Full wwPDB X-ray Structure Validation Report (i)

Sep 17, 2023 – 07:06 PM EDT

PDB ID	:	4ZHG
Title	:	Siderocalin-mediated recognition and cellular uptake of actinides
Authors	:	Allred, B.E.; Rupert, P.B.; Gauny, S.S.; An, D.D.; Ralston, C.Y.; Sturzbecher-Hoehne, M.; Strong, R.K.; Abergel, R.J.
Deposited on	:	2015-04-24
Resolution	:	2.05 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:

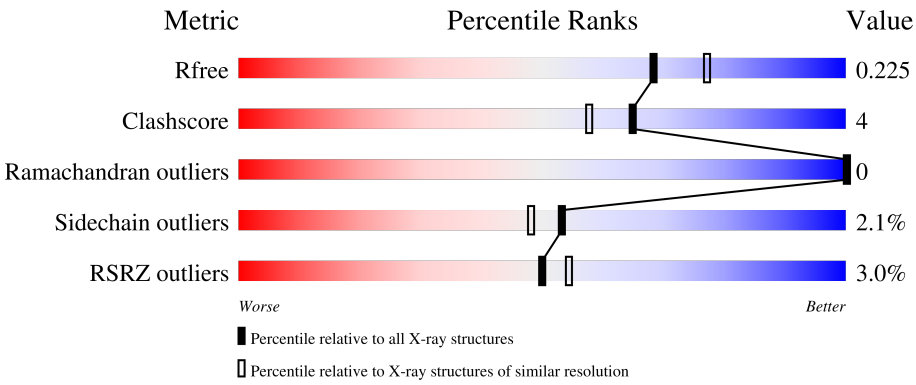
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	180	3% 89% 9% •
1	B	180	2% 89% 7% • •
1	C	180	2% 88% 9% • •
1	D	180	5% 91% 6% • •
1	E	180	3% 93% 5% •

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Mol	Chain	Length	Quality of chain
1	F	180	3% 89% 8%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 9246 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 Neutrophil gelatinase-associated lipocalin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	177	1436	930	241	261	4	0	2	0
1	B	175	1443	936	239	264	4	0	5	0
1	C	175	1412	917	237	254	4	0	1	0
1	D	177	1436	928	238	266	4	0	3	0
1	E	176	1424	923	236	261	4	0	2	0
1	F	175	1433	928	239	262	4	0	3	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P80188
A	0	SER	-	expression tag	UNP P80188
A	87	SER	CYS	engineered mutation	UNP P80188
B	-1	GLY	-	expression tag	UNP P80188
B	0	SER	-	expression tag	UNP P80188
B	87	SER	CYS	engineered mutation	UNP P80188
C	-1	GLY	-	expression tag	UNP P80188
C	0	SER	-	expression tag	UNP P80188
C	87	SER	CYS	engineered mutation	UNP P80188
D	-1	GLY	-	expression tag	UNP P80188
D	0	SER	-	expression tag	UNP P80188
D	87	SER	CYS	engineered mutation	UNP P80188
E	-1	GLY	-	expression tag	UNP P80188
E	0	SER	-	expression tag	UNP P80188
E	87	SER	CYS	engineered mutation	UNP P80188
F	-1	GLY	-	expression tag	UNP P80188
F	0	SER	-	expression tag	UNP P80188

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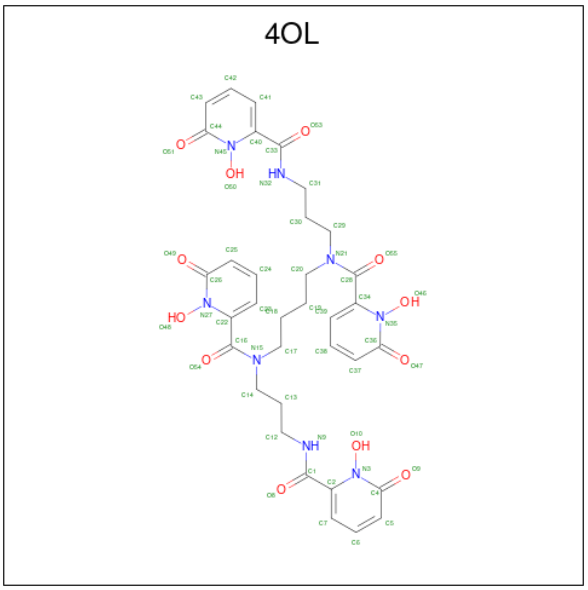
Chain	Residue	Modelled	Actual	Comment	Reference
F	87	SER	CYS	engineered mutation	UNP P80188

- Molecule 2 is AMERICIUM ION (three-letter code: AM) (formula: Am).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Am 1 1	0	0
2	B	1	Total Am 1 1	0	0
2	C	1	Total Am 1 1	0	0
2	D	1	Total Am 1 1	0	0
2	E	1	Total Am 1 1	0	0
2	F	1	Total Am 1 1	0	0

- Molecule 3 is N,N'-butane-1,4-diylbis[1-hydroxy-N-(3-{[(1-hydroxy-6-oxo-1,6-dihydropyridin-2-yl)carbonyl]amino}propyl)-6-oxo-1,6-dihydropyridine-2-carboxamide] (three-letter code: 4OL) (formula: $C_{34}H_{38}N_8O_{12}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 54 34 8 12	0	0
3	B	1	Total C N O 54 34 8 12	0	0

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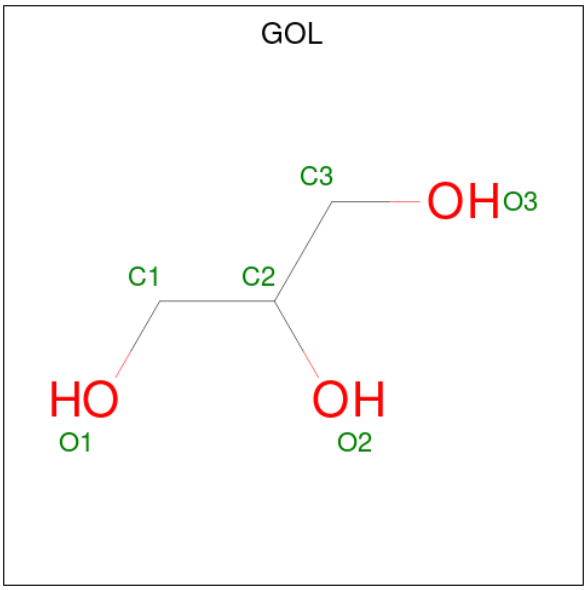
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	C	1	54	34	8	12	0	0
			Total	C	N	O		
3	D	1	54	34	8	12	0	0
			Total	C	N	O		
3	E	1	54	34	8	12	0	0
			Total	C	N	O		
3	F	1	54	34	8	12	0	0

- 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	F	1	6	3	3		0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
5	A	1	1	1	0	0
			Total	Cl		
5	B	1	1	1	0	0
			Total	Cl		
5	C	1	1	1	0	0

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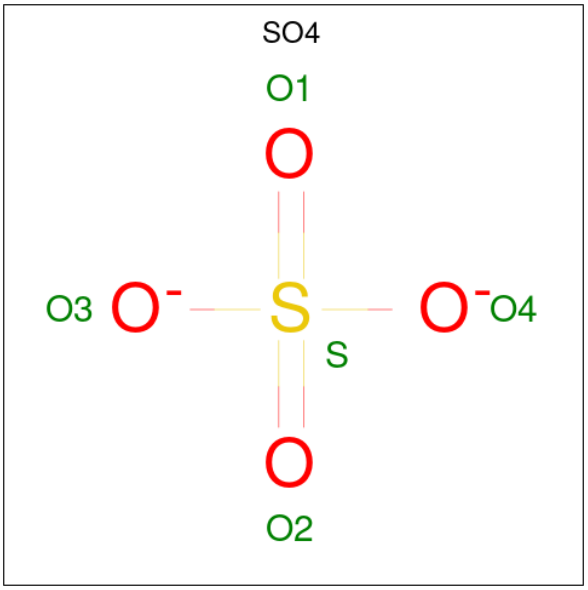
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total Cl 1 1	0	0
5	E	1	Total Cl 1 1	0	0
5	F	1	Total Cl 1 1	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
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	53	Total O 53 53	0	0
7	B	56	Total O 56 56	0	0
7	C	61	Total O 61 61	0	0

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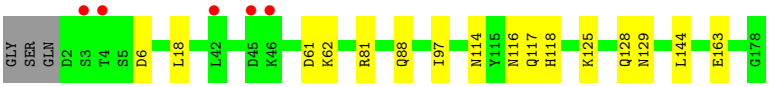
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	D	45	45	45	0	0
			Total	O		
7	E	39	39	39	0	0
			Total	O		
7	F	45	45	45	0	0

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: Neutrophil gelatinase-associated lipocalin

Chain A:

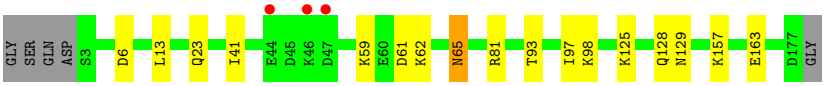


• Molecule 1: Neutrophil gelatinase-associated lipocalin

Chain B:

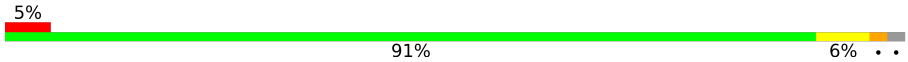
• Molecule 1: Neutrophil gelatinase-associated lipocalin

