



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:53 AM UTC

PDB ID : 5QSM / pdb_00005qsm
Title : PanDDA analysis group deposition – Crystal Structure of human STAG1 in complex with Z57261895
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 : 2.74 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

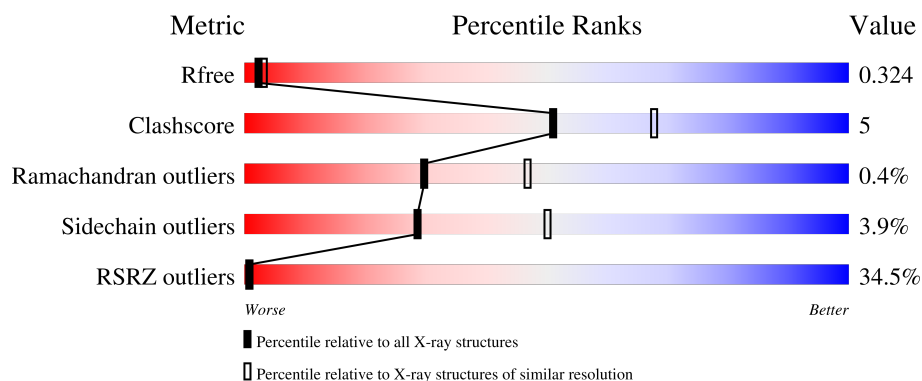
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.74 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	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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	459	29% 80% 14% • 5%
1	B	459	36% 77% 14% • 7%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7047 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.

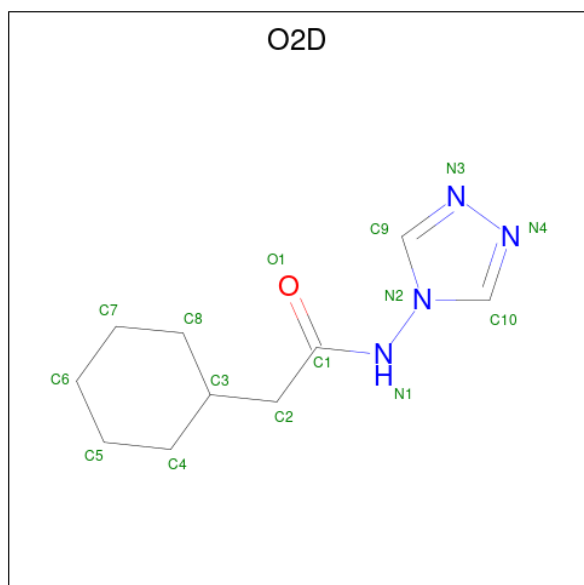
- Molecule 1 is a protein called Cohesin subunit SA-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	435	Total	C	N	O	S	0	0	0
			3483	2220	578	663	22			
1	B	425	Total	C	N	O	S	0	0	0
			3409	2176	563	648	22			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	457	SER	-	expression tag	UNP Q8WVM7
A	458	MET	-	expression tag	UNP Q8WVM7
B	457	SER	-	expression tag	UNP Q8WVM7
B	458	MET	-	expression tag	UNP Q8WVM7

- Molecule 2 is 2-cyclohexyl-N-(4H-1,2,4-triazol-4-yl)acetamide (CCD ID: O2D) (formula: C₁₀H₁₆N₄O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	10	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	102	Total	O	0	0
			102	102		
3	B	38	Total	O	0	0
			38	38		

