Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 01:05 PM EDT

PDB ID	:	5BSW
Title	:	Crystal structure of 4-coumarate:CoA ligase delta-V341 mutant complexed with feruloyl adenylate
Authors	:	Li, Z.; Nair, S.K.
Deposited on	:	2015-06-02
Resolution	:	2.10 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:

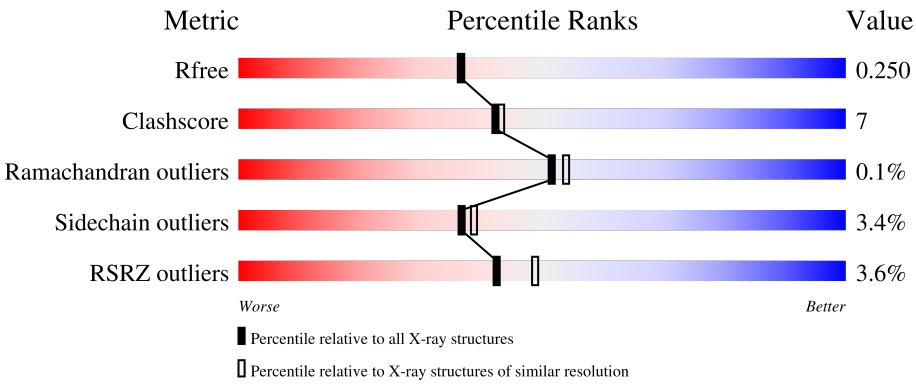
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	541	3% 83% 13% • •
1	B	541	4% 82% 14% • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8763 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.

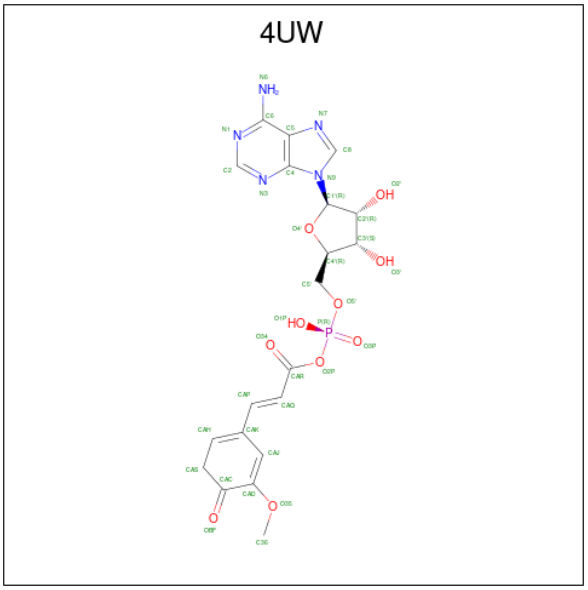
- Molecule 1 is a protein called 4-coumarate–CoA ligase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	526	4061	2605	673	761	22	0	0	0
1	B	526	4059	2604	672	761	22	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	VAL	deletion	UNP O24146
B	?	-	VAL	deletion	UNP O24146

- Molecule 2 is 5'-O-[(R)-hydroxy{[(2E)-3-(5-methoxy-4-oxocyclohexa-1,5-dien-1-yl)prop-2-enoyl]oxy}phosphoryl]adenosine (three-letter code: 4UW) (formula: $C_{20}H_{22}N_5O_{10}P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	36	20	5	10	1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	B	1	36	20	5	10	1	0	0

- Molecule 3 is water.

