wwPDB X-ray Structure Validation Summary Report (i)

Oct 31, 2023 – 07:14 PM JST

PDB ID	:	5GWV
Title	:	Structure of MoeN5-Sso7d fusion protein in complex with a substrate analogue
Authors	:	Ko, T.-P.; Guo, R.-T.; Chen, C.-C.
Deposited on	:	2016-09-14
Resolution	:	2.40 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:

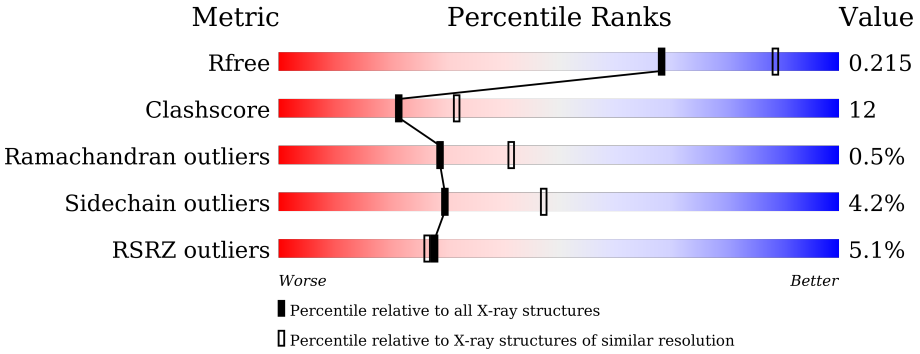
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	343	3%, 61%, 14%, •, 23%
1	B	343	4%, 79%, 16%, • •
1	C	343	59%, 15%, •, 24%
1	D	343	10%, 74%, 22%, • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10016 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 MoeN5,DNA-binding protein 7d.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	264	2013	1243	374	385	11	0	0	0
1	B	332	2533	1571	463	485	14	0	0	0
1	C	262	1998	1234	372	381	11	0	0	0
1	D	333	2544	1579	466	485	14	0	0	0

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP A0A010
A	-12	ALA	-	expression tag	UNP A0A010
A	-11	HIS	-	expression tag	UNP A0A010
A	-10	HIS	-	expression tag	UNP A0A010
A	-9	HIS	-	expression tag	UNP A0A010
A	-8	HIS	-	expression tag	UNP A0A010
A	-7	HIS	-	expression tag	UNP A0A010
A	-6	HIS	-	expression tag	UNP A0A010
A	-5	VAL	-	expression tag	UNP A0A010
A	-4	ASP	-	expression tag	UNP A0A010
A	-3	ASP	-	expression tag	UNP A0A010
A	-2	ASP	-	expression tag	UNP A0A010
A	-1	ASP	-	expression tag	UNP A0A010
A	0	LYS	-	expression tag	UNP A0A010
A	261	ALA	-	linker	UNP A0A010
A	262	GLY	-	linker	UNP A0A010
A	263	ALA	-	linker	UNP A0A010
A	264	GLY	-	linker	UNP A0A010
A	265	ALA	-	linker	UNP A0A010
B	-13	MET	-	expression tag	UNP A0A010
B	-12	ALA	-	expression tag	UNP A0A010

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	HIS	-	expression tag	UNP A0A010
B	-10	HIS	-	expression tag	UNP A0A010
B	-9	HIS	-	expression tag	UNP A0A010
B	-8	HIS	-	expression tag	UNP A0A010
B	-7	HIS	-	expression tag	UNP A0A010
B	-6	HIS	-	expression tag	UNP A0A010
B	-5	VAL	-	expression tag	UNP A0A010
B	-4	ASP	-	expression tag	UNP A0A010
B	-3	ASP	-	expression tag	UNP A0A010
B	-2	ASP	-	expression tag	UNP A0A010
B	-1	ASP	-	expression tag	UNP A0A010
B	0	LYS	-	expression tag	UNP A0A010
B	261	ALA	-	linker	UNP A0A010
B	262	GLY	-	linker	UNP A0A010
B	263	ALA	-	linker	UNP A0A010
B	264	GLY	-	linker	UNP A0A010
B	265	ALA	-	linker	UNP A0A010
C	-13	MET	-	expression tag	UNP A0A010
C	-12	ALA	-	expression tag	UNP A0A010
C	-11	HIS	-	expression tag	UNP A0A010
C	-10	HIS	-	expression tag	UNP A0A010
C	-9	HIS	-	expression tag	UNP A0A010
C	-8	HIS	-	expression tag	UNP A0A010
C	-7	HIS	-	expression tag	UNP A0A010
C	-6	HIS	-	expression tag	UNP A0A010
C	-5	VAL	-	expression tag	UNP A0A010
C	-4	ASP	-	expression tag	UNP A0A010
C	-3	ASP	-	expression tag	UNP A0A010
C	-2	ASP	-	expression tag	UNP A0A010
C	-1	ASP	-	expression tag	UNP A0A010
C	0	LYS	-	expression tag	UNP A0A010
C	261	ALA	-	linker	UNP A0A010
C	262	GLY	-	linker	UNP A0A010
C	263	ALA	-	linker	UNP A0A010
C	264	GLY	-	linker	UNP A0A010
C	265	ALA	-	linker	UNP A0A010
D	-13	MET	-	expression tag	UNP A0A010
D	-12	ALA	-	expression tag	UNP A0A010
D	-11	HIS	-	expression tag	UNP A0A010
D	-10	HIS	-	expression tag	UNP A0A010
D	-9	HIS	-	expression tag	UNP A0A010
D	-8	HIS	-	expression tag	UNP A0A010

