Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 07:18 AM EDT

PDB ID	:	1OU6
Title	:	Biosynthetic thiolase from Zoogloea ramigera in complex with acetyl-O-pantetheine-11-pivalate
Authors	:	Kursula, P.; Schmitz, W.; Wierenga, R.K.
Deposited on	:	2003-03-24
Resolution	:	2.07 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:

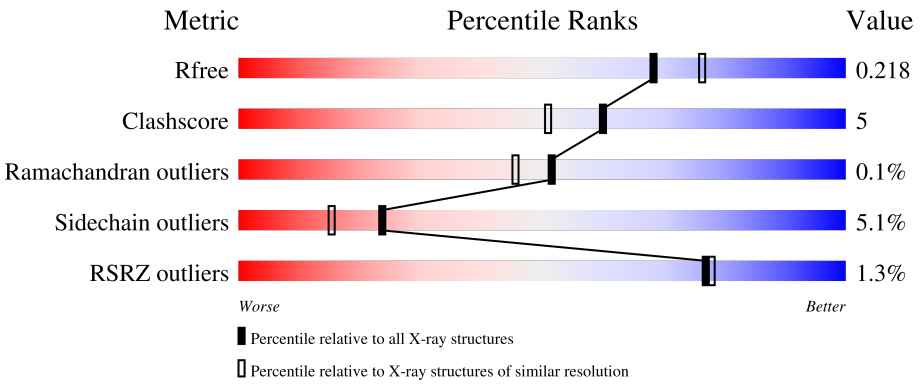
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.07 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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	392	.% 91% 8% •
1	B	392	.% 86% 12% •
1	C	392	.% 88% 12%
1	D	392	2% 86% 14% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12967 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.

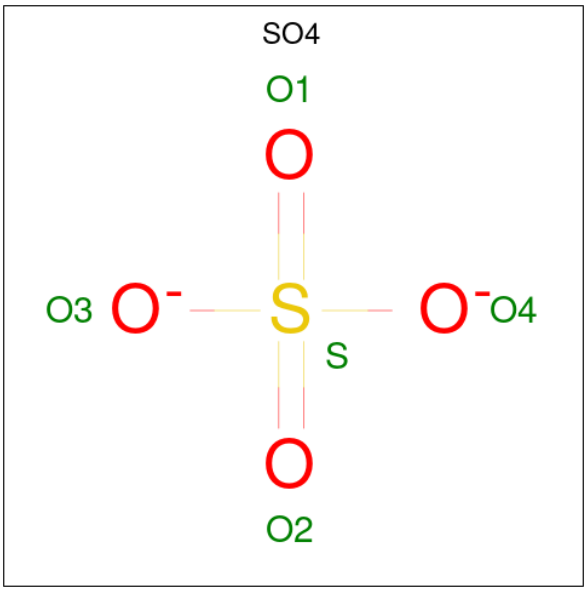
- Molecule 1 is a protein called Acetyl-CoA acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	392	2834	1758	512	543	21	0	0	0
1	B	392	2834	1758	512	543	21	0	0	0
1	C	392	2834	1758	512	543	21	0	0	0
1	D	392	2834	1758	512	543	21	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

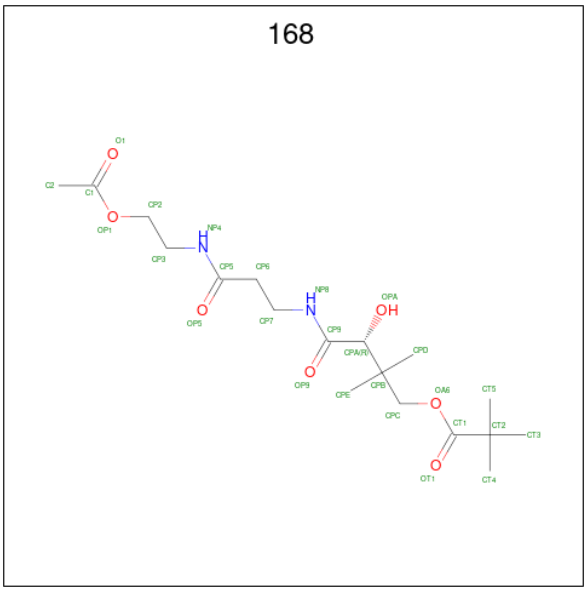
Chain	Residue	Modelled	Actual	Comment	Reference
A	10	ALA	-	SEE REMARK 999	UNP P07097
A	89	CSO	CYS	MODIFIED RESIDUE	UNP P07097
A	129	ARG	ALA	SEE REMARK 999	UNP P07097
B	10	ALA	-	SEE REMARK 999	UNP P07097
B	89	CSO	CYS	MODIFIED RESIDUE	UNP P07097
B	129	ARG	ALA	SEE REMARK 999	UNP P07097
C	10	ALA	-	SEE REMARK 999	UNP P07097
C	89	CSO	CYS	MODIFIED RESIDUE	UNP P07097
C	129	ARG	ALA	SEE REMARK 999	UNP P07097
D	10	ALA	-	SEE REMARK 999	UNP P07097
D	89	CSO	CYS	MODIFIED RESIDUE	UNP P07097
D	129	ARG	ALA	SEE REMARK 999	UNP P07097

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

- Molecule 3 is PANTOTHENYL-AMINOETHANOL-ACETATE PIVALIC ACID (three-letter code: 168) (formula: $C_{18}H_{32}N_2O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	27	18	2	7	0	0
3	B	1	27	18	2	7	0	0

- Molecule 4 is water.