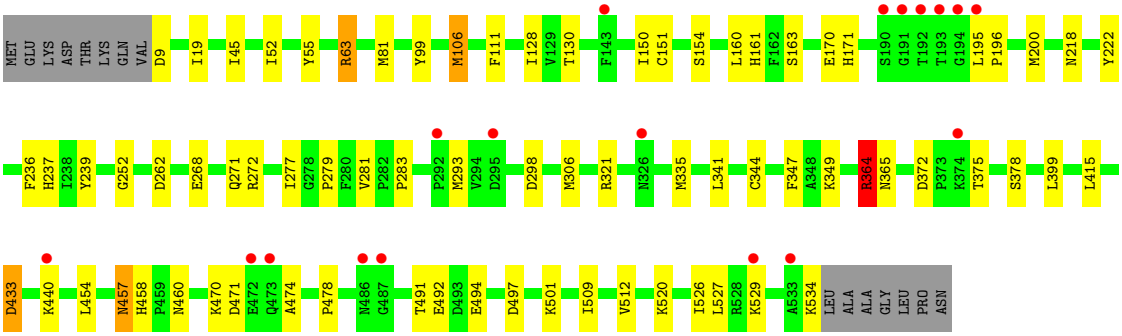
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	287	287	287	0	0
			Total	O		
3	B	284	284	284	0	0

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.

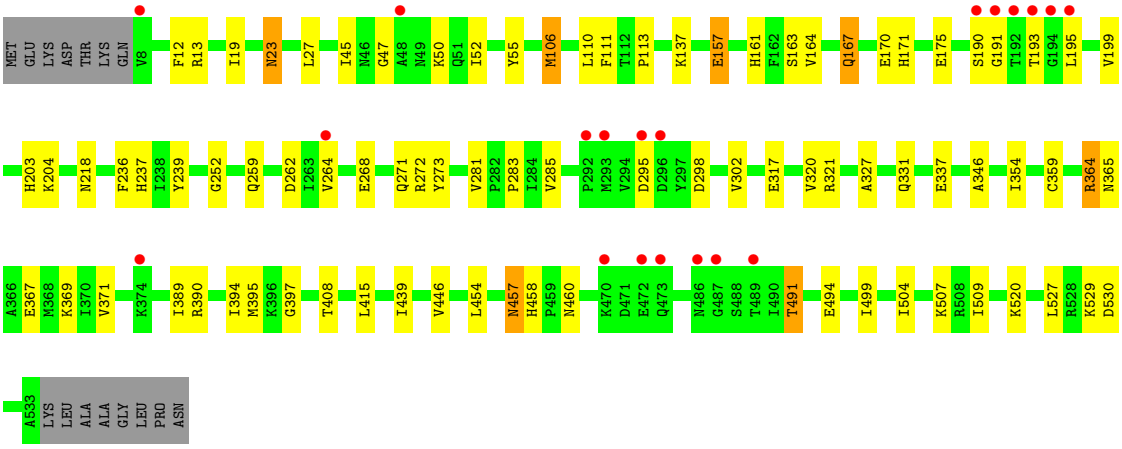
- Molecule 1: 4-coumarate–CoA ligase 2

Chain A:



- Molecule 1: 4-coumarate–CoA ligase 2

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	93.28Å 97.19Å 124.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.10 45.76 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.9 (25.00-2.10) 97.9 (45.76-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.93 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.197 , 0.246 0.198 , 0.250	Depositor DCC
R_{free} test set	3306 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	24.5	Xtriage
Anisotropy	0.595	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 48.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8763	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.34% 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: 4UW

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	0.53	0/4145	0.62	1/5624 (0.0%)
1	B	0.52	0/4143	0.63	1/5623 (0.0%)
All	All	0.52	0/8288	0.63	2/11247 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	171	HIS	CB-CA-C	-9.04	92.31	110.40
1	A	364	ARG	NE-CZ-NH2	-5.25	117.68	120.30

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	4061	0	4127	55	0
1	B	4059	0	4123	58	0
2	A	36	0	0	1	0
2	B	36	0	0	2	0
3	A	287	0	0	4	0
3	B	284	0	0	10	0
All	All	8763	0	8250	113	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 7.

