Full wwPDB X-ray Structure Validation Report (i)

Nov 2, 2023 – 03:55 AM EDT

PDB ID	:	3TZZ
Title	:	Crystal structure of a fragment containing the acyltransferase domain of Pks13 from Mycobacterium tuberculosis in the carboxypalmitoylated form at 2.5 A
Authors	:	Bergeret, F.; Pedelacq, J.D.; Mourey, L.; Bon, C.
Deposited on	:	2011-09-28
Resolution	:	2.49 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 (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:

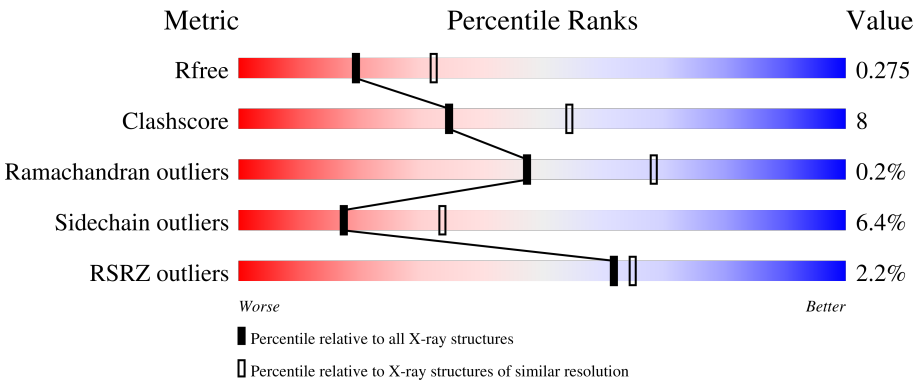
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.49 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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	491	2%, 78%, 15%, • 6%
1	B	491	2%, 75%, 19%, • 5%
2	C	12	8%, 33%, 42%, 8%, 17%

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
6	SO4	B	2005	-	X	-	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 7166 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 Polyketide synthase PKS13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	463	3454	2189	594	660	11	0	0	0
1	B	465	3434	2179	585	658	12	0	0	0

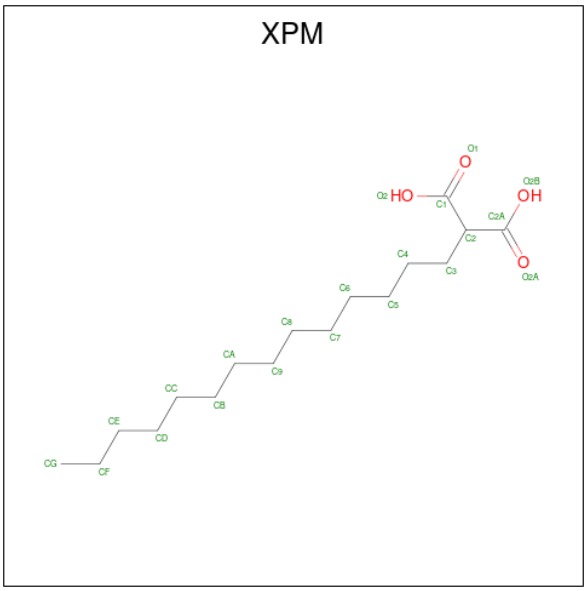
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	572	GLY	-	expression tag	UNP O53579
A	573	SER	-	expression tag	UNP O53579
A	574	HIS	-	expression tag	UNP O53579
A	575	MET	-	expression tag	UNP O53579
B	572	GLY	-	expression tag	UNP O53579
B	573	SER	-	expression tag	UNP O53579
B	574	HIS	-	expression tag	UNP O53579
B	575	MET	-	expression tag	UNP O53579

- Molecule 2 is a protein called 12-mer peptide.

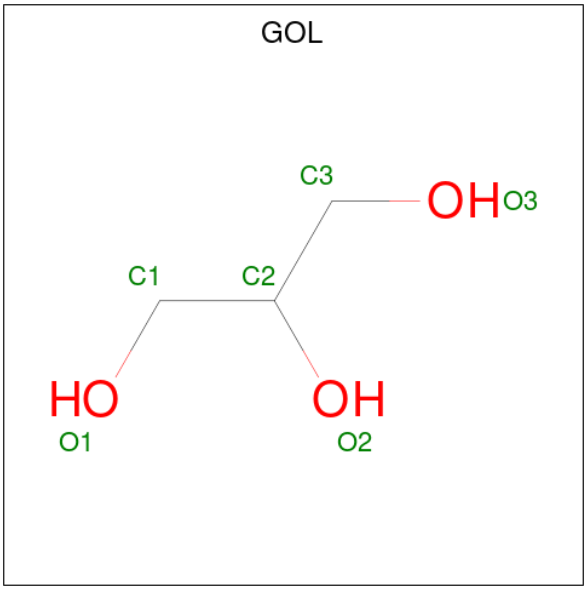
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	10	73	47	12	13	1	0	0	0