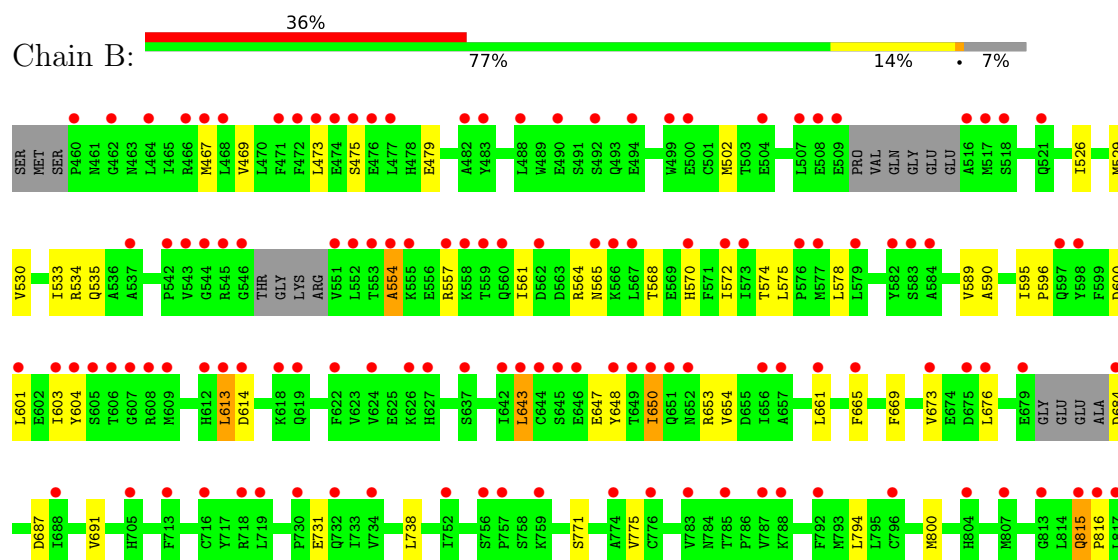
3 Residue-property plots [i](#)

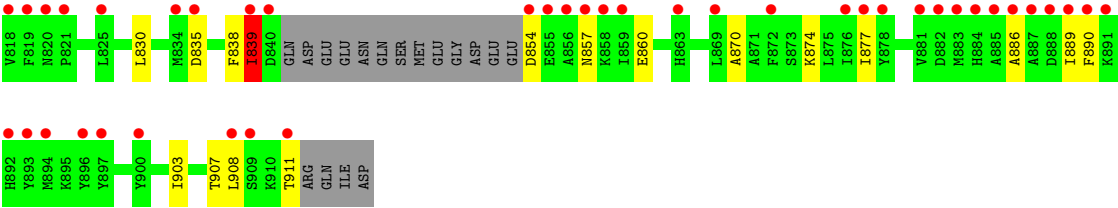
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Cohesin subunit SA-1



• Molecule 1: Cohesin subunit SA-1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	155.14Å 168.17Å 46.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	114.03 – 2.74 114.03 – 2.74	Depositor EDS
% Data completeness (in resolution range)	99.5 (114.03-2.74) 99.9 (114.03-2.74)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.260 , 0.299 0.290 , 0.324	Depositor DCC
R_{free} test set	1688 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	55.1	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 66.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7047	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: O2D

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	0.92	0/3544	1.14	3/4791 (0.1%)
1	B	0.91	1/3469 (0.0%)	1.09	2/4687 (0.0%)
All	All	0.92	1/7013 (0.0%)	1.11	5/9478 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	839	ILE	CA-C	5.92	1.58	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	613	LEU	N-CA-C	-5.93	104.89	111.71
1	A	627	HIS	N-CA-C	5.43	118.44	109.85
1	B	889	ILE	N-CA-C	5.29	116.77	111.00
1	A	645	SER	CA-C-N	-5.06	115.12	122.86
1	A	645	SER	C-N-CA	-5.06	115.12	122.86