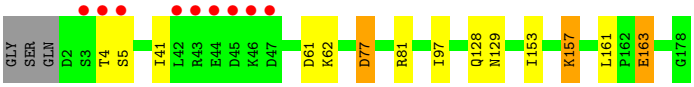
Chain C:



• Molecule 1: Neutrophil gelatinase-associated lipocalin

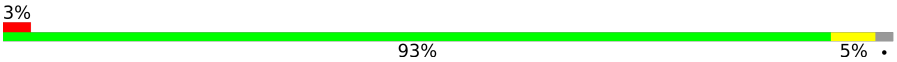
Chain D:

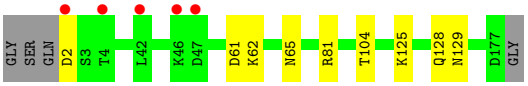




• Molecule 1: Neutrophil gelatinase-associated lipocalin

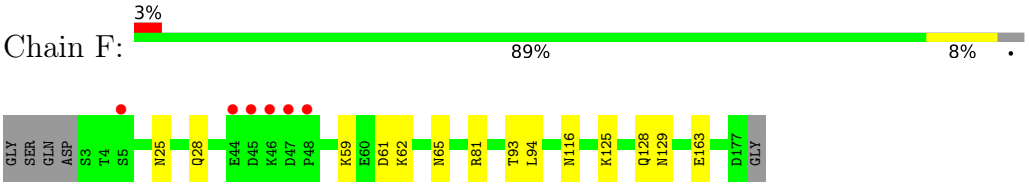
Chain E:





• Molecule 1: Neutrophil gelatinase-associated lipocalin

Chain F:


3%
89%
8%
GLY
SER
GLN
ASP
S3
T4
S5
N25
Q28
E44
D45
K46
D47
P48
K59
E60
D61
K62
N65
R81
T93
L94
N116
K125
Q128
N129
E163
D177
GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	107.73Å 117.69Å 121.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.05 48.19 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-2.05) 99.5 (48.19-2.05)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.76 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.195 , 0.217 0.203 , 0.225	Depositor DCC
R_{free} test set	4848 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	22.7	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 42.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.039 for -h,l,k	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9246	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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: GOL, 4OL, AM, CL, 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	0.46	0/1480	0.57	0/2007
1	B	0.44	0/1493	0.57	0/2028
1	C	0.44	0/1452	0.57	0/1970
1	D	0.46	0/1482	0.56	0/2011
1	E	0.44	0/1467	0.59	0/1991
1	F	0.44	0/1479	0.56	0/2006
All	All	0.45	0/8853	0.57	0/12013

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	E	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	2	ASP	Peptide

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	1436	0	1419	10	1
1	B	1443	0	1419	11	1
1	C	1412	0	1398	16	0
1	D	1436	0	1412	11	0
1	E	1424	0	1404	4	0
1	F	1433	0	1420	8	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
3	A	54	0	36	7	0
3	B	54	0	35	6	0
3	C	54	0	35	5	0
3	D	54	0	36	4	0
3	E	54	0	35	4	0
3	F	54	0	36	4	0
4	A	6	0	8	1	0
4	F	6	0	8	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
6	C	5	0	0	0	0
7	A	53	0	0	0	1
7	B	56	0	0	3	0
7	C	61	0	0	1	0
7	D	45	0	0	4	0
7	E	39	0	0	0	1
7	F	45	0	0	0	0
All	All	9246	0	8701	73	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 4.

All (73) 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:6:ASP:OD1	1:D:77[A]:ASP:OD2	2.07	0.73
1:D:77[A]:ASP:OD2	7:D:301:HOH:O	2.08	0.71
1:C:157:LYS:CE	1:C:163:GLU:HG3	2.23	0.68
3:D:202:4OL:O8	7:D:302:HOH:O	2.12	0.65
1:A:114:ASN:HD21	1:A:117:GLN:HE21	1.45	0.64
1:C:93:THR:HB	7:C:306:HOH:O	1.98	0.63
1:F:116:ASN:HD22	4:F:203:GOL:H2	1.67	0.60
1:D:153:ILE:O	1:D:157:LYS:HD3	2.03	0.59
1:A:125:LYS:HE2	3:A:202:4OL:H18	1.84	0.59
1:C:59:LYS:HD3	1:C:65:ASN:HD22	1.68	0.59
1:D:163:GLU:OE1	7:D:303:HOH:O	2.17	0.57
3:A:202:4OL:H23	3:A:202:4OL:O46	2.06	0.56
1:C:157:LYS:HE3	1:C:163:GLU:HG3	1.88	0.55
1:A:117:GLN:OE1	4:A:203:GOL:H11	2.07	0.54
1:D:153:ILE:HG23	1:D:157:LYS:HE3	1.89	0.54
1:A:118[B]:HIS:ND1	1:A:144:LEU:HD22	2.22	0.54
3:A:202:4OL:N9	3:A:202:4OL:O10	2.41	0.54
1:F:125:LYS:HE2	3:F:202:4OL:H18	1.89	0.54
3:F:202:4OL:N9	3:F:202:4OL:O10	2.41	0.54
3:E:202:4OL:N9	3:E:202:4OL:O10	2.39	0.53
3:D:202:4OL:O10	3:D:202:4OL:N9	2.31	0.53
1:C:125:LYS:HE2	3:C:202:4OL:H18	1.89	0.52
1:A:117:GLN:HB3	1:A:118[B]:HIS:CE1	2.45	0.52
1:D:157:LYS:HD2	1:D:161:LEU:O	2.09	0.52
1:B:60:GLU:OE2	1:C:98:LYS:NZ	2.43	0.52
1:D:41:ILE:HD11	3:D:202:4OL:H4	1.92	0.52
1:A:116:ASN:HA	1:C:23:GLN:HE22	1.74	0.51
1:C:157:LYS:HE2	1:C:163:GLU:HG3	1.92	0.51
3:A:202:4OL:H6	3:A:202:4OL:C22	2.41	0.50
1:B:41:ILE:HD11	3:B:202:4OL:H4	1.92	0.50
3:E:202:4OL:H23	3:E:202:4OL:O46	2.12	0.49
1:C:125:LYS:HE2	3:C:202:4OL:C25	2.43	0.49
1:D:5:SER:C	7:D:313:HOH:O	2.51	0.49
3:A:202:4OL:H6	3:A:202:4OL:C23	2.42	0.49
3:A:202:4OL:O50	3:A:202:4OL:N32	2.29	0.49
1:A:125:LYS:HE2	3:A:202:4OL:C25	2.42	0.49
3:D:202:4OL:O50	3:D:202:4OL:N32	2.35	0.48
3:E:202:4OL:O50	3:E:202:4OL:N32	2.38	0.48
1:F:125:LYS:HE2	3:F:202:4OL:C25	2.44	0.47
1:F:59:LYS:HD3	1:F:65[B]:ASN:ND2	2.29	0.47
1:B:93:THR:HB	7:B:316:HOH:O	2.16	0.45
3:B:202:4OL:N32	3:B:202:4OL:O50	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:25:ASN:OD1	1:F:28:GLN:NE2	2.49	0.45
1:B:88[B]:GLN:HE22	1:C:13:LEU:HD11	1.82	0.45
1:D:128:GLN:O	1:D:129:ASN:HB2	2.17	0.45
1:A:61:ASP:O	1:A:62:LYS:HB2	2.17	0.44
1:D:61:ASP:O	1:D:62:LYS:HB2	2.17	0.44
1:A:128:GLN:O	1:A:129:ASN:HB2	2.16	0.44
1:A:18:LEU:HD22	1:A:88:GLN:CD	2.37	0.44
1:B:61:ASP:O	1:B:62:LYS:HB2	2.18	0.43
1:F:61:ASP:O	1:F:62:LYS:HB2	2.17	0.43
1:B:88[B]:GLN:NE2	1:C:13:LEU:CD1	2.82	0.43
1:E:128:GLN:O	1:E:129:ASN:HB2	2.18	0.43
1:D:4:THR:O	1:D:5:SER:HB2	2.19	0.43
1:B:88[B]:GLN:HE22	1:C:13:LEU:CD1	2.32	0.42
1:B:97:ILE:HD11	7:B:316:HOH:O	2.19	0.42
1:C:128:GLN:O	1:C:129:ASN:HB2	2.19	0.42
1:C:61:ASP:O	1:C:62:LYS:HB2	2.19	0.42
1:B:100:TYR:CD2	3:B:202:4OL:H32	2.55	0.42
3:C:202:4OL:O50	3:C:202:4OL:N32	2.46	0.42
1:E:125:LYS:HE2	3:E:202:4OL:H18	2.02	0.42
3:F:202:4OL:O50	3:F:202:4OL:N32	2.37	0.42
1:E:61:ASP:O	1:E:62:LYS:HB2	2.19	0.42
1:E:65[A]:ASN:HD22	1:E:65[A]:ASN:HA	1.66	0.42
3:B:202:4OL:H21	7:B:349:HOH:O	2.19	0.42
1:B:128:GLN:O	1:B:129:ASN:HB2	2.20	0.41
3:B:202:4OL:H23	3:B:202:4OL:O46	2.20	0.41
3:C:202:4OL:N9	3:C:202:4OL:O10	2.48	0.41
1:F:93:THR:OG1	1:F:94:LEU:N	2.53	0.41
3:B:202:4OL:N9	3:B:202:4OL:O10	2.48	0.41
1:F:128:GLN:O	1:F:129:ASN:HB2	2.21	0.41
1:C:41:ILE:HD11	3:C:202:4OL:H4	2.03	0.40
1:B:65[A]:ASN:HD22	1:B:65[A]:ASN:HA	1.69	0.40