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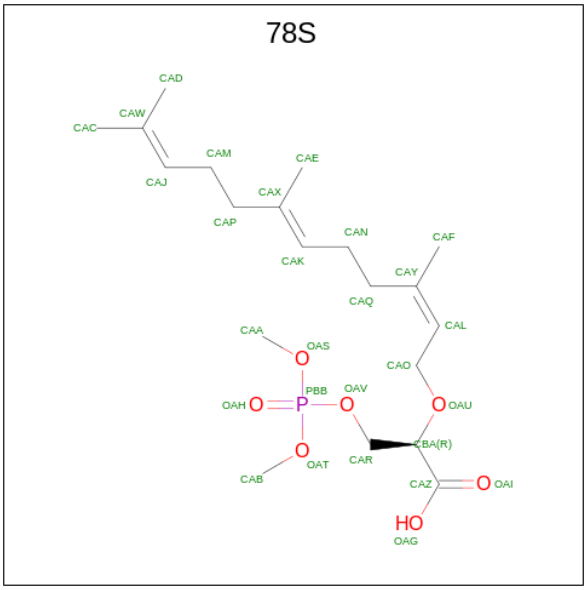
Chain	Residue	Modelled	Actual	Comment	Reference
D	-7	HIS	-	expression tag	UNP A0A010
D	-6	HIS	-	expression tag	UNP A0A010
D	-5	VAL	-	expression tag	UNP A0A010
D	-4	ASP	-	expression tag	UNP A0A010
D	-3	ASP	-	expression tag	UNP A0A010
D	-2	ASP	-	expression tag	UNP A0A010
D	-1	ASP	-	expression tag	UNP A0A010
D	0	LYS	-	expression tag	UNP A0A010
D	261	ALA	-	linker	UNP A0A010
D	262	GLY	-	linker	UNP A0A010
D	263	ALA	-	linker	UNP A0A010
D	264	GLY	-	linker	UNP A0A010
D	265	ALA	-	linker	UNP A0A010

- Molecule 2 is (2R)-3-dimethoxyphosphoryloxy-2-[(2Z,6E)-3,7,11-trimethyldodeca-2,6,10-trienoxy]propanoic acid (three-letter code: 78S) (formula: $C_{20}H_{35}O_7P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
2	D	1	28	20	7	1	0	0
			Total	C	O	P		
2	D	1	18	10	7	1	0	0

- Molecule 3 is water.

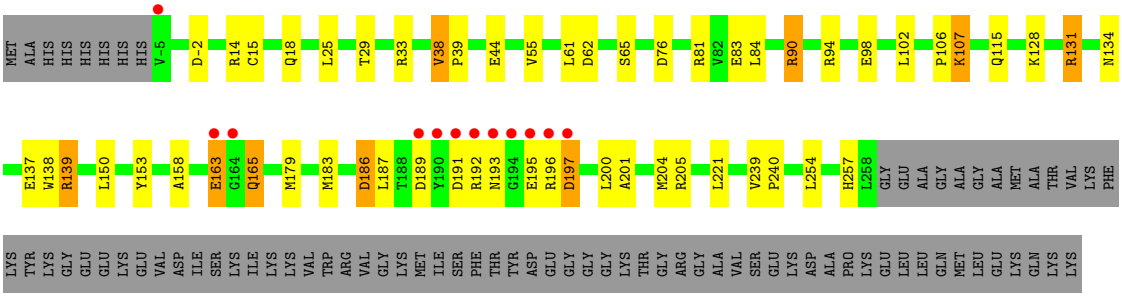
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	223	223	223	0	0
			Total	O		
3	B	243	243	243	0	0
			Total	O		
3	C	175	175	175	0	0
			Total	O		
3	D	241	241	241	0	0

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.