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3483	0	3458	32	0
1	B	3409	0	3386	40	0
2	A	15	0	0	5	0
3	A	102	0	0	0	0
3	B	38	0	0	0	0
All	All	7047	0	6844	72	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 (72) 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:A:689:TYR:CD1	2:A:1001:O2D:C2	2.37	1.08
1:B:604:TYR:CE1	1:B:613:LEU:HB2	1.93	1.01
1:A:689:TYR:HD1	2:A:1001:O2D:C2	1.72	1.00
1:A:696:LYS:HE2	2:A:1001:O2D:C6	1.92	0.98
1:B:604:TYR:CD1	1:B:613:LEU:HB2	2.06	0.90
1:B:614:ASP:OD1	1:B:653:ARG:HD3	1.81	0.80
1:B:469:VAL:O	1:B:473:LEU:HD23	1.89	0.72
1:B:604:TYR:HB3	1:B:650:ILE:HG21	1.69	0.71
1:A:689:TYR:CE1	2:A:1001:O2D:C2	2.74	0.71
1:A:677:LEU:HD12	1:A:718:ARG:NH2	2.06	0.70
1:A:696:LYS:CE	2:A:1001:O2D:C6	2.74	0.65
1:A:766:ARG:NH1	1:A:816:PRO:O	2.30	0.65
1:A:676:LEU:HD22	1:A:691:VAL:HG21	1.79	0.63
1:B:604:TYR:CE1	1:B:613:LEU:CB	2.78	0.58
1:B:601:LEU:HB2	1:B:648:TYR:CE2	2.39	0.58
1:B:564:ARG:HD3	1:B:600:ASP:HB2	1.87	0.56
1:A:800:MET:HE3	1:A:874:LYS:HB3	1.87	0.56
1:B:604:TYR:CB	1:B:650:ILE:HG21	2.36	0.55
1:B:533:ILE:O	1:B:534:ARG:C	2.51	0.53
1:B:877:ILE:HD11	1:B:907:THR:HA	1.89	0.53
1:A:552:LEU:HD22	1:A:556:GLU:HB3	1.89	0.53
1:B:643:LEU:HB3	1:B:654:VAL:HG11	1.91	0.53
1:A:742:HIS:CG	1:A:794:LEU:HD22	2.45	0.51
1:A:600:ASP:OD1	1:A:602:GLU:HG2	2.11	0.51
1:B:568:THR:HG22	1:B:572:ILE:CD1	2.40	0.51
1:B:534:ARG:O	1:B:535:GLN:C	2.55	0.50
1:B:561:ILE:O	1:B:565:ASN:ND2	2.44	0.50
1:B:502:MET:SD	1:B:529:MET:HG3	2.52	0.50
1:A:604:TYR:CD1	1:A:613:LEU:HB2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:677:LEU:CD1	1:A:718:ARG:NH2	2.75	0.49
1:B:568:THR:HG22	1:B:572:ILE:HD11	1.95	0.49
1:B:676:LEU:HD22	1:B:691:VAL:HG21	1.95	0.49
1:B:771:SER:O	1:B:775:VAL:HG23	2.13	0.49
1:B:469:VAL:O	1:B:473:LEU:CD2	2.58	0.48
1:B:554:ALA:HA	1:B:557:ARG:HB3	1.93	0.48
1:B:570:HIS:CE1	1:B:574:THR:HG21	2.48	0.48
1:B:830:LEU:CD1	1:B:886:ALA:HA	2.43	0.48
1:B:857:ASN:O	1:B:860:GLU:HB3	2.14	0.48
1:A:533:ILE:HD11	1:A:571:PHE:CE2	2.49	0.48
1:A:746:LEU:O	1:A:750:VAL:HG23	2.14	0.48
1:B:684:ASP:HB3	1:B:687:ASP:OD2	2.14	0.47
1:B:661:LEU:HD11	1:B:665:PHE:CZ	2.50	0.47
1:A:902:ASP:N	1:A:902:ASP:OD1	2.47	0.47
1:A:677:LEU:HD12	1:A:718:ARG:CZ	2.45	0.46
1:A:465:ILE:HG13	1:A:495:LEU:HD11	1.98	0.46
1:A:570:HIS:CE1	1:A:574:THR:HG21	2.51	0.46
1:B:526:ILE:O	1:B:530:VAL:HG23	2.16	0.46
1:B:815:GLN:N	1:B:816:PRO:HD2	2.32	0.45
1:A:830:LEU:HD11	1:A:886:ALA:HA	1.99	0.45
1:B:838:PHE:C	1:B:839:ILE:HD13	2.41	0.44
1:B:589:VAL:O	1:B:590:ALA:C	2.60	0.44
1:B:575:LEU:HA	1:B:578:LEU:HD12	1.99	0.44
1:B:467:MET:HE2	1:B:467:MET:HB3	1.94	0.44
1:B:870:ALA:HB2	1:B:903:ILE:HD12	2.00	0.44
1:A:719:LEU:O	1:A:729:MET:HE3	2.18	0.43
1:A:600:ASP:HB3	1:A:603:ILE:HD12	2.00	0.43
1:B:603:ILE:HG22	1:B:603:ILE:O	2.17	0.43
1:A:574:THR:HA	1:A:577:MET:HE2	2.01	0.43
1:A:594:GLN:O	1:A:597:GLN:HG2	2.18	0.42
1:A:785:THR:N	1:A:786:PRO:CD	2.82	0.42
1:A:621:LYS:HG3	1:A:661:LEU:HD13	2.01	0.42
1:A:669:PHE:O	1:A:673:VAL:HG23	2.20	0.42
1:A:601:LEU:HD12	1:A:646:GLU:HB2	2.02	0.41
1:A:689:TYR:CD2	1:A:689:TYR:C	2.99	0.41
1:A:498:ASP:CG	1:A:501:CYS:HB2	2.45	0.41
1:B:669:PHE:O	1:B:673:VAL:HG23	2.19	0.41
1:B:800:MET:HE3	1:B:874:LYS:HG2	2.02	0.41
1:A:575:LEU:N	1:A:576:PRO:CD	2.84	0.41
1:B:738:LEU:HB3	1:B:794:LEU:CD1	2.51	0.40
1:B:890:PHE:CD1	1:B:908:LEU:HD21	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:643:LEU:HD12	1:B:643:LEU:HA	1.80	0.40
1:B:595:ILE:HB	1:B:596:PRO:HD3	2.02	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	425/459 (93%)	406 (96%)	17 (4%)	2 (0%)	24	40
1	B	415/459 (90%)	385 (93%)	29 (7%)	1 (0%)	43	62
All	All	840/918 (92%)	791 (94%)	46 (6%)	3 (0%)	30	47