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)
1:A:6:ASP:OD1	1:B:77[A]:ASP:OD2[3_555]	1.68	0.52
7:A:350:HOH:O	7:E:338:HOH:O[4_445]	2.11	0.09

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	177/180 (98%)	173 (98%)	4 (2%)	0	100	100
1	B	178/180 (99%)	175 (98%)	3 (2%)	0	100	100
1	C	174/180 (97%)	170 (98%)	4 (2%)	0	100	100
1	D	178/180 (99%)	174 (98%)	4 (2%)	0	100	100
1	E	176/180 (98%)	173 (98%)	3 (2%)	0	100	100
1	F	176/180 (98%)	173 (98%)	3 (2%)	0	100	100
All	All	1059/1080 (98%)	1038 (98%)	21 (2%)	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	159/164 (97%)	156 (98%)	3 (2%)	57	53
1	B	160/164 (98%)	154 (96%)	6 (4%)	33	26
1	C	155/164 (94%)	152 (98%)	3 (2%)	57	53
1	D	160/164 (98%)	154 (96%)	6 (4%)	33	26
1	E	158/164 (96%)	156 (99%)	2 (1%)	69	67
1	F	160/164 (98%)	158 (99%)	2 (1%)	69	67
All	All	952/984 (97%)	930 (98%)	22 (2%)	53	44

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	ARG
1	A	97	ILE
1	A	163	GLU
1	B	77[A]	ASP
1	B	77[B]	ASP
1	B	81	ARG
1	B	97	ILE
1	B	157	LYS
1	B	163	GLU
1	C	65	ASN
1	C	81	ARG
1	C	97	ILE
1	D	77[A]	ASP
1	D	77[B]	ASP
1	D	81	ARG
1	D	97	ILE
1	D	157	LYS
1	D	163	GLU
1	E	81	ARG
1	E	104	THR
1	F	81	ARG
1	F	163	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	GLN
1	B	116	ASN
1	B	129	ASN
1	C	23	GLN
1	C	65	ASN
1	C	116	ASN
1	D	21	ASN
1	F	116	ASN

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)

Of 23 ligands modelled in this entry, 12 are monoatomic - leaving 11 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	$\#\|Z\| > 2$
3	4OL	F	202	-	57,57,57	1.69	8 (14%)	72,78,78	2.82	18 (25%)
4	GOL	A	203	-	5,5,5	0.26	0	5,5,5	0.44	0
4	GOL	F	203	-	5,5,5	0.27	0	5,5,5	0.38	0
6	SO4	B	203	-	4,4,4	0.33	0	6,6,6	0.49	0
6	SO4	C	203	-	4,4,4	0.41	0	6,6,6	0.23	0
3	4OL	E	202	-	57,57,57	2.17	9 (15%)	72,78,78	2.76	14 (19%)
3	4OL	A	202	-	57,57,57	2.00	7 (12%)	72,78,78	2.50	16 (22%)
3	4OL	D	202	-	57,57,57	2.28	8 (14%)	72,78,78	2.74	18 (25%)
3	4OL	C	202	-	57,57,57	2.00	10 (17%)	72,78,78	2.47	12 (16%)
6	SO4	A	205	-	4,4,4	0.39	0	6,6,6	0.23	0
3	4OL	B	202	-	57,57,57	2.46	9 (15%)	72,78,78	2.98	19 (26%)

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
3	4OL	F	202	-	-	5/43/45/45	0/4/4/4
4	GOL	A	203	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	F	203	-	-	2/4/4/4	-
3	4OL	E	202	-	-	3/43/45/45	0/4/4/4
3	4OL	A	202	-	-	6/43/45/45	0/4/4/4
3	4OL	D	202	-	-	4/43/45/45	0/4/4/4
3	4OL	C	202	-	-	6/43/45/45	0/4/4/4
3	4OL	B	202	-	-	5/43/45/45	0/4/4/4

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	202	4OL	C36-N35	11.95	1.43	1.38
3	E	202	4OL	C36-N35	9.92	1.42	1.38
3	B	202	4OL	C44-N45	8.69	1.41	1.38
3	D	202	4OL	C26-N27	8.01	1.41	1.38
3	D	202	4OL	C44-N45	7.95	1.41	1.38
3	C	202	4OL	C36-N35	7.91	1.41	1.38
3	C	202	4OL	C44-N45	7.67	1.41	1.38
3	A	202	4OL	C26-N27	7.42	1.41	1.38
3	D	202	4OL	C4-N3	7.33	1.41	1.38
3	E	202	4OL	C4-N3	6.69	1.41	1.38
3	A	202	4OL	C4-N3	6.02	1.41	1.38
3	A	202	4OL	C44-N45	5.54	1.40	1.38
3	A	202	4OL	C36-N35	5.45	1.40	1.38
3	E	202	4OL	C26-N27	5.38	1.40	1.38
3	F	202	4OL	C36-N35	5.31	1.40	1.38
3	F	202	4OL	C26-N27	5.21	1.40	1.38
3	F	202	4OL	O48-N27	5.12	1.45	1.38
3	B	202	4OL	O48-N27	4.98	1.44	1.38
3	D	202	4OL	C36-N35	4.70	1.40	1.38
3	D	202	4OL	O10-N3	4.59	1.44	1.38
3	B	202	4OL	C26-N27	4.36	1.40	1.38
3	C	202	4OL	C26-N27	4.20	1.40	1.38
3	A	202	4OL	O48-N27	4.12	1.43	1.38
3	E	202	4OL	O46-N35	4.07	1.43	1.38
3	D	202	4OL	O50-N45	4.03	1.43	1.38
3	E	202	4OL	O50-N45	3.96	1.43	1.38
3	D	202	4OL	O48-N27	3.90	1.43	1.38
3	A	202	4OL	O10-N3	3.90	1.43	1.38
3	B	202	4OL	O46-N35	3.83	1.43	1.38
3	E	202	4OL	O48-N27	3.69	1.43	1.38
3	C	202	4OL	O48-N27	3.57	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	202	4OL	O10-N3	3.52	1.43	1.38
3	B	202	4OL	O10-N3	3.45	1.42	1.38
3	C	202	4OL	O10-N3	3.42	1.42	1.38
3	F	202	4OL	O50-N45	3.34	1.42	1.38
3	E	202	4OL	O10-N3	3.29	1.42	1.38
3	A	202	4OL	O50-N45	3.23	1.42	1.38
3	C	202	4OL	C4-N3	3.23	1.40	1.38
3	F	202	4OL	O46-N35	3.22	1.42	1.38
3	C	202	4OL	O50-N45	3.17	1.42	1.38
3	F	202	4OL	C4-N3	3.15	1.40	1.38
3	B	202	4OL	C4-N3	3.10	1.40	1.38
3	B	202	4OL	O50-N45	3.00	1.42	1.38
3	F	202	4OL	C44-N45	2.89	1.39	1.38
3	C	202	4OL	C34-N35	2.87	1.43	1.38
3	E	202	4OL	C44-N45	2.49	1.39	1.38
3	C	202	4OL	O46-N35	2.45	1.41	1.38
3	B	202	4OL	C34-N35	2.27	1.42	1.38
3	C	202	4OL	C22-N27	2.27	1.42	1.38
3	D	202	4OL	O46-N35	2.23	1.41	1.38
3	E	202	4OL	C34-N35	2.09	1.41	1.38