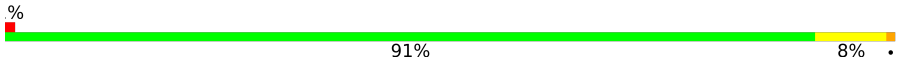
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	455	455	455	0	0
4	B	508	508	508	0	0
4	C	337	337	337	0	0
4	D	257	257	257	0	0

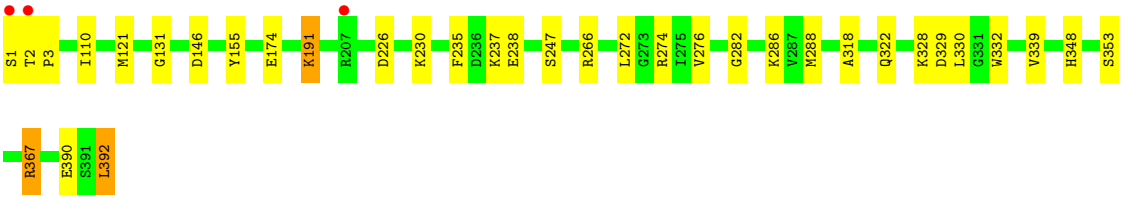
3 Residue-property plots (i)

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: Acetyl-CoA acetyltransferase

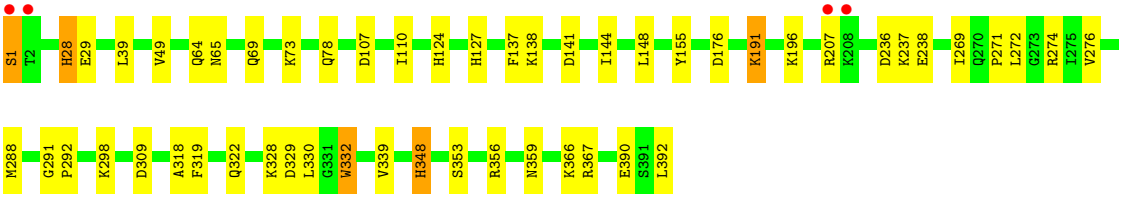
Chain A:





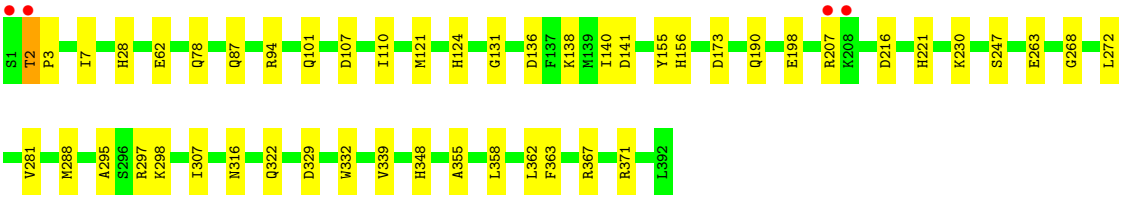
• Molecule 1: Acetyl-CoA acetyltransferase

Chain B:



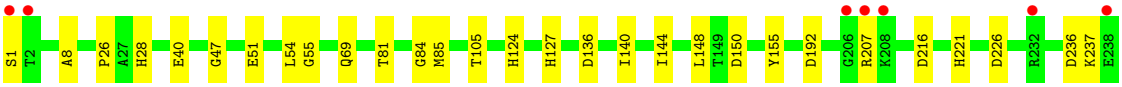
• Molecule 1: Acetyl-CoA acetyltransferase

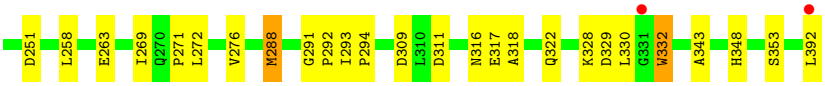
Chain C:



• Molecule 1: Acetyl-CoA acetyltransferase

Chain D:




D251
L258
E263
I269
Q270
P271
L272
V276
M288
G291
P292
I293
P294
D309
L310
D311
N316
E317
A318
Q322
K328
D329
L330
G331
W332
A343
H348
S353
L392

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	84.38Å 78.95Å 148.82Å 90.00° 92.96° 90.00°	Depositor
Resolution (Å)	20.00 – 2.07 19.39 – 2.07	Depositor EDS
% Data completeness (in resolution range)	94.3 (20.00-2.07) 81.4 (19.39-2.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.74 (at 2.07Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.161 , 0.212 0.171 , 0.218	Depositor DCC
R_{free} test set	4876 reflections (4.36%)	wwPDB-VP
Wilson B-factor (Å^2)	14.7	Xtriage
Anisotropy	0.936	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 36.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.105 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12967	wwPDB-VP
Average B, all atoms (Å^2)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% 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: SO4, CSO, 168