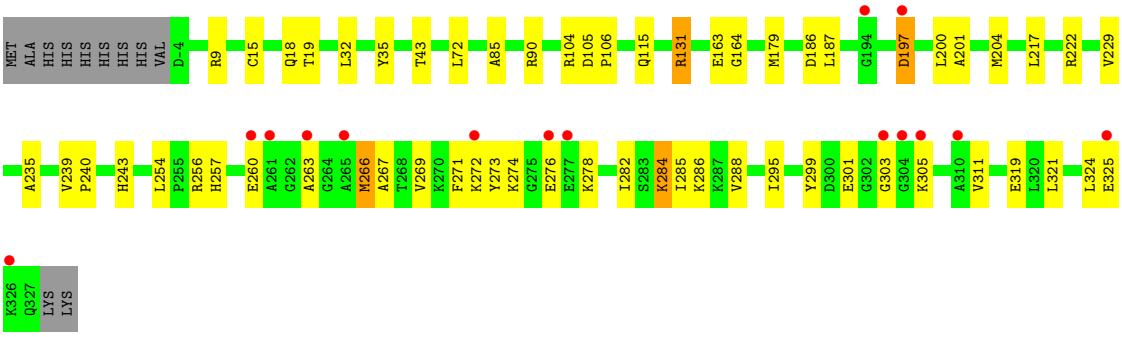
• Molecule 1: MoeN5,DNA-binding protein 7d

Chain A:



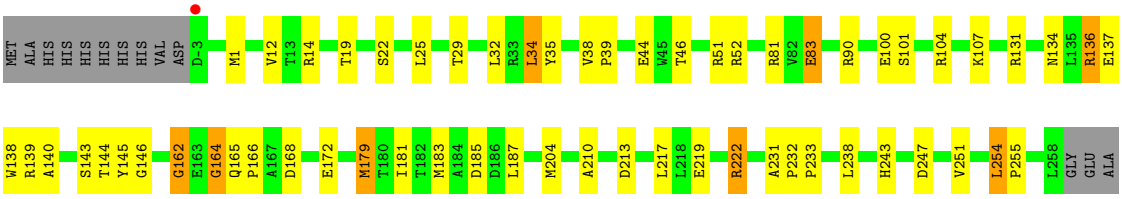
• Molecule 1: MoeN5,DNA-binding protein 7d

Chain B:



• Molecule 1: MoeN5,DNA-binding protein 7d

Chain C:



GLY ALA GLY ALA MET ALA THR VAL LYS PHE LYS TYR LYS GLY GLU GLU LYS GLU VAL ASP ILE SER LYS ILE LYS LYS VAL TRP ARG VAL GLY LYS MET ILE SER PHE THR TYR ASP GLU GLY GLY GLY LYS THR GLY ARG GLY ALA VAL SER GLU LYS ASP ALA PRO LYS GLU LEU LEU

GLN MET LEU GLU LYS GLN LYS LYS

- Molecule 1: MoeN5,DNA-binding protein 7d

Chain D: 10% 74% 22%

MET ALA HIS HIS HIS HIS HIS HIS VAL ASP D-3 M1 D10 H11 V12 T13 R14 C15 V16 A17 Q18 T19 L34 Y35 L36 R37 V38 P39 H40 W45 L61 D70 D75 R81 R90 R94 E98 L99 E100 R104 D105 P106 Q115 G123 T127

R131 W138 R139 A142 L150 Y153 G164 D168 S169 V170 R171 E172 T182 M183 H202 L203 T206 G207 A208 L217 R222 G223 R224 P233 H243 D247 V251 R252 L253 L254 P255 R256 H257 L258 G259 E260 A261 G262 A263 G264 A265 M266 A267 T268

V269 K270 F271 K272 Y273 K274 G275 E276 E277 K278 E279 V280 D281 I282 S283 K284 I285 Y299 D300 E301 G302 G303 G304 K305 T306 G307 R308 V311 K314 Q322 E325 K326 Q327 K328 K329