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	202	4OL	O46-N35-C36	14.76	129.62	116.75
3	D	202	4OL	O46-N35-C36	10.28	125.72	116.75
3	C	202	4OL	O46-N35-C36	10.05	125.52	116.75
3	D	202	4OL	O10-N3-C4	10.05	125.52	116.75
3	E	202	4OL	O46-N35-C36	10.05	125.52	116.75
3	F	202	4OL	O46-N35-C36	9.09	124.68	116.75
3	A	202	4OL	O46-N35-C36	9.02	124.62	116.75
3	F	202	4OL	O10-N3-C4	8.86	124.47	116.75
3	F	202	4OL	C22-N27-C26	-8.03	118.41	125.94
3	B	202	4OL	C22-N27-C26	-8.02	118.42	125.94
3	F	202	4OL	O50-N45-C44	8.01	123.73	116.75
3	E	202	4OL	O10-N3-C4	7.73	123.49	116.75
3	E	202	4OL	C40-N45-C44	-7.59	118.83	125.94
3	C	202	4OL	C2-N3-C4	-7.30	119.09	125.94
3	E	202	4OL	C34-N35-C36	-7.27	119.12	125.94
3	E	202	4OL	O50-N45-C44	7.19	123.02	116.75
3	E	202	4OL	C22-N27-C26	-7.10	119.28	125.94
3	D	202	4OL	C2-N3-C4	-7.07	119.31	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	202	4OL	O10-N3-C4	7.02	122.87	116.75
3	F	202	4OL	C34-N35-C36	-6.94	119.43	125.94
3	A	202	4OL	O50-N45-C44	6.91	122.78	116.75
3	A	202	4OL	C22-N27-C26	-6.84	119.53	125.94
3	C	202	4OL	C22-N27-C26	-6.77	119.59	125.94
3	F	202	4OL	C2-N3-C4	-6.76	119.60	125.94
3	B	202	4OL	C34-N35-C36	-6.72	119.64	125.94
3	B	202	4OL	O47-C36-N35	6.63	126.62	118.94
3	F	202	4OL	C40-N45-C44	-6.60	119.75	125.94
3	A	202	4OL	C2-N3-C4	-6.50	119.84	125.94
3	B	202	4OL	C40-N45-C44	-6.35	119.99	125.94
3	B	202	4OL	O10-N3-C4	6.20	122.16	116.75
3	D	202	4OL	C22-N27-C26	-5.89	120.42	125.94
3	A	202	4OL	C40-N45-C44	-5.87	120.43	125.94
3	C	202	4OL	C40-N45-C44	-5.85	120.46	125.94
3	E	202	4OL	C2-N3-C4	-5.78	120.52	125.94
3	D	202	4OL	C34-N35-C36	-5.65	120.64	125.94
3	C	202	4OL	C34-N35-C36	-5.61	120.67	125.94
3	C	202	4OL	O10-N3-C4	5.56	121.60	116.75
3	D	202	4OL	C40-N45-C44	-5.54	120.74	125.94
3	D	202	4OL	O50-N45-C44	5.47	121.52	116.75
3	C	202	4OL	O50-N45-C44	5.45	121.51	116.75
3	B	202	4OL	C2-N3-C4	-5.37	120.90	125.94
3	D	202	4OL	O48-N27-C26	5.33	121.40	116.75
3	A	202	4OL	C34-N35-C36	-5.15	121.11	125.94
3	A	202	4OL	O48-N27-C26	4.68	120.83	116.75
3	E	202	4OL	O48-N27-C26	4.68	120.83	116.75
3	F	202	4OL	O48-N27-C26	4.58	120.75	116.75
3	B	202	4OL	O46-N35-C34	-4.45	110.74	117.06
3	E	202	4OL	O47-C36-N35	4.32	123.94	118.94
3	B	202	4OL	O48-N27-C22	4.30	123.17	117.06
3	D	202	4OL	C7-C2-N3	4.28	121.60	118.47
3	B	202	4OL	O50-N45-C44	4.14	120.36	116.75
3	C	202	4OL	C7-C2-N3	3.97	121.37	118.47
3	C	202	4OL	O47-C36-N35	3.95	123.52	118.94
3	D	202	4OL	O47-C36-N35	3.95	123.51	118.94
3	C	202	4OL	O48-N27-C22	3.67	122.27	117.06
3	F	202	4OL	C23-C22-N27	3.61	121.11	118.47
3	F	202	4OL	C7-C2-N3	3.60	121.11	118.47
3	E	202	4OL	C39-C34-N35	3.56	121.07	118.47
3	B	202	4OL	O47-C36-C37	-3.23	114.67	124.37
3	F	202	4OL	C41-C40-N45	3.10	120.74	118.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	202	4OL	C7-C2-N3	3.02	120.68	118.47
3	A	202	4OL	O47-C36-N35	3.02	122.43	118.94
3	F	202	4OL	C39-C34-N35	2.98	120.65	118.47
3	A	202	4OL	C23-C22-N27	2.86	120.56	118.47
3	D	202	4OL	O9-C4-N3	2.84	122.22	118.94
3	D	202	4OL	C1-C2-N3	-2.83	116.70	122.25
3	E	202	4OL	O9-C4-N3	2.83	122.21	118.94
3	A	202	4OL	C7-C2-N3	2.81	120.53	118.47
3	E	202	4OL	C41-C40-N45	2.68	120.43	118.47
3	B	202	4OL	O51-C44-N45	2.68	122.04	118.94
3	E	202	4OL	C23-C22-N27	2.64	120.40	118.47
3	A	202	4OL	C33-C40-N45	-2.63	117.10	122.25
3	B	202	4OL	C23-C22-N27	2.56	120.34	118.47
3	F	202	4OL	O48-N27-C22	2.56	120.71	117.06
3	B	202	4OL	C41-C40-N45	2.51	120.31	118.47
3	D	202	4OL	O46-N35-C34	-2.42	113.63	117.06
3	F	202	4OL	O9-C4-N3	2.40	121.72	118.94
3	C	202	4OL	O46-N35-C34	-2.34	113.73	117.06
3	D	202	4OL	O55-C28-N21	-2.34	118.94	122.67
3	E	202	4OL	O47-C36-C37	-2.33	117.36	124.37
3	D	202	4OL	C23-C22-N27	2.30	120.15	118.47
3	F	202	4OL	O47-C36-N35	2.25	121.55	118.94
3	D	202	4OL	C33-C40-N45	-2.22	117.90	122.25
3	A	202	4OL	C41-C40-C33	2.21	123.47	119.28
3	A	202	4OL	C1-C2-N3	-2.17	117.99	122.25
3	B	202	4OL	C2-C1-N9	2.17	121.15	117.39
3	D	202	4OL	O47-C36-C37	-2.14	117.95	124.37
3	F	202	4OL	C19-C20-N21	-2.13	105.76	112.44
3	B	202	4OL	C39-C34-N35	2.13	120.03	118.47
3	A	202	4OL	O46-N35-C34	-2.11	114.07	117.06
3	D	202	4OL	O49-C26-N27	2.10	121.38	118.94
3	B	202	4OL	C29-N21-C28	2.08	126.69	120.61
3	B	202	4OL	O9-C4-N3	2.08	121.35	118.94
3	F	202	4OL	C33-C40-N45	-2.03	118.26	122.25
3	A	202	4OL	O9-C4-N3	2.01	121.27	118.94
3	F	202	4OL	O51-C44-N45	2.01	121.27	118.94
3	C	202	4OL	O47-C36-C37	-2.00	118.36	124.37

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	203	GOL	O1-C1-C2-C3
4	F	203	GOL	O1-C1-C2-C3
3	E	202	4OL	N15-C17-C18-C19
4	A	203	GOL	O1-C1-C2-O2
4	F	203	GOL	O1-C1-C2-O2
3	C	202	4OL	N15-C17-C18-C19
3	B	202	4OL	N15-C17-C18-C19
3	D	202	4OL	C18-C19-C20-N21
3	F	202	4OL	N15-C17-C18-C19
3	A	202	4OL	N15-C17-C18-C19
3	B	202	4OL	O55-C28-C34-C39
3	A	202	4OL	O55-C28-C34-N35
3	B	202	4OL	O55-C28-C34-N35
3	D	202	4OL	O55-C28-C34-N35
3	F	202	4OL	C18-C19-C20-N21
3	C	202	4OL	C18-C19-C20-N21
3	A	202	4OL	O54-C16-C22-C23
3	A	202	4OL	O55-C28-C34-C39
3	C	202	4OL	O54-C16-C22-C23
3	D	202	4OL	O55-C28-C34-C39
3	E	202	4OL	O55-C28-C34-C39
3	F	202	4OL	O55-C28-C34-C39
3	A	202	4OL	O54-C16-C22-N27
3	C	202	4OL	O54-C16-C22-N27
3	C	202	4OL	O55-C28-C34-N35
3	E	202	4OL	O55-C28-C34-N35
3	F	202	4OL	O55-C28-C34-N35
3	A	202	4OL	C18-C19-C20-N21
3	C	202	4OL	O55-C28-C34-C39
3	B	202	4OL	C30-C29-N21-C28
3	B	202	4OL	C18-C19-C20-N21
3	D	202	4OL	O54-C16-C22-C23
3	F	202	4OL	O54-C16-C22-N27

There are no ring outliers.

8 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	202	4OL	4	0
4	A	203	GOL	1	0
4	F	203	GOL	1	0
3	E	202	4OL	4	0
3	A	202	4OL	7	0