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	0.72	0/2868	0.88	7/3872 (0.2%)
1	B	0.73	0/2868	0.85	6/3872 (0.2%)
1	C	0.58	1/2868 (0.0%)	0.79	5/3872 (0.1%)
1	D	0.52	0/2868	0.78	9/3872 (0.2%)
All	All	0.64	1/11472 (0.0%)	0.83	27/15488 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	136	ASP	CB-CG	5.67	1.63	1.51

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	309	ASP	CB-CG-OD2	8.25	125.72	118.30
1	A	266	ARG	NE-CZ-NH2	-8.17	116.22	120.30
1	A	266	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	D	136	ASP	CB-CG-OD2	7.22	124.80	118.30
1	C	107	ASP	CB-CG-OD2	6.96	124.56	118.30
1	D	236	ASP	CB-CG-OD2	6.72	124.35	118.30
1	B	329	ASP	CB-CG-OD2	6.49	124.14	118.30
1	D	226	ASP	CB-CG-OD2	6.45	124.10	118.30
1	D	309	ASP	CB-CG-OD2	6.37	124.03	118.30
1	A	329	ASP	CB-CG-OD2	6.33	124.00	118.30
1	C	136	ASP	CB-CG-OD2	6.30	123.97	118.30
1	C	216	ASP	CB-CG-OD2	6.25	123.92	118.30
1	A	392	LEU	CA-CB-CG	6.21	129.59	115.30
1	D	311	ASP	CB-CG-OD2	6.13	123.82	118.30
1	A	146	ASP	CB-CG-OD2	5.85	123.57	118.30
1	A	367	ARG	NE-CZ-NH1	5.76	123.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	329	ASP	CB-CG-OD2	5.73	123.45	118.30
1	B	107	ASP	CB-CG-OD2	5.72	123.45	118.30
1	C	329	ASP	CB-CG-OD2	5.53	123.28	118.30
1	D	216	ASP	CB-CG-OD2	5.51	123.26	118.30
1	B	236	ASP	CB-CG-OD2	5.46	123.21	118.30
1	A	226	ASP	CB-CG-OD2	5.43	123.19	118.30
1	B	176	ASP	CB-CG-OD2	5.43	123.19	118.30
1	B	367	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	D	150	ASP	CB-CG-OD2	5.20	122.98	118.30
1	D	251	ASP	CB-CG-OD2	5.13	122.92	118.30
1	C	173	ASP	CB-CG-OD2	5.08	122.88	118.30

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	2834	0	2841	17	0
1	B	2834	0	2841	40	0
1	C	2834	0	2841	31	0
1	D	2834	0	2841	24	0
2	A	10	0	0	0	0
2	B	10	0	0	1	0
3	A	27	0	32	3	0
3	B	27	0	32	2	0
4	A	455	0	0	5	0
4	B	508	0	0	14	0
4	C	337	0	0	12	1
4	D	257	0	0	5	1
All	All	12967	0	11428	105	1

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 5.

