



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:18 AM UTC

PDB ID : 5QST / pdb_00005qst
Title : PanDDA analysis group deposition – Crystal Structure of human STAG1 in complex with Z2447286438
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 : 2.58 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

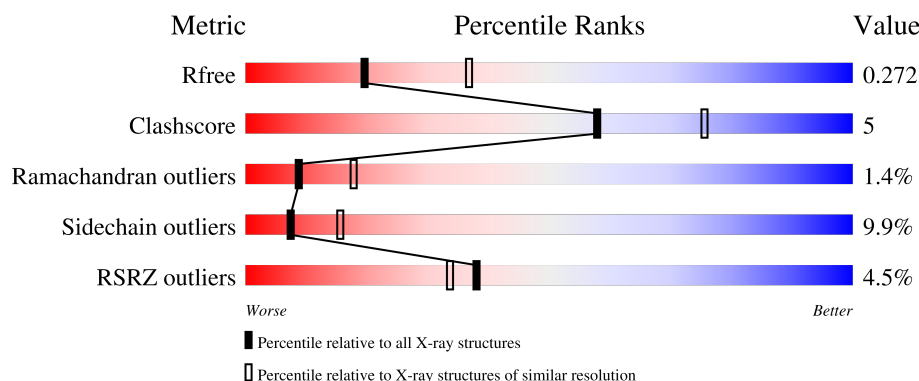
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.58 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	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (2.60-2.56)

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	5% 71% 14% • 12%
1	B	339	4% 71% 15% • 12%
1	C	339	5% 75% 16% • 7%
1	D	339	3% 76% 13% • 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10206 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.

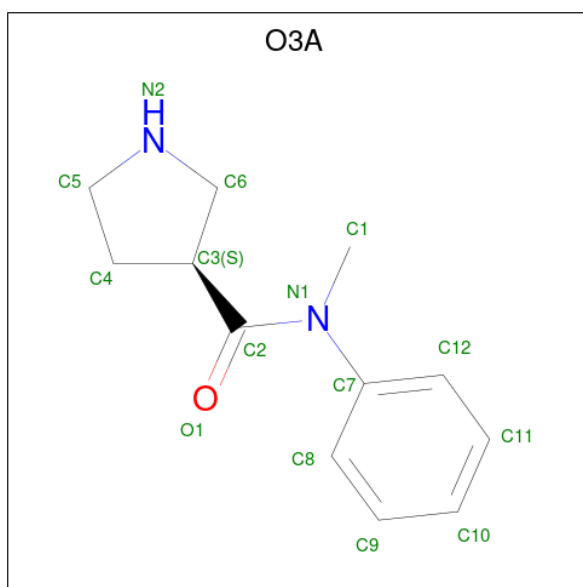
- Molecule 1 is a protein called Cohesin subunit SA-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	315	Total	C	N	O	S	0	0	0
			2587	1644	447	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 (3S)-N-methyl-N-phenylpyrrolidine-3-carboxamide (CCD ID: O3A) (formula: $C_{12}H_{16}N_2O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			15	12	2	1		

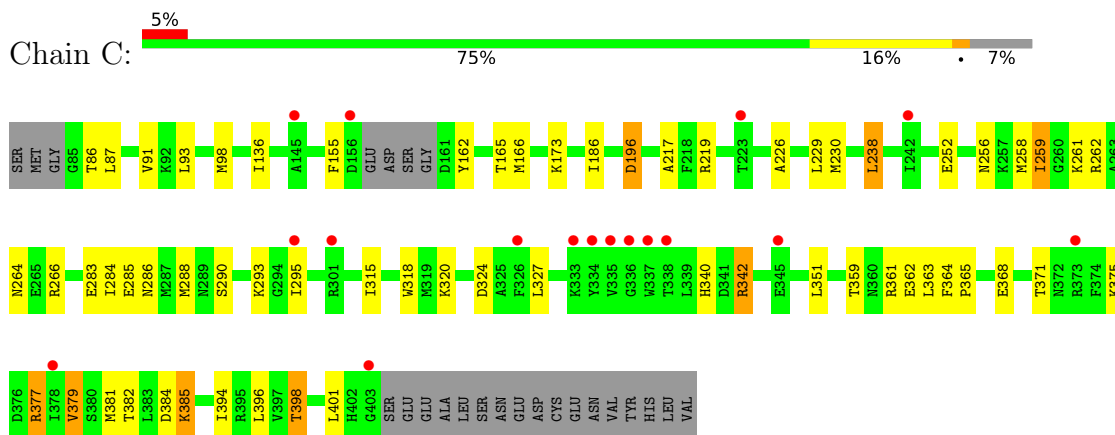
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	41	Total	O	0	0
			41	41		
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		

