Full wwPDB X-ray Structure Validation Report (i)

May 25, 2020 – 03:49 pm BST

PDB ID	:	5QSO
Title	:	PanDDA analysis group deposition – Crystal Structure of human STAG1 in complex with Z466628048
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	:	2.70 Å(reported)

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

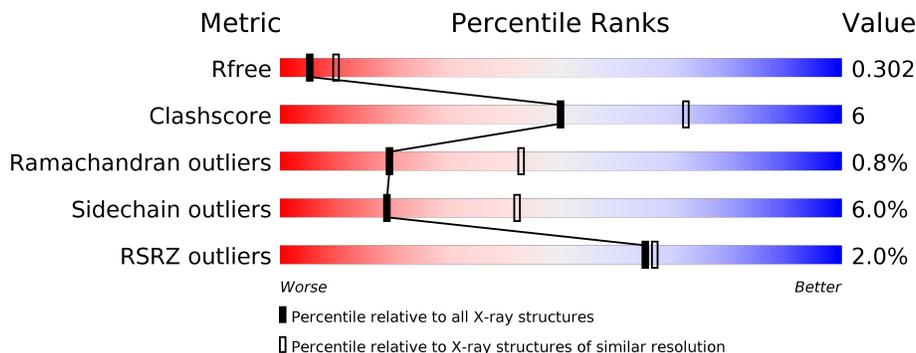|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.70 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	Percentile Ranks	Value
Rfree		0.302
Clashscore		6
Ramachandran outliers		0.8%
Sidechain outliers		6.0%
RSRZ outliers		2.0%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	459	81% 13% 5%
1	B	459	3% 75% 15% • 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7074 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 3490	C 2224	N 581	O 663	S 22	0	0	0
1	B	425	Total 3423	C 2180	N 570	O 651	S 22	0	0	0

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	457	SER	ARG	conflict	UNP Q8WVM7
A	458	MET	ASN	conflict	UNP Q8WVM7
A	901	GLY	-	expression tag	UNP Q8WVM7
A	902	ASP	-	expression tag	UNP Q8WVM7
A	903	ILE	-	expression tag	UNP Q8WVM7
A	904	ILE	-	expression tag	UNP Q8WVM7
A	905	LYS	-	expression tag	UNP Q8WVM7
A	906	GLU	-	expression tag	UNP Q8WVM7
A	907	THR	-	expression tag	UNP Q8WVM7
A	908	LEU	-	expression tag	UNP Q8WVM7
A	909	SER	-	expression tag	UNP Q8WVM7
A	910	LYS	-	expression tag	UNP Q8WVM7
A	911	THR	-	expression tag	UNP Q8WVM7
A	912	ARG	-	expression tag	UNP Q8WVM7
A	913	GLN	-	expression tag	UNP Q8WVM7
A	914	ILE	-	expression tag	UNP Q8WVM7
A	915	ASP	-	expression tag	UNP Q8WVM7
B	457	SER	ARG	conflict	UNP Q8WVM7
B	458	MET	ASN	conflict	UNP Q8WVM7
B	901	GLY	-	expression tag	UNP Q8WVM7
B	902	ASP	-	expression tag	UNP Q8WVM7
B	903	ILE	-	expression tag	UNP Q8WVM7
B	904	ILE	-	expression tag	UNP Q8WVM7
B	905	LYS	-	expression tag	UNP Q8WVM7
B	906	GLU	-	expression tag	UNP Q8WVM7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	907	THR	-	expression tag	UNP Q8WVM7
B	908	LEU	-	expression tag	UNP Q8WVM7
B	909	SER	-	expression tag	UNP Q8WVM7
B	910	LYS	-	expression tag	UNP Q8WVM7
B	911	THR	-	expression tag	UNP Q8WVM7
B	912	ARG	-	expression tag	UNP Q8WVM7
B	913	GLN	-	expression tag	UNP Q8WVM7
B	914	ILE	-	expression tag	UNP Q8WVM7
B	915	ASP	-	expression tag	UNP Q8WVM7