All (113) 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:199:VAL:HG13	1:B:395:MET:HE3	1.16	1.12
1:A:63:ARG:HG3	1:A:63:ARG:HH11	1.29	0.96
1:B:27:LEU:H	1:B:203:HIS:HD2	1.16	0.92
1:A:63:ARG:HH11	1:A:63:ARG:CG	1.83	0.91
1:A:458:HIS:HD2	1:A:460:ASN:H	1.17	0.91
1:A:200:MET:HE2	1:A:399:LEU:HD13	1.52	0.90
1:B:199:VAL:CG1	1:B:395:MET:HE3	2.03	0.89
1:B:19:ILE:H	1:B:365:ASN:HD21	1.23	0.86
1:B:199:VAL:HG13	1:B:395:MET:CE	2.03	0.85
1:A:19:ILE:H	1:A:365:ASN:HD21	1.22	0.84
1:A:497:ASP:O	1:A:501:LYS:HG2	1.79	0.81
1:A:271:GLN:HE21	1:A:298:ASP:H	1.27	0.79
1:B:491:THR:HG22	1:B:494:GLU:H	1.49	0.78
1:A:271:GLN:NE2	1:A:298:ASP:H	1.83	0.76
1:A:200:MET:CE	1:A:399:LEU:HD13	2.18	0.74
1:A:491:THR:HG21	3:A:970:HOH:O	1.88	0.72
1:B:27:LEU:H	1:B:203:HIS:CD2	2.06	0.68
1:B:191:GLY:HA2	1:B:337:GLU:OE2	1.94	0.67
1:B:264:VAL:O	1:B:268:GLU:HG2	1.94	0.67
1:A:200:MET:CE	1:A:399:LEU:CD1	2.73	0.67
1:B:408:THR:HG22	1:B:415:LEU:HD12	1.78	0.66
1:A:45:ILE:HG12	1:A:52:ILE:HD12	1.77	0.66
1:B:19:ILE:HG12	1:B:364:ARG:HD2	1.77	0.65
1:A:200:MET:HE2	1:A:399:LEU:CD1	2.24	0.65
1:B:458:HIS:HD2	1:B:460:ASN:H	1.42	0.65
1:A:161:HIS:HD2	1:A:163:SER:H	1.44	0.64
1:A:470:LYS:HG2	3:A:871:HOH:O	1.97	0.63
1:A:63:ARG:HG3	1:A:63:ARG:NH1	2.06	0.63
1:A:277:ILE:CG2	1:A:306:MET:HE3	2.29	0.62
1:B:161:HIS:CD2	1:B:163:SER:H	2.18	0.61
1:A:458:HIS:CD2	1:A:460:ASN:H	2.09	0.61
1:B:170:GLU:OE2	3:B:701:HOH:O	2.15	0.61
1:B:161:HIS:HD2	1:B:163:SER:H	1.49	0.61
1:A:491:THR:HG23	1:A:494:GLU:H	1.67	0.60
1:A:271:GLN:HE21	1:A:298:ASP:N	2.00	0.58
1:A:161:HIS:CD2	1:A:163:SER:H	2.20	0.58
1:B:23:ASN:C	1:B:23:ASN:HD22	2.08	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:ILE:HG12	1:A:364:ARG:HD2	1.86	0.57
1:A:200:MET:HE3	1:A:399:LEU:HD12	1.87	0.56
1:B:389:ILE:HG23	1:B:394:ILE:HD11	1.86	0.56
1:A:200:MET:HE1	3:A:986:HOH:O	2.05	0.56
1:B:167:GLN:HA	1:B:167:GLN:OE1	2.06	0.56
1:B:113:PRO:HG3	1:B:137:LYS:HG2	1.87	0.56
1:A:237:HIS:HE1	2:A:600:4UW:O2P	1.90	0.55
1:B:50:LYS:HD3	1:B:273:TYR:OH	2.05	0.55
1:B:530:ASP:HB3	3:B:943:HOH:O	2.06	0.55
1:B:454:LEU:O	1:B:457:ASN:HB2	2.05	0.55
1:A:478:PRO:HB2	1:A:509:ILE:HD13	1.89	0.54
1:B:504:ILE:HG22	1:B:507:LYS:HE2	1.90	0.53
1:A:63:ARG:NH1	1:A:170:GLU:HG2	2.24	0.53
1:B:218:ASN:O	1:B:364:ARG:NH2	2.42	0.53
1:B:237:HIS:HE1	2:B:600:4UW:O2P	1.92	0.52
1:B:164:VAL:HA	1:B:167:GLN:HG2	1.92	0.52
1:B:458:HIS:CD2	1:B:460:ASN:H	2.26	0.51
1:A:491:THR:HG22	1:A:494:GLU:HG3	1.93	0.51
1:A:268:GLU:O	1:A:272:ARG:HG3	2.11	0.50
1:A:195:LEU:HB3	1:A:196:PRO:HD2	1.93	0.50
1:A:63:ARG:HD3	1:A:99:TYR:CZ	2.47	0.50
1:A:520:LYS:HE2	1:A:526:ILE:CD1	2.43	0.49
