



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:43 AM UTC

PDB ID : 8QD4 / pdb_00008qd4
Title : Aylp active site converted to tetrahedral sulfonate ester
Authors : Schmalhofer, M.; Vagstad, A.L.; Zhou, Q.; Bode, H.B.; Groll, M.
Deposited on : 2023-08-28
Resolution : 1.80 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

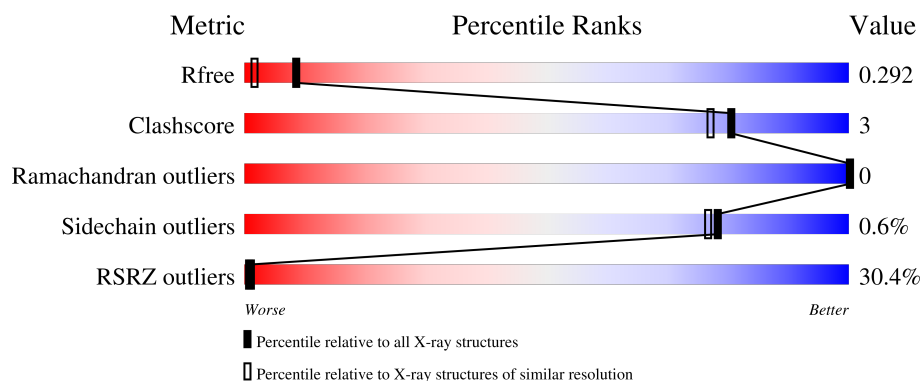
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	423	24% 89% 5% 6%
1	B	423	29% 87% 6% 6%
1	C	423	26% 87% 6% 6%
1	D	423	36% 87% 7% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12870 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 Pigment biosynthesis protein yellowish-green 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	S	0	3	0
			3115	1998	535	573	9			
1	B	398	Total	C	N	O	S	0	4	0
			3112	1996	538	569	9			
1	C	398	Total	C	N	O	S	0	3	0
			3078	1978	522	569	9			
1	D	398	Total	C	N	O	S	0	3	0
			3091	1985	530	567	9			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	initiating methionine	UNP Q9UVV1
A	-15	ARG	-	expression tag	UNP Q9UVV1
A	-14	GLY	-	expression tag	UNP Q9UVV1
A	-13	SER	-	expression tag	UNP Q9UVV1
A	-12	HIS	-	expression tag	UNP Q9UVV1
A	-11	HIS	-	expression tag	UNP Q9UVV1
A	-10	HIS	-	expression tag	UNP Q9UVV1
A	-9	HIS	-	expression tag	UNP Q9UVV1
A	-8	HIS	-	expression tag	UNP Q9UVV1
A	-7	HIS	-	expression tag	UNP Q9UVV1
A	-6	GLU	-	expression tag	UNP Q9UVV1
A	-5	ASN	-	expression tag	UNP Q9UVV1
A	-4	LEU	-	expression tag	UNP Q9UVV1
A	-3	TYR	-	expression tag	UNP Q9UVV1
A	-2	PHE	-	expression tag	UNP Q9UVV1
A	-1	GLN	-	expression tag	UNP Q9UVV1
A	0	GLY	-	expression tag	UNP Q9UVV1
A	1	SER	-	expression tag	UNP Q9UVV1
B	-16	MET	-	initiating methionine	UNP Q9UVV1
B	-15	ARG	-	expression tag	UNP Q9UVV1
B	-14	GLY	-	expression tag	UNP Q9UVV1

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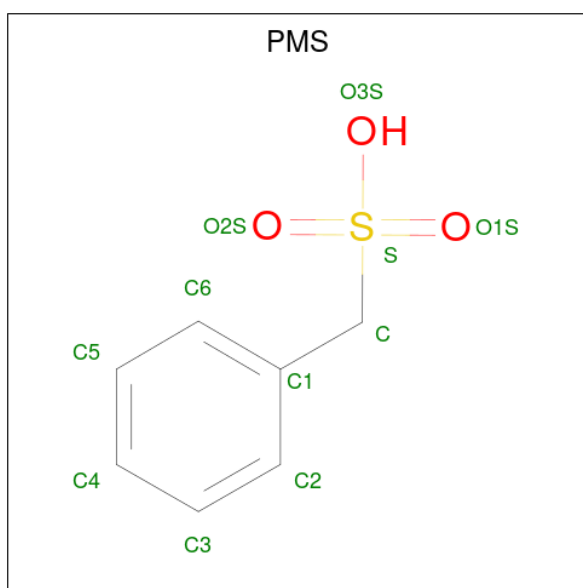
Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	SER	-	expression tag	UNP Q9UVV1
B	-12	HIS	-	expression tag	UNP Q9UVV1
B	-11	HIS	-	expression tag	UNP Q9UVV1
B	-10	HIS	-	expression tag	UNP Q9UVV1
B	-9	HIS	-	expression tag	UNP Q9UVV1
B	-8	HIS	-	expression tag	UNP Q9UVV1
B	-7	HIS	-	expression tag	UNP Q9UVV1
B	-6	GLU	-	expression tag	UNP Q9UVV1
B	-5	ASN	-	expression tag	UNP Q9UVV1
B	-4	LEU	-	expression tag	UNP Q9UVV1
B	-3	TYR	-	expression tag	UNP Q9UVV1
B	-2	PHE	-	expression tag	UNP Q9UVV1
B	-1	GLN	-	expression tag	UNP Q9UVV1
B	0	GLY	-	expression tag	UNP Q9UVV1
B	1	SER	-	expression tag	UNP Q9UVV1
C	-16	MET	-	initiating methionine	UNP Q9UVV1
C	-15	ARG	-	expression tag	UNP Q9UVV1
C	-14	GLY	-	expression tag	UNP Q9UVV1
C	-13	SER	-	expression tag	UNP Q9UVV1
C	-12	HIS	-	expression tag	UNP Q9UVV1
C	-11	HIS	-	expression tag	UNP Q9UVV1
C	-10	HIS	-	expression tag	UNP Q9UVV1
C	-9	HIS	-	expression tag	UNP Q9UVV1
C	-8	HIS	-	expression tag	UNP Q9UVV1
C	-7	HIS	-	expression tag	UNP Q9UVV1
C	-6	GLU	-	expression tag	UNP Q9UVV1
C	-5	ASN	-	expression tag	UNP Q9UVV1
C	-4	LEU	-	expression tag	UNP Q9UVV1
C	-3	TYR	-	expression tag	UNP Q9UVV1
C	-2	PHE	-	expression tag	UNP Q9UVV1
C	-1	GLN	-	expression tag	UNP Q9UVV1
C	0	GLY	-	expression tag	UNP Q9UVV1
C	1	SER	-	expression tag	UNP Q9UVV1
D	-16	MET	-	initiating methionine	UNP Q9UVV1
D	-15	ARG	-	expression tag	UNP Q9UVV1
D	-14	GLY	-	expression tag	UNP Q9UVV1
D	-13	SER	-	expression tag	UNP Q9UVV1
D	-12	HIS	-	expression tag	UNP Q9UVV1
D	-11	HIS	-	expression tag	UNP Q9UVV1
D	-10	HIS	-	expression tag	UNP Q9UVV1
D	-9	HIS	-	expression tag	UNP Q9UVV1
D	-8	HIS	-	expression tag	UNP Q9UVV1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-7	HIS	-	expression tag	UNP Q9UVV1
D	-6	GLU	-	expression tag	UNP Q9UVV1
D	-5	ASN	-	expression tag	UNP Q9UVV1
D	-4	LEU	-	expression tag	UNP Q9UVV1
D	-3	TYR	-	expression tag	UNP Q9UVV1
D	-2	PHE	-	expression tag	UNP Q9UVV1
D	-1	GLN	-	expression tag	UNP Q9UVV1
D	0	GLY	-	expression tag	UNP Q9UVV1
D	1	SER	-	expression tag	UNP Q9UVV1

- Molecule 2 is phenylmethanesulfonic acid (CCD ID: PMS) (formula: $C_7H_8O_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			10	7	2	1		
2	B	1	Total	C	O	S	0	0
			10	7	2	1		
2	C	1	Total	C	O	S	0	0
			10	7	2	1		
2	D	1	Total	C	O	S	0	0
			10	7	2	1		

