wwPDB X-ray Structure Validation Summary Report (i)

Mar 5, 2026 – 11:35 AM UTC

PDB ID	:	6A9O / pdb_00006a9o
Title	:	Rational discovery of a SOD1 tryptophan oxidation inhibitor with therapeutic potential for amyotrophic lateral sclerosis
Authors	:	Manjula, R.; Padmanabhan, B.
Deposited on	:	2018-07-14
Resolution	:	2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

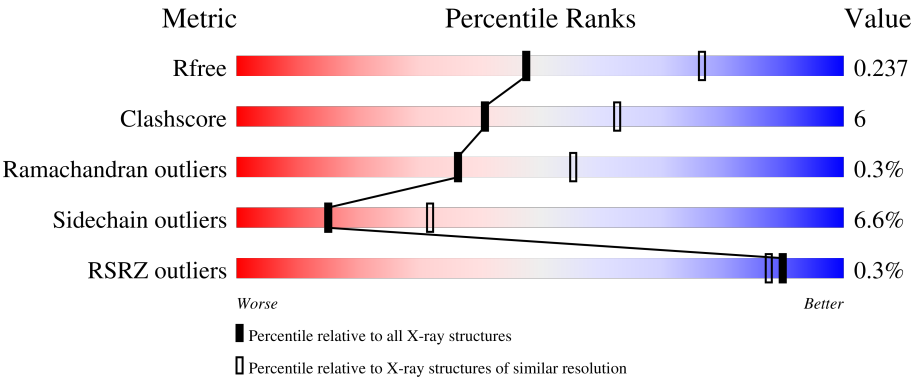
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 <=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	154	81% 18%
1	B	154	79% 19%
1	C	154	79% 18%
1	D	154	88% 10%
1	E	154	76% 20%

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Mol	Chain	Length	Quality of chain
1	F	154	80% 16%
1	G	154	% 56% 22% 18%
1	H	154	86% 13%
1	I	154	% 71% 25%
1	J	154	70% 28%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	D	203	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 12322 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 Superoxide dismutase [Cu-Zn].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	154	Total	C	N	O	S	0	0	0
			1115	682	204	225	4			
1	B	154	Total	C	N	O	S	0	2	0
			1130	690	206	230	4			
1	C	154	Total	C	N	O	S	0	0	0
			1118	684	204	225	5			
1	D	154	Total	C	N	O	S	0	1	0
			1123	687	207	225	4			
1	E	154	Total	C	N	O	S	0	1	0
			1115	681	205	225	4			
1	F	154	Total	C	N	O	S	0	1	0
			1121	685	205	227	4			
1	G	127	Total	C	N	O	S	0	1	0
			927	572	167	184	4			
1	H	153	Total	C	N	O	S	0	0	0
			1106	676	202	224	4			
1	I	154	Total	C	N	O	S	0	0	0
			1108	678	203	223	4			
1	J	154	Total	C	N	O	S	0	0	0
			1115	682	204	225	4			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		

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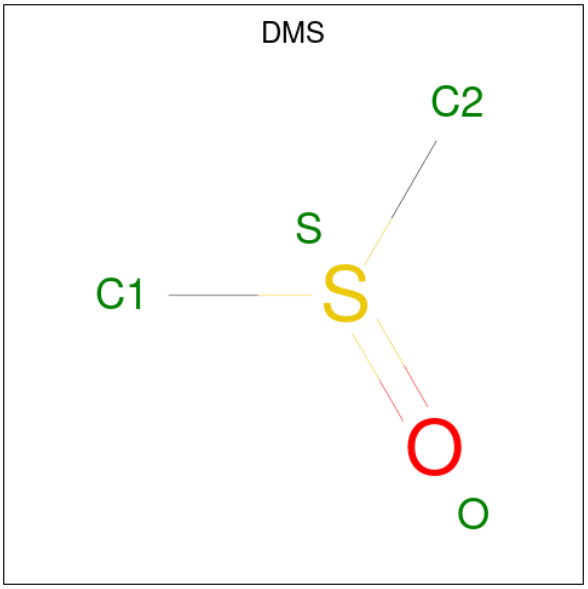
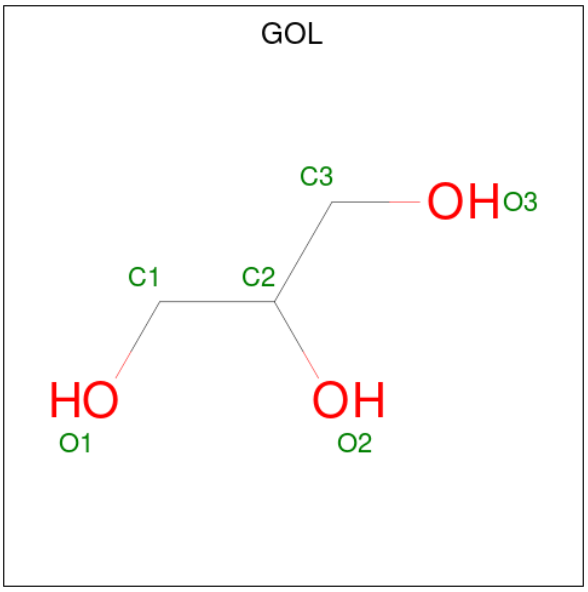
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total Zn 1 1	0	0
2	F	1	Total Zn 1 1	0	0
2	H	1	Total Zn 1 1	0	0
2	I	1	Total Zn 1 1	0	0
2	J	1	Total Zn 1 1	0	0