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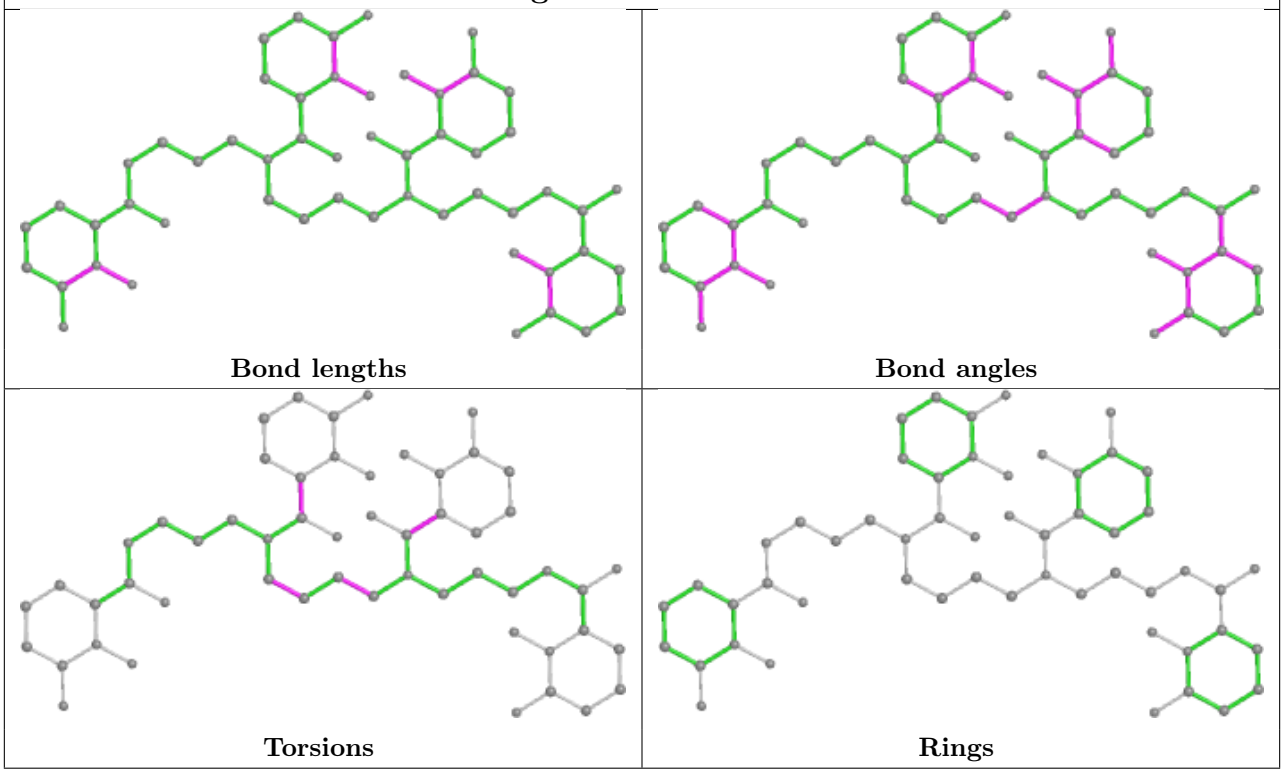
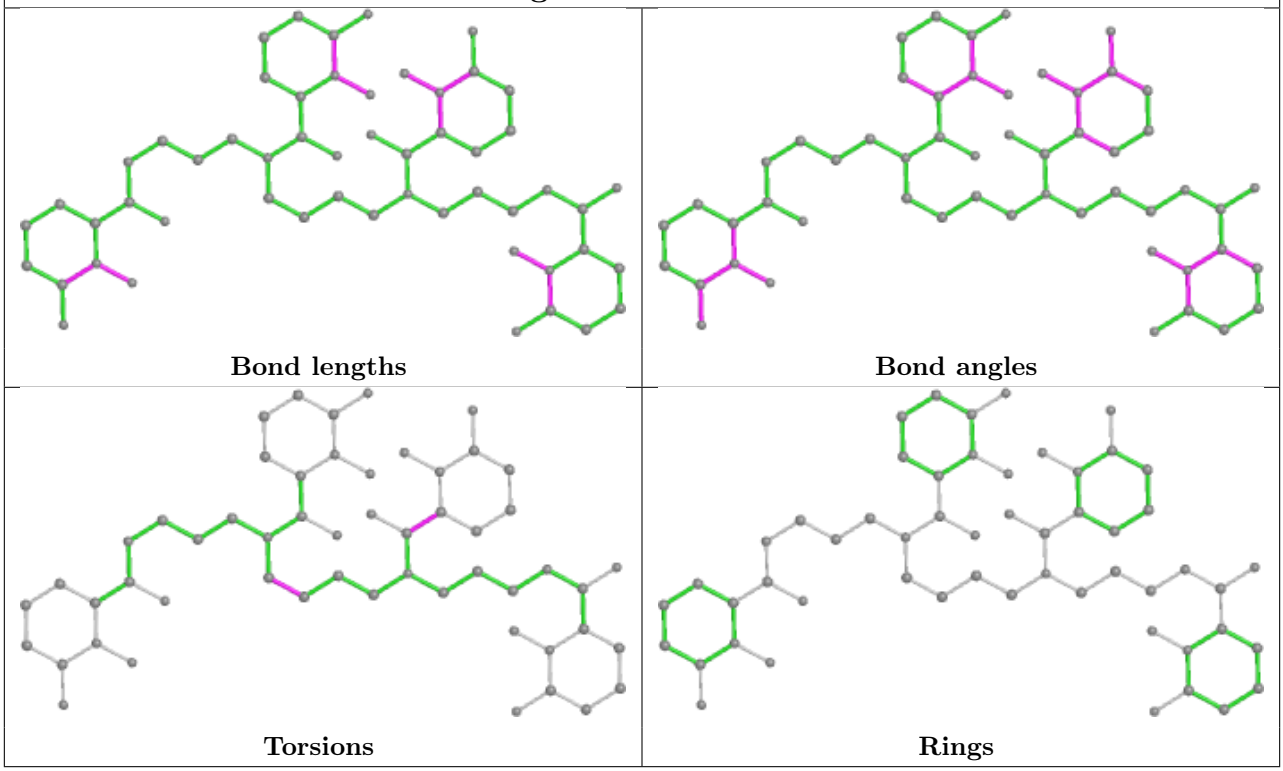
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	202	4OL	4	0
3	C	202	4OL	5	0
3	B	202	4OL	6	0

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.