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	137.94Å 217.70Å 104.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.40 25.04 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.6 (25.00-2.40) 95.2 (25.04-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 2.39Å)	Xtriage
Refinement program	CNS 1.21	Depositor
R, R_{free}	0.174 , 0.216 0.170 , 0.215	Depositor DCC
R_{free} test set	2976 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	38.8	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 52.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10016	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 78S

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	0.61	1/2045 (0.0%)	0.75	0/2780
1	B	0.59	1/2572 (0.0%)	0.74	0/3478
1	C	0.62	0/2030	0.76	2/2759 (0.1%)
1	D	0.57	0/2583	0.73	0/3489
All	All	0.60	2/9230 (0.0%)	0.75	2/12506 (0.0%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	15	CYS	CB-SG	-5.29	1.73	1.81
1	A	15	CYS	CB-SG	-5.16	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	83	GLU	CB-CA-C	-5.71	98.97	110.40
1	C	222	ARG	NE-CZ-NH2	-5.26	117.67	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	153	TYR	Sidechain
1	D	153	TYR	Sidechain

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	2013	0	1996	47	0
1	B	2533	0	2532	49	0
1	C	1998	0	1983	48	0
1	D	2544	0	2554	78	0
2	D	46	0	0	1	0
3	A	223	0	0	9	0
3	B	243	0	0	10	0
3	C	175	0	0	4	0
3	D	241	0	0	8	0
All	All	10016	0	9065	218	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 12.

The worst 5 of 218 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:ARG:HH11	1:C:136:ARG:HB3	1.07	1.10
1:D:325:GLU:HB2	1:D:329:LYS:HD3	1.48	0.92
1:C:136:ARG:HB3	1:C:136:ARG:NH1	1.86	0.88
1:C:131:ARG:HG2	1:C:131:ARG:HH11	1.42	0.82
1:C:136:ARG:HH11	1:C:136:ARG:CB	1.89	0.82

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	262/343 (76%)	256 (98%)	6 (2%)	0	100	100
1	B	330/343 (96%)	313 (95%)	16 (5%)	1 (0%)	41	55
1	C	260/343 (76%)	251 (96%)	7 (3%)	2 (1%)	19	29
1	D	331/343 (96%)	311 (94%)	17 (5%)	3 (1%)	17	25
All	All	1183/1372 (86%)	1131 (96%)	46 (4%)	6 (0%)	29	41

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	260	GLU
1	C	162	GLY
1	D	263	ALA
1	D	261	ALA
1	D	267	ALA

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	208/270 (77%)	192 (92%)	16 (8%)	13	20
1	B	260/270 (96%)	251 (96%)	9 (4%)	36	55
1	C	206/270 (76%)	199 (97%)	7 (3%)	37	56
1	D	261/270 (97%)	254 (97%)	7 (3%)	44	65
All	All	935/1080 (87%)	896 (96%)	39 (4%)	30	47

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	136	ARG
1	D	115	GLN
1	C	179	MET
1	D	1	MET
1	D	224	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	193	ASN
1	D	243	HIS
1	C	124	GLN
1	C	165	GLN
1	C	243	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are 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	78S	D	502	-	17,17,27	2.07	1 (5%)	16,22,34	2.11	3 (18%)
2	78S	D	501	-	27,27,27	2.88	3 (11%)	28,34,34	2.07	7 (25%)

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	78S	D	502	-	-	8/22/22/34	-
2	78S	D	501	-	-	10/34/34/34	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	78S	CAK-CAX	8.56	1.53	1.33
2	D	501	78S	CAL-CAY	8.50	1.53	1.33
2	D	502	78S	CAL-CAY	7.34	1.53	1.32
2	D	501	78S	CAJ-CAW	7.33	1.53	1.32

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	502	78S	CAO-CAL-CAY	-7.16	115.17	126.75
2	D	501	78S	CAO-CAL-CAY	-6.08	115.53	126.04
2	D	501	78S	CAN-CAK-CAX	-5.16	115.24	127.66
2	D	501	78S	CAM-CAJ-CAW	-3.70	115.09	127.75
2	D	501	78S	CAF-CAY-CAQ	3.31	120.84	115.27