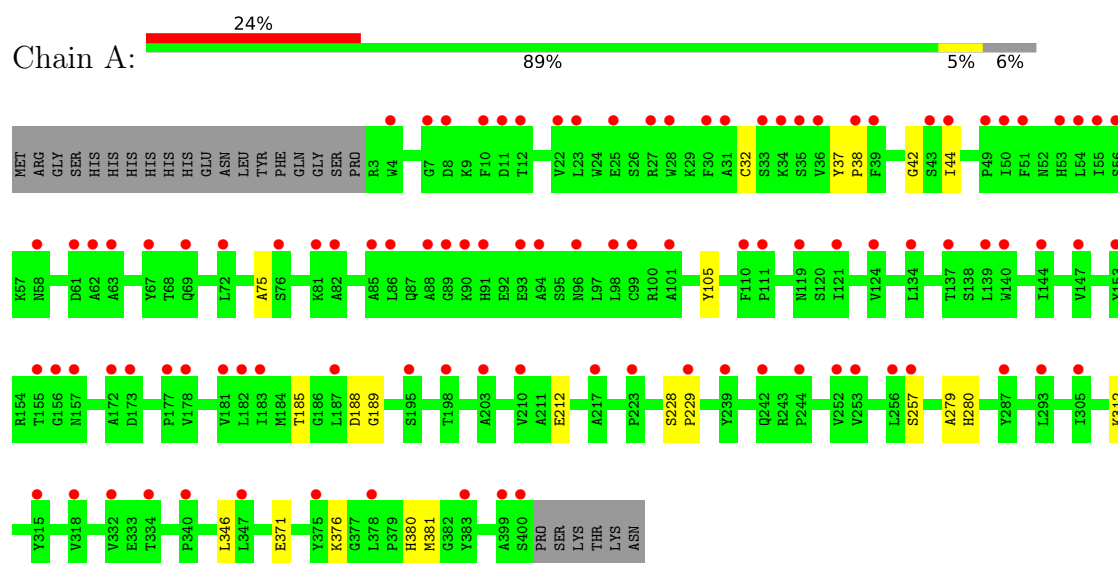
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	113	Total 113	O 113	0	0
3	B	110	Total 110	O 110	0	0
3	C	107	Total 107	O 107	0	0
3	D	104	Total 104	O 104	0	0

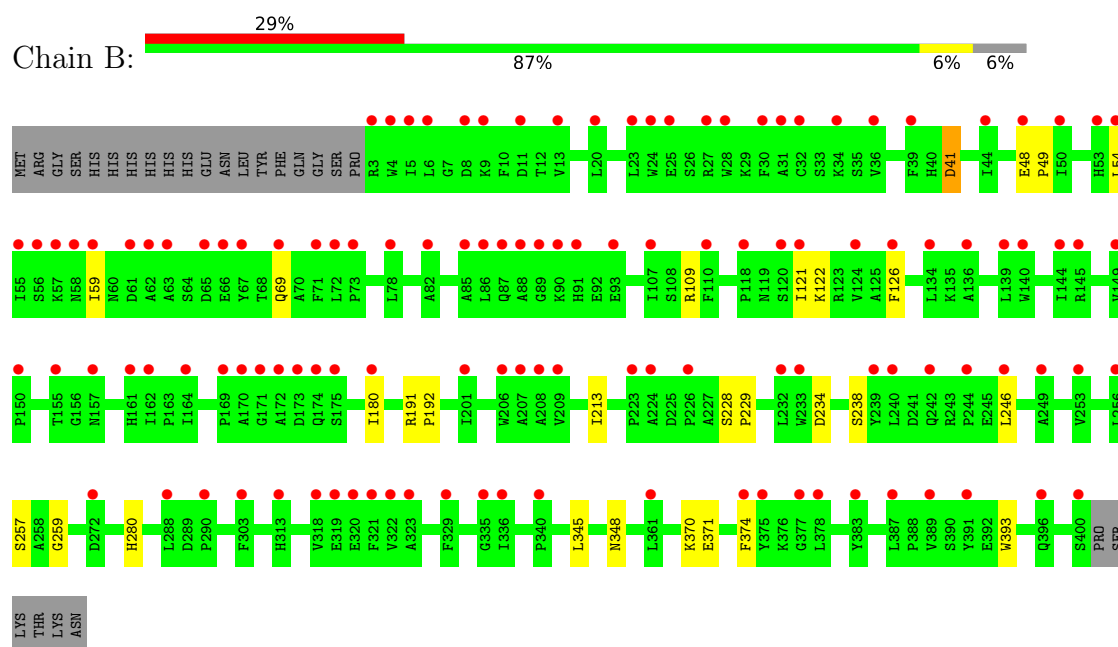
3 Residue-property plots [i](#)

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.

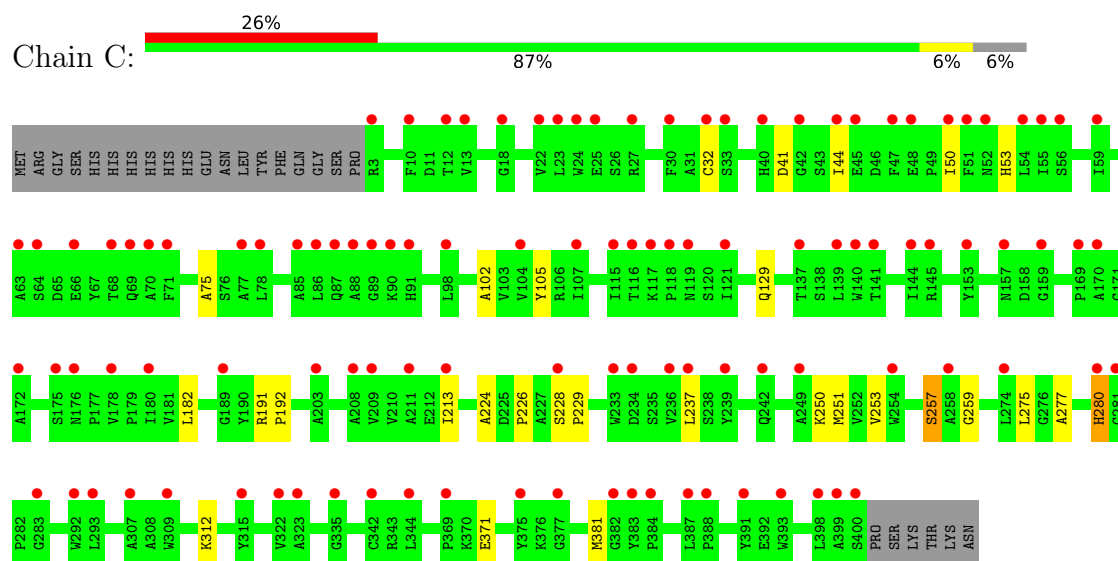
- Molecule 1: Pigment biosynthesis protein yellowish-green 1