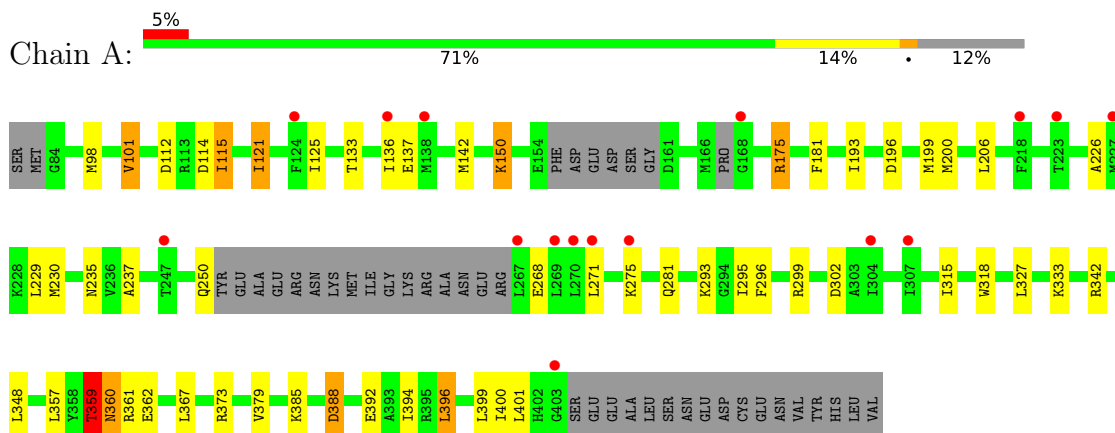
3 Residue-property plots

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

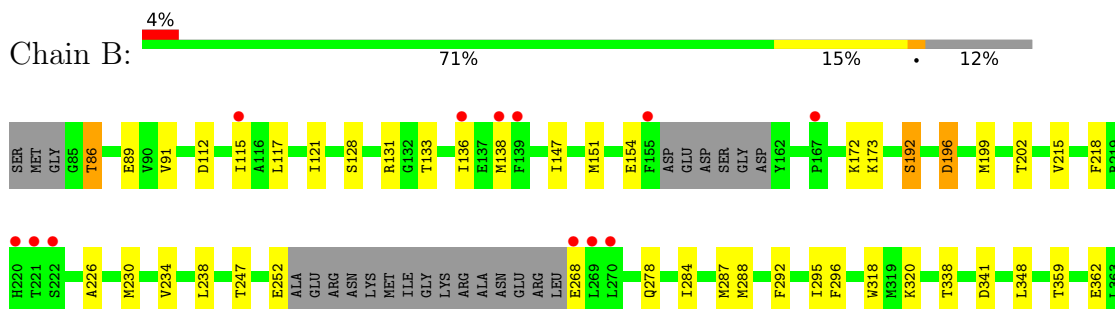
- Molecule 1: Cohesin subunit SA-1

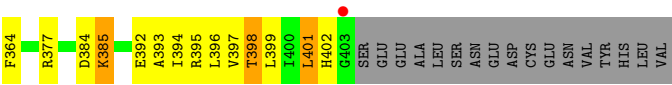


- Molecule 1: Cohesin subunit SA-1

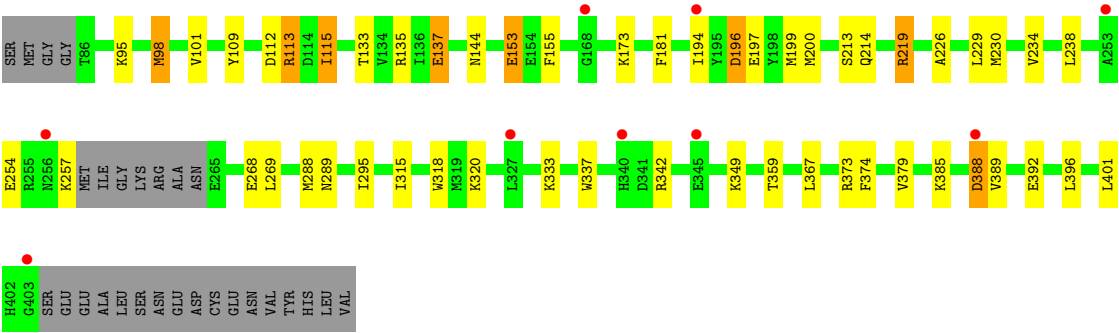
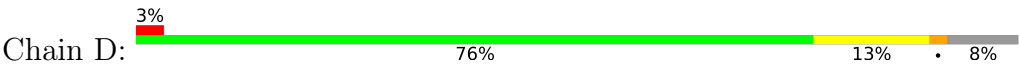