1:B:395:MET:HE2	1:B:397:GLY:O	2.13	0.49
1:A:454:LEU:O	1:A:457:ASN:HB2	2.13	0.49
1:B:167:GLN:OE1	1:B:167:GLN:CA	2.60	0.48
1:B:175:GLU:HG3	3:B:871:HOH:O	2.13	0.48
1:B:439:ILE:HB	1:B:446:VAL:HB	1.95	0.48
1:A:218:ASN:O	1:A:364:ARG:NH2	2.46	0.48
1:A:63:ARG:HH11	1:A:63:ARG:CB	2.27	0.48
1:B:47:GLY:O	1:B:50:LYS:NZ	2.46	0.48
1:B:199:VAL:HA	1:B:395:MET:CE	2.44	0.47
1:A:81:MET:HB3	1:A:128:ILE:HD12	1.97	0.47
1:A:471:ASP:HB3	1:A:474:ALA:HB3	1.97	0.47
1:B:271:GLN:HE21	1:B:298:ASP:H	1.60	0.47
1:B:203:HIS:HE1	3:B:730:HOH:O	1.97	0.47
1:A:321:ARG:NH1	3:A:709:HOH:O	2.48	0.47
1:A:150:ILE:HD13	1:A:160:LEU:HB2	1.97	0.46
1:B:157:GLU:HG2	3:B:939:HOH:O	2.15	0.46
1:B:281:VAL:HG23	1:B:283:PRO:HD2	1.95	0.46
1:A:491:THR:HG22	1:A:494:GLU:CG	2.45	0.46
1:B:23:ASN:HB2	1:B:204:LYS:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:THR:O	1:A:151:CYS:HA	2.16	0.46
1:A:222:TYR:CE1	1:A:349:LYS:HD2	2.51	0.46
1:A:344:CYS:HB3	1:A:347:PHE:CE2	2.51	0.46
1:B:193:THR:HG23	3:B:764:HOH:O	2.16	0.45
1:B:12:PHE:HB3	3:B:898:HOH:O	2.17	0.45
1:B:285:VAL:HG13	1:B:320:VAL:HG21	1.99	0.45
1:B:45:ILE:HG12	1:B:52:ILE:HG12	1.99	0.45
1:B:331:GLN:HB2	1:B:359:CYS:HA	1.99	0.44
1:B:367:GLU:OE1	1:B:390:ARG:HD2	2.17	0.44
1:B:395:MET:CE	1:B:397:GLY:O	2.66	0.44
1:B:13:ARG:HD3	3:B:925:HOH:O	2.17	0.44
1:B:369:LYS:HE3	1:B:371:VAL:HG21	2.00	0.44
1:A:281:VAL:HG23	1:A:283:PRO:HD2	2.00	0.44
1:B:237:HIS:CE1	2:B:600:4UW:O2P	2.70	0.43
1:A:491:THR:CG2	1:A:494:GLU:H	2.31	0.43
1:B:302:VAL:O	1:B:327:ALA:HB2	2.19	0.42
1:B:346:ALA:HB2	1:B:354:ILE:HG12	2.01	0.42
1:B:529:LYS:HD2	1:B:529:LYS:HA	1.67	0.42
1:A:55:TYR:CZ	1:A:252:GLY:HA2	2.54	0.42
1:A:492:GLU:HG3	1:A:512:VAL:HB	2.00	0.42
1:B:106:MET:HG3	1:B:236:PHE:HA	2.01	0.42
1:A:529:LYS:HD2	1:A:529:LYS:HA	1.74	0.42
1:A:457:ASN:HD22	1:A:457:ASN:HA	1.64	0.42
1:A:106:MET:HG3	1:A:236:PHE:HA	2.01	0.42
1:A:277:ILE:O	1:A:279:PRO:HD3	2.20	0.42
1:B:317:GLU:OE2	1:B:321:ARG:NH2	2.51	0.42
1:A:9:ASP:HA	1:A:378:SER:OG	2.19	0.41
1:B:19:ILE:N	1:B:365:ASN:HD21	2.04	0.41
1:B:190:SER:HB3	3:B:888:HOH:O	2.19	0.41
1:B:520:LYS:NZ	3:B:724:HOH:O	2.54	0.41
1:A:81:MET:HB3	1:A:128:ILE:CD1	2.50	0.41
1:B:55:TYR:CZ	1:B:252:GLY:HA2	2.56	0.41
1:A:372:ASP:HB3	1:A:375:THR:OG1	2.21	0.41
1:B:499:ILE:HG21	1:B:509:ILE:HG12	2.03	0.40
1:A:335:MET:HE1	1:A:341:LEU:HD21	2.02	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	524/541 (97%)	502 (96%)	21 (4%)	1 (0%)	47	49
1	B	524/541 (97%)	505 (96%)	19 (4%)	0	100	100
All	All	1048/1082 (97%)	1007 (96%)	40 (4%)	1 (0%)	51	54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	433	ASP