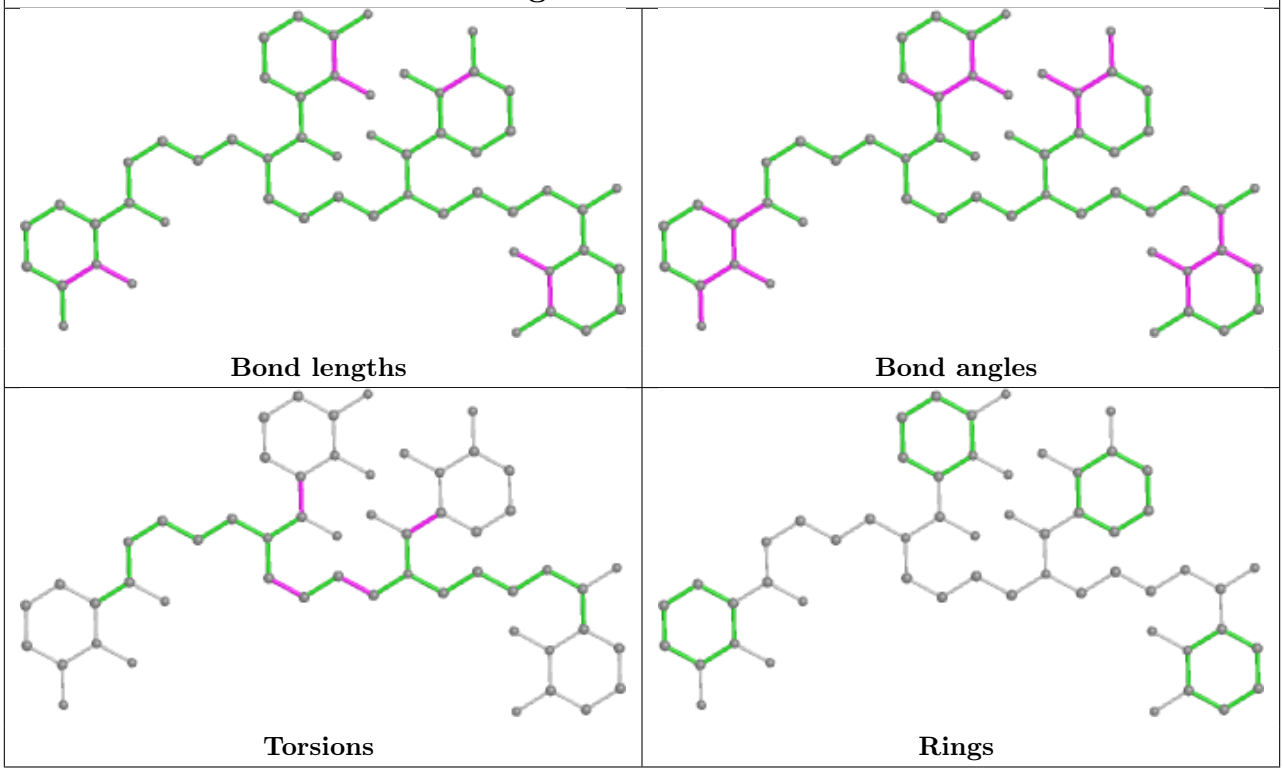
Ligand 4OL F 202



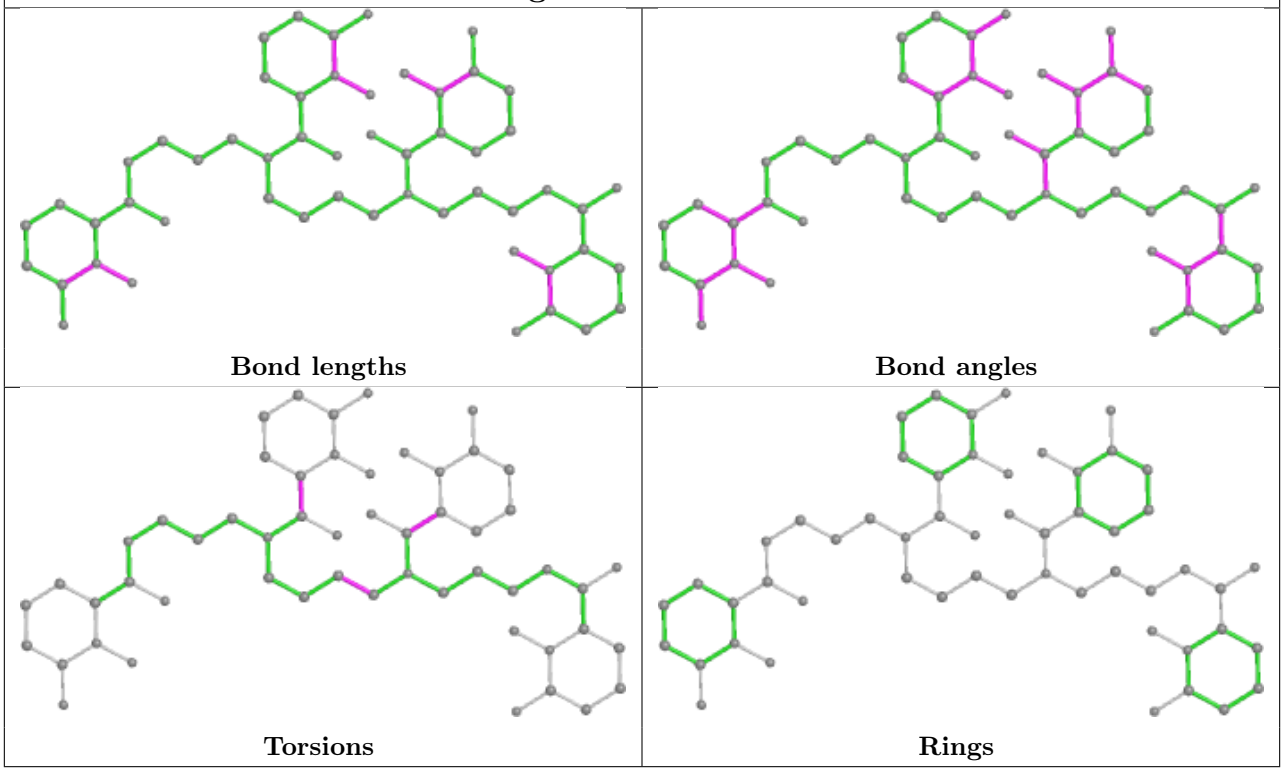
Ligand 4OL E 202



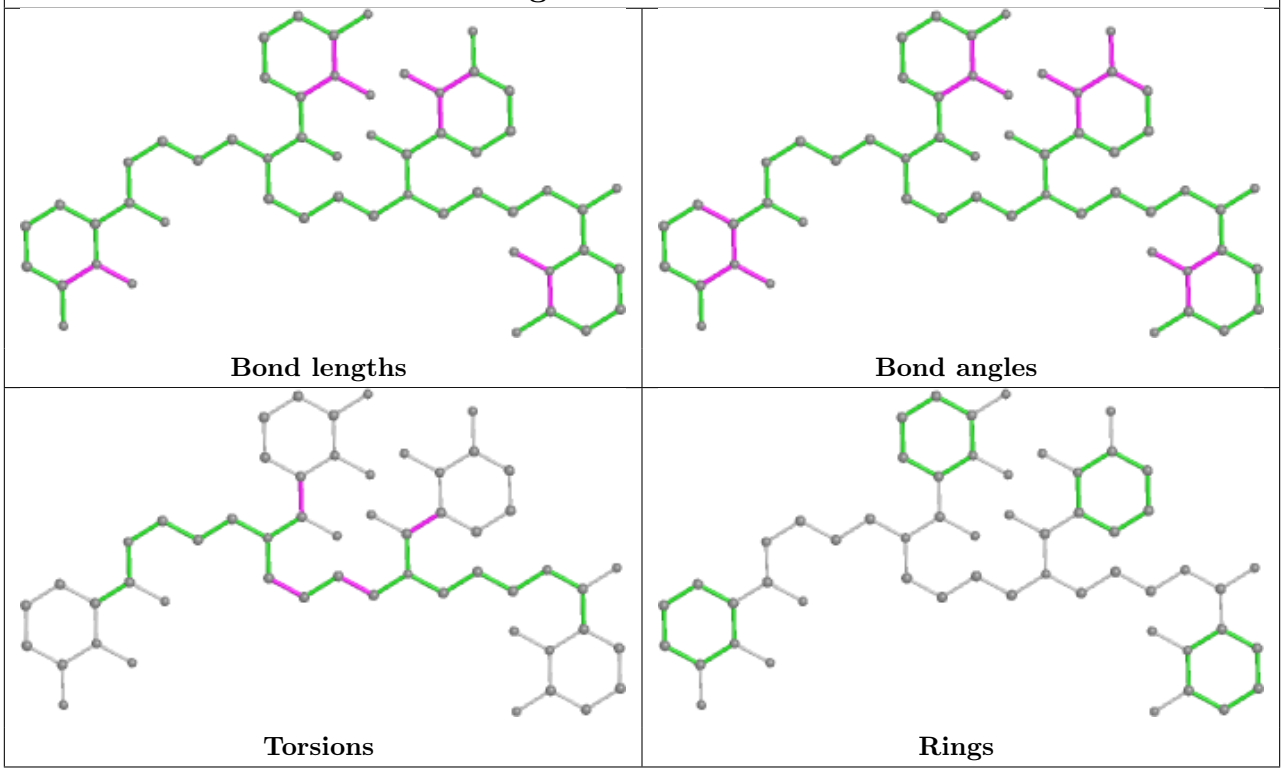
Ligand 4OL A 202

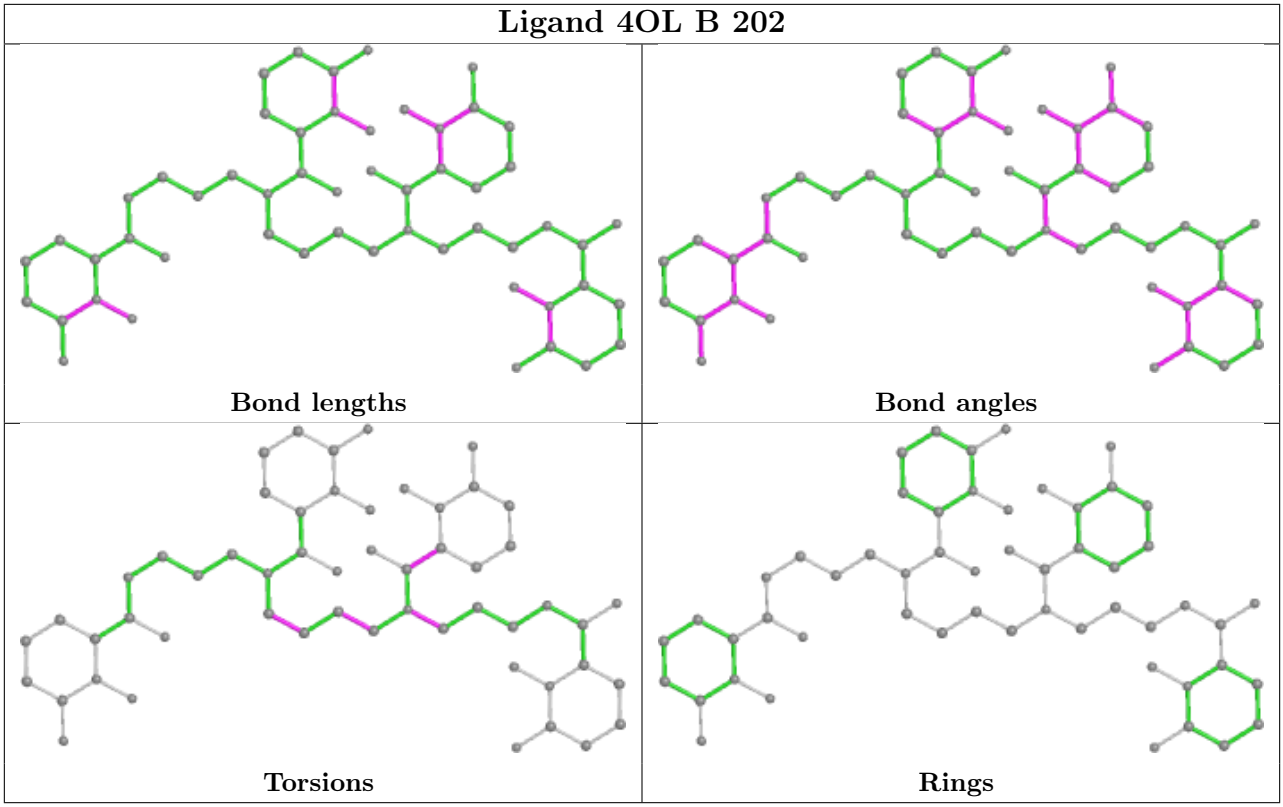


Ligand 4OL D 202



Ligand 4OL C 202





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	177/180 (98%)	-0.22	5 (2%)	53	58	13, 23, 52, 68	0
1	B	175/180 (97%)	-0.27	4 (2%)	60	64	12, 22, 48, 89	0
1	C	175/180 (97%)	-0.31	3 (1%)	70	73	13, 22, 45, 87	0
1	D	177/180 (98%)	-0.13	9 (5%)	28	30	14, 23, 54, 87	1 (0%)
1	E	176/180 (97%)	-0.19	5 (2%)	53	58	14, 26, 56, 78	0
1	F	175/180 (97%)	-0.21	6 (3%)	45	49	13, 23, 54, 79	0
All	All	1055/1080 (97%)	-0.22	32 (3%)	50	54	12, 23, 53, 89	1 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	46	LYS	4.9
1	B	46	LYS	4.7
1	D	4	THR	4.5
1	F	5	SER	4.4
1	B	3	SER	3.9
1	D	5	SER	3.9
1	B	47	ASP	3.7
1	D	45	ASP	3.3
1	F	47	ASP	3.2
1	A	42	LEU	3.1
1	C	46	LYS	3.1
1	F	45	ASP	3.1
1	E	2	ASP	3.0
1	D	42	LEU	2.8
1	A	4	THR	2.8
1	E	47	ASP	2.7
1	F	46	LYS	2.7
1	E	46	LYS	2.6
1	F	44	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	47	ASP	2.5
1	B	45	ASP	2.5
1	D	3	SER	2.4
1	D	43	ARG	2.3
1	A	3	SER	2.3
1	E	4	THR	2.2
1	E	42	LEU	2.2
1	A	45	ASP	2.1
1	F	48	PRO	2.1
1	A	46	LYS	2.1
1	C	44	GLU	2.1
1	D	44	GLU	2.0
1	D	47	ASP	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	F	203	6/6	0.76	0.26	32,41,54,59	0