- Molecule 2 is N-[(4-methyl-1,3-thiazol-2-yl)methyl]-1H-pyrazole-5-carboxamide (three-letter code: O2M) (formula: $C_9H_{10}N_4OS$) (labeled as "Ligand of Interest" by author).
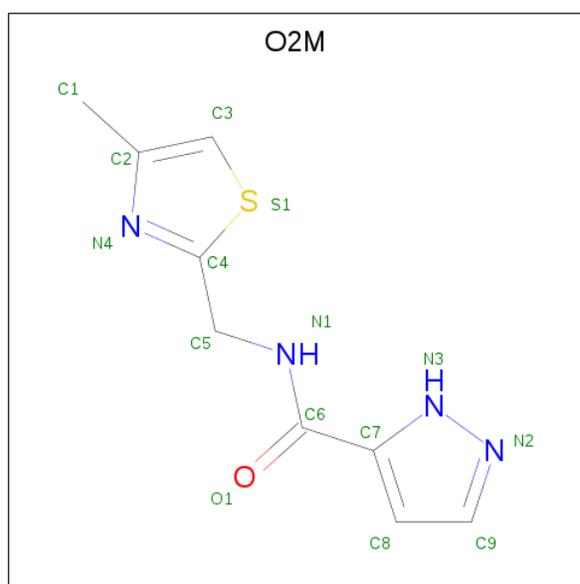
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 15	C 9	N 4	O 1	S 1	0	0

- Molecule 3 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	106	Total 106	O 106	0	0
3	B	40	Total 40	O 40	0	0

3 Residue-property plots ⓘ

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 A:

- Molecule 1: Cohesin subunit SA-1

Chain B:
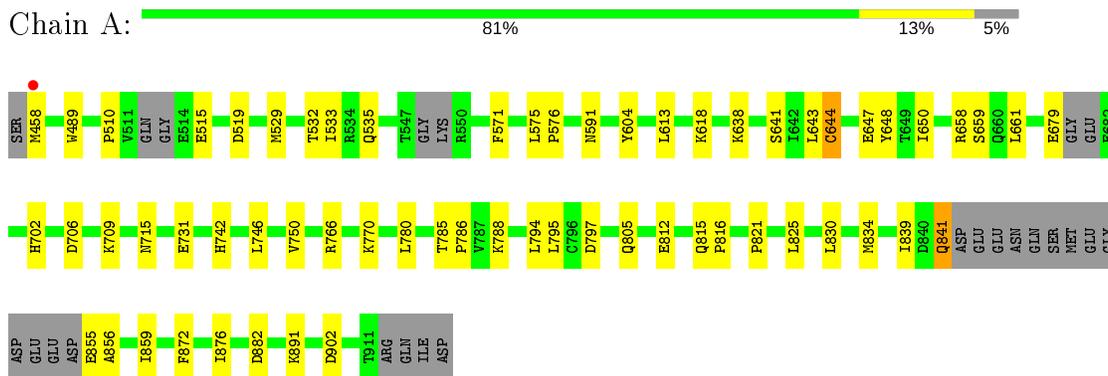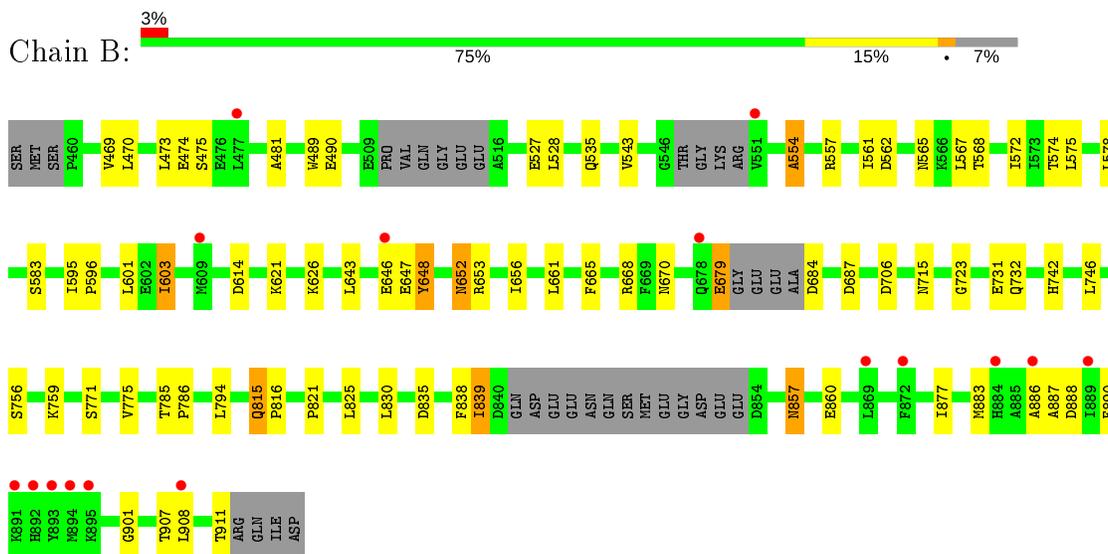
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	155.55Å 167.54Å 48.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	83.91 – 2.70 83.77 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (83.91-2.70) 99.8 (83.77-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.39 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.228 , 0.295 0.239 , 0.302	Depositor DCC
R_{free} test set	1797 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	68.7	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 48.6	EDS
L-test for twinning[2]	$<|L|> = 0.52$, $<L^2> = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7074	wwPDB-VP
Average B, all atoms (Å^2)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.62% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: O2M