- Molecule 3 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



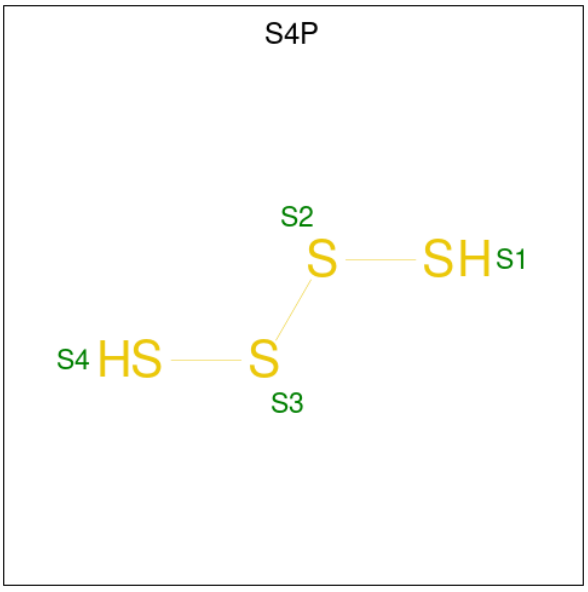
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O S 4 2 1 1	0	0
3	D	1	Total C O S 4 2 1 1	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



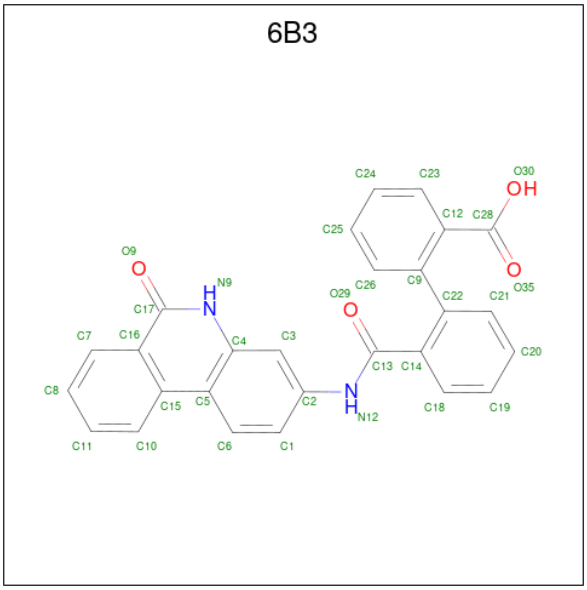
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0

- Molecule 5 is Dihydrogen tetrasulfide (CCD ID: S4P) (formula: H_2S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total S 4 4	0	0
5	C	1	Total S 4 4	0	0
5	F	1	Total S 4 4	0	0

- Molecule 6 is 2'-[(6-oxo-5,6-dihydrophenanthridin-3-yl)carbamoyl][1,1'-biphenyl]-2-carboxylic acid (CCD ID: 6B3) (formula: $C_{27}H_{18}N_2O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	1	Total C N O 24 20 2 2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	111	Total O 114 114	0	3
7	B	161	Total O 169 169	0	8
7	C	133	Total O 138 138	0	4
7	D	169	Total O 175 175	0	6
7	E	116	Total O 118 118	0	2