All (105) 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:191:LYS:HZ2	1:B:191:LYS:HB3	1.34	0.92
1:B:191:LYS:HB3	1:B:191:LYS:NZ	1.82	0.91
1:C:156:HIS:ND1	4:C:436:HOH:O	2.09	0.86
1:C:156:HIS:CE1	4:C:436:HOH:O	2.31	0.82
1:C:358:LEU:HD23	4:C:495:HOH:O	1.82	0.78
1:A:2:THR:HG22	1:A:3:PRO:HD2	1.67	0.74
1:D:288:MET:HE3	4:D:644:HOH:O	1.89	0.72
1:B:196:LYS:HB2	4:B:6466:HOH:O	1.91	0.70
1:D:28:HIS:HD2	1:D:69:GLN:HB3	1.57	0.68
1:C:94:ARG:HG2	4:C:696:HOH:O	1.93	0.68
1:B:144:ILE:HD12	3:B:6001:168:HT41	1.78	0.66
2:B:2003:SO4:O1	4:B:6461:HOH:O	2.12	0.65
1:C:281:VAL:HG23	4:C:710:HOH:O	1.97	0.65
1:A:121:MET:HA	1:B:127:HIS:CD2	2.32	0.64
1:A:121:MET:SD	1:B:127:HIS:CD2	2.90	0.63
1:C:316:ASN:HD21	1:C:348:HIS:CE1	2.17	0.61
1:B:28:HIS:HD2	1:B:29:GLU:N	1.97	0.61
1:A:318:ALA:HA	4:A:5190:HOH:O	2.00	0.61
1:C:295:ALA:HA	4:C:710:HOH:O	2.03	0.58
1:B:191:LYS:NZ	1:B:191:LYS:CB	2.62	0.58
1:C:121:MET:SD	1:D:127:HIS:CE1	2.97	0.58
1:B:348:HIS:CD2	4:B:6472:HOH:O	2.58	0.57
1:C:298:LYS:HB3	4:C:710:HOH:O	2.05	0.56
1:C:2:THR:HG22	1:C:3:PRO:HD2	1.87	0.56
1:B:298:LYS:NZ	4:B:6493:HOH:O	2.38	0.56
1:A:348:HIS:CE1	1:A:353:SER:HG	2.24	0.55
1:B:274:ARG:NH2	1:B:390:GLU:OE1	2.40	0.54
1:B:138:LYS:NZ	4:B:6394:HOH:O	2.40	0.54
1:A:191:LYS:NZ	4:A:5181:HOH:O	2.23	0.54
1:A:121:MET:SD	1:B:127:HIS:HD2	2.31	0.54
1:A:174:GLU:OE1	4:A:5075:HOH:O	2.19	0.53
1:D:8:ALA:HB1	1:D:269:ILE:HG21	1.89	0.52
1:B:191:LYS:CD	4:B:6217:HOH:O	2.57	0.52
1:B:28:HIS:CE1	1:B:69:GLN:OE1	2.63	0.51
1:B:330:LEU:HD13	1:B:332:TRP:CH2	2.46	0.51
1:B:144:ILE:HD13	1:B:148:LEU:HD12	1.92	0.51
1:C:124:HIS:HD1	1:C:141:ASP:HA	1.76	0.50
1:D:28:HIS:HD2	1:D:69:GLN:CB	2.22	0.50
1:B:269:ILE:O	1:B:271:PRO:HD3	2.11	0.50
1:B:191:LYS:HD3	4:B:6217:HOH:O	2.11	0.50
1:B:28:HIS:CD2	1:B:29:GLU:N	2.79	0.49
1:D:271:PRO:HG2	1:D:392:LEU:HD12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ARG:NH2	1:A:390:GLU:OE1	2.46	0.49
1:B:274:ARG:HB2	1:B:392:LEU:HD21	1.95	0.48
1:B:1:SER:O	1:B:1:SER:OG	2.27	0.48
1:A:286:LYS:NZ	4:A:5427:HOH:O	2.38	0.48
1:C:121:MET:HA	1:D:127:HIS:CE1	2.49	0.48
1:C:297:ARG:NH1	1:C:307:ILE:HD11	2.28	0.48
1:C:121:MET:SD	1:D:127:HIS:ND1	2.87	0.47
1:D:316:ASN:HD21	1:D:348:HIS:CE1	2.31	0.47
1:C:110:ILE:HD11	1:C:263:GLU:OE2	2.14	0.47
1:C:268:GLY:HA2	4:C:402:HOH:O	2.13	0.47
1:C:355:ALA:HA	4:C:495:HOH:O	2.14	0.47
1:D:47:GLY:C	4:D:648:HOH:O	2.53	0.47
1:D:144:ILE:HD13	1:D:148:LEU:HD12	1.95	0.47
1:D:54:LEU:O	1:D:84:GLY:HA2	2.15	0.47
1:B:28:HIS:CD2	1:B:29:GLU:HG3	2.50	0.47
1:C:316:ASN:ND2	1:C:348:HIS:CE1	2.82	0.47
1:C:124:HIS:ND1	1:C:141:ASP:HA	2.31	0.46
1:D:26:PRO:HB2	1:D:28:HIS:CE1	2.50	0.46
1:B:28:HIS:ND1	1:B:69:GLN:OE1	2.48	0.46
3:A:5001:168:HT31	4:A:5414:HOH:O	2.16	0.46
1:D:317:GLU:O	1:D:343:ALA:HB3	2.15	0.46
1:B:73:LYS:NZ	4:B:6421:HOH:O	2.46	0.46
1:C:87:GLN:HB2	4:C:696:HOH:O	2.16	0.46
1:A:2:THR:HG22	1:A:3:PRO:CD	2.42	0.45
1:D:291:GLY:N	1:D:292:PRO:CD	2.79	0.45
1:B:238:GLU:HB3	4:B:6156:HOH:O	2.15	0.45
1:A:235:PHE:HE1	3:A:5001:168:HT32	1.80	0.45
1:B:319:PHE:CZ	3:B:6001:168:HP22	2.52	0.45
1:C:7:ILE:HD13	1:C:362:LEU:HD11	1.99	0.45
1:D:258:LEU:HD22	4:D:451:HOH:O	2.15	0.44
1:C:101:GLN:HG2	1:D:105:THR:HG21	1.99	0.44
1:C:198:GLU:HB3	1:C:363:PHE:CD2	2.53	0.44
1:C:78:GLN:NE2	4:C:714:HOH:O	2.51	0.43
1:D:330:LEU:HD13	1:D:332:TRP:CH2	2.53	0.43
1:B:137:PHE:CE1	1:C:124:HIS:HD2	2.36	0.43
1:C:28:HIS:ND1	1:C:62:GLU:OE2	2.47	0.43
1:C:358:LEU:HB3	4:C:495:HOH:O	2.18	0.43
1:D:318:ALA:CB	4:D:644:HOH:O	2.65	0.43
1:B:291:GLY:N	1:B:292:PRO:CD	2.82	0.42
1:C:124:HIS:HA	1:C:140:ILE:O	2.19	0.42
1:D:124:HIS:HA	1:D:140:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:GLY:HA2	1:C:131:GLY:HA2	2.02	0.42
1:B:366:LYS:NZ	4:B:6507:HOH:O	2.51	0.42
1:B:191:LYS:HG3	4:B:6167:HOH:O	2.19	0.42
1:D:293:ILE:HB	1:D:294:PRO:CD	2.50	0.42
1:D:51:GLU:HA	1:D:81:THR:O	2.20	0.42
1:D:192:ASP:HB3	4:D:555:HOH:O	2.20	0.41
1:B:356:ARG:O	1:B:356:ARG:HD2	2.21	0.41
1:D:55:GLY:HA2	1:D:85:MET:O	2.21	0.41
1:A:247:SER:OG	1:A:348:HIS:HB2	2.20	0.41
1:B:124:HIS:CD2	1:B:141:ASP:HA	2.56	0.41
1:B:191:LYS:NZ	4:B:6450:HOH:O	2.49	0.41
1:A:237:LYS:HA	1:A:237:LYS:HD3	1.90	0.41
1:A:330:LEU:HD23	1:A:330:LEU:HA	1.91	0.41
1:B:64:GLN:O	1:B:65:ASN:C	2.58	0.41
1:B:348:HIS:CE1	1:B:353:SER:HG	2.31	0.41
1:A:282:GLY:HA3	1:B:78:GLN:O	2.21	0.40
3:A:5001:168:HT52	3:A:5001:168:CPC	2.51	0.40
1:B:196:LYS:NZ	4:B:6355:HOH:O	2.54	0.40
1:B:318:ALA:HA	4:B:6472:HOH:O	2.21	0.40
1:C:190:GLN:OE1	1:C:221:HIS:HE1	2.05	0.40
1:B:39:LEU:HD21	1:B:49:VAL:CG2	2.52	0.40
1:C:190:GLN:OE1	1:C:221:HIS:CE1	2.75	0.40