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	0.70	0/3551	0.81	0/4799
1	B	0.71	0/3483	0.80	0/4703
All	All	0.70	0/7034	0.81	0/9502

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	3490	0	3471	29	0
1	B	3423	0	3400	51	0
2	A	15	0	0	4	0
3	A	106	0	0	2	0
3	B	40	0	0	4	0
All	All	7074	0	6871	80	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 6.

All (80) 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:652:ASN:HD21	1:B:656:ILE:HD11	1.24	0.98
1:B:601:LEU:HB2	1:B:648:TYR:CE2	2.08	0.89
1:B:652:ASN:ND2	1:B:656:ILE:HD11	1.98	0.79
1:B:652:ASN:HD21	1:B:656:ILE:CD1	1.96	0.78
1:B:652:ASN:ND2	1:B:656:ILE:CD1	2.50	0.73
1:B:469:VAL:O	1:B:473:LEU:HD23	1.92	0.69
1:B:561:ILE:O	1:B:565:ASN:ND2	2.29	0.65
1:B:771:SER:O	1:B:775:VAL:HG23	1.97	0.65
1:B:679:GLU:OE2	1:B:684:ASP:N	2.31	0.64
1:B:601:LEU:CB	1:B:648:TYR:CE2	2.80	0.64
1:A:834:MET:CE	2:A:1001:O2M:C9	2.75	0.63
1:A:834:MET:HE1	2:A:1001:O2M:C9	2.28	0.62
1:B:489:TRP:CD2	1:B:535:GLN:HG2	2.36	0.61
1:B:857:ASN:O	1:B:860:GLU:HB3	2.01	0.61
1:A:839:ILE:HD12	1:A:839:ILE:O	2.01	0.60
1:B:684:ASP:HB3	1:B:687:ASP:OD2	2.03	0.59
1:B:601:LEU:HB3	1:B:648:TYR:CD2	2.40	0.56
1:A:902:ASP:N	1:A:902:ASP:OD1	2.38	0.56
1:B:648:TYR:CD1	1:B:648:TYR:N	2.72	0.55
1:A:715:ASN:ND2	3:A:1102:HOH:O	2.39	0.55
1:B:830:LEU:CD1	1:B:886:ALA:HA	2.37	0.54
1:A:872:PHE:CE2	1:A:876:ILE:HD11	2.43	0.54
1:B:815:GLN:N	1:B:816:PRO:HD2	2.23	0.53
1:B:652:ASN:ND2	1:B:652:ASN:O	2.42	0.53
1:A:766:ARG:NH1	1:A:816:PRO:O	2.42	0.53
1:A:841:GLN:OE1	1:A:841:GLN:C	2.48	0.52
1:B:603:ILE:HG22	1:B:603:ILE:O	2.10	0.52
1:B:732:GLN:NE2	3:B:1004:HOH:O	2.37	0.52
1:A:658:ARG:O	1:A:661:LEU:HB3	2.10	0.51
1:A:529:MET:O	1:A:532:THR:OG1	2.25	0.51
1:B:601:LEU:CB	1:B:648:TYR:CD2	2.95	0.50
1:B:481:ALA:CB	1:B:527:GLU:OE2	2.60	0.50
1:B:601:LEU:HB2	1:B:648:TYR:HE2	1.68	0.50
1:B:554:ALA:HA	1:B:557:ARG:HB3	1.92	0.49
1:B:601:LEU:CD1	1:B:648:TYR:HE2	2.24	0.49
1:A:742:HIS:CG	1:A:794:LEU:HD22	2.49	0.48
1:B:489:TRP:CE3	1:B:535:GLN:HG2	2.49	0.47
1:A:855:GLU:HG3	1:A:856:ALA:N	2.29	0.47
1:B:877:ILE:HD11	1:B:907:THR:HA	1.97	0.47
1:A:834:MET:HE2	2:A:1001:O2M:C9	2.45	0.47
1:B:830:LEU:HD13	1:B:886:ALA:HA	1.97	0.46