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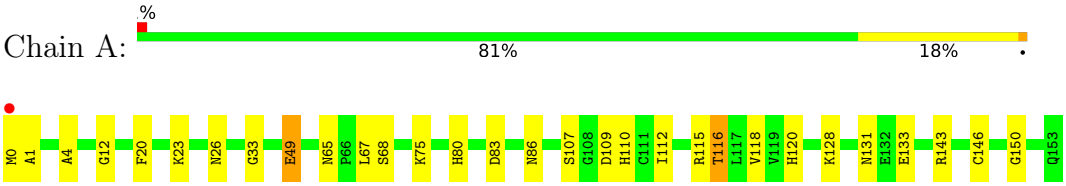
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	F	169	Total O 170 170	0	1
7	G	80	Total O 85 85	0	5
7	H	124	Total O 125 125	0	1
7	I	80	Total O 82 82	0	2
7	J	91	Total O 91 91	0	0

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.

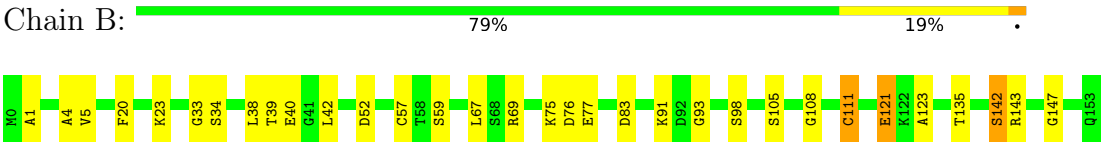
• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:



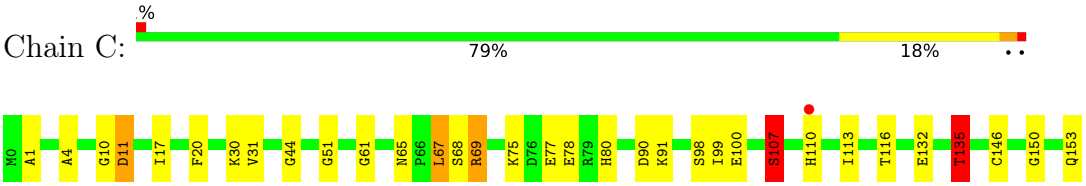
• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain B:



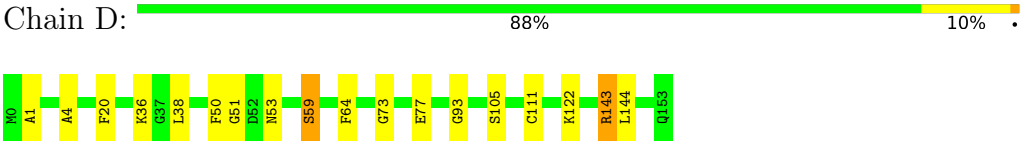
• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain C:



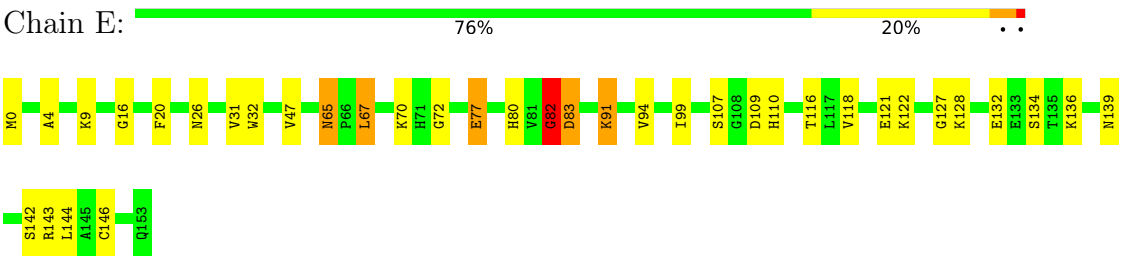
• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain D:



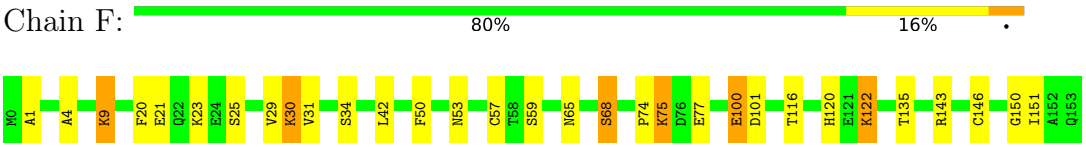
• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain E:



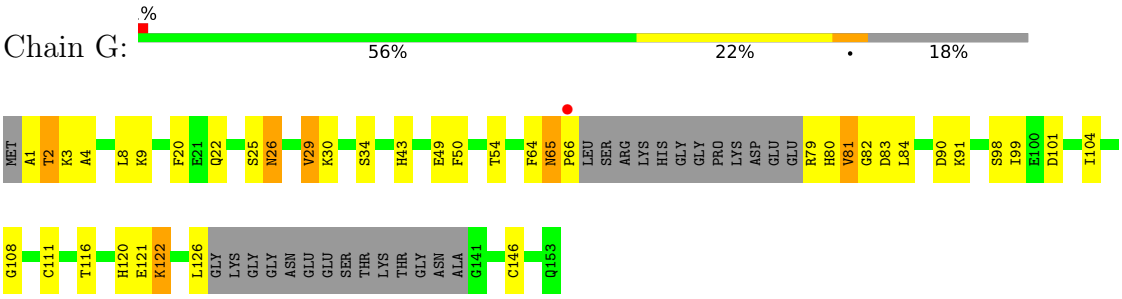
• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain F:



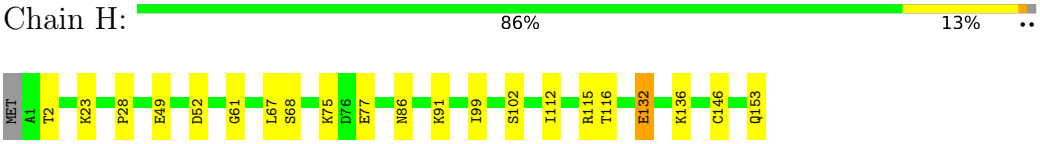
• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain G:



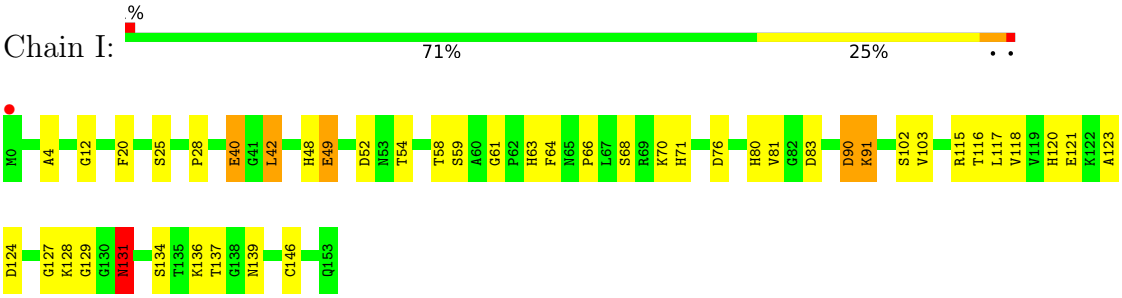
• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain H:



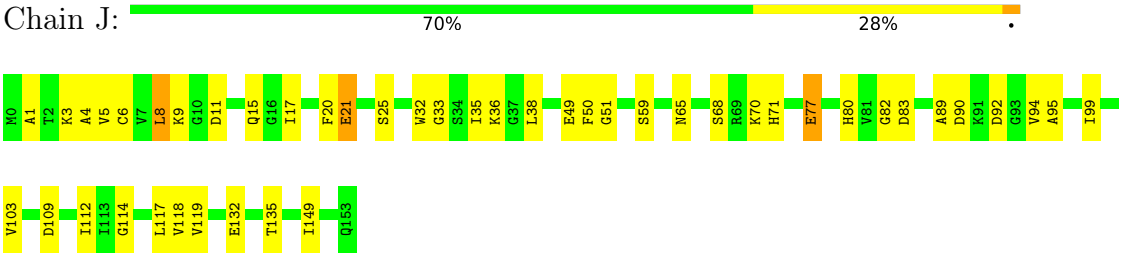
• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain I:



• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	164.37Å 203.69Å 144.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-2.50) 99.7 (20.00-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.163 , 0.237 0.168 , 0.237	Depositor DCC
R_{free} test set	4182 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	41.8	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 57.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12322	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.37% 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: DMS, ZN, S4P, 6B3, GOL

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	1.48	6/1133 (0.5%)	1.43	10/1527 (0.7%)
1	B	1.52	9/1148 (0.8%)	1.39	8/1547 (0.5%)
1	C	1.57	6/1136 (0.5%)	1.43	8/1530 (0.5%)
1	D	1.46	4/1144 (0.3%)	1.34	3/1541 (0.2%)
1	E	1.61	9/1133 (0.8%)	1.38	5/1529 (0.3%)
1	F	1.55	13/1139 (1.1%)	1.32	3/1535 (0.2%)
1	G	1.47	2/941 (0.2%)	1.51	9/1271 (0.7%)
1	H	1.44	3/1124 (0.3%)	1.43	7/1516 (0.5%)
1	I	1.53	6/1126 (0.5%)	1.48	11/1519 (0.7%)
1	J	1.42	4/1133 (0.4%)	1.47	11/1527 (0.7%)
All	All	1.51	62/11157 (0.6%)	1.42	75/15042 (0.5%)

The worst 5 of 62 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	78	GLU	CA-C	8.03	1.63	1.52
1	E	83	ASP	CA-C	-7.67	1.43	1.52
1	D	1	ALA	N-CA	7.14	1.54	1.46
1	B	5	VAL	N-CA	-7.09	1.38	1.46
1	A	150	GLY	C-O	6.87	1.32	1.23

The worst 5 of 75 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	142	SER	CA-CB-OG	-8.91	93.27	111.10
1	A	110	HIS	N-CA-C	-8.32	101.60	112.41
1	G	49	GLU	N-CA-C	8.24	120.34	111.36
1	I	12	GLY	CA-C-N	8.06	127.78	119.64
1	I	12	GLY	C-N-CA	8.06	127.78	119.64

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	1115	0	1078	11	0
1	B	1130	0	1087	12	0
1	C	1118	0	1085	13	0
1	D	1123	0	1091	14	0
1	E	1115	0	1068	23	0
1	F	1121	0	1082	10	0
1	G	927	0	892	23	0
1	H	1106	0	1066	7	0
1	I	1108	0	1066	20	0
1	J	1115	0	1079	12	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
3	A	4	0	6	0	0
3	D	4	0	6	1	0
4	A	6	0	8	1	0
4	B	6	0	8	2	0
4	C	6	0	8	1	0
4	D	6	0	8	6	0
5	A	4	0	0	0	0
5	C	4	0	0	0	0
5	F	4	0	0	0	0
6	F	24	0	0	3	0
7	A	114	0	0	4	0
7	B	169	0	0	2	0
7	C	138	0	0	3	1
7	D	175	0	0	4	1
7	E	118	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	F	170	0	0	6	1
7	G	85	0	0	3	0
7	H	125	0	0	3	0
7	I	82	0	0	0	0
7	J	91	0	0	1	0
All	All	12322	0	10638	140	2

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.

The worst 5 of 140 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:E:109:ASP:HB2	7:E:375:HOH:O	1.58	1.03
1:D:143:ARG:HH21	4:D:203:GOL:H32	1.24	1.00
1:B:39:THR:HA	4:B:202:GOL:H31	1.45	0.97
1:G:66:PRO:HD2	1:G:81:VAL:HG23	1.49	0.93
1:J:1:ALA:HB1	7:J:319:HOH:O	1.70	0.90

All (2) 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)
7:F:469:HOH:O	7:F:469:HOH:O[3_555]	1.91	0.29
7:C:407:HOH:O	7:D:434:HOH:O[4_575]	2.18	0.02