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	515	GLU
1	B	554	ALA
1	A	644	CYS

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	389/415 (94%)	370 (95%)	19 (5%)	22	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	381/415 (92%)	370 (97%)	11 (3%)	37 59
All	All	770/830 (93%)	740 (96%)	30 (4%)	28 50

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	523	SER
1	A	591	ASN
1	A	618	LYS
1	A	641	SER
1	A	642	ILE
1	A	645	SER
1	A	646	GLU
1	A	696	LYS
1	A	770	LYS
1	A	795	LEU
1	A	797	ASP
1	A	805	GLN
1	A	812	GLU
1	A	823	THR
1	A	830	LEU
1	A	840	ASP
1	A	859	ILE
1	A	868	LEU
1	A	891	LYS
1	B	475	SER
1	B	479	GLU
1	B	643	LEU
1	B	647	GLU
1	B	650	ILE
1	B	731	GLU
1	B	815	GLN
1	B	835	ASP
1	B	839	ILE
1	B	854	ASP
1	B	911	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	463	ASN

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Mol	Chain	Res	Type
1	A	591	ASN
1	A	619	GLN
1	A	651	GLN
1	A	778	GLN
1	A	784	ASN
1	A	790	GLN
1	A	815	GLN
1	B	591	ASN
1	B	612	HIS
1	B	660	GLN
1	B	703	ASN
1	B	732	GLN
1	B	736	GLN
1	B	739	GLN
1	B	782	ASN
1	B	790	GLN
1	B	804	HIS
1	B	863	HIS

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	O2D	A	1001	-	16,16,16	1.35	3 (18%)	18,20,20	1.92	3 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	O2D	A	1001	-	-	0/8/16/16	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	O2D	C1-N1	-2.77	1.31	1.35
2	A	1001	O2D	O1-C1	-2.46	1.18	1.23
2	A	1001	O2D	C5-C4	-2.01	1.48	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	O2D	C3-C2-C1	-6.32	104.26	113.22
2	A	1001	O2D	C8-C3-C2	-2.45	108.28	111.48
2	A	1001	O2D	C5-C4-C3	-2.41	107.01	112.08

There are no chirality outliers.