- Molecule 3 is tetradecylpropanedioic acid (three-letter code: XPM) (formula: $C_{17}H_{32}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	27	24	3	0	1
			Total	C	O		
3	B	1	20	17	3	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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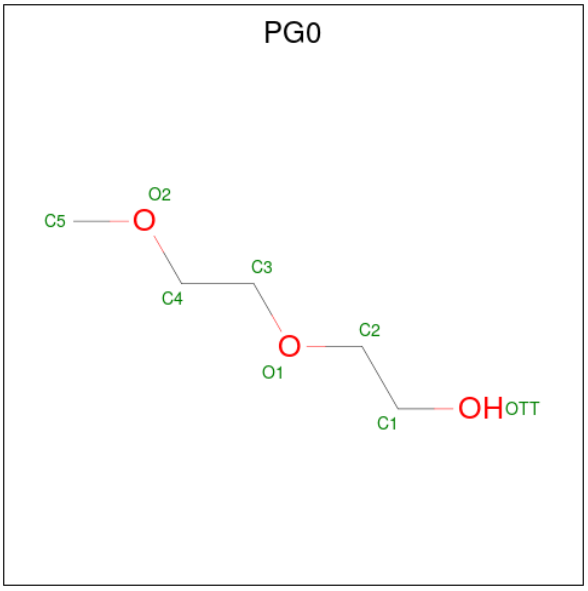
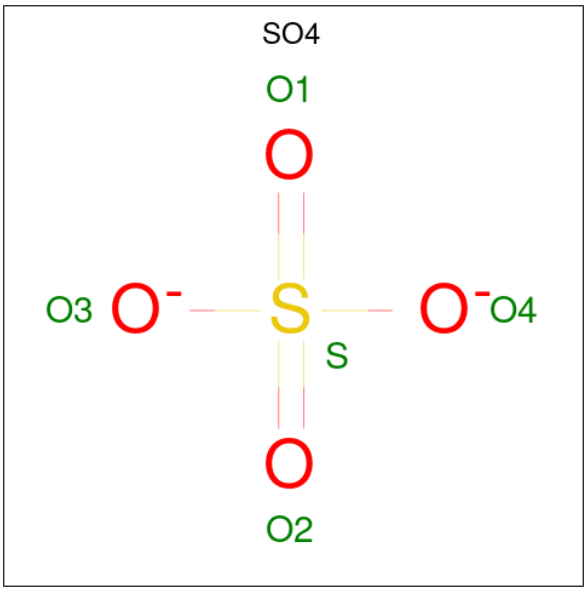
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	6	3	3	0	0
			Total	C	O		
4	A	1	6	3	3	0	0
			Total	C	O		
4	B	1	6	3	3	0	0
			Total	C	O		
4	B	1	6	3	3	0	0
			Total	C	O		
4	B	1	6	3	3	0	0

- Molecule 5 is 2-(2-METHOXYETHOXY)ETHANOL (three-letter code: PG0) (formula: $C_5H_{12}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	8	5	3	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0

- Molecule 7 is water.

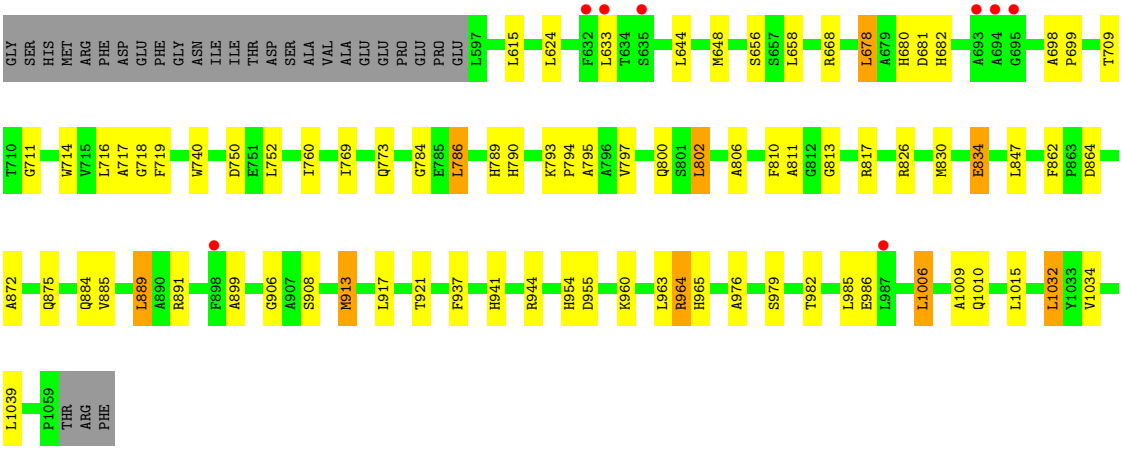
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	64	Total O 64 64	0	0
7	B	34	Total O 34 34	0	0

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.

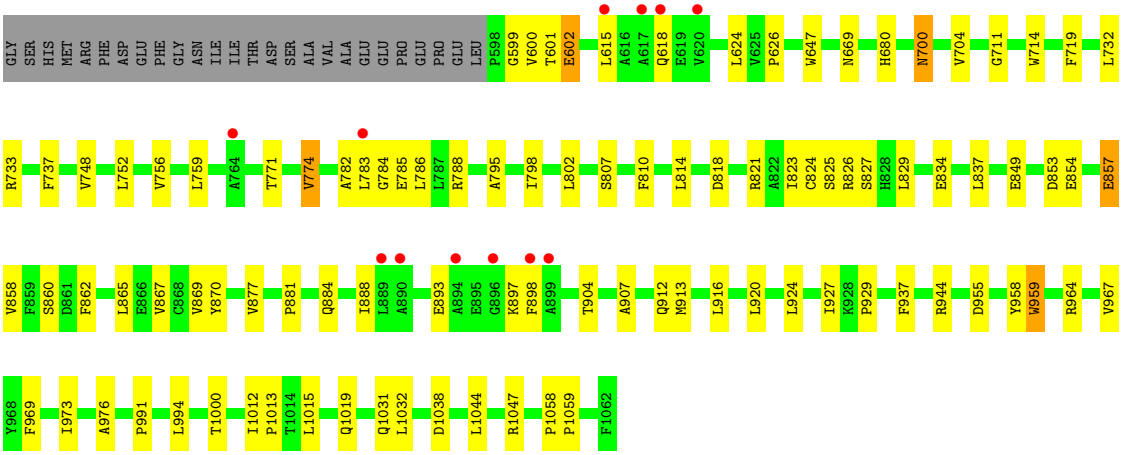
• Molecule 1: Polyketide synthase PKS13

Chain A:



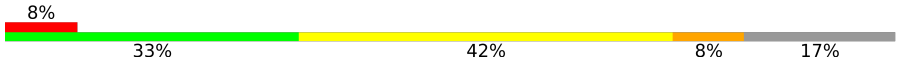
• Molecule 1: Polyketide synthase PKS13

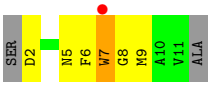
Chain B:



• Molecule 2: 12-mer peptide

Chain C:




SER
D2
N5
F6
W7
G8
M9
A10
V11
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	106.33Å 106.33Å 261.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.96 – 2.49 47.55 – 2.50	Depositor EDS
% Data completeness (in resolution range)	92.6 (46.96-2.49) 92.8 (47.55-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.03 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.228 , 0.278 0.227 , 0.275	Depositor DCC
R_{free} test set	2524 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	52.9	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 31.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7166	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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: XPM, GOL, PG0, SO4