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	152/154 (99%)	148 (97%)	4 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	154/154 (100%)	153 (99%)	1 (1%)	0	100 100
1	C	152/154 (99%)	148 (97%)	4 (3%)	0	100 100
1	D	153/154 (99%)	152 (99%)	1 (1%)	0	100 100
1	E	153/154 (99%)	146 (95%)	6 (4%)	1 (1%)	18 34
1	F	153/154 (99%)	149 (97%)	4 (3%)	0	100 100
1	G	122/154 (79%)	112 (92%)	8 (7%)	2 (2%)	7 14
1	H	151/154 (98%)	147 (97%)	4 (3%)	0	100 100
1	I	152/154 (99%)	138 (91%)	13 (9%)	1 (1%)	18 34
1	J	152/154 (99%)	142 (93%)	10 (7%)	0	100 100
All	All	1494/1540 (97%)	1435 (96%)	55 (4%)	4 (0%)	36 55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	131	ASN
1	E	82	GLY
1	G	81	VAL
1	G	90	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	118/119 (99%)	114 (97%)	4 (3%)	32 60
1	B	120/119 (101%)	117 (98%)	3 (2%)	42 69
1	C	119/119 (100%)	110 (92%)	9 (8%)	12 26
1	D	119/119 (100%)	116 (98%)	3 (2%)	42 69
1	E	117/119 (98%)	112 (96%)	5 (4%)	26 51
1	F	119/119 (100%)	109 (92%)	10 (8%)	10 22
1	G	99/119 (83%)	85 (86%)	14 (14%)	3 7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	117/119 (98%)	112 (96%)	5 (4%)	26 51
1	I	116/119 (98%)	107 (92%)	9 (8%)	11 24
1	J	118/119 (99%)	104 (88%)	14 (12%)	5 11
All	All	1162/1190 (98%)	1086 (94%)	76 (6%)	15 32

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	70	LYS
1	J	70	LYS
1	I	91	LYS
1	J	15	GLN
1	J	119	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	80	HIS
1	J	53	ASN
1	E	139	ASN
1	F	53	ASN
1	F	110	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)

Of 19 ligands modelled in this entry, 9 are monoatomic - leaving 10 for Mogul analysis.

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	$\#\|Z\| > 2$
4	GOL	B	202	-	5,5,5	0.77	0	5,5,5	0.89	0
5	S4P	A	204	-	1,3,3	0.66	0	0,2,2	-	-
3	DMS	A	202	-	3,3,3	0.49	0	3,3,3	1.38	1 (33%)
4	GOL	C	202	-	5,5,5	1.11	0	5,5,5	0.68	0
6	6B3	F	201	-	27,27,37	2.50	11 (40%)	38,38,53	2.45	11 (28%)
5	S4P	C	203	-	1,3,3	0.36	0	0,2,2	-	-
5	S4P	F	203	-	1,3,3	0.18	0	0,2,2	-	-
4	GOL	A	203	-	5,5,5	0.82	0	5,5,5	1.13	0
4	GOL	D	203	-	5,5,5	0.88	0	5,5,5	1.96	1 (20%)
3	DMS	D	202	-	3,3,3	0.65	0	3,3,3	2.19	2 (66%)

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
4	GOL	B	202	-	-	2/4/4/4	-
5	S4P	A	204	-	-	0/0/1/1	-
4	GOL	C	202	-	-	0/4/4/4	-
6	6B3	F	201	-	-	4/8/8/16	0/4/4/5
5	S4P	C	203	-	-	0/0/1/1	-
5	S4P	F	203	-	-	0/0/1/1	-
4	GOL	A	203	-	-	3/4/4/4	-
4	GOL	D	203	-	-	4/4/4/4	-

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	201	6B3	C18-C14	5.01	1.47	1.39
6	F	201	6B3	C5-C4	4.80	1.47	1.40
6	F	201	6B3	C6-C5	4.72	1.47	1.40
6	F	201	6B3	C16-C15	4.24	1.47	1.40
6	F	201	6B3	C17-N9	3.70	1.42	1.36

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	201	6B3	C21-C22-C14	-7.66	112.84	120.36
6	F	201	6B3	C20-C19-C18	-5.48	113.48	120.24
6	F	201	6B3	C22-C14-C18	5.03	124.96	118.57
4	D	203	GOL	O3-C3-C2	3.85	127.72	110.38
6	F	201	6B3	C6-C1-C2	-3.85	115.87	120.30

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	203	GOL	O1-C1-C2-C3
4	B	202	GOL	O1-C1-C2-O2
4	B	202	GOL	O1-C1-C2-C3
4	D	203	GOL	O1-C1-C2-C3
4	D	203	GOL	C1-C2-C3-O3

There are no ring outliers.