- Molecule 1: Cohesin subunit SA-1





● Molecule 1: Cohesin subunit SA-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	66.60Å 72.05Å 118.41Å 94.81° 98.61° 115.22°	Depositor
Resolution (Å)	60.65 – 2.58 60.65 – 2.58	Depositor EDS
% Data completeness (in resolution range)	97.8 (60.65-2.58) 97.8 (60.65-2.58)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.230 , 0.271 0.234 , 0.272	Depositor DCC
R_{free} test set	3045 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	74.8	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.7	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	10206	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: O3A

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	1.00	0/2470	1.62	0/3319
1	B	0.99	0/2493	1.60	0/3353
1	C	0.99	0/2629	1.60	0/3535
1	D	0.98	0/2603	1.58	0/3501
All	All	0.99	0/10195	1.60	0/13708

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	359	THR	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	27	0
1	B	2452	0	2471	24	0
1	C	2587	0	2602	25	0
1	D	2561	0	2568	23	0
2	C	15	0	0	0	0
3	A	38	0	0	1	0
3	B	26	0	0	0	0
3	C	41	0	0	0	0
3	D	53	0	0	0	0
All	All	10206	0	10098	91	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 5.

All (91) 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:B:394:ILE:O	1:B:398:THR:HG22	1.87	0.73
1:C:91:VAL:HG22	1:A:98:MET:HE1	1.71	0.70
1:C:226:ALA:CB	1:C:295:ILE:HD13	2.21	0.70
1:B:384:ASP:O	1:B:385:LYS:HB2	1.93	0.68
1:A:226:ALA:CB	1:A:295:ILE:HD13	2.28	0.64
1:D:226:ALA:CB	1:D:295:ILE:HD13	2.28	0.63
1:C:379:VAL:HG13	1:D:379:VAL:HG13	1.81	0.63
1:D:230:MET:HG2	1:D:318:TRP:CZ2	2.34	0.62
1:B:230:MET:HG2	1:B:318:TRP:CZ2	2.35	0.60
1:A:237:ALA:HB1	1:A:281:GLN:HE22	1.67	0.60
1:D:226:ALA:HB2	1:D:295:ILE:HD13	1.83	0.59
1:B:359:THR:HA	1:B:399:LEU:HD22	1.83	0.59
1:D:135:ARG:NH1	1:D:137:GLU:OE1	2.35	0.59
1:C:226:ALA:HB2	1:C:295:ILE:HD13	1.83	0.58
1:A:361:ARG:O	3:A:501:HOH:O	2.17	0.57
1:A:226:ALA:HB2	1:A:295:ILE:HD13	1.86	0.56
1:C:375:LYS:O	1:C:379:VAL:HB	2.06	0.55
1:C:230:MET:HG2	1:C:318:TRP:CE2	2.42	0.55
1:B:226:ALA:CB	1:B:295:ILE:HD13	2.38	0.54
1:A:359:THR:O	1:A:360:ASN:HB2	2.07	0.54
1:C:384:ASP:O	1:C:385:LYS:HB2	2.08	0.54
1:C:315:ILE:HA	1:C:318:TRP:CE3	2.43	0.54
1:A:142:MET:HE1	1:A:150:LYS:HD2	1.91	0.53
1:B:226:ALA:HB2	1:B:295:ILE:HD13	1.89	0.53
1:D:98:MET:HE2	1:D:181:PHE:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:ARG:O	1:A:302:ASP:HB2	2.10	0.52
1:C:284:ILE:HG22	1:C:288:MET:HE2	1.91	0.51
1:A:175:ARG:HH11	1:A:175:ARG:HG3	1.74	0.51
1:A:121:ILE:HD12	1:A:206:LEU:HD22	1.93	0.51
1:D:388:ASP:OD2	1:D:389:VAL:N	2.44	0.51
1:A:327:LEU:HD22	1:A:357:LEU:HD22	1.93	0.51
1:A:112:ASP:HB3	1:A:115:ILE:HD12	1.94	0.50
1:D:315:ILE:HA	1:D:318:TRP:CE3	2.47	0.50
1:D:213:SER:O	1:D:219:ARG:HD3	2.12	0.49