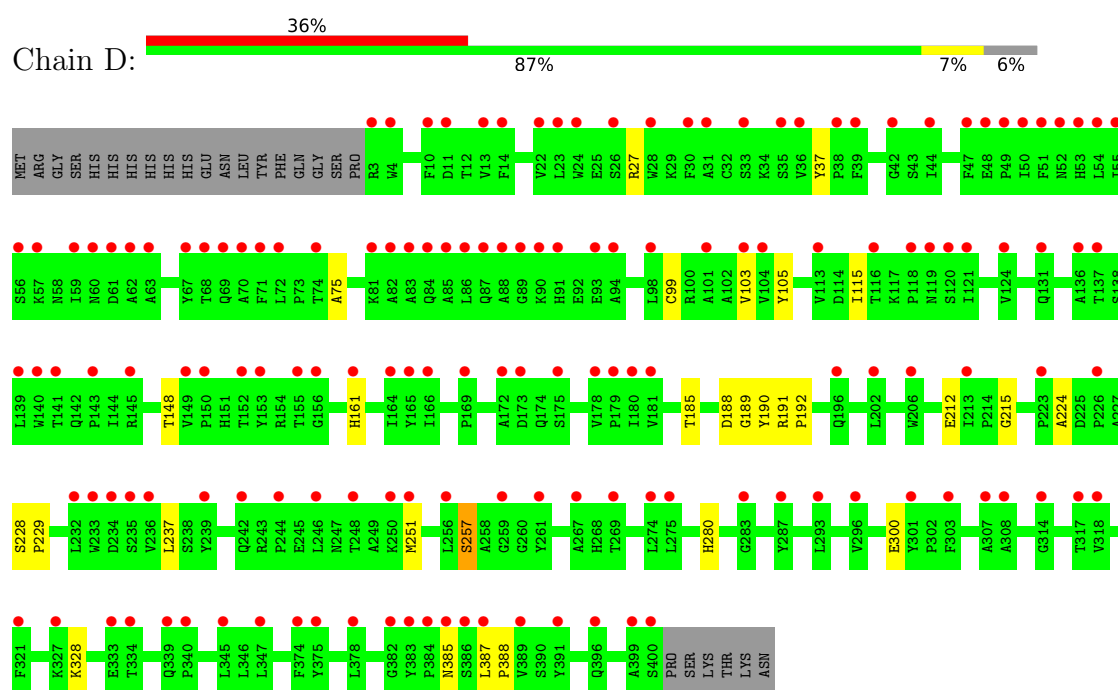
- Molecule 1: Pigment biosynthesis protein yellowish-green 1



• Molecule 1: Pigment biosynthesis protein yellowish-green 1



• Molecule 1: Pigment biosynthesis protein yellowish-green 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.64Å 107.55Å 92.54Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	46.49 – 1.80 46.49 – 1.80	Depositor EDS
% Data completeness (in resolution range)	95.9 (46.49-1.80) 99.5 (46.49-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.235 , 0.246 0.276 , 0.292	Depositor DCC
R_{free} test set	7658 reflections (3.94%)	wwPDB-VP
Wilson B-factor (Å ²)	26.8	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 22.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.56$, $\langle L^2 \rangle = 0.40$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12870	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.21 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5765e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: PMS

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	1.02	1/3211 (0.0%)	1.43	2/4390 (0.0%)
1	B	1.02	1/3212 (0.0%)	1.43	1/4391 (0.0%)
1	C	1.03	1/3177 (0.0%)	1.44	0/4348
1	D	1.03	1/3194 (0.0%)	1.44	0/4370
All	All	1.02	4/12794 (0.0%)	1.44	3/17499 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	257	SER	C-O	-7.91	1.17	1.24
1	C	257	SER	C-O	-7.30	1.17	1.24
1	A	257	SER	C-O	-6.34	1.18	1.24
1	B	257	SER	C-O	-5.29	1.17	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	41	ASP	CA-CB-CG	6.10	118.70	112.60
1	A	380	HIS	CA-C-N	5.46	131.97	121.54
1	A	380	HIS	C-N-CA	5.46	131.97	121.54

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	3115	0	2989	16	0
1	B	3112	0	2981	16	0
1	C	3078	0	2916	16	0
1	D	3091	0	2951	16	0
2	A	10	0	7	3	0
2	B	10	0	7	1	0
2	C	10	0	7	1	0
2	D	10	0	7	3	0
3	A	113	0	0	2	0
3	B	110	0	0	1	0
3	C	107	0	0	2	0
3	D	104	0	0	2	0
All	All	12870	0	11865	62	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 3.

All (62) 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:371[A]:GLU:CG	1:B:371[A]:GLU:HG2	1.75	1.16
1:A:371[A]:GLU:HG2	1:B:371[A]:GLU:CG	1.75	1.15
1:A:381:MET:HG3	2:A:501:PMS:C4	2.20	0.72
1:B:54:LEU:HD23	1:B:59:ILE:HD12	1.76	0.67
1:A:376:LYS:NZ	3:A:601:HOH:O	2.28	0.65
1:A:185:THR:HB	1:A:189:GLY:O	2.02	0.59
1:A:371[A]:GLU:HG2	1:B:371[A]:GLU:HG2	0.81	0.58
1:A:381:MET:HG3	2:A:501:PMS:C5	2.34	0.57
1:C:257:SER:HB2	2:C:501:PMS:C2	2.36	0.55
1:B:228:SER:N	1:B:229:PRO:HD2	2.21	0.55
1:D:27:ARG:NH1	3:D:605:HOH:O	2.42	0.52
1:B:234:ASP:O	1:B:238:SER:OG	2.25	0.52
1:C:228:SER:N	1:C:229:PRO:HD2	2.24	0.51
2:B:501:PMS:H2	3:B:652:HOH:O	2.10	0.51
1:A:228:SER:N	1:A:229:PRO:HD2	2.25	0.51
1:D:228:SER:N	1:D:229:PRO:HD2	2.25	0.51
1:B:345:LEU:HD22	1:B:393:TRP:CG	2.48	0.49
1:C:250:LYS:HA	1:C:275:LEU:CD1	2.42	0.48
1:C:182:LEU:HB2	1:C:251:MET:HE3	1.93	0.48
1:D:185:THR:HB	1:D:189:GLY:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:LYS:NZ	3:C:606:HOH:O	2.47	0.48
1:D:27:ARG:NH2	1:D:300:GLU:O	2.37	0.48
1:C:213:ILE:HG21	1:C:259:GLY:HA2	1.95	0.48
1:D:148:THR:HG23	1:D:161:HIS:HB3	1.95	0.47
1:D:75:ALA:HB1	1:D:105:TYR:CZ	2.49	0.47
1:C:280:HIS:HB3	1:C:381:MET:HE1	1.95	0.47
1:D:190:TYR:HB3	1:D:212:GLU:OE2	2.15	0.47
1:A:371[B]:GLU:HG3	1:B:370:LYS:O	2.15	0.47
1:A:42:GLY:C	3:A:625:HOH:O	2.59	0.46
1:D:188:ASP:OD2	2:D:501:PMS:H1	2.15	0.46
1:C:102:ALA:O	1:C:129:GLN:HG3	2.15	0.46
1:C:191:ARG:N	1:C:192:PRO:CD	2.79	0.46
1:D:191:ARG:N	1:D:192:PRO:CD	2.78	0.46
2:D:501:PMS:H5	3:D:688:HOH:O	2.15	0.46
1:C:50:ILE:O	1:C:53:HIS:HB3	2.16	0.45
1:D:224:ALA:O	1:D:328:LYS:NZ	2.45	0.45
1:A:75:ALA:HB1	1:A:105:TYR:CZ	2.52	0.44
1:C:224:ALA:O	1:C:226:PRO:HD3	2.18	0.44
1:B:180:ILE:HD11	1:B:246:LEU:HB3	2.00	0.44
1:B:191:ARG:N	1:B:192:PRO:CD	2.81	0.43
1:C:371[A]:GLU:HG3	3:C:677:HOH:O	2.17	0.43
1:A:32:CYS:SG	1:A:44:ILE:HA	2.59	0.43
1:A:185:THR:OG1	1:A:212:GLU:HA	2.19	0.43
1:C:75:ALA:HB1	1:C:105:TYR:CZ	2.53	0.43
1:B:109:ARG:HA	1:B:122:LYS:HG2	1.99	0.43
1:D:387:LEU:HB3	1:D:388:PRO:HD3	2.01	0.43
1:C:237:LEU:CD2	1:C:251:MET:HE1	2.49	0.42
1:D:257:SER:HB2	2:D:501:PMS:C1	2.49	0.42
1:D:115:ILE:HD13	1:D:215:GLY:HA2	2.00	0.42
1:B:48:GLU:N	1:B:49:PRO:CD	2.83	0.42
1:C:32:CYS:SG	1:C:44:ILE:HA	2.60	0.42
1:B:109:ARG:HD3	1:B:126:PHE:HB2	2.02	0.41
1:D:99:CYS:O	1:D:103:VAL:HG23	2.20	0.41
1:A:279:ALA:HB3	1:A:346:LEU:HD23	2.02	0.41
1:A:188:ASP:OD2	2:A:501:PMS:H2A	2.21	0.41
1:B:69:GLN:HG2	1:B:121:ILE:HG21	2.02	0.41
1:C:253:VAL:O	1:C:277:ALA:HA	2.21	0.41
1:B:348:ASN:O	1:B:374:PHE:HA	2.21	0.41
1:A:37:TYR:HA	1:A:38:PRO:HA	1.89	0.40
1:D:237:LEU:CD2	1:D:251:MET:HE1	2.51	0.40
1:D:37:TYR:CD2	1:D:37:TYR:C	2.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:ILE:HG21	1:B:259:GLY:HA2	2.03	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	399/423 (94%)	381 (96%)	18 (4%)	0	100	100
1	B	400/423 (95%)	378 (94%)	22 (6%)	0	100	100
1	C	399/423 (94%)	381 (96%)	18 (4%)	0	100	100
1	D	399/423 (94%)	377 (94%)	22 (6%)	0	100	100
All	All	1597/1692 (94%)	1517 (95%)	80 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	321/354 (91%)	319 (99%)	2 (1%)	78	77
1	B	319/354 (90%)	317 (99%)	2 (1%)	78	77
1	C	311/354 (88%)	309 (99%)	2 (1%)	78	77
1	D	316/354 (89%)	314 (99%)	2 (1%)	78	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1267/1416 (90%)	1259 (99%)	8 (1%)	78	77