There are no torsion outliers.

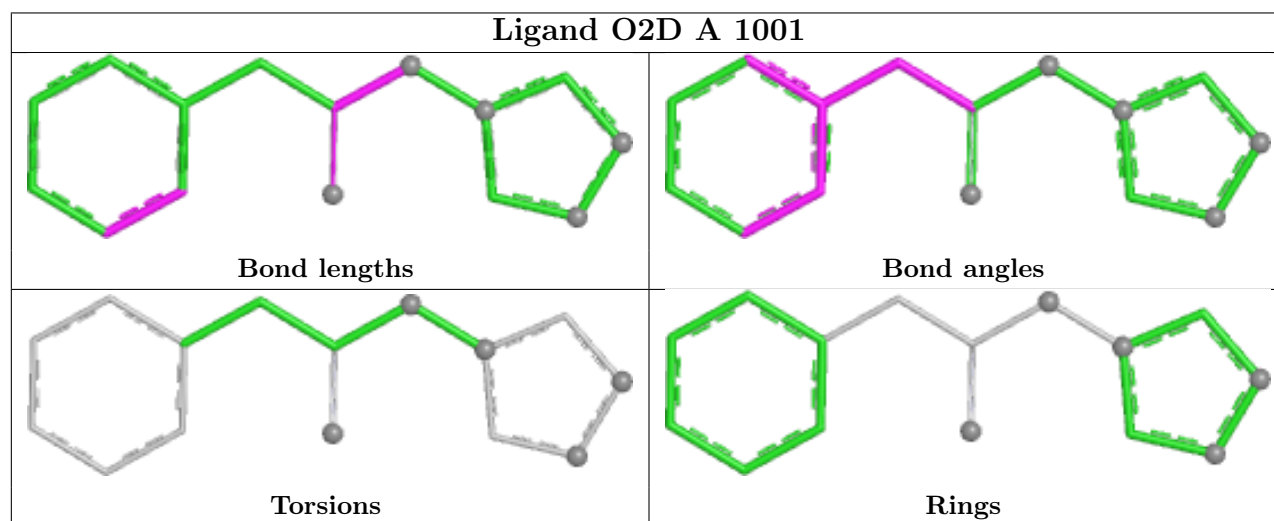
There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	O2D	5	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, 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	435/459 (94%)	1.65	133 (30%)  	56, 82, 122, 143	0
1	B	425/459 (92%)	1.87	164 (38%)  	62, 101, 143, 173	0
All	All	860/918 (93%)	1.76	297 (34%)  	56, 92, 137, 173	0