1:A:98:MET:HA	1:A:98:MET:HE3	1.95	0.49
1:A:98:MET:HE2	1:A:181:PHE:HB2	1.93	0.49
1:D:112:ASP:HB3	1:D:115:ILE:HD12	1.94	0.49
1:B:91:VAL:HA	1:D:98:MET:HE1	1.94	0.49
1:A:315:ILE:HA	1:A:318:TRP:CE3	2.48	0.48
1:B:284:ILE:HA	1:B:287:MET:HE3	1.96	0.48
1:B:91:VAL:HG22	1:D:98:MET:CE	2.44	0.48
1:A:394:ILE:HD12	1:B:401:LEU:HD12	1.97	0.47
1:D:333:LYS:HD2	1:D:337:TRP:CH2	2.49	0.47
1:D:373:ARG:HG2	1:D:374:PHE:CE2	2.50	0.47
1:C:87:LEU:O	1:C:91:VAL:HG23	2.15	0.47
1:B:338:THR:O	1:B:341:ASP:HB2	2.15	0.47
1:D:234:VAL:HA	1:D:288:MET:CE	2.45	0.47
1:D:153:GLU:O	1:D:155:PHE:N	2.49	0.45
1:D:196:ASP:OD1	1:D:196:ASP:C	2.60	0.45
1:C:379:VAL:CG1	1:D:379:VAL:HG13	2.47	0.44
1:C:196:ASP:C	1:C:196:ASP:OD1	2.60	0.44
1:C:226:ALA:CB	1:C:295:ILE:CD1	2.92	0.44
1:C:162:TYR:CD1	1:C:217:ALA:HB2	2.52	0.44
1:C:394:ILE:O	1:C:398:THR:HG22	2.18	0.43
1:A:112:ASP:HB3	1:A:115:ILE:CD1	2.48	0.43
1:A:388:ASP:O	1:A:392:GLU:HG2	2.18	0.43
1:A:296:PHE:CZ	1:A:315:ILE:HD12	2.53	0.43
1:B:230:MET:HG2	1:B:318:TRP:CE2	2.53	0.43
1:B:393:ALA:O	1:B:397:VAL:HG23	2.19	0.43
1:C:91:VAL:HG22	1:A:98:MET:CE	2.46	0.43
1:C:351:LEU:HD11	1:C:381:MET:HE2	2.00	0.43
1:B:196:ASP:OD1	1:B:196:ASP:C	2.61	0.43
1:B:117:LEU:O	1:B:121:ILE:HG12	2.19	0.42
1:B:112:ASP:HB3	1:B:115:ILE:HG12	2.02	0.42
1:D:388:ASP:O	1:D:392:GLU:HG2	2.20	0.42
1:C:364:PHE:HB3	1:C:365:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:371:THR:O	1:C:375:LYS:HB3	2.20	0.42
1:A:193:ILE:HG22	1:A:199:MET:HE3	2.01	0.41
1:B:215:VAL:HB	1:B:218:PHE:HD2	1.85	0.41
1:D:230:MET:HG2	1:D:318:TRP:CE2	2.55	0.41
1:C:340:HIS:CE1	1:C:377:ARG:HG3	2.56	0.41
1:A:359:THR:HA	1:A:399:LEU:HD22	2.02	0.41
1:B:86:THR:HG22	1:B:89:GLU:H	1.86	0.41
1:B:121:ILE:HD11	1:B:202:THR:HG22	2.01	0.41
1:B:128:SER:HB3	1:B:218:PHE:CD1	2.55	0.41
1:C:238:LEU:HD12	1:C:238:LEU:HA	1.91	0.41
1:A:396:LEU:HD22	1:A:400:ILE:HD11	2.02	0.41
1:B:234:VAL:HA	1:B:288:MET:HE1	2.03	0.41
1:C:162:TYR:CE2	1:C:165:THR:HG23	2.56	0.41
1:A:98:MET:HA	1:A:101:VAL:HG13	2.02	0.41
1:B:147:ILE:HG22	1:B:151:MET:HE2	2.02	0.41
1:D:200:MET:HE1	1:D:229:LEU:HD11	2.03	0.41
1:C:382:THR:OG1	1:D:379:VAL:CG2	2.69	0.41
1:A:230:MET:HG2	1:A:318:TRP:CZ2	2.56	0.41
1:C:285:GLU:HA	1:C:288:MET:HE3	2.03	0.40
1:C:342:ARG:CD	1:C:342:ARG:H	2.34	0.40
1:D:109:TYR:CZ	1:D:113:ARG:HG2	2.56	0.40
1:A:121:ILE:O	1:A:125:ILE:HG12	2.21	0.40
1:A:200:MET:HE1	1:A:229:LEU:HD11	2.02	0.40
1:B:292:PHE:CE1	1:B:296:PHE:CD1	3.09	0.40
1:B:392:GLU:OE1	1:B:395:ARG:NH1	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	266 (92%)	19 (7%)	4 (1%)	9 18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	292/339 (86%)	275 (94%)	13 (4%)	4 (1%)	9	18
1	C	311/339 (92%)	299 (96%)	6 (2%)	6 (2%)	6	12
1	D	307/339 (91%)	294 (96%)	10 (3%)	3 (1%)	12	26
All	All	1199/1356 (88%)	1134 (95%)	48 (4%)	17 (1%)	9	18