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	280	HIS
1	A	312	LYS
1	B	41	ASP
1	B	280	HIS
1	C	41	ASP
1	C	280	HIS
1	D	280	HIS
1	D	385	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	366	HIS
1	B	60	ASN
1	B	326	GLN
1	D	339	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	PMS	C	501	1	7,10,11	0.28	0	11,12,15	0.48	0
2	PMS	B	501	1	7,10,11	0.28	0	11,12,15	1.55	2 (18%)
2	PMS	A	501	1	7,10,11	0.19	0	11,12,15	0.84	1 (9%)
2	PMS	D	501	1	7,10,11	0.26	0	11,12,15	0.53	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	PMS	C	501	1	-	1/4/4/5	0/1/1/1
2	PMS	B	501	1	-	2/4/4/5	0/1/1/1
2	PMS	A	501	1	-	2/4/4/5	0/1/1/1
2	PMS	D	501	1	-	1/4/4/5	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	PMS	C1-C-S	4.44	121.94	110.71
2	A	501	PMS	O2S-S-C	2.54	109.93	105.55
2	B	501	PMS	O2S-S-C	2.46	109.79	105.55

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	PMS	C1-C-S-O1S
2	B	501	PMS	C1-C-S-O1S
2	D	501	PMS	C1-C-S-O2S
2	B	501	PMS	C1-C-S-O2S

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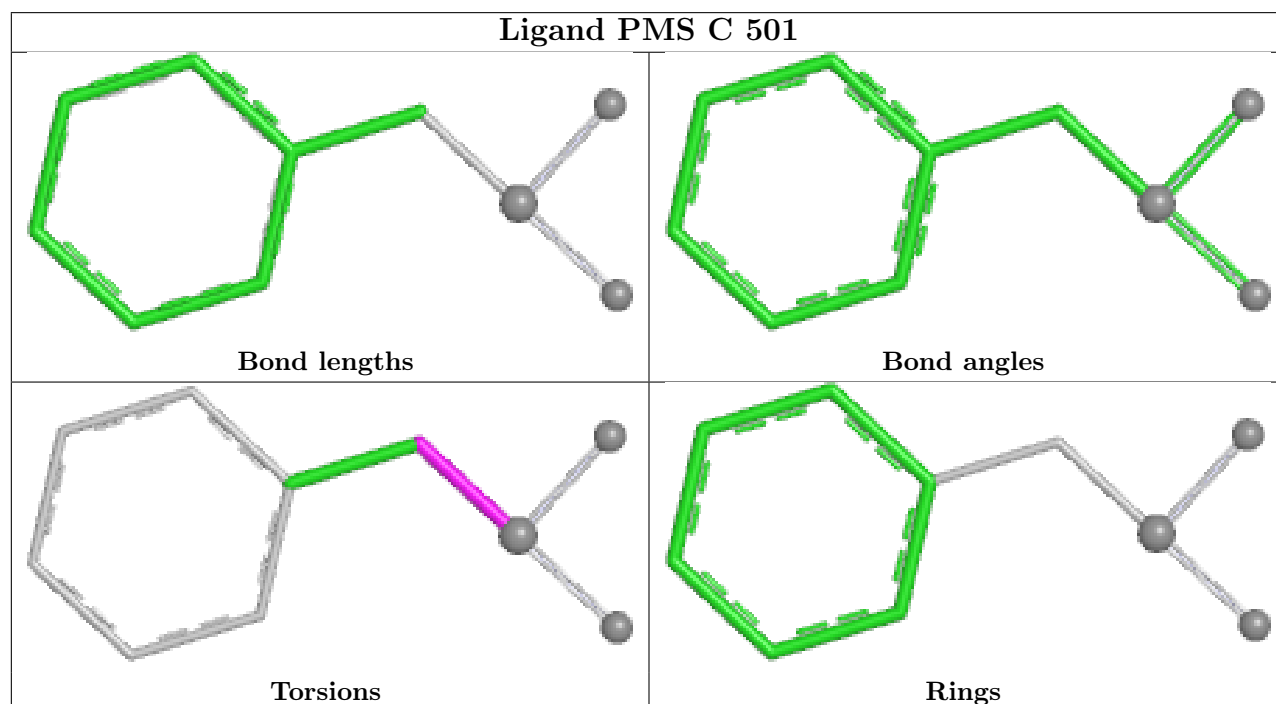
Mol	Chain	Res	Type	Atoms
2	C	501	PMS	C1-C-S-O2S
2	A	501	PMS	S-C-C1-C6