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	0.51	1/3527 (0.0%)	0.63	1/4802 (0.0%)
1	B	0.51	3/3507 (0.1%)	0.62	0/4781
2	C	0.92	1/75 (1.3%)	0.71	0/101
All	All	0.52	5/7109 (0.1%)	0.63	1/9684 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	740	TRP	CD2-CE2	5.79	1.48	1.41
1	B	959	TRP	CD2-CE2	5.26	1.47	1.41
1	B	647	TRP	CD2-CE2	5.11	1.47	1.41
2	C	7	TRP	CD2-CE2	5.11	1.47	1.41
1	B	714	TRP	CD2-CE2	5.01	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	802	LEU	CA-CB-CG	5.03	126.88	115.30

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	3454	0	3380	46	0
1	B	3434	0	3321	67	0
2	C	73	0	51	6	0
3	A	27	0	43	4	0
3	B	20	0	30	7	0
4	A	24	0	32	1	0
4	B	18	0	24	3	0
5	A	8	0	12	2	0
6	B	5	0	0	0	0
6	C	5	0	0	1	0
7	A	64	0	0	2	0
7	B	34	0	0	0	0
All	All	7166	0	6893	116	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 8.

All (116) 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:823:ILE:O	1:B:827:SER:HB2	1.54	1.08
1:B:748:VAL:HG11	1:B:756:VAL:HG23	1.54	0.89
1:B:719:PHE:HB2	3:B:2001:XPM:O2	1.72	0.87
1:B:904:THR:HG21	3:B:2001:XPM:H7	1.61	0.82
1:A:913:MET:HG2	1:A:963:LEU:HG	1.62	0.82
1:A:681:ASP:HB2	5:A:2006:PG0:H12	1.65	0.77
1:A:889:LEU:HD12	1:A:899:ALA:HB1	1.69	0.74
1:B:964:ARG:HH22	4:B:2002:GOL:H2	1.51	0.73
1:B:602:GLU:H	1:B:602:GLU:CD	1.93	0.72
1:B:700:ASN:HD22	1:B:700:ASN:H	1.42	0.66
1:B:600:VAL:HG12	1:B:601:THR:H	1.61	0.65
1:A:864:ASP:H	1:A:884:GLN:HE22	1.44	0.65
1:B:825:SER:HB3	1:B:920:LEU:HD12	1.79	0.65
1:B:869:VAL:HB	1:B:877:VAL:HB	1.78	0.65
1:A:718:GLY:HA3	1:A:802:LEU:HD22	1.79	0.63
1:B:955:ASP:O	1:B:959:TRP:CD1	2.52	0.63
1:B:854:GLU:O	1:B:858:VAL:HB	1.99	0.62
1:A:908:SER:HA	1:A:913:MET:SD	2.41	0.60
1:A:624:LEU:HD21	1:A:678:LEU:HG	1.84	0.60
1:B:907:ALA:H	1:B:912:GLN:NE2	1.99	0.60
1:B:955:ASP:CB	1:B:958:TYR:H	2.16	0.59
1:B:680:HIS:HE2	2:C:6:PHE:HE2	1.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:985:LEU:HD12	1:A:1032:LEU:HD11	1.84	0.58
1:A:885:VAL:O	1:A:889:LEU:HD22	2.04	0.57
1:B:913:MET:HE1	3:B:2001:XPM:HB	1.88	0.56
1:A:862:PHE:HB3	1:A:884:GLN:HE21	1.71	0.56
1:A:797:VAL:HG21	1:A:811:ALA:HB2	1.88	0.56
1:B:955:ASP:HB2	1:B:958:TYR:H	1.72	0.55
1:A:789:HIS:ND1	7:A:2141:HOH:O	2.33	0.55
1:B:700:ASN:HD22	1:B:700:ASN:N	2.05	0.55
1:A:872:ALA:HB3	1:A:875:GLN:HB2	1.90	0.54
1:B:785:GLU:HA	1:B:785:GLU:OE1	2.08	0.53
1:A:784:GLY:HA3	1:A:810:PHE:CZ	2.44	0.53
1:A:826:ARG:O	1:A:830:MET:HG3	2.09	0.52
1:A:624:LEU:HD13	1:A:680:HIS:CE1	2.45	0.52
1:A:769:ILE:CD1	1:A:834:GLU:HG2	2.39	0.52
1:B:862:PHE:CD1	1:B:884:GLN:HG2	2.45	0.52
1:B:829:LEU:HB3	1:B:916:LEU:HD22	1.90	0.52
1:A:982:THR:OG1	1:A:1010:GLN:NE2	2.32	0.52
1:B:711:GLY:HA3	1:B:795:ALA:HB2	1.92	0.51
1:B:802:LEU:C	1:B:802:LEU:HD23	2.32	0.50
1:A:682:HIS:HB2	5:A:2006:PG0:H11	1.92	0.50
1:B:913:MET:CE	3:B:2001:XPM:HB	2.42	0.50
1:A:769:ILE:HD12	1:A:834:GLU:HG2	1.94	0.50
1:B:1013:PRO:HG2	2:C:8:GLY:HA3	1.94	0.50
1:A:847:LEU:HD11	1:A:875:GLN:HB3	1.94	0.49
1:B:862:PHE:HB3	1:B:884:GLN:HG2	1.95	0.49
1:A:716:LEU:HD22	1:A:806:ALA:HB3	1.95	0.48
1:B:626:PRO:HG3	1:B:1044:LEU:HD23	1.94	0.48
1:B:600:VAL:HG12	1:B:601:THR:N	2.28	0.48
1:B:869:VAL:HG22	1:B:967:VAL:HB	1.94	0.48
1:B:853:ASP:O	1:B:857:GLU:HB2	2.14	0.47
1:B:1019:GLN:OE1	2:C:6:PHE:HB3	2.14	0.47
1:B:752:LEU:HD13	1:B:824:CYS:HB3	1.97	0.47
1:B:756:VAL:HA	1:B:759:LEU:HD12	1.97	0.47
2:C:5:ASN:ND2	2:C:7:TRP:HD1	2.12	0.47
1:B:784:GLY:O	1:B:788:ARG:HG3	2.16	0.46
1:B:867:VAL:HG11	1:B:870:TYR:CE1	2.51	0.46