All (1) 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)
4:C:553:HOH:O	4:D:481:HOH:O[2_646]	2.16	0.04

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	389/392 (99%)	374 (96%)	15 (4%)	0	100	100
1	B	389/392 (99%)	378 (97%)	11 (3%)	0	100	100
1	C	389/392 (99%)	376 (97%)	12 (3%)	1 (0%)	41	32
1	D	389/392 (99%)	377 (97%)	12 (3%)	0	100	100
All	All	1556/1568 (99%)	1505 (97%)	50 (3%)	1 (0%)	51	45

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	247	SER

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	278/278 (100%)	263 (95%)	15 (5%)	22	14
1	B	278/278 (100%)	262 (94%)	16 (6%)	20	11
1	C	278/278 (100%)	266 (96%)	12 (4%)	29	22
1	D	278/278 (100%)	264 (95%)	14 (5%)	24	16
All	All	1112/1112 (100%)	1055 (95%)	57 (5%)	24	15

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	110	ILE
1	A	155	TYR
1	A	191	LYS
1	A	230	LYS
1	A	238	GLU
1	A	272	LEU
1	A	276	VAL
1	A	288	MET
1	A	322	GLN

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Mol	Chain	Res	Type
1	A	328	LYS
1	A	332	TRP
1	A	339	VAL
1	A	367	ARG
1	A	392	LEU
1	B	1	SER
1	B	28	HIS
1	B	110	ILE
1	B	155	TYR
1	B	191	LYS
1	B	207	ARG
1	B	237	LYS
1	B	272	LEU
1	B	276	VAL
1	B	288	MET
1	B	322	GLN
1	B	328	LYS
1	B	332	TRP
1	B	339	VAL
1	B	348	HIS
1	B	359	ASN
1	C	2	THR
1	C	138	LYS
1	C	155	TYR
1	C	207	ARG
1	C	230	LYS
1	C	272	LEU
1	C	288	MET
1	C	322	GLN
1	C	332	TRP
1	C	339	VAL
1	C	367	ARG
1	C	371	ARG
1	D	1	SER
1	D	40	GLU
1	D	155	TYR
1	D	207	ARG
1	D	221	HIS
1	D	237	LYS
1	D	263	GLU
1	D	272	LEU
1	D	276	VAL

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Mol	Chain	Res	Type
1	D	288	MET
1	D	322	GLN
1	D	328	LYS
1	D	332	TRP
1	D	353	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	156	HIS
1	A	184	ASN
1	B	78	GLN
1	C	78	GLN
1	C	124	HIS
1	C	169	GLN
1	C	175	GLN
1	C	184	ASN
1	C	221	HIS
1	C	316	ASN
1	C	348	HIS
1	D	28	HIS
1	D	78	GLN
1	D	184	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)

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	CSO	D	89	1	3,6,7	0.68	0	0,6,8	-	-
1	CSO	B	89	1	3,6,7	0.81	0	0,6,8	-	-
1	CSO	A	89	1	3,6,7	0.63	0	0,6,8	-	-
1	CSO	C	89	1	3,6,7	0.44	0	0,6,8	-	-