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	450/462 (97%)	435 (97%)	15 (3%)	38	40
1	B	450/462 (97%)	434 (96%)	16 (4%)	35	36
All	All	900/924 (97%)	869 (97%)	31 (3%)	37	39

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	ARG
1	A	106	MET
1	A	111	PHE
1	A	154	SER
1	A	171	HIS

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Mol	Chain	Res	Type
1	A	239	TYR
1	A	262	ASP
1	A	293	MET
1	A	364	ARG
1	A	415	LEU
1	A	433	ASP
1	A	440	LYS
1	A	457	ASN
1	A	527	LEU
1	A	534	LYS
1	B	23	ASN
1	B	106	MET
1	B	110	LEU
1	B	111	PHE
1	B	157	GLU
1	B	167	GLN
1	B	195	LEU
1	B	239	TYR
1	B	259	GLN
1	B	262	ASP
1	B	272	ARG
1	B	295	ASP
1	B	364	ARG
1	B	457	ASN
1	B	491	THR
1	B	527	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	75	GLN
1	A	119	GLN
1	A	161	HIS
1	A	179	GLN
1	A	237	HIS
1	A	271	GLN
1	A	365	ASN
1	A	457	ASN
1	A	458	HIS
1	A	460	ASN
1	A	502	GLN

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Mol	Chain	Res	Type
1	B	23	ASN
1	B	34	ASN
1	B	61	ASN
1	B	161	HIS
1	B	203	HIS
1	B	237	HIS
1	B	271	GLN
1	B	331	GLN
1	B	365	ASN
1	B	382	ASN
1	B	457	ASN
1	B	458	HIS
1	B	486	ASN
1	B	502	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)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	4UW	A	600	-	35,39,39	3.23	7 (20%)	40,57,57	2.97	14 (35%)
2	4UW	B	600	-	35,39,39	3.17	6 (17%)	40,57,57	3.00	12 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	4UW	A	600	-	-	4/16/51/51	0/4/4/4
2	4UW	B	600	-	-	5/16/51/51	0/4/4/4