1:A:760:ILE:HA	7:A:2132:HOH:O	2.14	0.46
1:A:913:MET:HA	1:A:913:MET:CE	2.45	0.46
1:B:955:ASP:O	1:B:959:TRP:HD1	1.96	0.46
1:A:979:SER:HB2	4:A:2003:GOL:H2	1.98	0.46
1:B:1012:ILE:HG12	1:B:1031:GLN:NE2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:865:LEU:HD11	1:B:888:ILE:CD1	2.47	0.45
1:B:783:LEU:HD21	1:B:1015:LEU:CD1	2.46	0.45
1:B:834:GLU:HB2	3:B:2001:XPM:HA	1.98	0.45
1:B:814:LEU:HD23	1:B:929:PRO:HA	1.99	0.45
1:B:973:ILE:HB	1:B:1000:THR:HG21	1.99	0.45
1:A:698:ALA:HB1	1:A:699:PRO:HD2	1.97	0.45
1:A:964:ARG:HB3	1:A:965:HIS:CD2	2.52	0.45
1:B:907:ALA:H	1:B:912:GLN:HE22	1.63	0.44
1:B:964:ARG:NH2	4:B:2002:GOL:H2	2.26	0.44
1:B:865:LEU:HD11	1:B:888:ILE:HD11	1.99	0.44
1:A:921:THR:OG1	1:A:960:LYS:HD2	2.16	0.44
1:A:941:HIS:O	1:A:944:ARG:HG2	2.17	0.44
1:A:1006:LEU:HD13	1:A:1009:ALA:HB2	1.99	0.44
1:B:870:TYR:O	1:B:969:PHE:HB3	2.17	0.44
1:B:849:GLU:OE1	1:B:898:PHE:N	2.48	0.44
1:B:798:ILE:HG23	1:B:798:ILE:O	2.18	0.44
1:B:862:PHE:HD1	1:B:884:GLN:HG2	1.82	0.43
1:A:797:VAL:CG2	1:A:811:ALA:HB2	2.48	0.43
1:B:881:PRO:HG2	1:B:884:GLN:NE2	2.33	0.43
1:B:1038:ASP:H	4:B:2003:GOL:H11	1.82	0.43
1:B:955:ASP:HB3	1:B:958:TYR:H	1.84	0.43
1:B:849:GLU:HB3	1:B:897:LYS:HB3	2.00	0.43
1:A:714:TRP:CG	1:A:794:PRO:HB3	2.54	0.43
1:B:784:GLY:HA3	1:B:810:PHE:CZ	2.54	0.43
1:A:716:LEU:HD22	1:A:806:ALA:CB	2.49	0.43
1:B:1019:GLN:OE1	1:B:1019:GLN:HA	2.18	0.43
1:B:821:ARG:NH1	1:B:927:ILE:HG23	2.33	0.43
1:B:837:LEU:HD11	3:B:2001:XPM:HD	2.00	0.43
1:A:937:PHE:CZ	1:A:976:ALA:HA	2.53	0.43
1:A:716:LEU:CD2	1:A:806:ALA:HB3	2.49	0.42
1:A:813:GLY:HA3	1:A:954:HIS:HD2	1.84	0.42
1:B:624:LEU:HD11	2:C:7:TRP:HZ3	1.83	0.42
1:A:786:LEU:O	1:A:789:HIS:HB3	2.19	0.42
1:A:813:GLY:HA3	1:A:954:HIS:CD2	2.54	0.42
1:B:924:LEU:O	1:B:927:ILE:HG12	2.19	0.42
1:A:906:GLY:HA3	3:A:2001[A]:XPM:HA	2.00	0.42
1:A:773:GLN:HE21	3:A:2001[B]:XPM:H6A	1.84	0.42
1:B:700:ASN:H	1:B:700:ASN:ND2	2.15	0.42
1:A:717:ALA:CB	1:A:800:GLN:HB3	2.50	0.41
1:A:644:LEU:O	1:A:648:MET:HG3	2.21	0.41
1:B:771:THR:HA	1:B:774:VAL:CG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:6:PHE:HD1	6:C:101:SO4:O1	2.02	0.41
1:B:913:MET:HE2	3:B:2001:XPM:HDA	2.02	0.41
1:A:790:HIS:O	1:A:1039:LEU:HD22	2.21	0.41
1:B:937:PHE:CZ	1:B:976:ALA:HA	2.56	0.41
1:A:719:PHE:HD1	3:A:2001[B]:XPM:H5A	1.86	0.41
1:B:994:LEU:HD12	1:B:994:LEU:HA	1.80	0.41
1:B:1058:PRO:HA	1:B:1059:PRO:HD3	1.97	0.41
1:A:711:GLY:HA3	1:A:795:ALA:HB2	2.03	0.40
1:B:737:PHE:CE2	1:B:782:ALA:HB3	2.56	0.40
1:B:818:ASP:O	1:B:821:ARG:HB2	2.21	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	461/491 (94%)	447 (97%)	14 (3%)	0	100 100
1	B	463/491 (94%)	431 (93%)	30 (6%)	2 (0%)	34 54
2	C	8/12 (67%)	7 (88%)	1 (12%)	0	100 100
All	All	932/994 (94%)	885 (95%)	45 (5%)	2 (0%)	47 68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	599	GLY
1	B	991	PRO

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	348/387 (90%)	324 (93%)	24 (7%)	15	30
1	B	339/387 (88%)	321 (95%)	18 (5%)	22	43
2	C	5/9 (56%)	3 (60%)	2 (40%)	0	0
All	All	692/783 (88%)	648 (94%)	44 (6%)	17	33

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	615	LEU
1	A	633	LEU
1	A	656	SER
1	A	658	LEU
1	A	668	ARG
1	A	678	LEU
1	A	709	THR
1	A	750	ASP
1	A	752	LEU
1	A	786	LEU
1	A	793	LYS
1	A	817	ARG
1	A	834	GLU
1	A	889	LEU
1	A	891	ARG
1	A	913	MET
1	A	917	LEU
1	A	955	ASP
1	A	964	ARG
1	A	986	GLU
1	A	1006	LEU
1	A	1015	LEU
1	A	1032	LEU
1	A	1034	VAL
1	B	602	GLU
1	B	615	LEU