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
1	CSO	D	89	1	-	0/1/5/7	-
1	CSO	B	89	1	-	0/1/5/7	-
1	CSO	A	89	1	-	0/1/5/7	-
1	CSO	C	89	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	SO4	A	2004	-	4,4,4	0.17	0	6,6,6	0.21	0
3	168	B	6001	-	23,26,26	1.32	2 (8%)	34,36,36	1.61	6 (17%)
3	168	A	5001	-	23,26,26	1.35	2 (8%)	34,36,36	1.92	9 (26%)
2	SO4	A	2002	-	4,4,4	0.14	0	6,6,6	0.36	0
2	SO4	B	2001	-	4,4,4	0.17	0	6,6,6	0.15	0
2	SO4	B	2003	-	4,4,4	0.19	0	6,6,6	0.47	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
3	168	B	6001	-	-	15/35/35/35	-
3	168	A	5001	-	-	17/35/35/35	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	6001	168	OA6-CT1	5.24	1.45	1.33
3	A	5001	168	OA6-CT1	5.13	1.44	1.33
3	A	5001	168	OP1-C1	2.39	1.45	1.33
3	B	6001	168	OP1-C1	2.27	1.44	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	5001	168	OA6-CT1-CT2	5.78	124.10	112.56
3	B	6001	168	OA6-CT1-CT2	4.33	121.20	112.56
3	A	5001	168	OA6-CT1-OT1	-4.29	115.72	124.54
3	A	5001	168	CP6-CP7-NP8	-3.50	104.83	111.90
3	A	5001	168	CPC-OA6-CT1	-3.31	112.13	116.81
3	A	5001	168	CP7-NP8-CP9	3.22	128.33	122.59
3	B	6001	168	CP3-NP4-CP5	-3.21	116.87	122.84
3	A	5001	168	OA6-CPC-CPB	3.07	115.18	109.39
3	B	6001	168	CP7-NP8-CP9	2.92	127.80	122.59
3	B	6001	168	OA6-CPC-CPB	2.91	114.88	109.39
3	B	6001	168	CP6-CP7-NP8	-2.84	106.17	111.90
3	B	6001	168	OA6-CT1-OT1	-2.65	119.09	124.54
3	A	5001	168	CT5-CT2-CT1	2.32	115.62	109.16
3	A	5001	168	CPA-CP9-NP8	-2.28	112.05	116.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	5001	168	OP1-CP2-CP3	2.11	114.60	108.30

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	5001	168	CP9-CPA-CPB-CPD
3	A	5001	168	CP9-CPA-CPB-CPE
3	A	5001	168	OPA-CPA-CPB-CPD
3	A	5001	168	OPA-CPA-CPB-CPE
3	B	6001	168	CP3-CP2-OP1-C1
3	B	6001	168	CP9-CPA-CPB-CPE
3	B	6001	168	CT2-CT1-OA6-CPC
3	B	6001	168	OT1-CT1-OA6-CPC
3	B	6001	168	C2-C1-OP1-CP2
3	A	5001	168	CT2-CT1-OA6-CPC
3	A	5001	168	OT1-CT1-OA6-CPC
3	B	6001	168	O1-C1-OP1-CP2
3	A	5001	168	OP1-CP2-CP3-NP4
3	A	5001	168	C2-C1-OP1-CP2
3	B	6001	168	OPA-CPA-CPB-CPD
3	B	6001	168	OPA-CPA-CPB-CPE
3	A	5001	168	O1-C1-OP1-CP2
3	B	6001	168	CP9-CPA-CPB-CPD
3	A	5001	168	OA6-CT1-CT2-CT5
3	A	5001	168	CP9-CPA-CPB-CPC
3	A	5001	168	OPA-CPA-CPB-CPC
3	B	6001	168	OPA-CPA-CPB-CPC
3	A	5001	168	OA6-CT1-CT2-CT3
3	A	5001	168	OA6-CT1-CT2-CT4
3	A	5001	168	OP5-CP5-CP6-CP7
3	B	6001	168	OP9-CP9-CPA-OPA
3	A	5001	168	OT1-CT1-CT2-CT5
3	B	6001	168	NP8-CP9-CPA-OPA
3	A	5001	168	NP4-CP5-CP6-CP7
3	B	6001	168	OA6-CT1-CT2-CT4
3	B	6001	168	OA6-CT1-CT2-CT3
3	B	6001	168	CP9-CPA-CPB-CPC