All (297) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	550	ARG	6.3
1	A	547	THR	6.2
1	B	460	PRO	6.2
1	B	551	VAL	5.2
1	A	908	LEU	5.1
1	B	893	TYR	5.1
1	A	511	VAL	5.1
1	A	551	VAL	5.0
1	A	647	GLU	4.9
1	B	552	LEU	4.9
1	B	911	THR	4.6
1	A	458	MET	4.5
1	B	651	GLN	4.5
1	B	892	HIS	4.3
1	A	546	GLY	4.3
1	A	544	GLY	4.1
1	A	557	ARG	4.1
1	B	883	MET	4.0
1	B	603	ILE	4.0
1	B	656	ILE	3.9
1	A	671	HIS	3.9
1	A	816	PRO	3.8
1	B	554	ALA	3.8
1	B	646	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	618	LYS	3.8
1	B	516	ALA	3.8
1	B	475	SER	3.8
1	A	543	VAL	3.8
1	A	648	TYR	3.7
1	B	890	PHE	3.7
1	A	471	PHE	3.7
1	B	884	HIS	3.6
1	A	813	GLY	3.6
1	A	628	VAL	3.6
1	B	856	ALA	3.6
1	B	804	HIS	3.6
1	B	650	ILE	3.6
1	A	911	THR	3.6
1	B	604	TYR	3.6
1	B	601	LEU	3.5
1	B	908	LEU	3.5
1	B	583	SER	3.5
1	B	553	THR	3.5
1	A	881	VAL	3.5
1	B	887	ALA	3.5
1	A	759	LYS	3.4
1	B	606	THR	3.4
1	B	886	ALA	3.4
1	B	477	LEU	3.4
1	B	665	PHE	3.4
1	A	514	GLU	3.3
1	B	507	LEU	3.3
1	B	544	GLY	3.3
1	B	555	LYS	3.3
1	B	839	ILE	3.3
1	B	509	GLU	3.2
1	B	807	MET	3.2
1	A	811	ARG	3.2
1	B	558	LYS	3.2
1	B	546	GLY	3.2
1	A	644	CYS	3.2
1	A	817	LEU	3.2
1	B	863	HIS	3.2
1	A	688	ILE	3.2
1	B	543	VAL	3.2
1	B	584	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	552	LEU	3.1
1	A	545	ARG	3.1
1	A	904	ILE	3.1
1	B	622	PHE	3.1
1	B	872	PHE	3.1
1	A	459	SER	3.1
1	A	741	SER	3.1
1	A	682	GLU	3.0
1	A	561	ILE	3.0
1	A	900	TYR	3.0
1	B	627	HIS	3.0
1	A	727	GLY	3.0
1	A	859	ILE	3.0
1	A	893	TYR	3.0
1	A	649	THR	3.0
1	A	763	LEU	3.0
1	B	869	LEU	3.0
1	B	652	ASN	3.0
1	A	799	LEU	2.9
1	A	510	PRO	2.9
1	B	645	SER	2.9
1	B	909	SER	2.9
1	A	565	ASN	2.9
1	B	613	LEU	2.9
1	A	752	ILE	2.9
1	A	516	ALA	2.9
1	B	881	VAL	2.9
1	A	726	HIS	2.9
1	A	591	ASN	2.9
1	A	467	MET	2.8
1	A	483	TYR	2.8
1	A	808	THR	2.8
1	B	885	ALA	2.8
1	A	622	PHE	2.8
1	B	612	HIS	2.8
1	A	807	MET	2.8
1	B	813	GLY	2.8
1	A	554	ALA	2.8
1	A	724	ILE	2.8
1	B	573	ILE	2.8
1	A	645	SER	2.8
1	A	806	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	809	GLY	2.8
1	B	825	LEU	2.8
1	B	648	TYR	2.8
1	A	728	ALA	2.8
1	B	483	TYR	2.8
1	B	644	CYS	2.7
1	B	894	MET	2.7
1	A	631	ASP	2.7
1	A	711	ASP	2.7
1	A	856	ALA	2.7
1	A	819	PHE	2.7
1	B	559	THR	2.7
1	A	767	LYS	2.7
1	A	804	HIS	2.7
1	B	462	GLY	2.7
1	B	619	GLN	2.7
1	B	676	LEU	2.7
1	A	494	GLU	2.7
1	B	796	CYS	2.7
1	A	652	ASN	2.7
1	A	818	VAL	2.7
1	B	566	LYS	2.7
1	B	897	TYR	2.6
1	A	740	CYS	2.6
1	B	473	LEU	2.6
1	A	606	THR	2.6
1	B	649	THR	2.6
1	B	752	ILE	2.6
1	B	557	ARG	2.6
1	B	608	ARG	2.6
1	B	857	ASN	2.6
1	B	605	SER	2.6
1	B	840	ASP	2.6
1	B	888	ASP	2.6
1	A	883	MET	2.6
1	B	889	ILE	2.6
1	B	900	TYR	2.6
1	B	494	GLU	2.6
1	A	665	PHE	2.6
1	B	472	PHE	2.6
1	B	609	MET	2.6