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Mol	Chain	Res	Type
1	B	618	GLN
1	B	669	ASN
1	B	700	ASN
1	B	704	VAL
1	B	732	LEU
1	B	733	ARG
1	B	774	VAL
1	B	786	LEU
1	B	807	SER
1	B	826	ARG
1	B	857	GLU
1	B	860	SER
1	B	893	GLU
1	B	944	ARG
1	B	1032	LEU
1	B	1047	ARG
2	C	2	ASP
2	C	9	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	654	GLN
1	A	884	GLN
1	A	954	HIS
1	A	965	HIS
1	A	1010	GLN
1	A	1019	GLN
1	B	700	ASN
1	B	723	HIS
1	B	749	GLN
1	B	780	GLN
1	B	912	GLN
1	B	1031	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

13 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	$\#\|Z\| > 2$
4	GOL	A	2005	-	5,5,5	0.46	0	5,5,5	0.41	0
3	XPM	B	2001	1	19,19,20	0.51	0	18,20,22	0.75	0
4	GOL	A	2002	-	5,5,5	0.45	0	5,5,5	0.38	0
6	SO4	B	2005	-	4,4,4	0.45	0	6,6,6	3.61	4 (66%)
4	GOL	B	2004	-	5,5,5	0.36	0	5,5,5	0.17	0
4	GOL	A	2004	-	5,5,5	0.52	0	5,5,5	0.35	0
6	SO4	C	101	-	4,4,4	0.34	0	6,6,6	0.18	0
3	XPM	A	2001[A]	-	19,19,20	0.45	0	18,20,22	1.38	3 (16%)
5	PG0	A	2006	-	7,7,7	0.53	0	6,6,6	0.49	0
3	XPM	A	2001[B]	-	19,14,20	46.72	1 (5%)	18,15,22	4.00	5 (27%)
4	GOL	B	2003	-	5,5,5	0.43	0	5,5,5	0.42	0
4	GOL	A	2003	-	5,5,5	0.49	0	5,5,5	0.37	0
4	GOL	B	2002	-	5,5,5	0.29	0	5,5,5	0.24	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
4	GOL	A	2005	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	XPM	B	2001	1	-	10/20/20/22	-
4	GOL	A	2002	-	-	2/4/4/4	-
4	GOL	B	2004	-	-	2/4/4/4	-
4	GOL	A	2004	-	-	0/4/4/4	-
3	XPM	A	2001[A]	-	-	10/20/20/22	-
5	PG0	A	2006	-	-	3/5/5/5	-
3	XPM	A	2001[B]	-	-	10/20/15/22	-
4	GOL	B	2003	-	-	2/4/4/4	-
4	GOL	A	2003	-	-	0/4/4/4	-
4	GOL	B	2002	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2001[B]	XPM	CC-CB	203.65	12.95	1.51

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2001[B]	XPM	CC-CB-CA	-15.41	36.20	114.42
6	B	2005	SO4	O4-S-O3	-5.35	86.23	109.06
6	B	2005	SO4	O4-S-O1	-4.57	85.44	109.31
6	B	2005	SO4	O4-S-O2	-4.37	86.51	109.31
3	A	2001[B]	XPM	CD-CC-CB	4.33	136.43	114.42
3	A	2001[A]	XPM	O2A-C2A-C2	-3.48	114.41	122.93
3	A	2001[B]	XPM	O2A-C2A-C2	-3.48	114.41	122.93
3	A	2001[A]	XPM	O2B-C2A-C2	3.12	122.38	114.21
3	A	2001[B]	XPM	O2B-C2A-C2	3.12	122.38	114.21
6	B	2005	SO4	O3-S-O1	2.11	120.32	109.31
3	A	2001[A]	XPM	C3-C2-C2A	2.08	115.74	111.01
3	A	2001[B]	XPM	C3-C2-C2A	2.08	115.74	111.01

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2001[A]	XPM	O2-C1-C2-C2A
3	A	2001[A]	XPM	C2A-C2-C3-C4
3	A	2001[B]	XPM	O2-C1-C2-C2A

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Mol	Chain	Res	Type	Atoms
3	A	2001[B]	XPM	C2A-C2-C3-C4
3	B	2001	XPM	O2-C1-C2-C3
3	B	2001	XPM	O2-C1-C2-C2A
4	A	2002	GOL	C1-C2-C3-O3
4	A	2005	GOL	O1-C1-C2-C3
4	B	2002	GOL	C1-C2-C3-O3
4	B	2004	GOL	O1-C1-C2-C3
5	A	2006	PG0	O1-C3-C4-O2
5	A	2006	PG0	OTT-C1-C2-O1
3	A	2001[A]	XPM	C5-C6-C7-C8
3	A	2001[A]	XPM	CC-CD-CE-CF
3	A	2001[B]	XPM	CA-CB-CC-CD
3	A	2001[B]	XPM	CC-CD-CE-CF
3	B	2001	XPM	C6-C7-C8-C9
3	B	2001	XPM	CB-CC-CD-CE
3	A	2001[A]	XPM	C6-C7-C8-C9
3	A	2001[B]	XPM	C9-CA-CB-CC
3	A	2001[A]	XPM	C3-C4-C5-C6
4	A	2002	GOL	O2-C2-C3-O3
4	A	2005	GOL	O1-C1-C2-O2
4	B	2004	GOL	O1-C1-C2-O2
3	B	2001	XPM	CA-CB-CC-CD
3	B	2001	XPM	CC-CD-CE-CF
3	A	2001[A]	XPM	C7-C8-C9-CA
3	A	2001[B]	XPM	CB-CC-CD-CE
3	B	2001	XPM	C8-C9-CA-CB
3	A	2001[B]	XPM	C4-C5-C6-C7
3	A	2001[B]	XPM	C5-C6-C7-C8
3	B	2001	XPM	C2-C3-C4-C5
4	B	2003	GOL	O2-C2-C3-O3
3	B	2001	XPM	C7-C8-C9-CA
4	A	2005	GOL	O2-C2-C3-O3
3	A	2001[A]	XPM	C8-C9-CA-CB
5	A	2006	PG0	C3-C4-O2-C5
3	B	2001	XPM	CD-CE-CF-CG
4	B	2002	GOL	O2-C2-C3-O3
3	A	2001[B]	XPM	C7-C8-C9-CA
3	A	2001[B]	XPM	C2-C3-C4-C5
3	A	2001[A]	XPM	CA-CB-CC-CD
3	A	2001[A]	XPM	C4-C5-C6-C7
4	B	2003	GOL	C1-C2-C3-O3