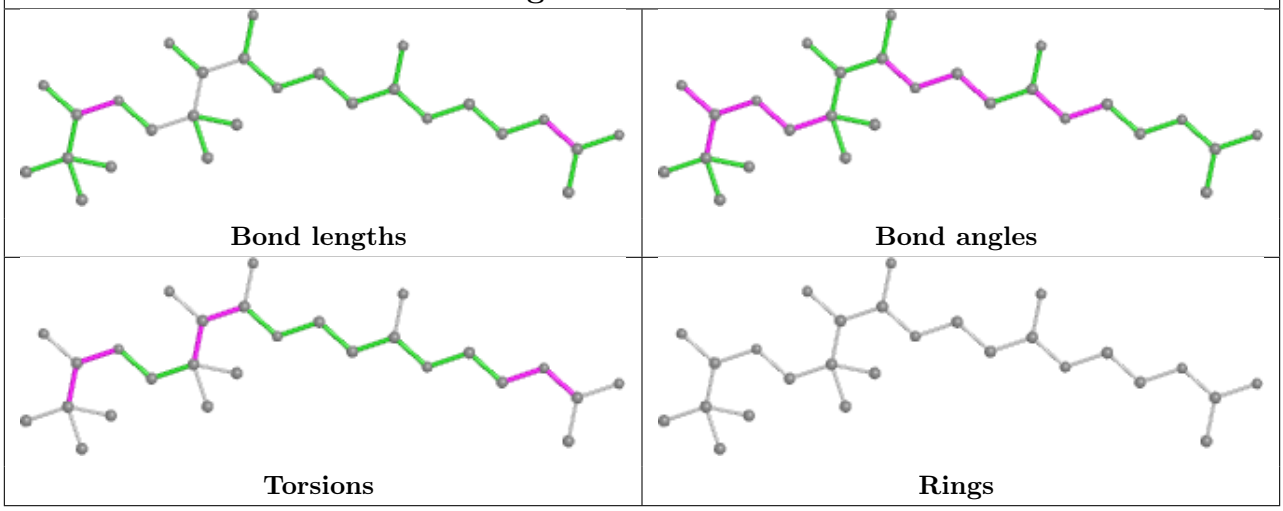
There are no ring outliers.

3 monomers are involved in 6 short contacts:

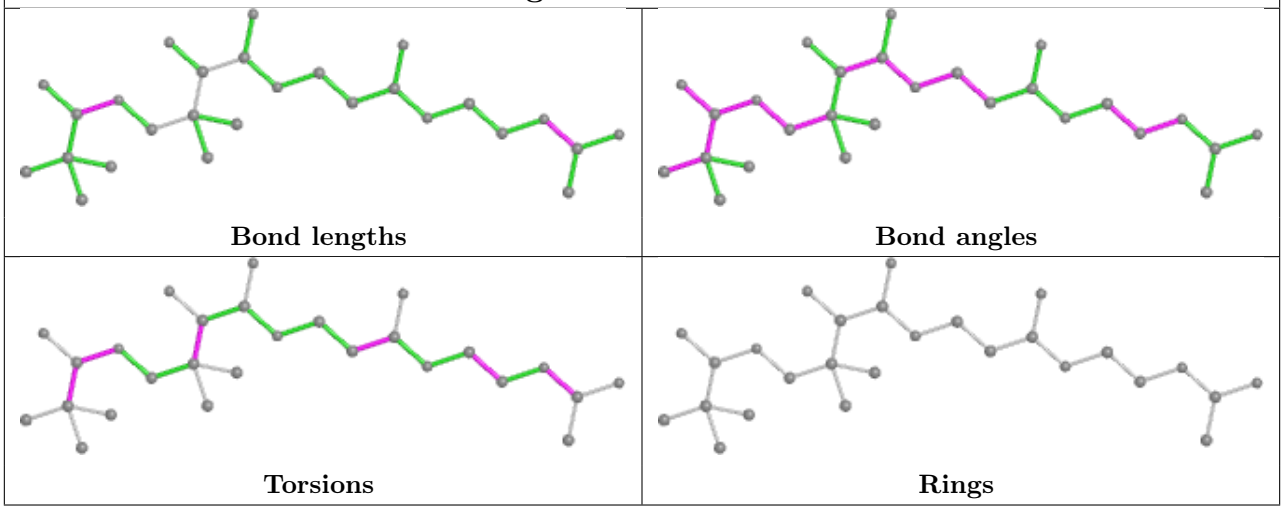
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	6001	168	2	0
3	A	5001	168	3	0
2	B	2003	SO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 168 B 6001



Ligand 168 A 5001



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	391/392 (99%)	-0.67	3 (0%)	86	87	2, 7, 21, 52	0
1	B	391/392 (99%)	-0.67	4 (1%)	82	83	2, 7, 20, 46	0
1	C	391/392 (99%)	-0.46	4 (1%)	82	83	3, 8, 18, 42	0
1	D	391/392 (99%)	-0.20	9 (2%)	60	63	2, 9, 19, 39	0
All	All	1564/1568 (99%)	-0.50	20 (1%)	77	78	2, 8, 20, 52	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	SER	6.7
1	D	1	SER	5.4
1	C	2	THR	5.0
1	D	2	THR	4.0
1	B	1	SER	4.0
1	D	206	GLY	3.4
1	C	207	ARG	3.2
1	D	392	LEU	2.9
1	A	2	THR	2.8
1	D	207	ARG	2.8
1	C	1	SER	2.8
1	D	208	LYS	2.7
1	D	232	ARG	2.6
1	B	2	THR	2.6
1	B	207	ARG	2.4
1	D	331	GLY	2.4
1	A	207	ARG	2.4
1	C	208	LYS	2.3
1	B	208	LYS	2.2
1	D	238	GLU	2.2