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	501	78S	CAJ-CAM-CAP-CAX
2	D	501	78S	CAR-CBA-OAU-CAO
2	D	501	78S	OAG-CAZ-CBA-OAU
2	D	501	78S	OAV-CAR-CBA-OAU
2	D	501	78S	OAV-CAR-CBA-CAZ

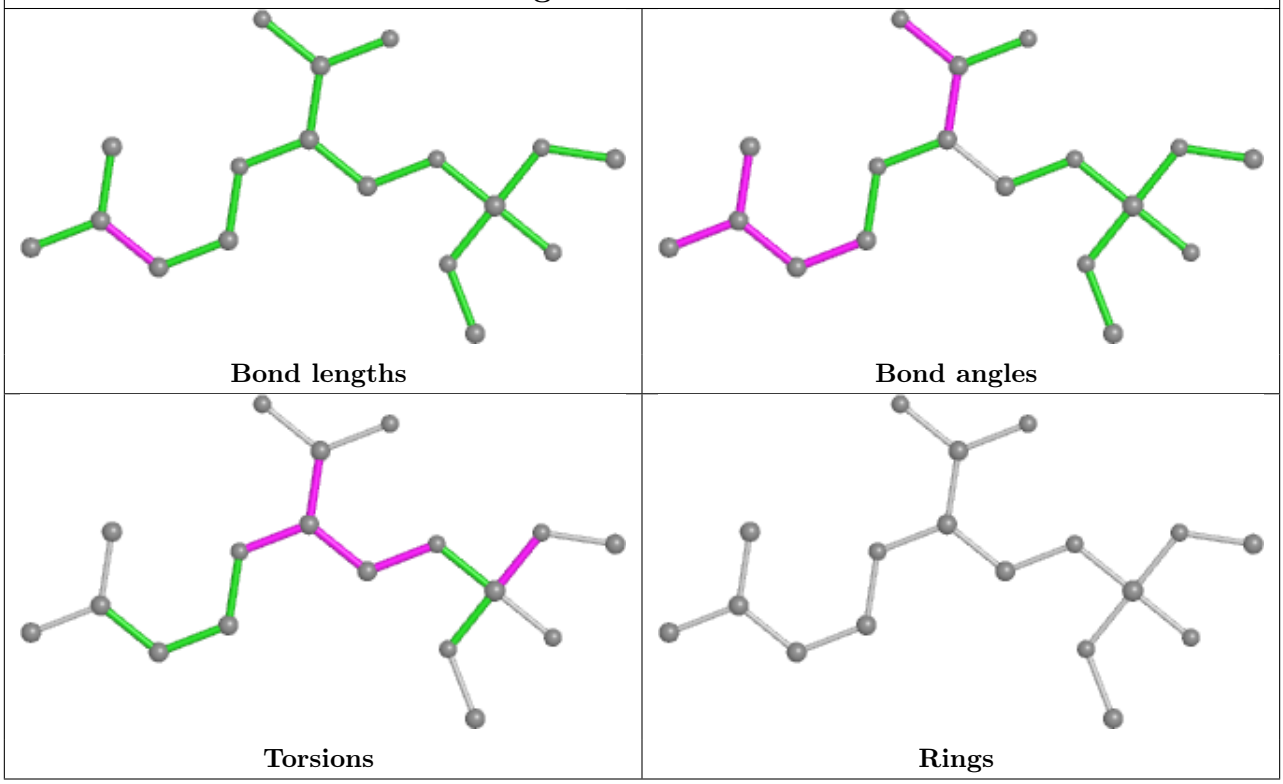
There are no ring outliers.

1 monomer is involved in 1 short contact:

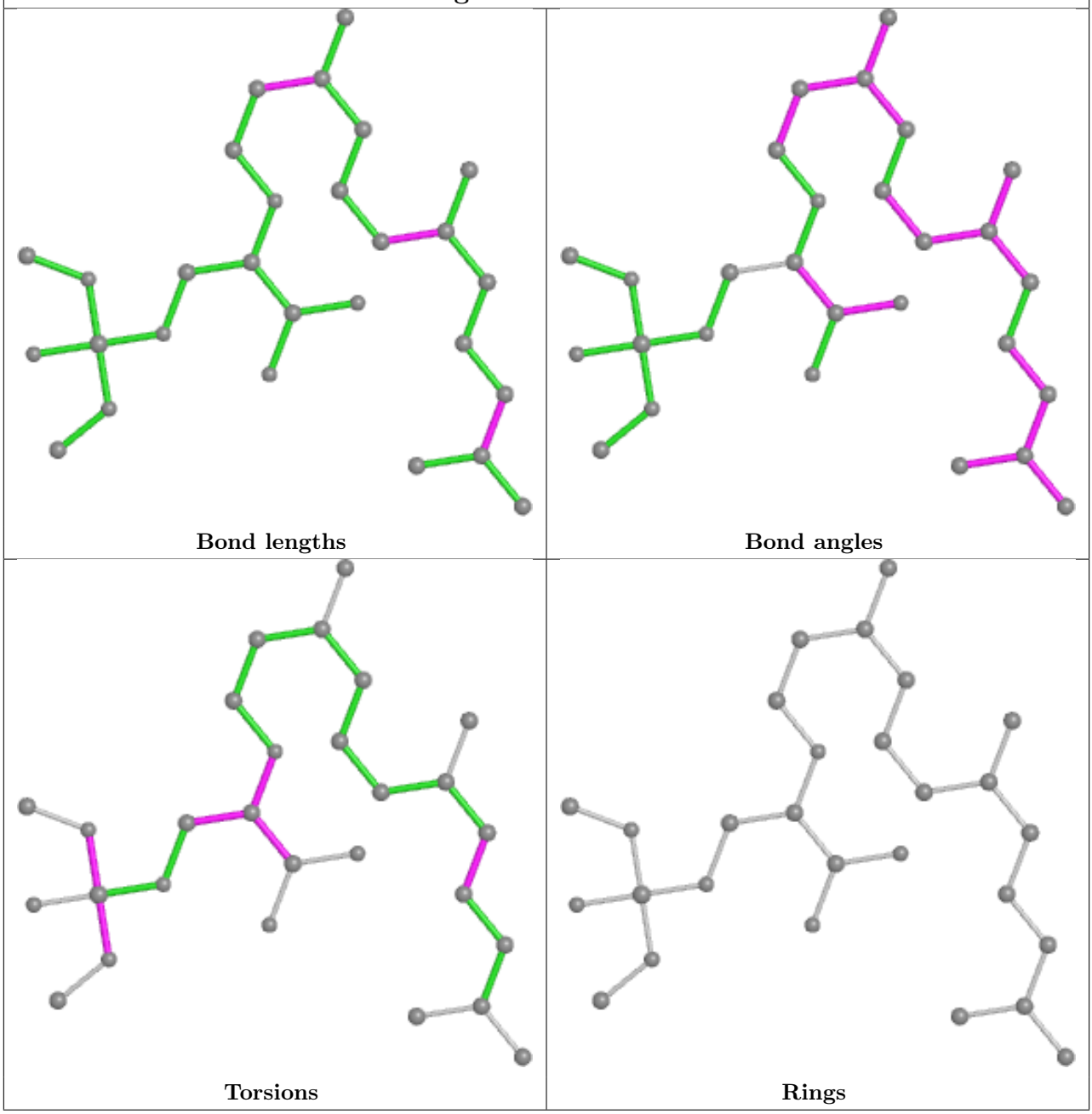
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	78S	1	0

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 78S D 502



Ligand 78S D 501



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	264/343 (76%)	-0.40	12 (4%)	33	31	27, 39, 72, 118	0
1	B	332/343 (96%)	-0.27	15 (4%)	33	31	27, 43, 87, 96	0
1	C	262/343 (76%)	-0.55	1 (0%)	92	91	24, 41, 58, 98	0
1	D	333/343 (97%)	0.03	33 (9%)	7	6	25, 42, 121, 143	0
All	All	1191/1372 (86%)	-0.28	61 (5%)	28	26	24, 41, 96, 143	0

The worst 5 of 61 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	265	ALA	8.9
1	D	264	GLY	8.8
1	D	266	MET	8.4
1	D	263	ALA	7.8
1	D	275	GLY	7.6

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 monosaccharides in this entry.