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	93	LEU
1	A	360	ASN
1	A	385	LYS
1	C	259	ILE
1	C	361	ARG
1	C	385	LYS
1	A	388	ASP
1	B	385	LYS
1	D	153	GLU
1	D	385	LYS
1	D	388	ASP
1	C	258	MET
1	C	362	GLU
1	B	402	HIS
1	A	359	THR
1	B	362	GLU
1	B	192	SER

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%)	244 (91%)	25 (9%)	8	18
1	B	271/306 (89%)	248 (92%)	23 (8%)	10	21
1	C	284/306 (93%)	250 (88%)	34 (12%)	5	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	283/306 (92%)	255 (90%)	28 (10%)	7	15
All	All	1107/1224 (90%)	997 (90%)	110 (10%)	7	15

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	86	THR
1	C	98	MET
1	C	136	ILE
1	C	155	PHE
1	C	166	MET
1	C	173	LYS
1	C	186	ILE
1	C	196	ASP
1	C	219	ARG
1	C	229	LEU
1	C	238	LEU
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	283	GLU
1	C	286	ASN
1	C	290	SER
1	C	293	LYS
1	C	320	LYS
1	C	324	ASP
1	C	327	LEU
1	C	342	ARG
1	C	359	THR
1	C	363	LEU
1	C	368	GLU
1	C	377	ARG
1	C	379	VAL
1	C	396	LEU
1	C	398	THR
1	C	401	LEU
1	A	101	VAL
1	A	114	ASP

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Mol	Chain	Res	Type
1	A	115	ILE
1	A	121	ILE
1	A	133	THR
1	A	136	ILE
1	A	137	GLU
1	A	150	LYS
1	A	175	ARG
1	A	196	ASP
1	A	235	ASN
1	A	250	GLN
1	A	268	GLU
1	A	271	LEU
1	A	275	LYS
1	A	293	LYS
1	A	333	LYS
1	A	342	ARG
1	A	348	LEU
1	A	362	GLU
1	A	367	LEU
1	A	373	ARG
1	A	379	VAL
1	A	396	LEU
1	A	401	LEU
1	B	86	THR
1	B	131	ARG
1	B	133	THR
1	B	136	ILE
1	B	138	MET
1	B	154	GLU
1	B	172	LYS
1	B	173	LYS
1	B	192	SER
1	B	196	ASP
1	B	199	MET
1	B	238	LEU
1	B	247	THR
1	B	252	GLU
1	B	268	GLU
1	B	278	GLN
1	B	320	LYS
1	B	348	LEU
1	B	364	PHE

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Mol	Chain	Res	Type
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	101	VAL
1	D	113	ARG
1	D	115	ILE
1	D	133	THR
1	D	137	GLU
1	D	144	ASN
1	D	173	LYS
1	D	194	ILE
1	D	196	ASP
1	D	197	GLU
1	D	199	MET
1	D	214	GLN
1	D	219	ARG
1	D	238	LEU
1	D	254	GLU
1	D	257	LYS
1	D	268	GLU
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	367	LEU
1	D	396	LEU
1	D	401	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	126	GLN
1	C	143	GLN
1	C	188	GLN
1	C	235	ASN
1	C	244	GLN
1	C	256	ASN