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	CSO	D	89	7/8	0.97	0.09	5,8,10,12	0
1	CSO	B	89	7/8	0.98	0.08	5,7,12,19	0
1	CSO	C	89	7/8	0.98	0.08	5,7,16,17	0
1	CSO	A	89	7/8	0.98	0.08	6,6,13,21	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

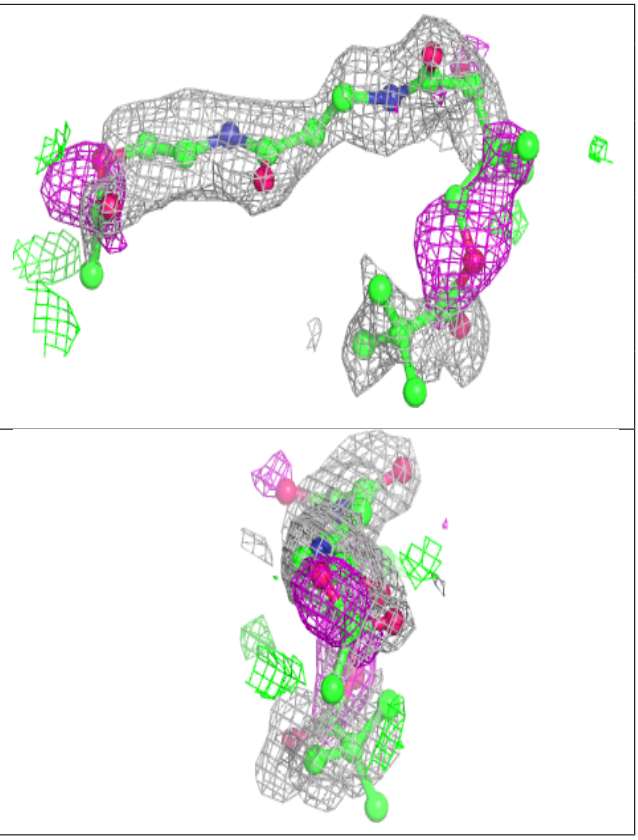
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

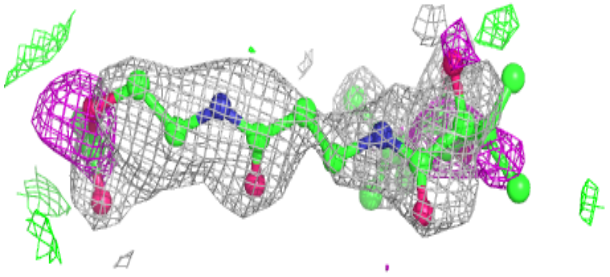
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	168	B	6001	27/27	0.71	0.33	40,49,55,57	0
3	168	A	5001	27/27	0.73	0.26	35,44,46,52	0
2	SO4	A	2004	5/5	0.95	0.18	67,68,69,71	0
2	SO4	A	2002	5/5	0.96	0.16	52,56,57,60	0
2	SO4	B	2001	5/5	0.97	0.12	66,66,68,69	0
2	SO4	B	2003	5/5	0.99	0.10	41,41,45,46	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 168 B 6001:

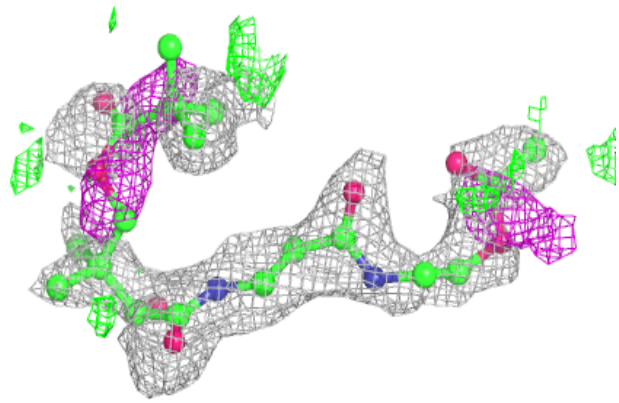
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

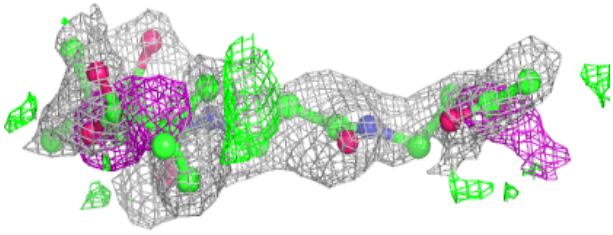


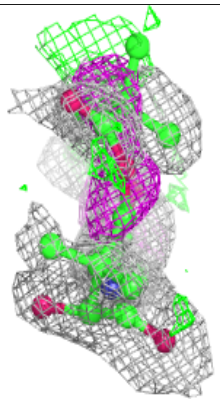


Electron density around 168 A 5001:

$2mF_o$-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.