A	136	ILE
1	A	137	GLU
1	A	144	ASN
1	A	175	ARG
1	A	196	ASP
1	A	211	SER
1	A	219	ARG
1	A	235	ASN
1	A	250	GLN
1	A	271	LEU
1	A	274	ARG
1	A	275	LYS
1	A	290	SER
1	A	293	LYS
1	A	300	TYR
1	A	330	SER
1	A	333	LYS
1	A	342	ARG
1	A	348	LEU
1	A	360	ASN
1	A	362	GLU
1	A	367	LEU
1	A	368	GLU
1	A	371	THR
1	A	379	VAL
1	A	396	LEU
1	A	401	LEU

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Mol	Chain	Res	Type
1	B	86	THR
1	B	131	ARG
1	B	136	ILE
1	B	137	GLU
1	B	138	MET
1	B	172	LYS
1	B	192	SER
1	B	196	ASP
1	B	211	SER
1	B	251	TYR
1	B	252	GLU
1	B	268	GLU
1	B	348	LEU
1	B	362	GLU
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	95	LYS
1	D	98	MET
1	D	101	VAL
1	D	115	ILE
1	D	133	THR
1	D	140	ARG
1	D	142	MET
1	D	172	LYS
1	D	173	LYS
1	D	175	ARG
1	D	194	ILE
1	D	196	ASP
1	D	198	TYR
1	D	199	MET
1	D	205	SER
1	D	218	PHE
1	D	254	GLU
1	D	257	LYS
1	D	268	GLU
1	D	269	LEU

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Mol	Chain	Res	Type
1	D	289	ASN
1	D	290	SER
1	D	299	ARG
1	D	320	LYS
1	D	348	LEU
1	D	349	LYS
1	D	359	THR
1	D	360	ASN
1	D	361	ARG
1	D	367	LEU
1	D	373	ARG
1	D	377	ARG
1	D	379	VAL
1	D	380	SER
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 (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	143	GLN
1	C	235	ASN
1	C	250	GLN
1	C	256	ASN
1	C	264	ASN
1	C	281	GLN
1	C	289	ASN
1	A	190	GLN
1	A	214	GLN
1	A	235	ASN
1	A	239	ASN
1	A	281	GLN
1	A	343	GLN
1	A	360	ASN
1	A	402	HIS
1	B	111	GLN
1	B	144	ASN
1	B	278	GLN
1	B	280	ASN
1	B	289	ASN
1	B	343	GLN

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Mol	Chain	Res	Type
1	D	99	GLN
1	D	144	ASN
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)

1 ligand is 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	O3G	D	501	-	17,17,17	0.19	0	21,21,21	0.30	0

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	O3G	D	501	-	-	1/6/6/6	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

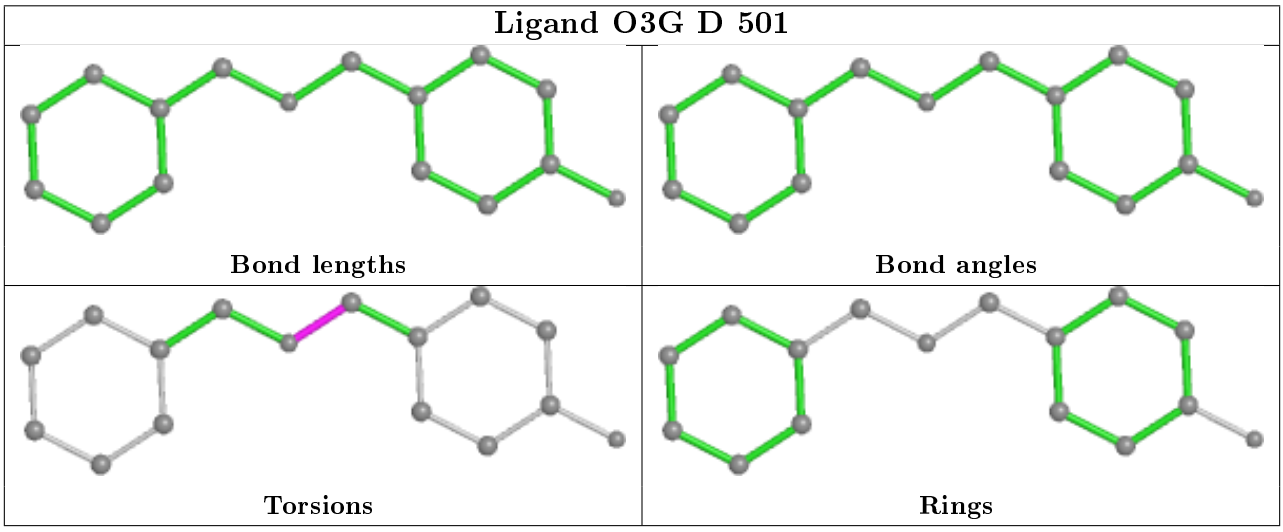
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	501	O3G	C4-C5-N1-C6

There are no ring outliers.

No monomer is involved in short contacts.