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Mol	Chain	Res	Type
1	C	264	ASN
1	C	278	GLN
1	C	289	ASN
1	C	360	ASN
1	C	402	HIS
1	A	126	GLN
1	A	239	ASN
1	A	281	GLN
1	A	286	ASN
1	A	289	ASN
1	A	340	HIS
1	A	360	ASN
1	B	280	ASN
1	B	402	HIS
1	D	99	GLN
1	D	214	GLN
1	D	235	ASN
1	D	281	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	O3A	C	501	-	15,16,16	0.74	0	18,21,21	0.91	1 (5%)

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	O3A	C	501	-	-	4/12/19/19	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	C	501	O3A	C4-C3-C6	-2.06	99.73	102.45

There are no chirality outliers.

All (4) torsion outliers are listed below:

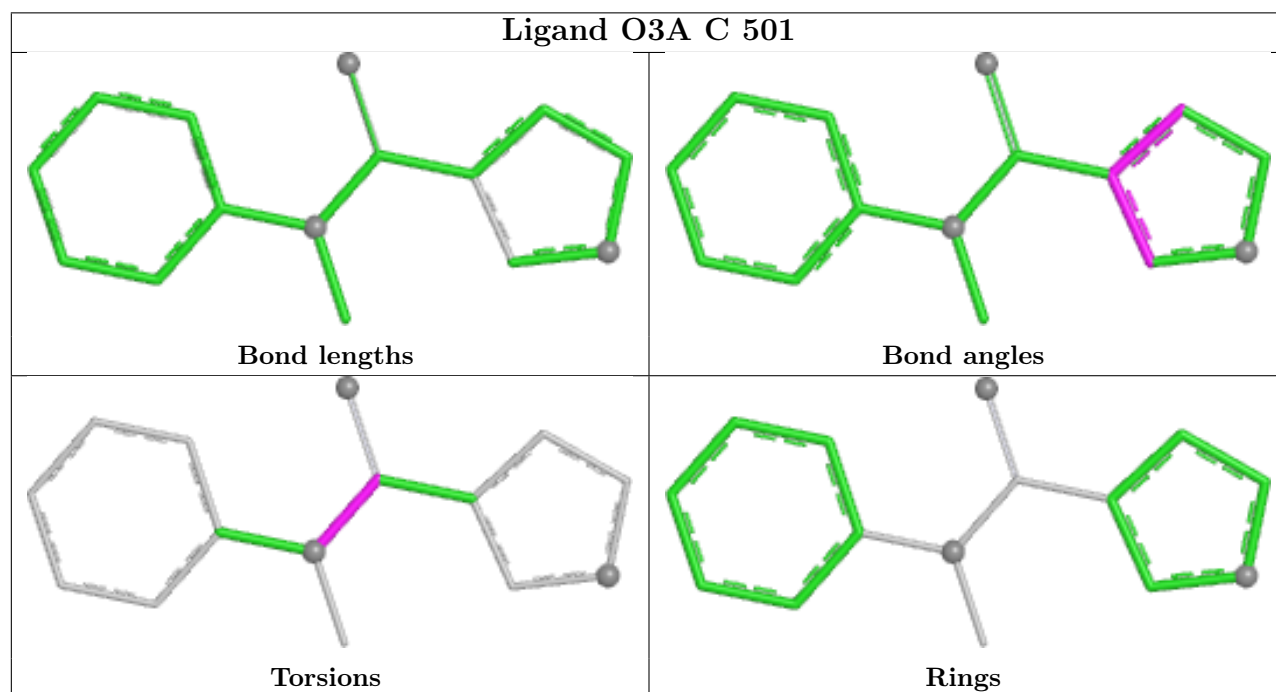
Mol	Chain	Res	Type	Atoms
2	C	501	O3A	C3-C2-N1-C7
2	C	501	O3A	O1-C2-N1-C7
2	C	501	O3A	C3-C2-N1-C1
2	C	501	O3A	O1-C2-N1-C1