3	4OL	A	202	54/54	0.86	0.15	21,29,35,41	0
6	SO4	A	205	5/5	0.87	0.30	51,60,63,67	0
6	SO4	C	203	5/5	0.87	0.34	61,63,80,80	0
3	4OL	E	202	54/54	0.88	0.13	19,28,35,36	0
3	4OL	D	202	54/54	0.88	0.15	23,33,37,43	0
3	4OL	F	202	54/54	0.89	0.12	20,26,32,33	0
3	4OL	C	202	54/54	0.90	0.12	18,26,29,31	0
4	GOL	A	203	6/6	0.91	0.16	29,35,46,46	0
3	4OL	B	202	54/54	0.91	0.13	17,25,32,33	0

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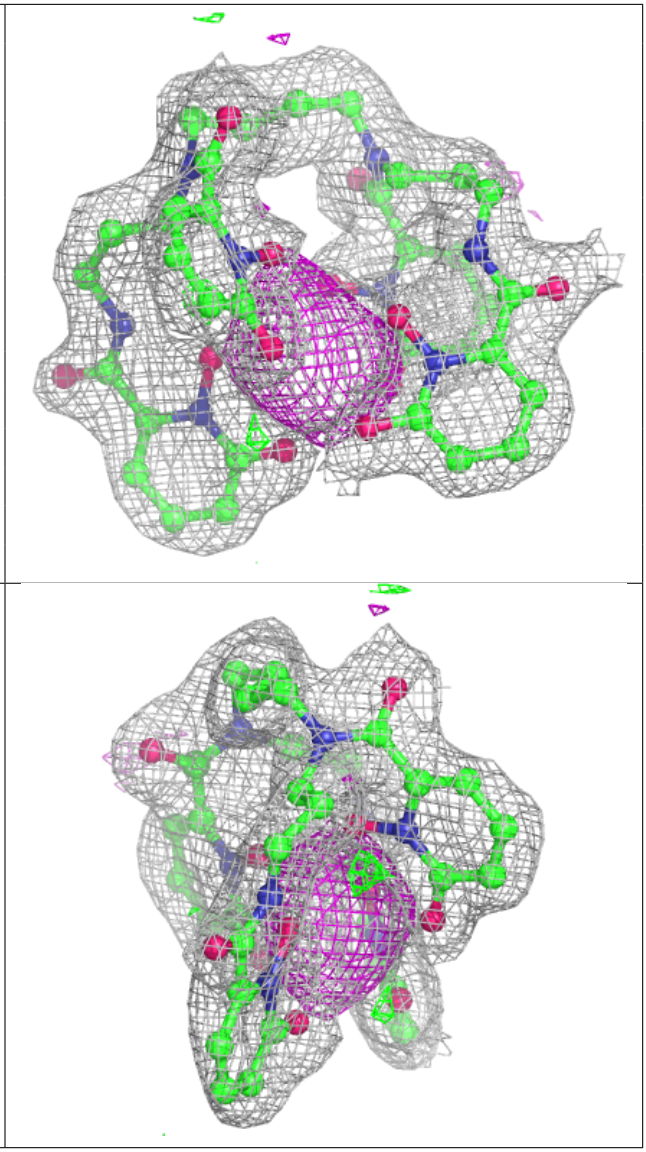
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	SO4	B	203	5/5	0.94	0.14	36,44,48,67	0
2	AM	F	201	1/1	0.99	0.03	37,37,37,37	0
5	CL	B	204	1/1	0.99	0.09	17,17,17,17	0
5	CL	E	203	1/1	0.99	0.09	20,20,20,20	0
2	AM	A	201	1/1	0.99	0.03	39,39,39,39	0
2	AM	B	201	1/1	0.99	0.04	34,34,34,34	0
2	AM	D	201	1/1	0.99	0.03	43,43,43,43	0
5	CL	D	203	1/1	1.00	0.08	20,20,20,20	0
2	AM	C	201	1/1	1.00	0.04	32,32,32,32	0
5	CL	F	204	1/1	1.00	0.06	17,17,17,17	0
5	CL	A	204	1/1	1.00	0.06	19,19,19,19	0
2	AM	E	201	1/1	1.00	0.03	37,37,37,37	0
5	CL	C	204	1/1	1.00	0.08	19,19,19,19	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.

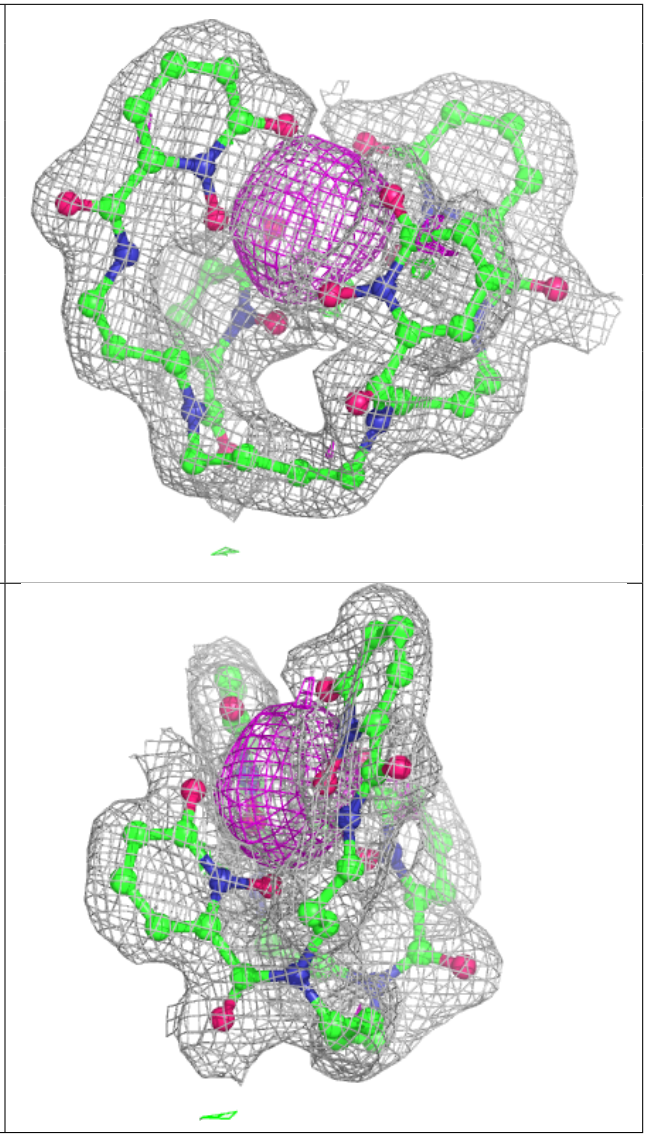
Electron density around 4OL A 202:

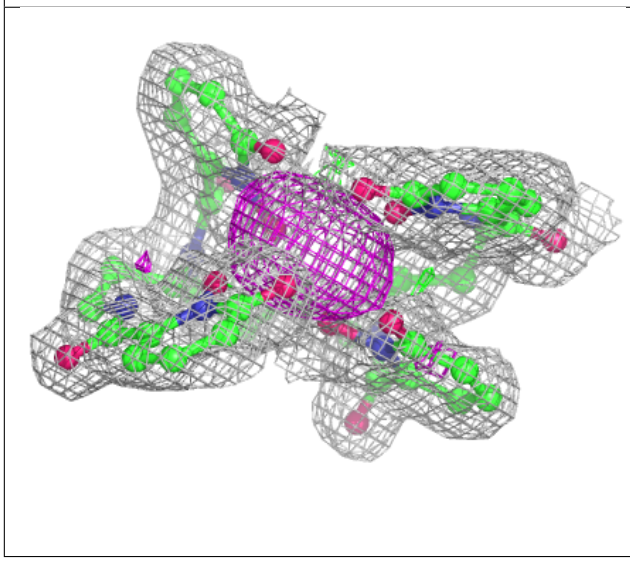
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 4OL E 202:

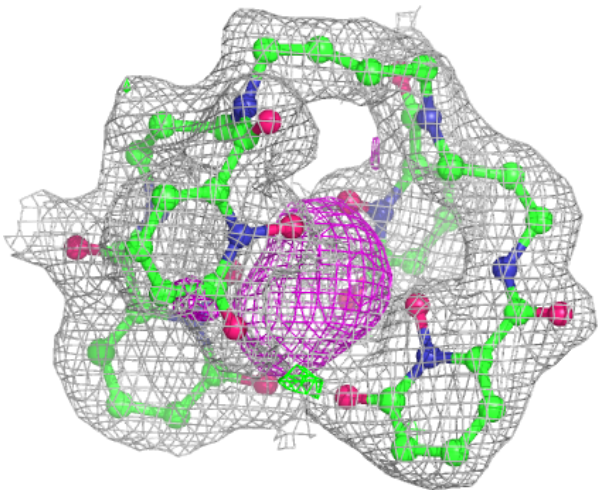
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