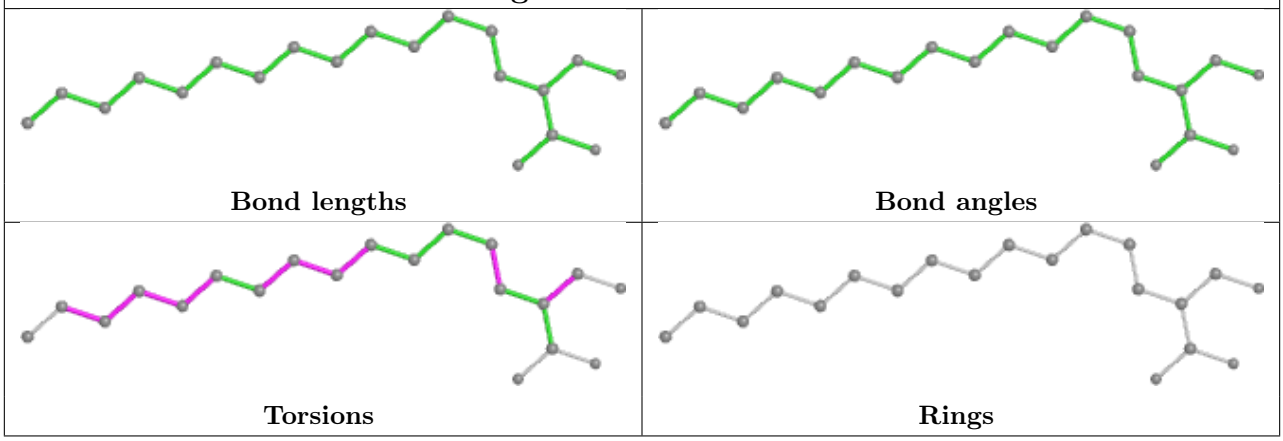
There are no ring outliers.

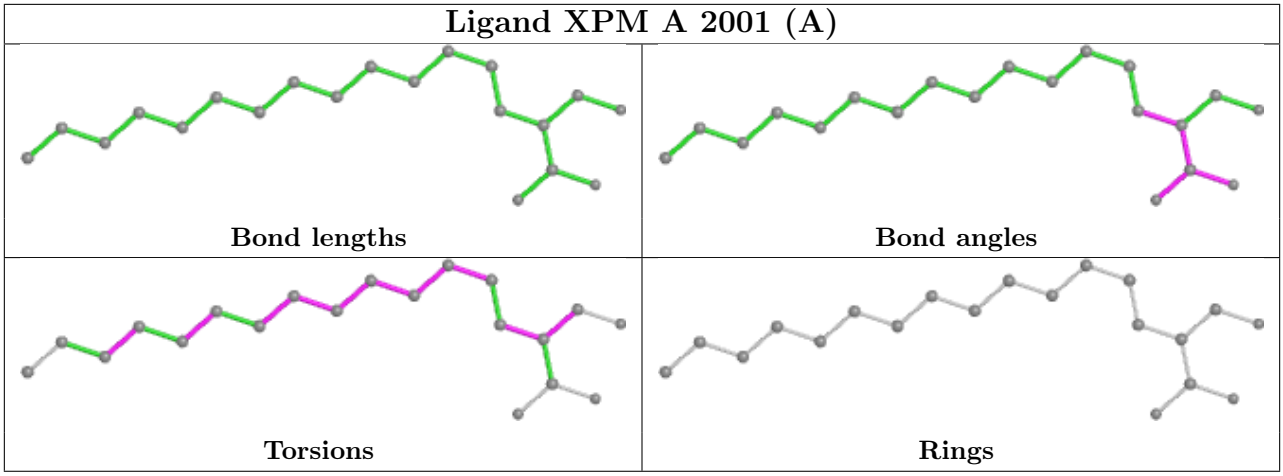
8 monomers are involved in 18 short contacts:

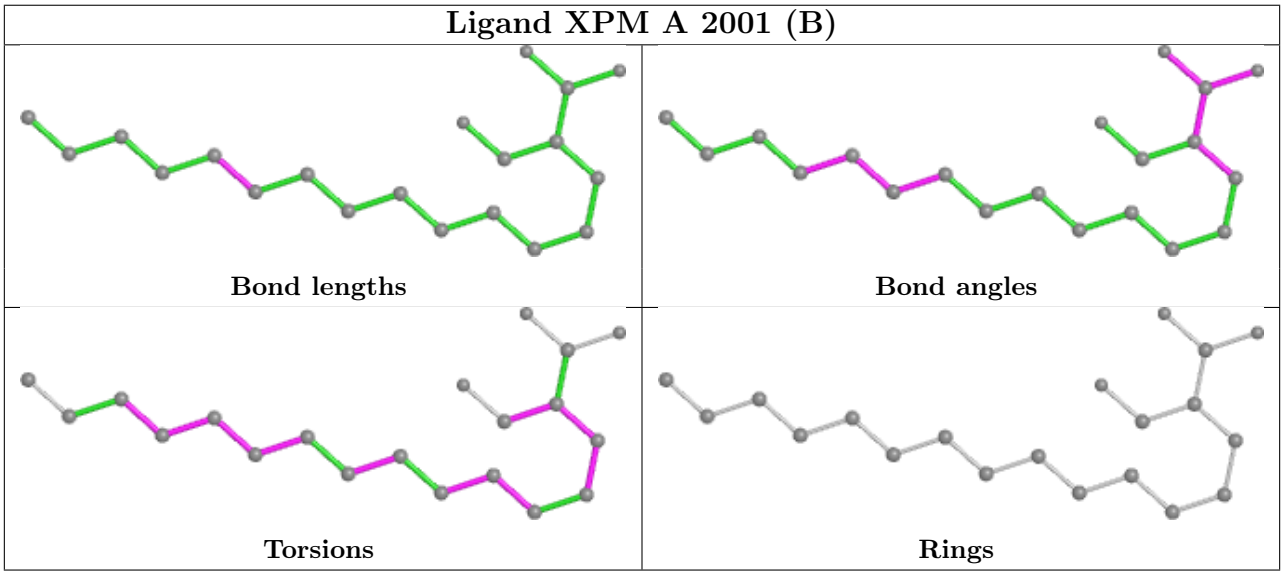
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2001	XPM	7	0
6	C	101	SO4	1	0
3	A	2001[A]	XPM	1	0
5	A	2006	PG0	2	0
3	A	2001[B]	XPM	3	0
4	B	2003	GOL	1	0
4	A	2003	GOL	1	0
4	B	2002	GOL	2	0