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 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, 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%)	0.56	16 (5%) 31 27	61, 96, 147, 175	0
1	B	298/339 (87%)	0.40	13 (4%) 39 34	55, 90, 135, 153	0
1	C	315/339 (92%)	0.68	17 (5%) 31 27	43, 84, 118, 156	8 (2%)
1	D	311/339 (91%)	0.29	9 (2%) 53 49	49, 80, 116, 143	0
All	All	1221/1356 (90%)	0.48	55 (4%) 38 34	43, 88, 131, 175	8 (0%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	337	TRP	13.9
1	C	301	ARG	11.2
1	C	335	VAL	9.7
1	C	333	LYS	9.3
1	C	336	GLY	9.1
1	C	334	TYR	9.0
1	C	338	THR	8.1
1	C	373	ARG	6.6
1	B	155	PHE	5.5
1	A	269	LEU	4.2
1	D	403	GLY	3.8
1	A	267	LEU	3.7
1	C	403	GLY	3.5
1	A	124	PHE	3.3
1	A	271	LEU	3.3
1	B	403	GLY	3.0
1	B	268	GLU	3.0
1	D	253	ALA	2.9
1	A	168	GLY	2.9
1	B	222	SER	2.9
1	A	247	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	269	LEU	2.8
1	A	138	MET	2.8
1	A	223	THR	2.7
1	B	136	ILE	2.7
1	A	403	GLY	2.6
1	A	307	ILE	2.6
1	D	194	ILE	2.6
1	B	270	LEU	2.6
1	A	270	LEU	2.5
1	C	156	ASP	2.5
1	C	145	ALA	2.5
1	C	378	ILE	2.4
1	D	388	ASP	2.4
1	A	136	ILE	2.4
1	D	345	GLU	2.4
1	B	221	THR	2.3
1	B	220	HIS	2.3
1	B	167	PRO	2.3
1	D	327	LEU	2.3
1	C	223	THR	2.2
1	A	275	LYS	2.2
1	C	326	PHE	2.1
1	C	345	GLU	2.1
1	D	256	ASN	2.1
1	D	340	HIS	2.1
1	B	139	PHE	2.1
1	C	242	ILE	2.1
1	D	168	GLY	2.0
1	A	304	ILE	2.0
1	A	227	MET	2.0
1	A	218	PHE	2.0
1	C	295	ILE	2.0
1	B	115	ILE	2.0
1	B	138	MET	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

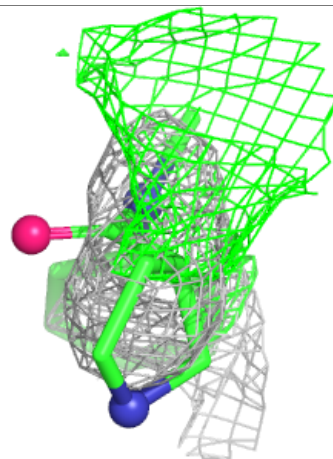
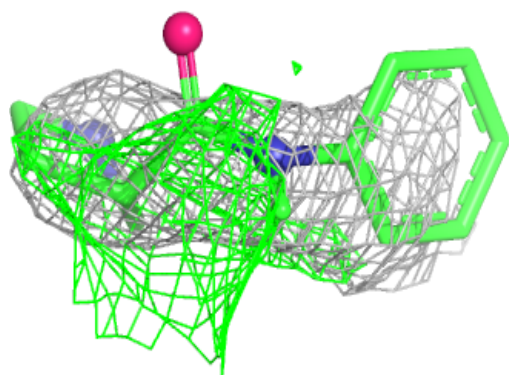
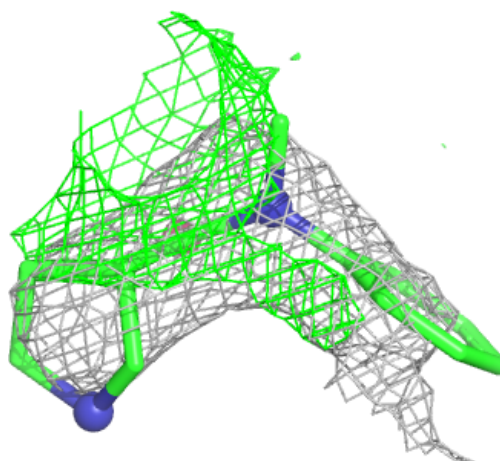
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	O3A	C	501	15/15	0.88	0.35	83,87,90,94	15

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 O3A 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.