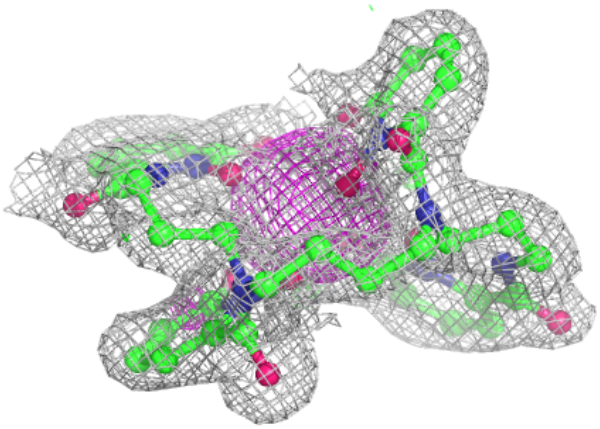


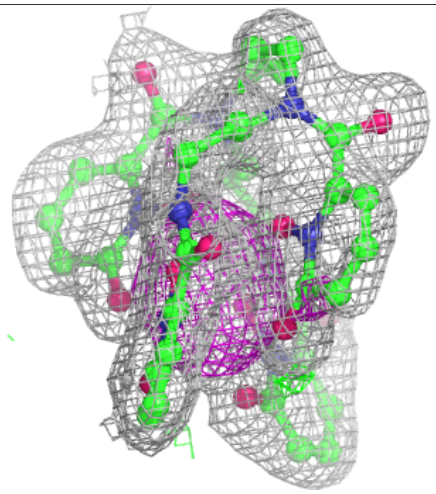


Electron density around 4OL D 202:

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

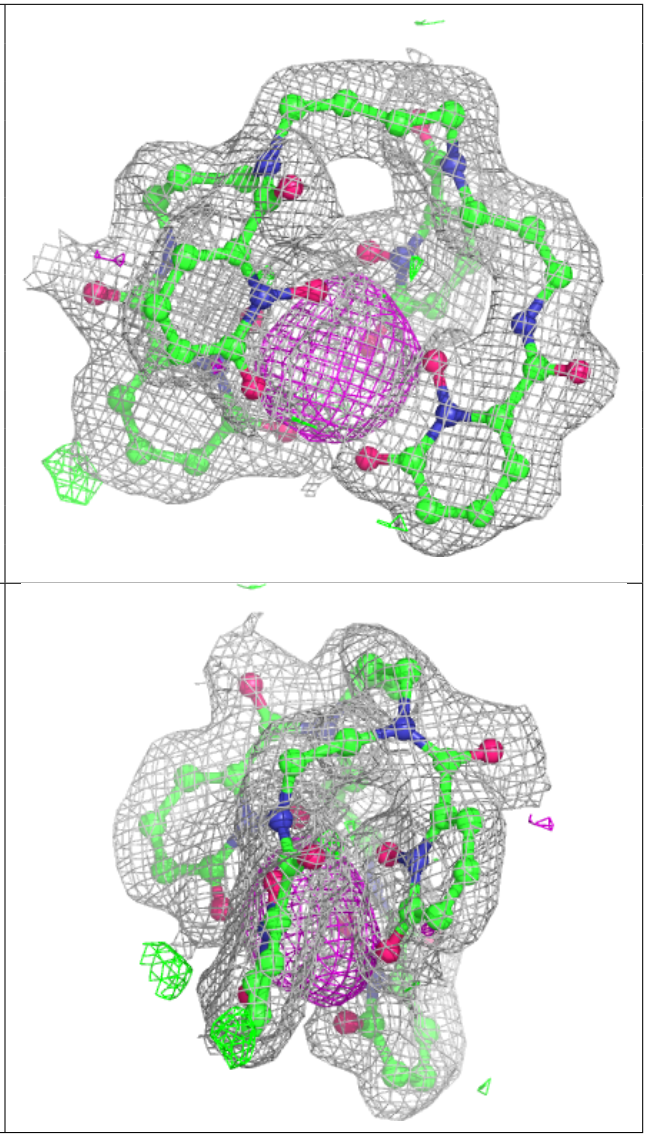






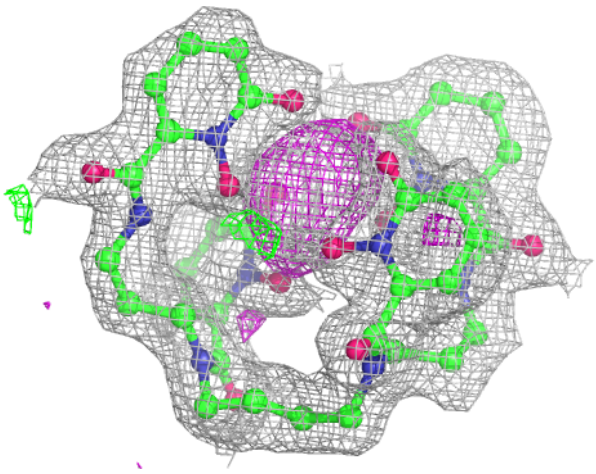
Electron density around 4OL F 202:

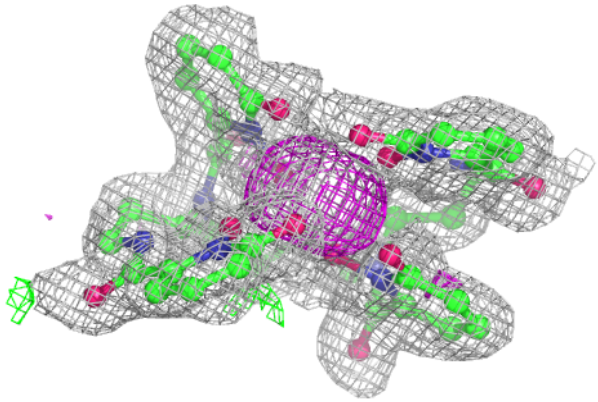
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

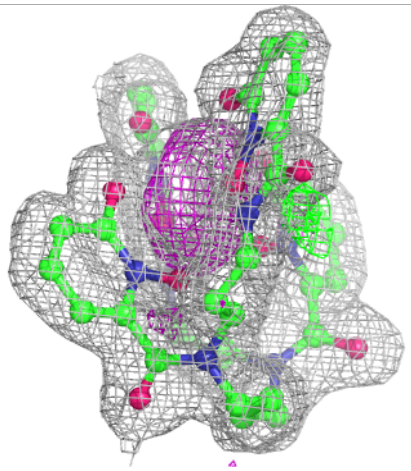


Electron density around 4OL C 202:

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

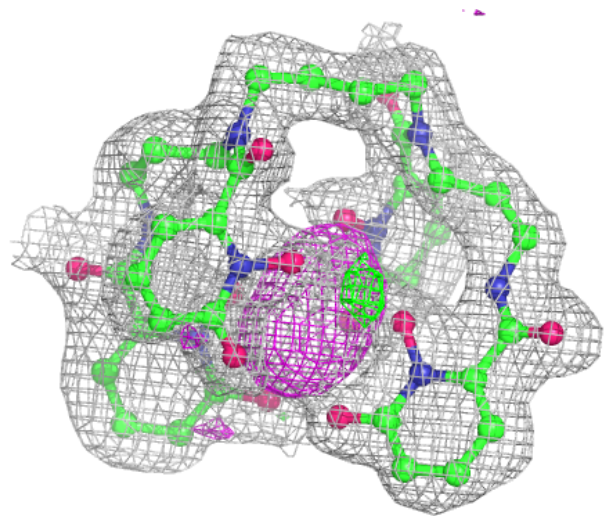


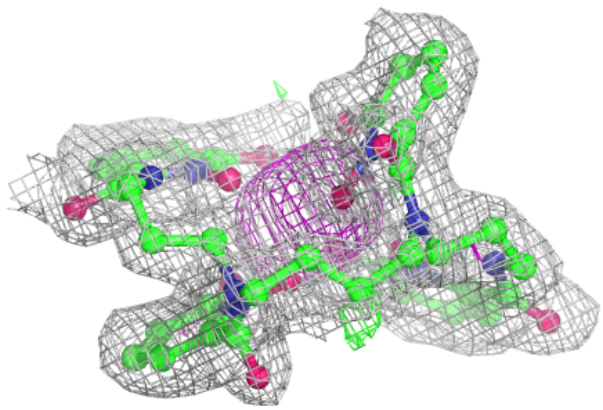


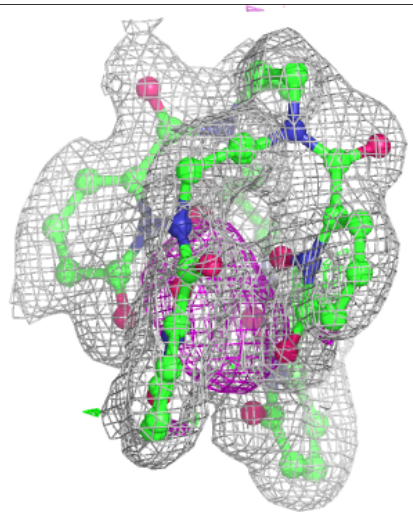


Electron density around 4OL B 202:

$2mF_o$-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.