1:B:746:LEU:HD11	3:B:1027:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:746:LEU:O	1:A:750:VAL:HG23	2.16	0.46
1:A:785:THR:N	1:A:786:PRO:CD	2.79	0.45
1:A:882:ASP:HB2	2:A:1001:O2M:C3	2.46	0.45
1:B:595:ILE:HB	1:B:596:PRO:HD3	1.98	0.45
1:A:648:TYR:CD1	1:A:648:TYR:O	2.70	0.45
1:B:568:THR:HG22	1:B:572:ILE:HD11	1.99	0.45
1:B:883:MET:CE	1:B:908:LEU:HD23	2.47	0.45
1:A:815:GLN:N	1:A:816:PRO:CD	2.80	0.45
1:B:723:GLY:HA3	3:B:1011:HOH:O	2.16	0.45
1:A:489:TRP:CE2	1:A:535:GLN:HG2	2.52	0.44
1:B:887:ALA:HA	1:B:890:PHE:CD2	2.53	0.44
1:B:603:ILE:CG2	1:B:603:ILE:O	2.66	0.44
1:B:583:SER:OG	1:B:626:LYS:NZ	2.39	0.44
1:B:785:THR:O	1:B:786:PRO:C	2.55	0.43
1:B:887:ALA:HA	1:B:890:PHE:CE2	2.53	0.43
1:B:821:PRO:HB3	1:B:825:LEU:HD23	1.99	0.43
1:B:742:HIS:CG	1:B:794:LEU:HD22	2.53	0.43
1:B:575:LEU:HA	1:B:578:LEU:HD12	2.00	0.43
1:B:661:LEU:HG	1:B:665:PHE:CE1	2.54	0.43
1:A:643:LEU:HD23	1:A:643:LEU:HA	1.88	0.43
1:B:614:ASP:OD1	1:B:653:ARG:CD	2.68	0.42
1:A:458:MET:HA	3:A:1151:HOH:O	2.18	0.42
1:B:652:ASN:ND2	1:B:652:ASN:C	2.73	0.42
1:B:670:ASN:OD1	1:B:715:ASN:ND2	2.52	0.42
1:A:533:ILE:HD11	1:A:571:PHE:CZ	2.55	0.42
1:B:621:LYS:HB2	3:B:1030:HOH:O	2.20	0.42
1:B:614:ASP:OD1	1:B:653:ARG:HD2	2.19	0.42
1:A:575:LEU:N	1:A:576:PRO:CD	2.82	0.41
1:A:533:ILE:HD11	1:A:571:PHE:CE2	2.54	0.41
1:B:661:LEU:HD11	1:B:665:PHE:CZ	2.55	0.41
1:A:702:HIS:ND1	1:A:702:HIS:O	2.52	0.41
1:B:481:ALA:HB2	1:B:527:GLU:OE2	2.21	0.41
1:B:815:GLN:N	1:B:816:PRO:CD	2.84	0.41
1:B:838:PHE:C	1:B:839:ILE:HD13	2.42	0.40
1:A:706:ASP:C	1:A:706:ASP:OD1	2.60	0.40
1:A:604:TYR:CD1	1:A:613:LEU:HB2	2.57	0.40
1:A:780:LEU:O	1:A:788:LYS:HG2	2.22	0.40
1:A:821:PRO:CB	1:A:825:LEU:HD23	2.51	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%)	400 (94%)	23 (5%)	2 (0%)	29	54
1	B	415/459 (90%)	375 (90%)	35 (8%)	5 (1%)	13	32
All	All	840/918 (92%)	775 (92%)	58 (7%)	7 (1%)	19	43

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	901	GLY
1	A	515	GLU
1	A	644	CYS
1	B	554	ALA
1	B	706	ASP
1	B	603	ILE
1	B	543	VAL

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	390/415 (94%)	368 (94%)	22 (6%)	21	45
1	B	383/415 (92%)	359 (94%)	24 (6%)	18	40
All	All	773/830 (93%)	727 (94%)	46 (6%)	19	42