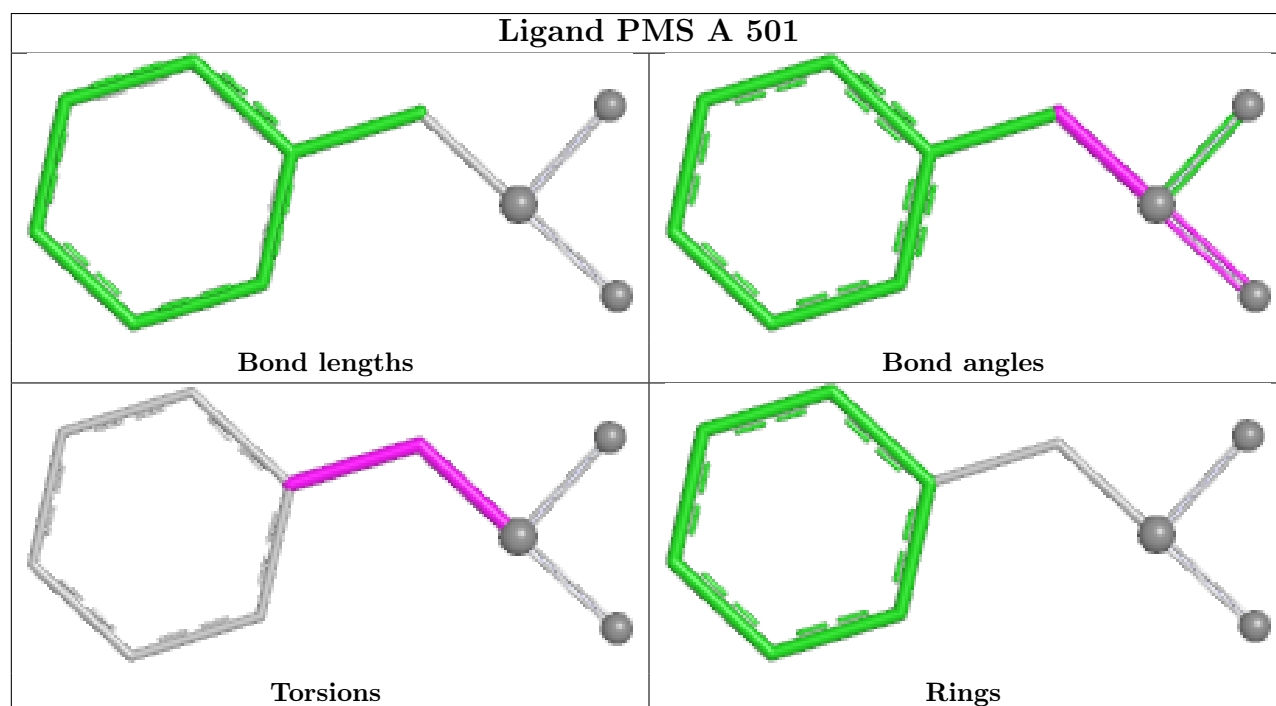
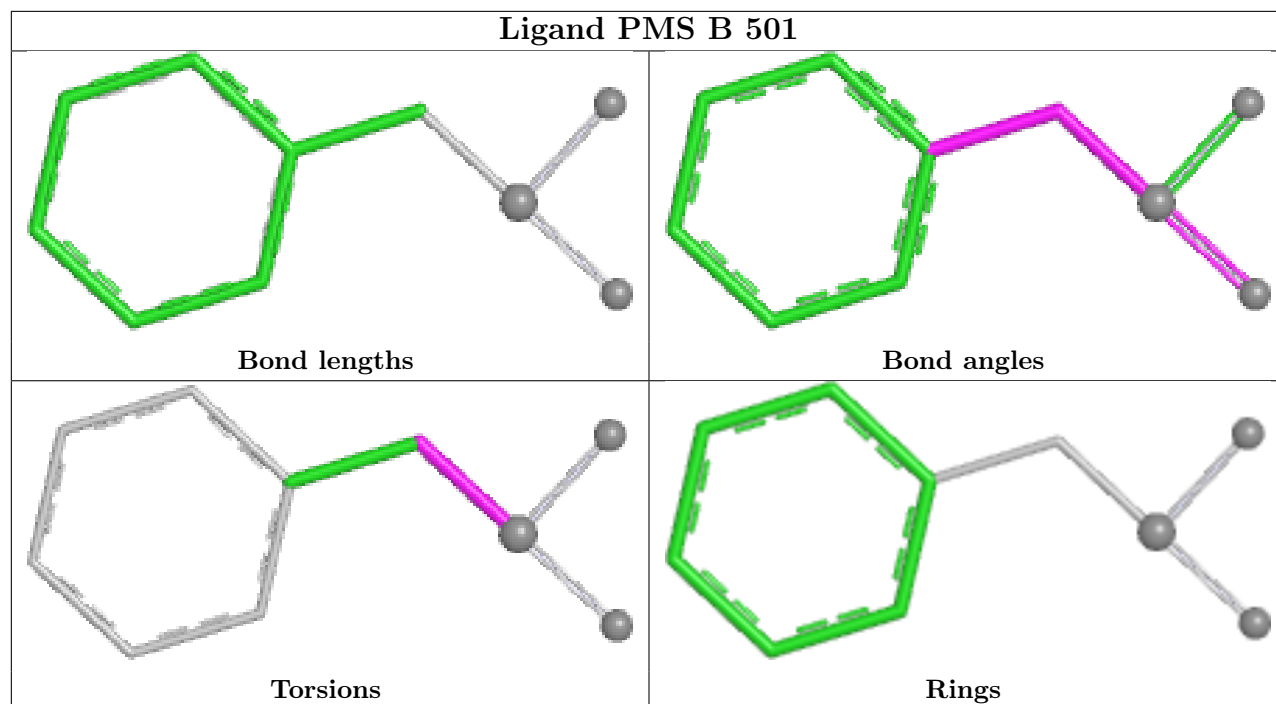
There are no ring outliers.

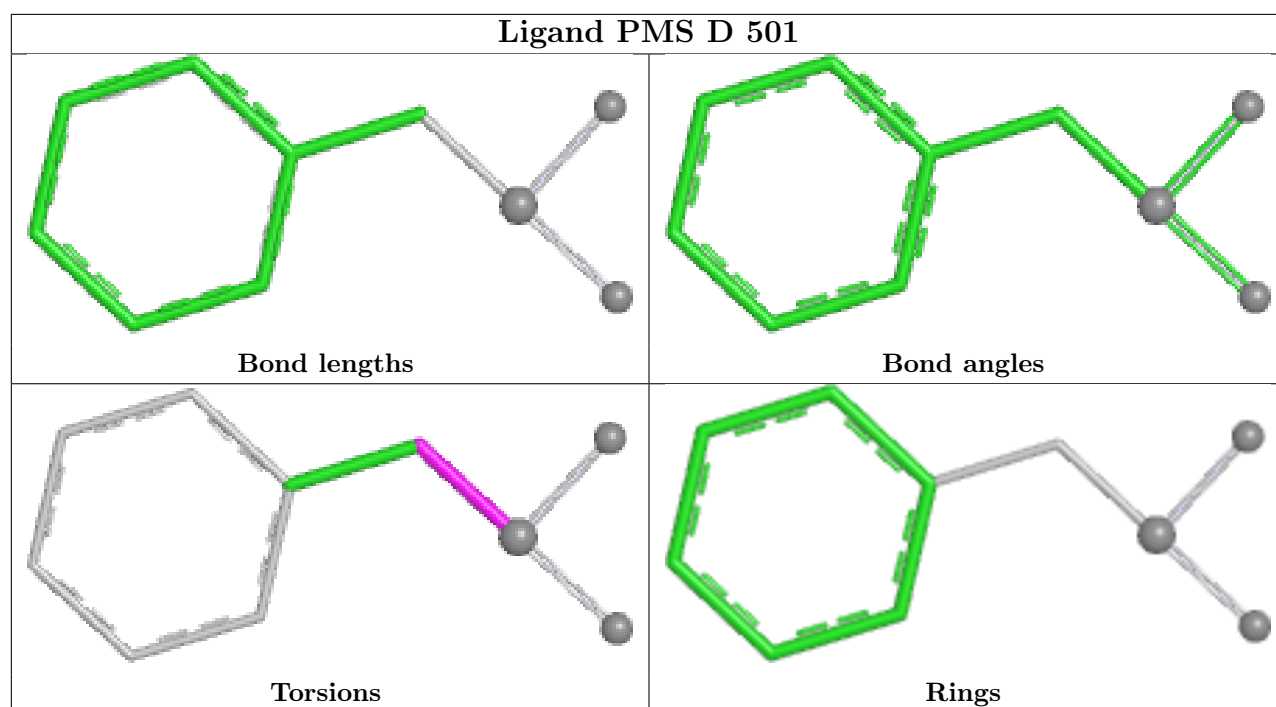
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	PMS	1	0
2	B	501	PMS	1	0
2	A	501	PMS	3	0
2	D	501	PMS	3	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	398/423 (94%)	1.49	101 (25%) 1 1	11, 27, 40, 48	3 (0%)
1	B	398/423 (94%)	1.63	122 (30%) 1 1	10, 29, 43, 55	4 (1%)
1	C	398/423 (94%)	1.58	110 (27%) 1 1	10, 29, 41, 49	3 (0%)
1	D	398/423 (94%)	1.73	151 (37%) 1 0	18, 29, 44, 55	3 (0%)
All	All	1592/1692 (94%)	1.61	484 (30%) 1 1	10, 28, 42, 55	13 (0%)