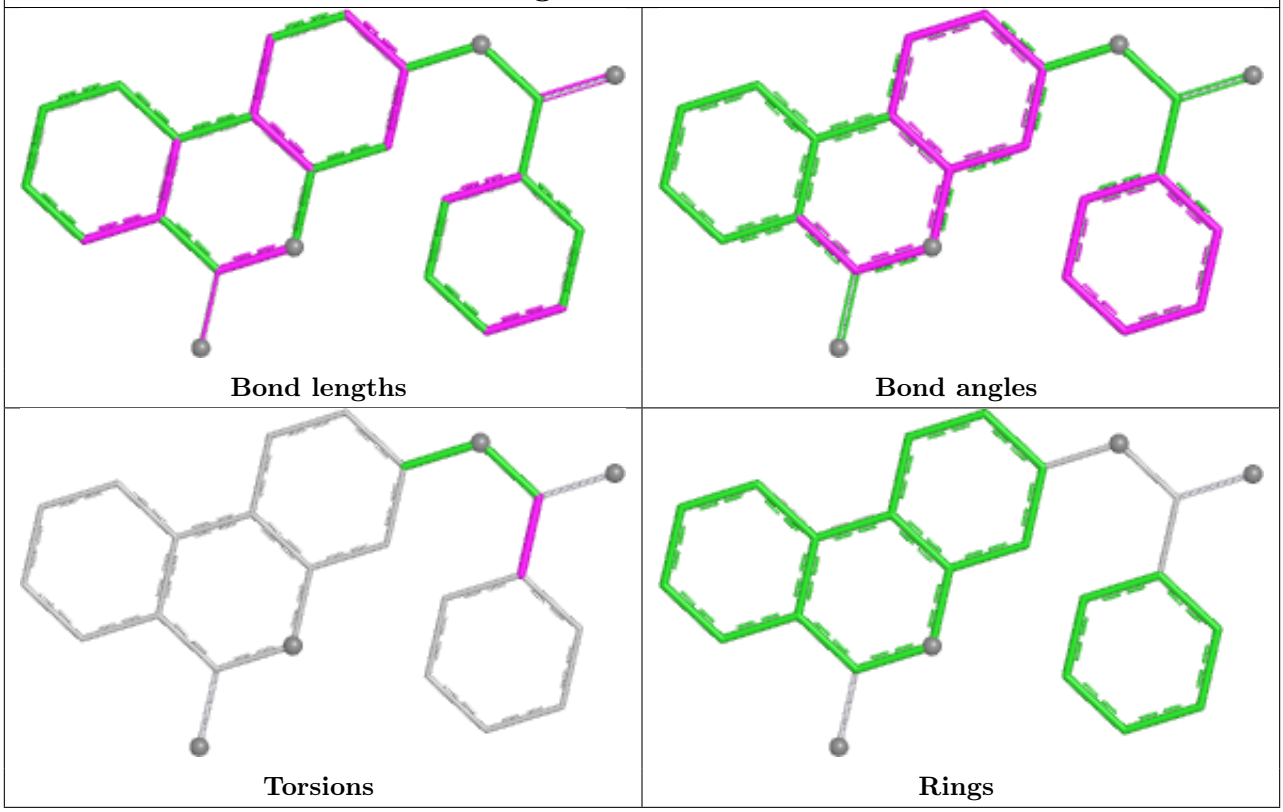
6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	202	GOL	2	0
4	C	202	GOL	1	0
6	F	201	6B3	3	0
4	A	203	GOL	1	0
4	D	203	GOL	6	0
3	D	202	DMS	1	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 6B3 F 201