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	510	PRO
1	A	519	ASP
1	A	591	ASN
1	A	618	LYS
1	A	638	LYS
1	A	641	SER
1	A	644	CYS
1	A	647	GLU
1	A	650	ILE
1	A	659	SER
1	A	679	GLU
1	A	709	LYS
1	A	731	GLU
1	A	770	LYS
1	A	795	LEU
1	A	797	ASP
1	A	805	GLN
1	A	812	GLU
1	A	830	LEU
1	A	841	GLN
1	A	859	ILE
1	A	891	LYS
1	B	470	LEU
1	B	474	GLU
1	B	475	SER
1	B	490	GLU
1	B	528	LEU
1	B	562	ASP
1	B	567	LEU
1	B	574	THR
1	B	643	LEU
1	B	646	GLU
1	B	647	GLU
1	B	648	TYR
1	B	652	ASN
1	B	668	ARG
1	B	679	GLU
1	B	731	GLU
1	B	756	SER
1	B	759	LYS
1	B	815	GLN
1	B	835	ASP
1	B	839	ILE

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Mol	Chain	Res	Type
1	B	857	ASN
1	B	888	ASP
1	B	911	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	493	GLN
1	A	790	GLN
1	B	565	ASN
1	B	619	GLN
1	B	652	ASN
1	B	748	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 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	O2M	A	1001	-	12,16,16	0.78	1 (8%)	9,21,21	0.90	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	O2M	A	1001	-	-	1/4/9/9	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	O2M	C8-C9	-2.03	1.35	1.38

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	O2M	O1-C6-C7-C8

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	O2M	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

Ligand O2M A 1001
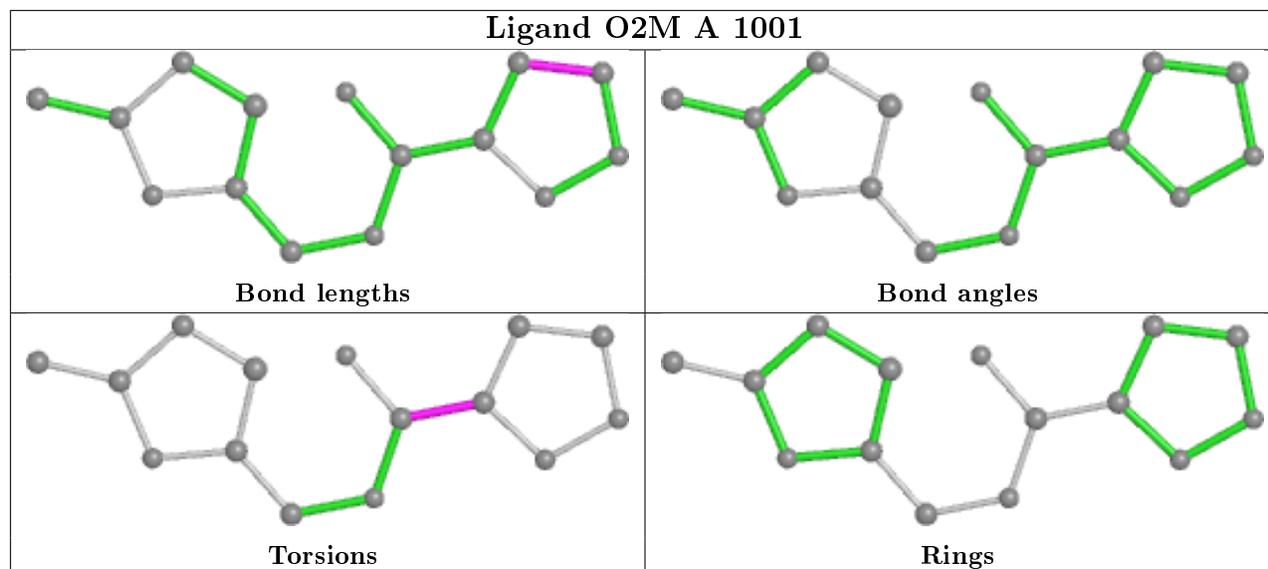
5.7 Other polymers (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.11	1 (0%)	95 96	50, 75, 119, 152	0
1	B	425/459 (92%)	0.34	16 (3%)	40 39	60, 97, 139, 179	0
All	All	860/918 (93%)	0.22	17 (1%)	65 67	50, 85, 131, 179	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	892	HIS	4.6
1	B	893	TYR	4.3
1	B	609	MET	3.1
1	B	872	PHE	3.0
1	B	886	ALA	2.7
1	B	889	ILE	2.7
1	B	551	VAL	2.6
1	B	678	GLN	2.6
1	B	646	GLU	2.5
1	B	894	MET	2.4
1	B	891	LYS	2.4
1	B	908	LEU	2.3
1	B	895	LYS	2.1
1	A	458	MET	2.1
1	B	869	LEU	2.1
1	B	884	HIS	2.1
1	B	477	LEU	2.0