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 XPM B 2001







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	463/491 (94%)	-0.04	8 (1%)	70	72	31, 43, 61, 77	0
1	B	465/491 (94%)	0.05	12 (2%)	56	59	29, 51, 73, 93	0
2	C	10/12 (83%)	0.65	1 (10%)	7	6	59, 67, 87, 99	0
All	All	938/994 (94%)	0.01	21 (2%)	62	65	29, 46, 70, 99	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	894	ALA	4.4
1	B	896	GLY	4.1
1	B	890	ALA	3.6
1	B	620	VAL	3.4
1	A	635	SER	3.3
2	C	7	TRP	3.2
1	B	899	ALA	3.1
1	B	898	PHE	2.9
1	B	617	ALA	2.7
1	A	694	ALA	2.6
1	A	632	PHE	2.4
1	B	764	ALA	2.4
1	B	618	GLN	2.3
1	A	693	ALA	2.2
1	A	898	PHE	2.2
1	B	783	LEU	2.2
1	A	633	LEU	2.1
1	A	987	LEU	2.1
1	B	615	LEU	2.1
1	B	889	LEU	2.1
1	A	695	GLY	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 monosaccharides in this entry.

6.4 Ligands (i)

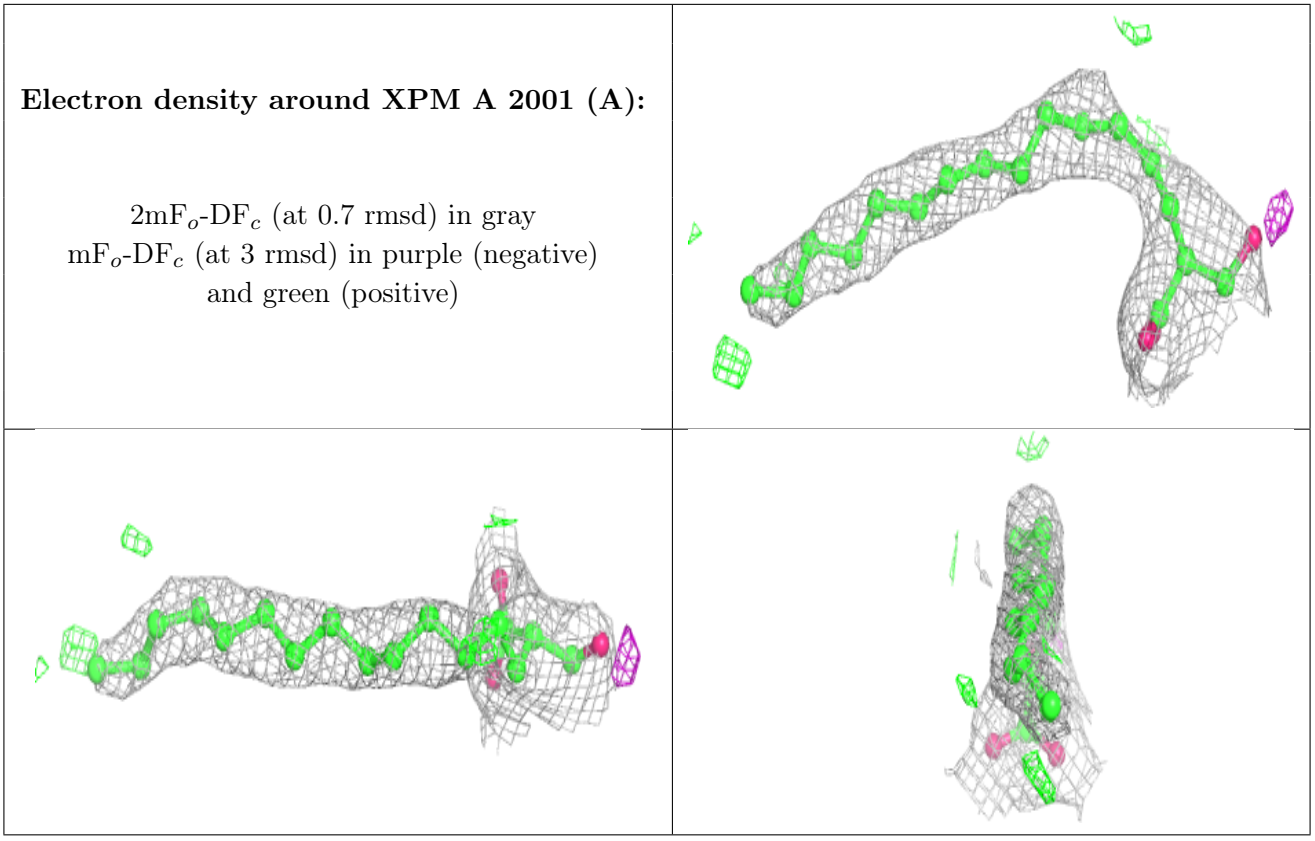
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	A	2003	6/6	0.69	0.33	79,81,85,87	0
4	GOL	A	2004	6/6	0.76	0.20	63,64,71,72	0
4	GOL	B	2003	6/6	0.77	0.27	65,71,72,74	0
5	PG0	A	2006	8/8	0.78	0.22	61,64,83,87	0
4	GOL	A	2005	6/6	0.79	0.28	65,67,69,70	0
4	GOL	A	2002	6/6	0.82	0.18	42,44,45,48	0
3	XPM	A	2001[A]	20/21	0.82	0.30	30,39,56,60	12
3	XPM	A	2001[B]	15/21	0.82	0.30	32,43,56,60	7
4	GOL	B	2004	6/6	0.83	0.19	62,68,71,74	0
4	GOL	B	2002	6/6	0.85	0.15	76,77,78,79	0
6	SO4	B	2005	5/5	0.90	0.23	129,131,134,134	0
6	SO4	C	101	5/5	0.93	0.15	94,96,97,98	0
3	XPM	B	2001	20/21	0.95	0.21	60,65,70,70	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.