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	154/154 (100%)	-0.77	1 (0%) 85 83	28, 37, 54, 62	0
1	B	154/154 (100%)	-0.93	0 100 100	15, 31, 48, 58	2 (1%)
1	C	154/154 (100%)	-0.62	1 (0%) 85 83	28, 38, 58, 70	0
1	D	154/154 (100%)	-0.96	0 100 100	18, 31, 47, 61	1 (0%)
1	E	154/154 (100%)	-0.48	0 100 100	16, 41, 70, 82	1 (0%)
1	F	154/154 (100%)	-0.93	0 100 100	17, 32, 49, 61	1 (0%)
1	G	127/154 (82%)	-0.32	1 (0%) 82 80	19, 46, 70, 82	1 (0%)
1	H	153/154 (99%)	-0.77	0 100 100	30, 40, 56, 71	0
1	I	154/154 (100%)	-0.38	1 (0%) 85 83	37, 50, 70, 77	0
1	J	154/154 (100%)	-0.58	0 100 100	35, 46, 66, 80	0
All	All	1512/1540 (98%)	-0.68	4 (0%) 90 87	15, 39, 64, 82	6 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	66	PRO	4.2
1	C	110	HIS	2.8
1	I	0	MET	2.4
1	A	0	MET	2.2

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

There are no oligosaccharides in this entry.

6.4 Ligands (i)

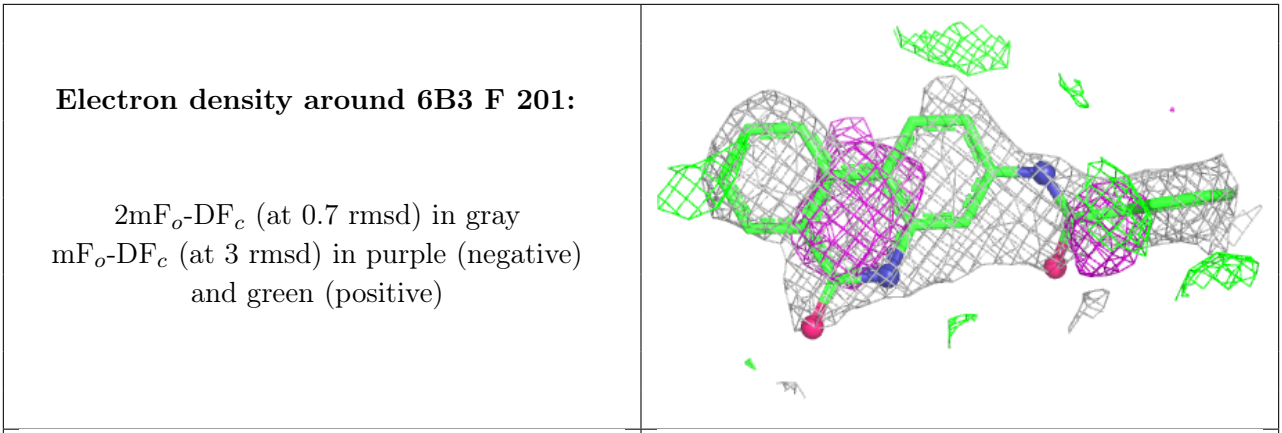
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
6	6B3	F	201	24/33	0.72	0.16	60,74,83,86	0
4	GOL	C	202	6/6	0.83	0.15	56,62,65,70	0
3	DMS	A	202	4/4	0.87	0.22	61,63,74,76	0
4	GOL	D	203	6/6	0.90	0.12	40,52,53,56	0
4	GOL	A	203	6/6	0.90	0.14	56,58,59,63	0
4	GOL	B	202	6/6	0.91	0.10	49,55,57,68	0
5	S4P	A	204	4/4	0.91	0.19	62,66,73,73	0
3	DMS	D	202	4/4	0.91	0.20	63,66,67,74	0
5	S4P	C	203	4/4	0.92	0.19	66,70,74,75	0
5	S4P	F	203	4/4	0.94	0.21	60,61,61,65	0
2	ZN	A	201	1/1	0.99	0.03	49,49,49,49	0
2	ZN	C	201	1/1	0.99	0.06	49,49,49,49	0
2	ZN	E	201	1/1	0.99	0.13	62,62,62,62	0
2	ZN	H	201	1/1	0.99	0.02	48,48,48,48	0
2	ZN	I	201	1/1	0.99	0.09	59,59,59,59	0
2	ZN	B	201	1/1	1.00	0.01	39,39,39,39	0
2	ZN	J	201	1/1	1.00	0.02	50,50,50,50	0
2	ZN	F	202	1/1	1.00	0.01	39,39,39,39	0
2	ZN	D	201	1/1	1.00	0.01	41,41,41,41	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.

Electron density around 6B3 F 201:

$2mF_o$-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.