1	A	839	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	638	LYS	2.6
1	B	673	VAL	2.6
1	B	783	VAL	2.6
1	A	478	HIS	2.5
1	A	878	TYR	2.5
1	B	896	TYR	2.5
1	B	607	GLY	2.5
1	B	816	PRO	2.5
1	A	492	SER	2.5
1	A	909	SER	2.5
1	A	895	LYS	2.5
1	A	476	GLU	2.5
1	A	812	GLU	2.5
1	B	474	GLU	2.5
1	B	521	GLN	2.5
1	A	756	SER	2.5
1	A	581	LYS	2.5
1	A	520	ARG	2.5
1	B	562	ASP	2.5
1	B	688	ILE	2.5
1	B	876	ILE	2.5
1	B	542	PRO	2.5
1	A	472	PHE	2.5
1	B	464	LEU	2.5
1	B	490	GLU	2.5
1	A	815	GLN	2.5
1	B	597	GLN	2.5
1	B	661	LEU	2.4
1	B	854	ASP	2.4
1	B	679	GLU	2.4
1	A	594	GLN	2.4
1	B	732	GLN	2.4
1	A	713	PHE	2.4
1	A	802	PHE	2.4
1	A	872	PHE	2.4
1	B	859	ILE	2.4
1	A	687	ASP	2.4
1	A	541	PRO	2.4
1	B	576	PRO	2.4
1	A	910	LYS	2.4
1	B	787	VAL	2.4
1	A	903	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	642	ILE	2.4
1	A	479	GLU	2.4
1	A	748	GLN	2.4
1	B	598	TYR	2.4
1	B	657	ALA	2.4
1	A	876	ILE	2.4
1	B	785	THR	2.4
1	B	637	SER	2.4
1	B	684	ASP	2.4
1	B	499	TRP	2.4
1	B	577	MET	2.4
1	B	891	LYS	2.4
1	A	679	GLU	2.3
1	A	855	GLU	2.3
1	A	709	LYS	2.3
1	B	835	ASP	2.3
1	A	678	GLN	2.3
1	A	477	LEU	2.3
1	A	760	GLU	2.3
1	B	730	PRO	2.3
1	B	719	LEU	2.3
1	A	745	ILE	2.3
1	B	572	ILE	2.3
1	B	788	LYS	2.3
1	B	716	CYS	2.3
1	B	819	PHE	2.3
1	A	683	ALA	2.3
1	A	737	ALA	2.3
1	A	517	MET	2.3
1	A	814	LEU	2.3
1	B	468	LEU	2.3
1	B	643	LEU	2.3
1	B	877	ILE	2.2
1	A	753	THR	2.2
1	B	718	ARG	2.2
1	A	542	PRO	2.2
1	B	518	SER	2.2
1	B	815	GLN	2.2
1	A	496	LEU	2.2
1	A	749	LEU	2.2
1	B	624	VAL	2.2
1	B	818	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	537	ALA	2.2
1	A	553	THR	2.2
1	B	675	ASP	2.2
1	A	751	LYS	2.2
1	B	759	LYS	2.2
1	B	517	MET	2.2
1	B	570	HIS	2.2
1	B	834	MET	2.2
1	A	587	GLU	2.2
1	A	699	THR	2.2
1	B	466	ARG	2.2
1	A	493	GLN	2.2
1	A	473	LEU	2.2
1	A	770	LYS	2.2
1	B	567	LEU	2.2
1	B	626	LYS	2.2
1	B	817	LEU	2.2
1	B	467	MET	2.2
1	A	884	HIS	2.2
1	B	476	GLU	2.2
1	B	776	CYS	2.2
1	A	875	LEU	2.2
1	A	800	MET	2.2
1	B	614	ASP	2.2
1	B	882	ASP	2.2
1	B	471	PHE	2.2
1	B	855	GLU	2.1
1	A	766	ARG	2.1
1	A	531	CYS	2.1
1	B	757	PRO	2.1
1	B	560	GLN	2.1
1	B	878	TYR	2.1
1	A	738	LEU	2.1
1	B	756	SER	2.1
1	B	774	ALA	2.1
1	A	689	TYR	2.1
1	B	582	TYR	2.1
1	B	734	VAL	2.1
1	A	630	SER	2.1
1	A	618	LYS	2.1
1	B	858	LYS	2.1
1	A	684	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	713	PHE	2.1
1	B	792	PHE	2.1
1	B	482	ALA	2.1
1	B	545	ARG	2.1
1	A	626	LYS	2.1
1	A	464	LEU	2.1
1	B	488	LEU	2.1
1	B	820	ASN	2.1
1	A	797	ASP	2.0
1	A	840	ASP	2.0
1	A	774	ALA	2.0
1	B	500	GLU	2.0
1	B	504	GLU	2.0
1	B	579	LEU	2.0
1	A	899	ASP	2.0
1	B	508	GLU	2.0
1	B	492	SER	2.0
1	B	821	PRO	2.0
1	A	863	HIS	2.0
1	B	705	HIS	2.0
1	B	565	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