All (484) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	30	PHE	5.4
1	D	399	ALA	5.1
1	C	139	LEU	4.8
1	D	88	ALA	4.4
1	D	70	ALA	4.3
1	C	400	SER	4.3
1	B	62	ALA	4.3
1	C	3	ARG	4.2
1	B	55	ILE	4.2
1	D	91	HIS	4.2
1	B	139	LEU	4.1
1	C	322	VAL	4.1
1	C	30	PHE	4.1
1	B	72	LEU	4.0
1	B	54	LEU	4.0
1	C	91	HIS	4.0
1	A	157	ASN	4.0
1	C	169	PRO	3.9
1	B	244	PRO	3.9
1	D	181	VAL	3.8
1	D	118	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	59	ILE	3.8
1	D	400	SER	3.7
1	D	396[A]	GLN	3.7
1	D	30	PHE	3.7
1	C	56	SER	3.7
1	D	54	LEU	3.6
1	D	386	SER	3.6
1	D	94	ALA	3.6
1	D	72	LEU	3.6
1	C	399	ALA	3.6
1	C	209	VAL	3.6
1	B	56	SER	3.6
1	A	28	TRP	3.5
1	D	33	SER	3.5
1	D	55	ILE	3.5
1	B	318	VAL	3.5
1	A	156	GLY	3.5
1	D	384	PRO	3.5
1	A	203	ALA	3.5
1	A	334	THR	3.4
1	D	119	ASN	3.4
1	C	44	ILE	3.4
1	C	66	GLU	3.4
1	B	63	ALA	3.4
1	C	170	ALA	3.4
1	A	56	SER	3.4
1	C	237	LEU	3.4
1	D	56	SER	3.4
1	A	44	ILE	3.3
1	D	85	ALA	3.3
1	D	139	LEU	3.3
1	D	293	LEU	3.3
1	A	8	ASP	3.3
1	D	274	LEU	3.3
1	D	39	PHE	3.3
1	D	150	PRO	3.3
1	B	171	GLY	3.3
1	A	67	TYR	3.3
1	B	44	ILE	3.3
1	D	57	LYS	3.3
1	D	202	LEU	3.3
1	C	42	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	175	SER	3.3
1	D	44	ILE	3.2
1	C	141	THR	3.2
1	D	140	TRP	3.2
1	B	107	ILE	3.2
1	C	107	ILE	3.2
1	D	166	ILE	3.2
1	D	63	ALA	3.2
1	D	152	THR	3.2
1	B	136	ALA	3.2
1	B	383	TYR	3.2
1	C	98	LEU	3.2
1	D	23	LEU	3.2
1	B	59	ILE	3.1
1	D	62	ALA	3.1
1	C	398	LEU	3.1
1	C	71	PHE	3.1
1	A	155	THR	3.1
1	A	88	ALA	3.1
1	D	121	ILE	3.1
1	A	182	LEU	3.1
1	D	275	LEU	3.1
1	D	169	PRO	3.1
1	A	121	ILE	3.1
1	B	65	ASP	3.1
1	C	22	VAL	3.1
1	B	58	ASN	3.1
1	C	119	ASN	3.1
1	A	35	SER	3.1
1	C	18	GLY	3.1
1	D	172	ALA	3.1
1	B	5	ILE	3.0
1	D	180	ILE	3.0
1	B	240	LEU	3.0
1	C	13	VAL	3.0
1	D	36	VAL	3.0
1	C	175	SER	3.0
1	A	82	ALA	3.0
1	A	305	ILE	3.0
1	D	246	LEU	3.0
1	D	391	TYR	3.0
1	A	89	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	11	ASP	3.0
1	B	32	CYS	3.0
1	A	110	PHE	3.0
1	B	87	GLN	3.0
1	C	382	GLY	3.0
1	D	89	GLY	3.0
1	A	90	LYS	2.9
1	B	110	PHE	2.9
1	B	53	HIS	2.9
1	A	239	TYR	2.9
1	D	383	TYR	2.9
1	B	73	PRO	2.9
1	B	140	TRP	2.9
1	C	233	TRP	2.9
1	C	145	ARG	2.9
1	D	67	TYR	2.9
1	C	63	ALA	2.9
1	D	82	ALA	2.9
1	D	308	ALA	2.9
1	D	50	ILE	2.9
1	D	59	ILE	2.9
1	A	318[A]	VAL	2.8
1	A	223	PRO	2.8
1	B	239	TYR	2.8
1	B	82	ALA	2.8
1	C	86	LEU	2.8
1	B	174	GLN	2.8
1	A	332	VAL	2.8
1	C	384	PRO	2.8
1	D	178	VAL	2.8
1	C	153	TYR	2.8
1	A	25	GLU	2.8
1	A	173	ASP	2.8
1	A	257	SER	2.8
1	B	88	ALA	2.8
1	C	249	ALA	2.8
1	A	7	GLY	2.8
1	C	89	GLY	2.8
1	C	144	ILE	2.8
1	C	203	ALA	2.8
1	C	208	ALA	2.8
1	D	11	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	24	TRP	2.8
1	B	27[A]	ARG	2.7
1	B	71	PHE	2.7
1	C	280	HIS	2.7
1	A	22	VAL	2.7
1	A	124	VAL	2.7
1	B	145	ARG	2.7
1	D	22	VAL	2.7
1	D	124	VAL	2.7
1	A	63	ALA	2.7
1	D	321	PHE	2.7
1	B	173	ASP	2.7
1	B	180	ILE	2.7
1	C	55	ILE	2.7
1	A	140	TRP	2.7
1	B	249	ALA	2.7
1	C	88	ALA	2.7
1	D	287	TYR	2.7
1	A	111	PRO	2.7
1	B	226	PRO	2.7
1	C	118	PRO	2.7
1	C	85	ALA	2.6
1	D	267	ALA	2.6
1	C	234	ASP	2.6
1	B	24	TRP	2.6
1	C	383	TYR	2.6
1	A	69	GLN	2.6
1	C	48	GLU	2.6
1	B	150	PRO	2.6
1	B	223	PRO	2.6
1	A	54	LEU	2.6
1	A	187	LEU	2.6
1	D	86	LEU	2.6
1	C	121	ILE	2.6
1	B	36	VAL	2.6
1	B	253	VAL	2.6
1	B	224	ALA	2.6
1	B	272	ASP	2.6
1	D	317	THR	2.6
1	C	47	PHE	2.6
1	A	340	PRO	2.6
1	A	50	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	11	ASP	2.6
1	D	382	GLY	2.6
1	A	36	VAL	2.6
1	C	25	GLU	2.6
1	D	31	ALA	2.6
1	D	389	VAL	2.6
1	D	68	THR	2.6
1	D	137	THR	2.6
1	D	165	TYR	2.6
1	A	38	PRO	2.6
1	D	47	PHE	2.6
1	C	254	TRP	2.6
1	B	25	GLU	2.6
1	B	93	GLU	2.6
1	A	62	ALA	2.6
1	A	181	VAL	2.6
1	C	104	VAL	2.6
1	B	161	HIS	2.5
1	A	99	CYS	2.5
1	C	32	CYS	2.5
1	D	239	TYR	2.5
1	D	301	TYR	2.5
1	A	242	GLN	2.5
1	B	39	PHE	2.5
1	B	319	GLU	2.5
1	B	361	LEU	2.5
1	B	387	LEU	2.5
1	A	183	ILE	2.5
1	D	283	GLY	2.5
1	B	157	ASN	2.5
1	C	33	SER	2.5
1	A	53	HIS	2.5
1	A	147	VAL	2.5
1	C	178	VAL	2.5
1	D	318	VAL	2.5
1	B	321	PHE	2.5
1	C	10	PHE	2.5
1	B	134	LEU	2.5
1	C	387	LEU	2.5
1	B	175	SER	2.5
1	D	35[A]	SER	2.5
1	D	269	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	177	PRO	2.5
1	A	347	LEU	2.5
1	B	23	LEU	2.5
1	B	86	LEU	2.5
1	B	246	LEU	2.5
1	B	256	LEU	2.5
1	B	91	HIS	2.5
1	D	69	GLN	2.5
1	D	206	TRP	2.5
1	B	31	ALA	2.5
1	B	170	ALA	2.5
1	D	104	VAL	2.5
1	D	296	VAL	2.5
1	D	250	LYS	2.5
1	D	143	PRO	2.5
1	C	157	ASN	2.4
1	D	375	TYR	2.4
1	A	293	LEU	2.4
1	B	378	LEU	2.4
1	C	87	GLN	2.4
1	B	34	LYS	2.4
1	B	206	TRP	2.4
1	D	28	TRP	2.4
1	D	52	ASN	2.4
1	A	86	LEU	2.4
1	B	67	TYR	2.4
1	D	235	SER	2.4
1	D	256	LEU	2.4
1	D	374	PHE	2.4
1	A	55	ILE	2.4
1	A	198	THR	2.4
1	D	83	ALA	2.4
1	A	27[A]	ARG	2.4
1	B	169	PRO	2.4
1	D	84	GLN	2.4
1	D	314	GLY	2.4
1	C	293	LEU	2.4
1	D	98	LEU	2.4
1	D	153	TYR	2.4
1	D	10	PHE	2.4
1	B	3	ARG	2.4
1	B	164	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	323	ALA	2.4
1	D	87	GLN	2.4
1	B	89	GLY	2.4
1	B	322	VAL	2.4
1	C	377	GLY	2.4
1	D	42	GLY	2.4
1	B	233	TRP	2.4
1	C	90	LYS	2.4
1	A	61	ASP	2.3
1	C	54	LEU	2.3
1	A	383	TYR	2.3
1	B	329	PHE	2.3
1	A	31	ALA	2.3
1	B	144	ILE	2.3
1	D	179	PRO	2.3
1	D	251	MET	2.3
1	B	389	VAL	2.3
1	C	236	VAL	2.3
1	D	103	VAL	2.3
1	B	66	GLU	2.3
1	A	139	LEU	2.3
1	B	20	LEU	2.3
1	B	232	LEU	2.3
1	C	23	LEU	2.3
1	C	344	LEU	2.3
1	A	137	THR	2.3
1	A	375	TYR	2.3
1	B	126	PHE	2.3
1	C	239	TYR	2.3
1	D	101	ALA	2.3
1	A	144	ILE	2.3
1	B	50	ILE	2.3
1	C	115	ILE	2.3
1	D	223	PRO	2.3
1	C	281	GLY	2.3
1	D	48	GLU	2.3
1	B	69	GLN	2.3
1	C	69	GLN	2.3
1	D	131	GLN	2.3
1	A	72	LEU	2.3
1	B	28	TRP	2.3
1	D	232	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	116	THR	2.3
1	B	375	TYR	2.3
1	D	90	LYS	2.3
1	B	118	PRO	2.3
1	B	290	PRO	2.3
1	B	121	ILE	2.3
1	B	162	ILE	2.3
1	C	180	ILE	2.3
1	B	120	SER	2.3
1	C	64	SER	2.3
1	D	120	SER	2.3
1	C	45	GLU	2.3
1	D	234	ASP	2.3
1	D	339	GLN	2.3
1	A	252	VAL	2.3
1	D	236	VAL	2.3
1	A	119	ASN	2.3
1	A	81	LYS	2.3
1	B	90	LYS	2.3
1	D	347	LEU	2.3
1	A	51	PHE	2.2
1	A	229	PRO	2.2
1	A	244	PRO	2.2
1	B	85	ALA	2.2
1	C	77	ALA	2.2
1	C	335	GLY	2.2
1	D	307	ALA	2.2
1	B	8	ASP	2.2
1	D	61	ASP	2.2
1	A	91	HIS	2.2
1	B	313	HIS	2.2
1	D	53	HIS	2.2
1	C	342	CYS	2.2
1	A	378	LEU	2.2
1	D	93	GLU	2.2
1	B	400	SER	2.2
1	C	228	SER	2.2
1	C	388	PRO	2.2
1	A	101	ALA	2.2
1	C	307	ALA	2.2
1	D	233	TRP	2.2
1	B	57	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	385	ASN	2.2
1	C	27	ARG	2.2
1	B	209	VAL	2.2
1	B	155	THR	2.2
1	C	68	THR	2.2
1	D	155	THR	2.2
1	D	242	GLN	2.2
1	B	61	ASP	2.2
1	C	189	GLY	2.2
1	C	283	GLY	2.2
1	B	340	PRO	2.2
1	B	172	ALA	2.2
1	B	208	ALA	2.2
1	B	303	PHE	2.2
1	B	374	PHE	2.2
1	B	201	ILE	2.2
1	A	4	TRP	2.2
1	B	9	LYS	2.2
1	C	24	TRP	2.2
1	C	52	ASN	2.2
1	C	117	LYS	2.2
1	D	145	ARG	2.2
1	B	48	GLU	2.2
1	A	210	VAL	2.2
1	A	253	VAL	2.2
1	D	196	GLN	2.2
1	C	12	THR	2.2
1	C	137	THR	2.2
1	A	23	LEU	2.2
1	D	156	GLY	2.2
1	D	387	LEU	2.2
1	D	244	PRO	2.2
1	D	340	PRO	2.2
1	A	94	ALA	2.2
1	A	217	ALA	2.2
1	C	70	ALA	2.2
1	A	30	PHE	2.1
1	A	58	ASN	2.1
1	A	96	ASN	2.1
1	C	51	PHE	2.1
1	D	303	PHE	2.1
1	C	391	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	213	ILE	2.1
1	A	12	THR	2.1
1	C	116	THR	2.1
1	D	141	THR	2.1
1	D	149	VAL	2.1
1	A	43	SER	2.1
1	A	134	LEU	2.1
1	B	6	LEU	2.1
1	B	78	LEU	2.1
1	C	369	PRO	2.1
1	D	327	LYS	2.1
1	C	40	HIS	2.1
1	C	176	ASN	2.1
1	C	258	ALA	2.1
1	C	323	ALA	2.1
1	D	136	ALA	2.1
1	A	39	PHE	2.1
1	D	71	PHE	2.1
1	A	153	TYR	2.1
1	A	287	TYR	2.1
1	C	50	ILE	2.1
1	D	173	ASP	2.1
1	A	33	SER	2.1
1	A	400	SER	2.1
1	B	4	TRP	2.1
1	C	393	TRP	2.1
1	D	4	TRP	2.1
1	A	178	VAL	2.1
1	C	159	GLY	2.1
1	D	113	VAL	2.1
1	A	34	LYS	2.1
1	A	93	GLU	2.1
1	D	378	LEU	2.1
1	A	10	PHE	2.1
1	C	315	TYR	2.1
1	A	76	SER	2.1
1	D	74	THR	2.1
1	D	81	LYS	2.1
1	D	333	GLU	2.1
1	B	377	GLY	2.1
1	B	124	VAL	2.1
1	B	149	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	292	TRP	2.1
1	C	309	TRP	2.1
1	D	60	ASN	2.1
1	B	396[A]	GLN	2.1
1	A	98	LEU	2.1
1	C	78	LEU	2.1
1	D	345	LEU	2.1
1	A	85	ALA	2.1
1	A	399	ALA	2.1
1	B	207	ALA	2.1
1	C	172	ALA	2.1
1	D	3	ARG	2.1
1	A	195	SER	2.0
1	B	336	ILE	2.0
1	D	14	PHE	2.0
1	D	213	ILE	2.0
1	A	315	TYR	2.0
1	C	375	TYR	2.0
1	D	261	TYR	2.0
1	D	334	THR	2.0
1	B	335	GLY	2.0
1	D	259	GLY	2.0
1	C	242	GLN	2.0
1	B	13	VAL	2.0
1	D	38	PRO	2.0
1	D	49	PRO	2.0
1	D	226	PRO	2.0
1	A	256	LEU	2.0
1	B	288	LEU	2.0
1	C	140	TRP	2.0
1	C	274	LEU	2.0
1	A	172	ALA	2.0
1	C	211	ALA	2.0
1	B	320	GLU	2.0
1	D	26	SER	2.0
1	D	51	PHE	2.0
1	D	161	HIS	2.0
1	D	164	ILE	2.0
1	B	242	GLN	2.0
1	D	248	THR	2.0
1	B	391	TYR	2.0
1	A	49	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	13	VAL	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](#)