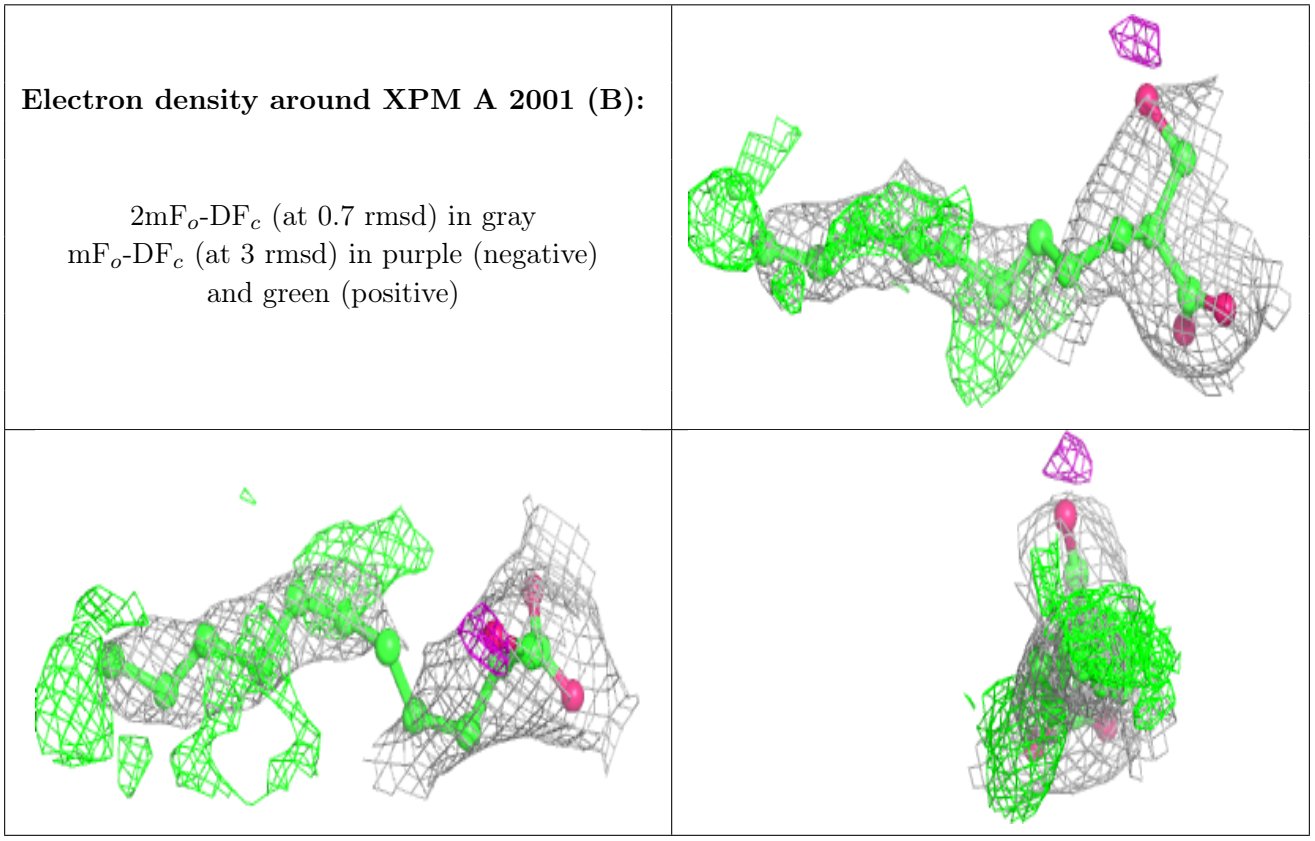
Electron density around XPM A 2001 (A):

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



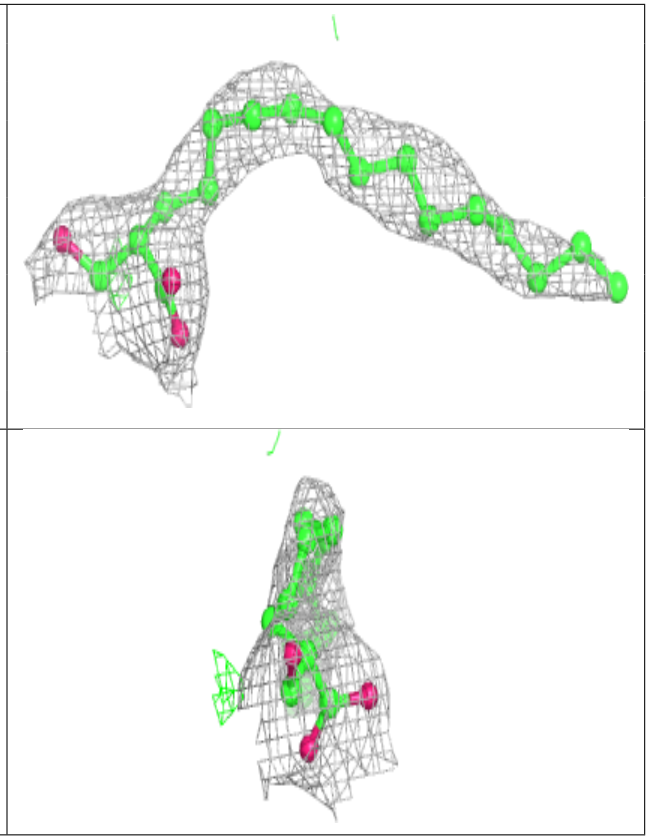
Electron density around XPM A 2001 (B):

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



Electron density around XPM B 2001:

$2mF_o$-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.