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 then 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

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^{th} 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%)	0.60	27 (9%) 9 10	65, 106, 156, 194	0
1	B	298/339 (87%)	0.35	18 (6%) 21 26	60, 103, 154, 191	0
1	C	315/339 (92%)	0.32	4 (1%) 77 84	52, 93, 135, 168	0
1	D	311/339 (91%)	0.45	15 (4%) 30 36	48, 86, 136, 172	9 (2%)
All	All	1221/1356 (90%)	0.43	64 (5%) 27 33	48, 98, 147, 194	9 (0%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	271	LEU	8.6
1	D	139	PHE	7.5
1	A	250	GLN	7.3
1	D	141	ASN	7.0
1	D	142	MET	7.0
1	D	138	MET	6.8
1	A	249	ARG	6.7
1	D	145	ALA	6.4
1	D	144	ASN	6.2
1	D	140	ARG	4.9
1	A	161	ASP	4.7
1	A	273	LYS	4.6
1	D	143	GLN	4.3
1	B	155	PHE	4.1
1	D	198	TYR	4.0
1	D	257	LYS	3.9
1	C	364	PHE	3.9
1	B	206	LEU	3.6
1	A	169	PRO	3.6
1	A	216	ARG	3.5
1	B	363	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	362	GLU	3.3
1	A	367	LEU	3.3
1	C	363	LEU	3.3
1	B	383	LEU	3.2
1	A	269	LEU	3.2
1	B	218	PHE	3.2
1	A	272	GLN	3.2
1	B	216	ARG	3.0
1	B	364	PHE	2.9
1	C	262	ARG	2.9
1	B	210	LEU	2.9
1	A	267	LEU	2.8
1	D	364	PHE	2.7
1	A	164	LEU	2.6
1	A	358	TYR	2.6
1	B	214	GLN	2.6
1	B	358	TYR	2.6
1	A	218	PHE	2.5
1	A	248	GLN	2.5
1	A	172	LYS	2.5
1	B	400	ILE	2.4
1	A	168	GLY	2.4
1	C	345	GLU	2.4
1	A	84	GLY	2.3
1	D	255	ARG	2.3
1	A	383	LEU	2.3
1	A	136	ILE	2.3
1	B	361	ARG	2.3
1	D	109	TYR	2.3
1	A	370	PHE	2.2
1	B	327	LEU	2.2
1	B	139	PHE	2.2
1	A	373	ARG	2.2
1	A	364	PHE	2.2
1	B	215	VAL	2.1
1	A	274	ARG	2.1
1	D	327	LEU	2.1
1	D	378	ILE	2.1
1	B	144	ASN	2.1
1	A	368	GLU	2.1
1	B	217	ALA	2.1
1	A	181	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	203	VAL	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)

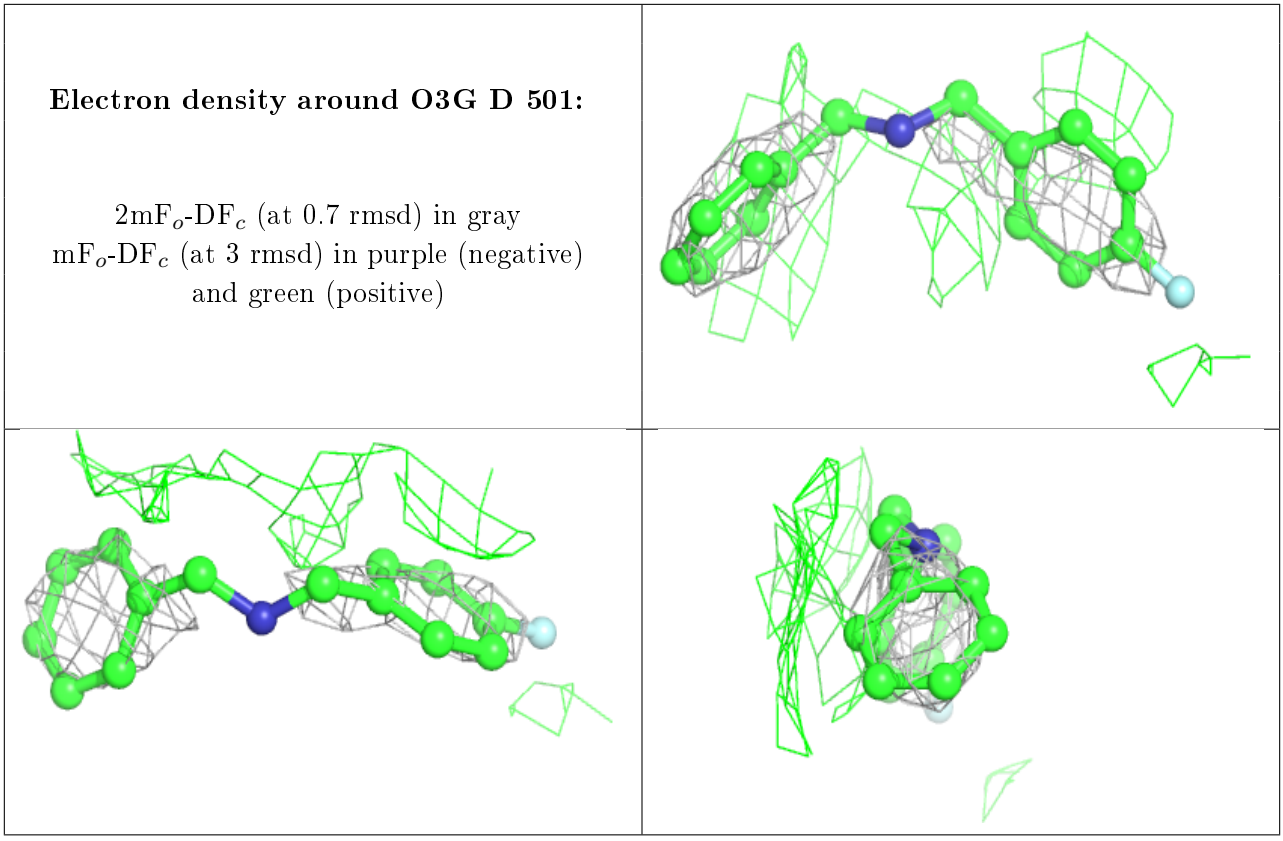
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	O3G	D	501	16/16	0.83	0.43	51,57,63,64	16

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 O3G 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)



6.5 Other polymers

There are no such residues in this entry.