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

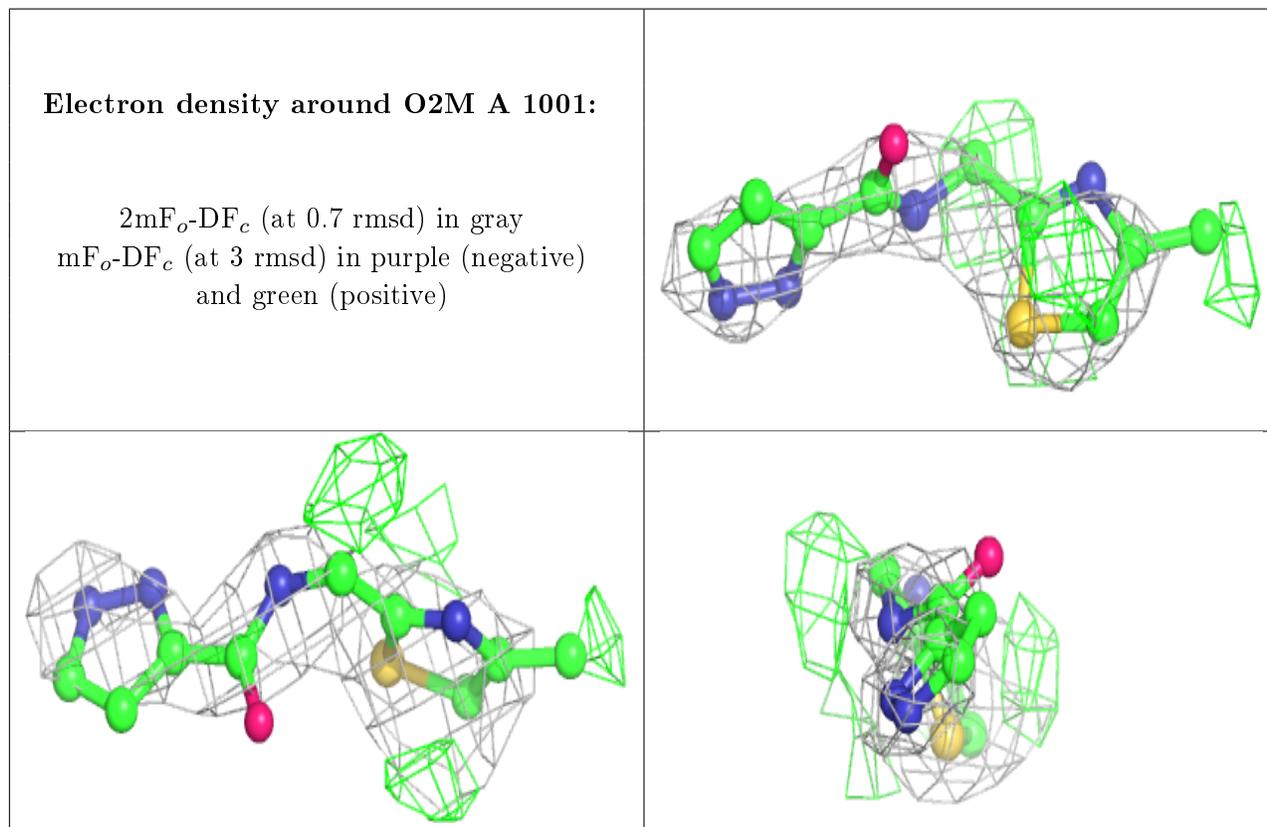There are no non-standard protein/DNA/RNA residues in this entry.

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, 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($Å^2$)	Q<0.9
2	O2M	A	1001	15/15	0.83	0.32	42,46,55,57	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 O2M A 1001:

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

6.5 Other polymers (i)

There are no such residues in this entry.