6.4 Ligands (i)

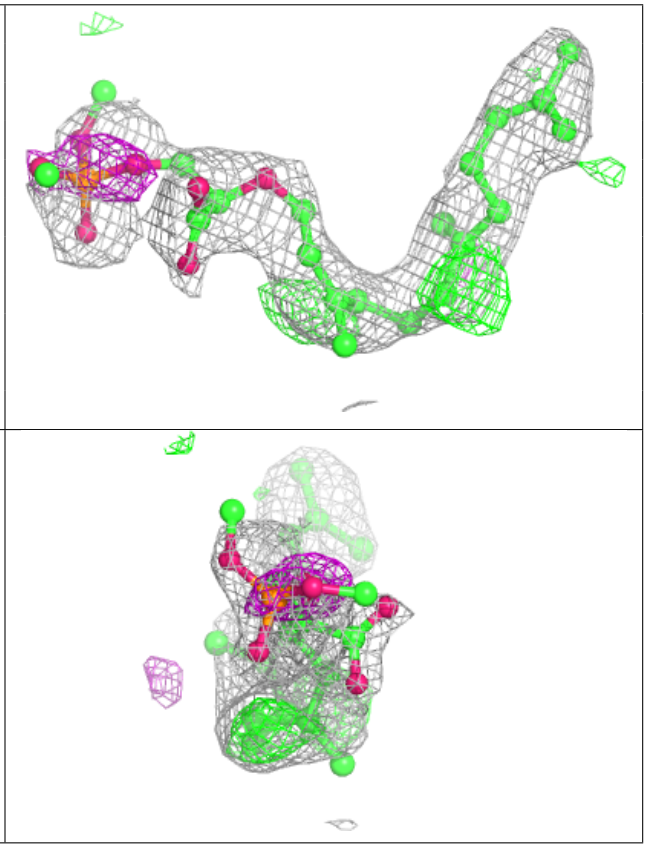
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	78S	D	501	28/28	0.73	0.29	49,83,116,118	0
2	78S	D	502	18/28	0.85	0.25	100,108,111,112	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.

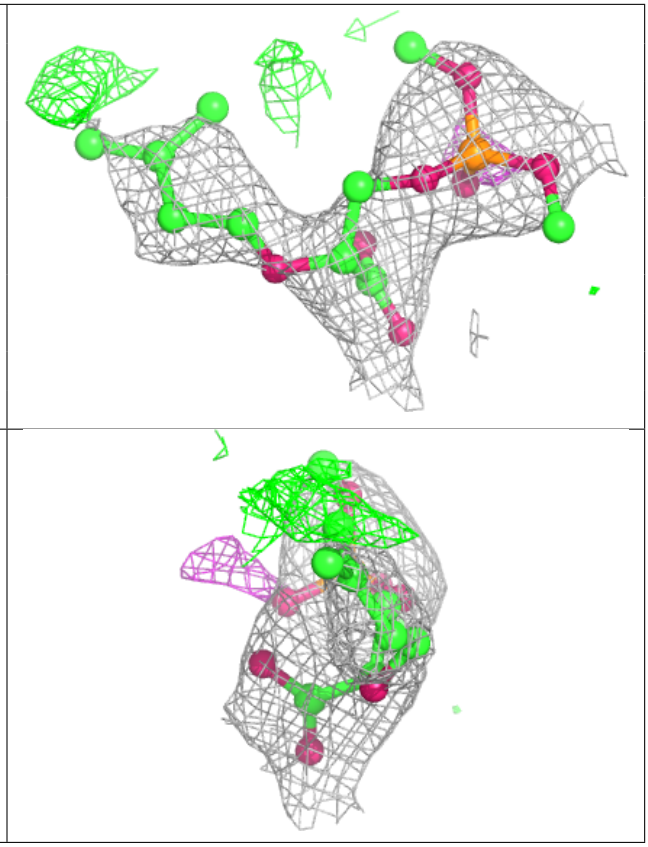
Electron density around 78S D 501:

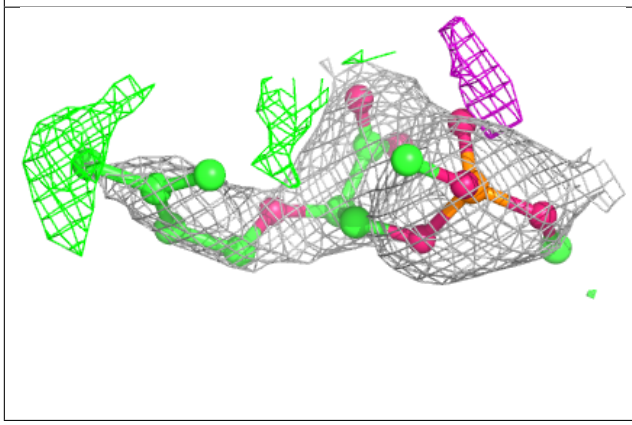
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



Electron density around 78S D 502:

$2mF_o$-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.