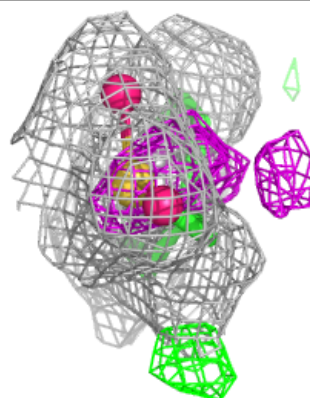
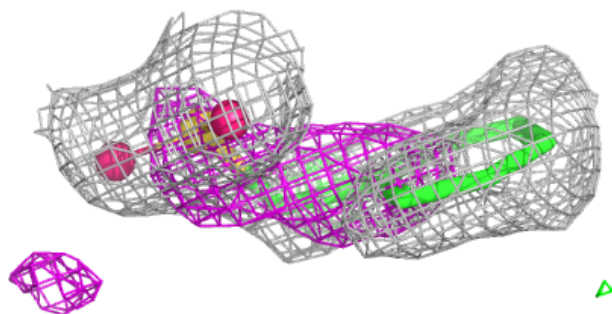
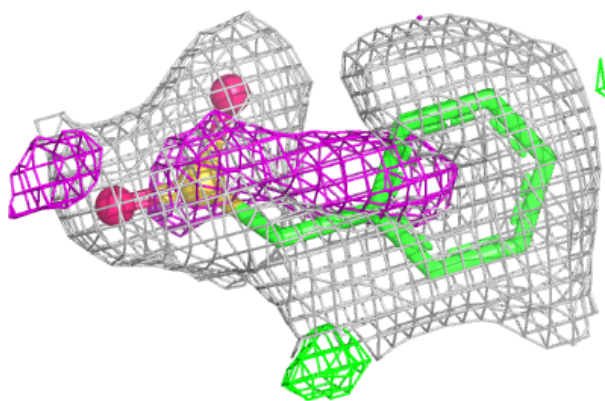
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PMS	C	501	10/11	0.81	0.18	29,32,32,33	0
2	PMS	A	501	10/11	0.83	0.17	25,27,28,28	0
2	PMS	D	501	10/11	0.86	0.15	29,29,31,31	0
2	PMS	B	501	10/11	0.91	0.13	26,30,31,31	0