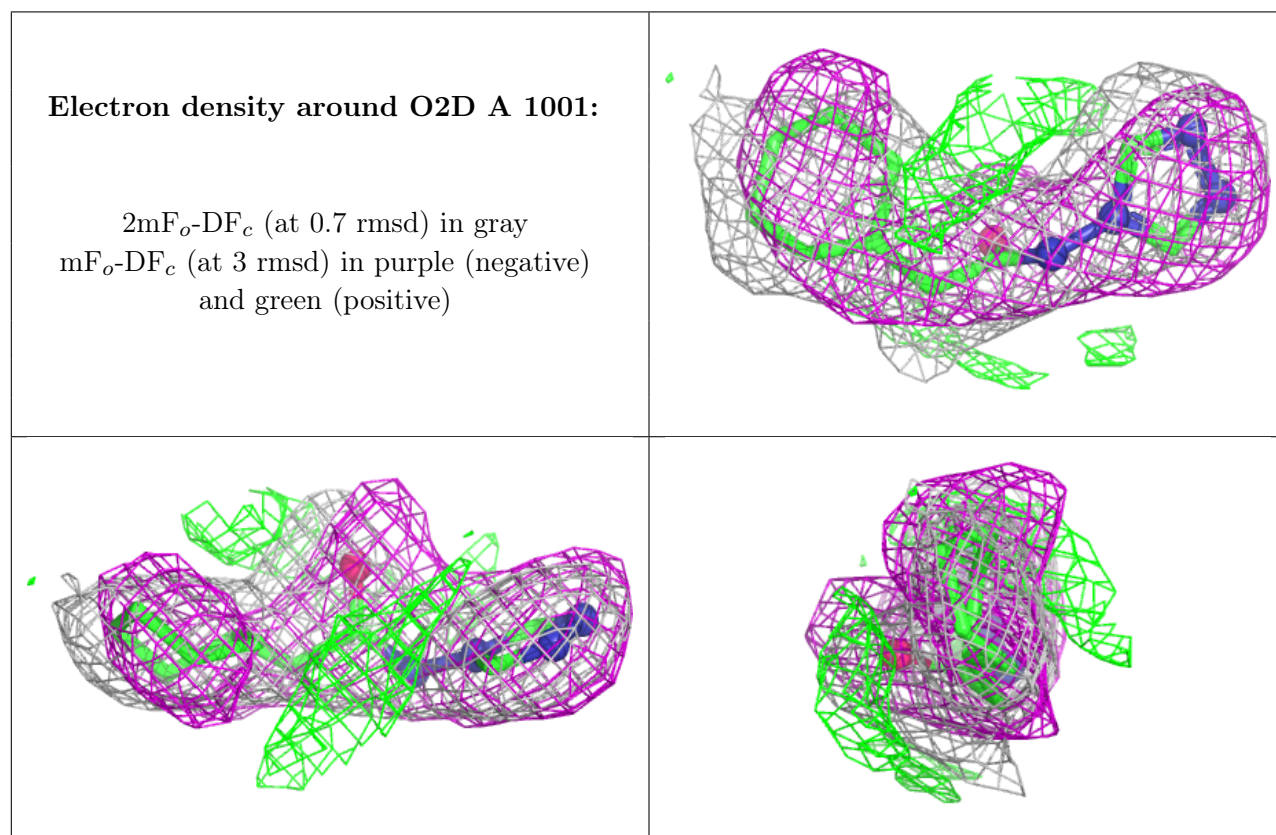
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	O2D	A	1001	15/15	0.85	0.33	20,20,20,20	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.