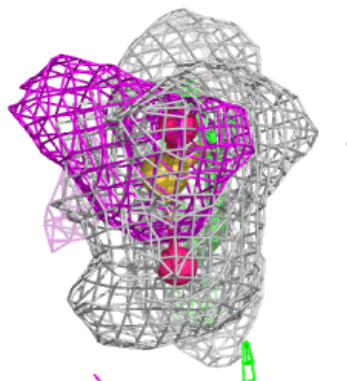
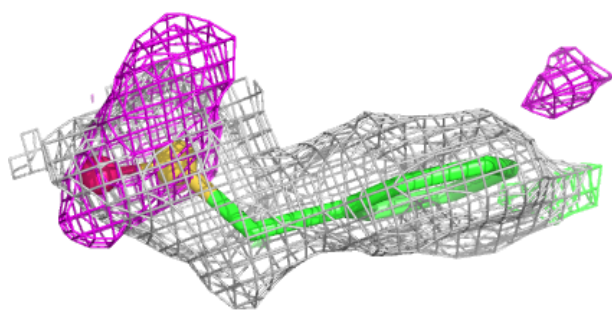
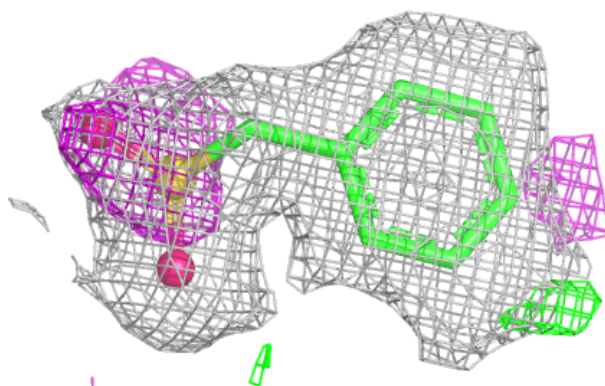
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PMS C 501:

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

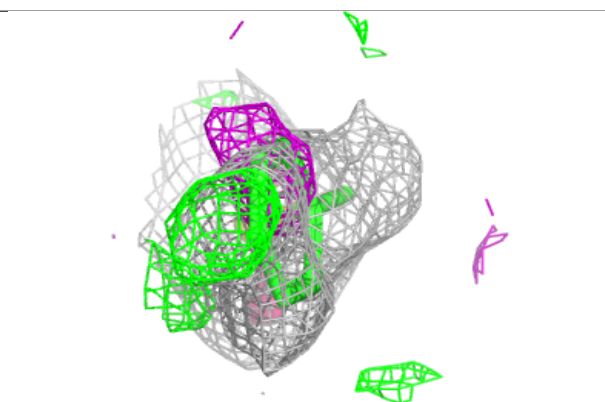
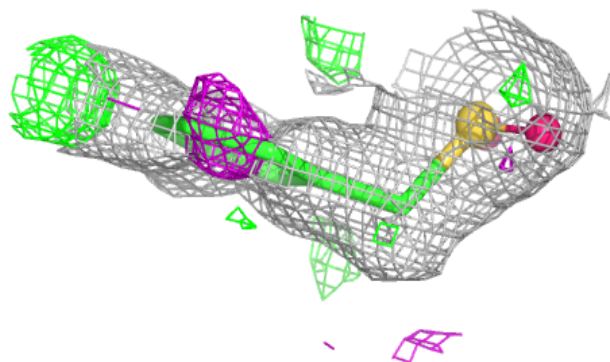
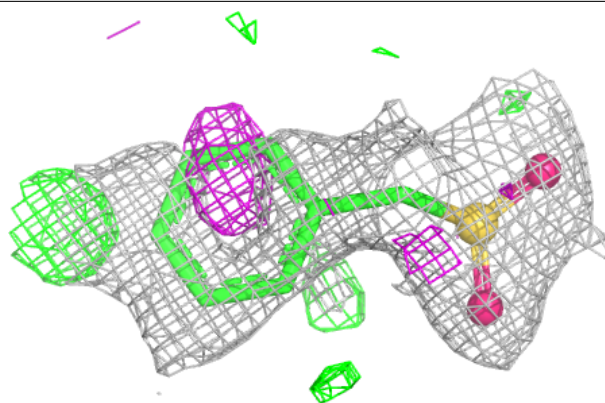
**Electron density around PMS A 501:**

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

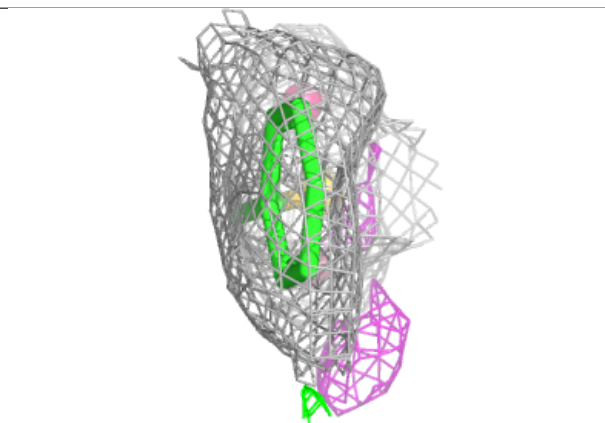
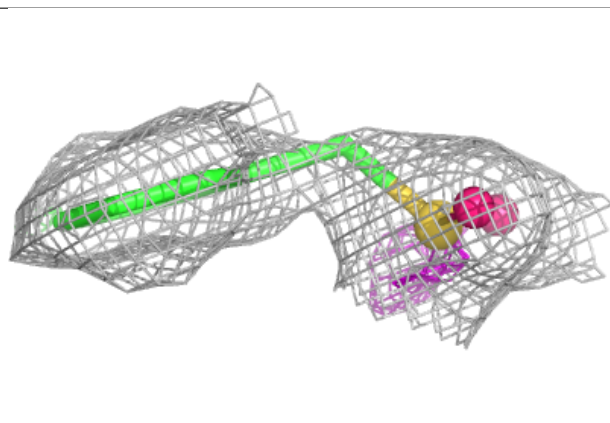
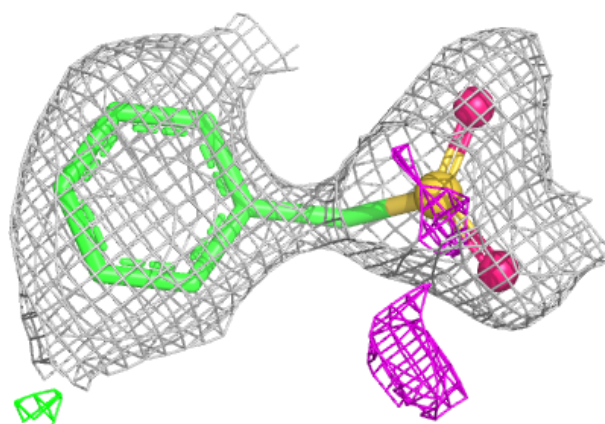


Electron density around PMS D 501:

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

**Electron density around PMS B 501:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.