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	4UW	O2P-CAR	16.26	1.54	1.37
2	B	600	4UW	O2P-CAR	15.62	1.54	1.37
2	B	600	4UW	CAD-CAC	-6.02	1.39	1.48
2	A	600	4UW	CAD-CAC	-5.70	1.39	1.48
2	A	600	4UW	CAS-CAH	-4.86	1.40	1.49
2	B	600	4UW	CAS-CAH	-4.37	1.41	1.49
2	B	600	4UW	P-O2P	3.59	1.67	1.60
2	B	600	4UW	CAP-CAK	3.22	1.52	1.45
2	A	600	4UW	P-O2P	3.09	1.66	1.60
2	A	600	4UW	CAP-CAK	2.69	1.51	1.45
2	B	600	4UW	CAJ-CAD	2.54	1.43	1.36
2	A	600	4UW	CAJ-CAD	2.39	1.43	1.36
2	A	600	4UW	O35-CAD	2.18	1.39	1.35

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	600	4UW	O35-CAD-CAC	9.77	117.92	112.09
2	B	600	4UW	O2P-CAR-CAQ	9.34	131.33	110.72
2	A	600	4UW	O2P-CAR-CAQ	9.33	131.30	110.72
2	B	600	4UW	O35-CAD-CAC	7.41	116.51	112.09
2	B	600	4UW	CAQ-CAP-CAK	6.52	135.96	126.23
2	B	600	4UW	N3-C2-N1	-5.54	120.02	128.68
2	B	600	4UW	C36-O35-CAD	5.16	126.50	116.96
2	A	600	4UW	N3-C2-N1	-5.11	120.70	128.68
2	A	600	4UW	O34-CAR-CAQ	-4.84	106.65	123.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	600	4UW	O2P-CAR-O34	-4.82	118.12	122.20
2	A	600	4UW	C36-O35-CAD	4.61	125.48	116.96
2	A	600	4UW	CAQ-CAP-CAK	4.31	132.66	126.23
2	B	600	4UW	CAJ-CAK-CAH	-4.18	115.51	119.07
2	B	600	4UW	O34-CAR-CAQ	-3.81	110.24	123.58
2	B	600	4UW	CAH-CAS-CAC	3.74	121.13	112.42
2	A	600	4UW	CAH-CAS-CAC	3.73	121.09	112.42
2	A	600	4UW	CAS-CAC-CAD	3.17	119.39	116.20
2	A	600	4UW	CAJ-CAK-CAH	-2.95	116.56	119.07
2	A	600	4UW	CAP-CAQ-CAR	-2.78	113.99	123.53
2	B	600	4UW	CAS-CAC-CAD	2.40	118.62	116.20
2	A	600	4UW	C4-C5-N7	-2.39	106.91	109.40
2	B	600	4UW	CAP-CAQ-CAR	-2.26	115.79	123.53
2	B	600	4UW	C2-N1-C6	2.25	122.61	118.75
2	A	600	4UW	O2P-P-O3P	2.23	116.32	109.45
2	A	600	4UW	C3'-C2'-C1'	2.15	104.22	100.98
2	A	600	4UW	CAJ-CAD-CAC	-2.05	119.35	121.56

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	4UW	CAC-CAD-O35-C36
2	A	600	4UW	CAJ-CAD-O35-C36
2	B	600	4UW	CAJ-CAD-O35-C36
2	B	600	4UW	CAC-CAD-O35-C36
2	B	600	4UW	CAR-O2P-P-O5'
2	B	600	4UW	CAJ-CAK-CAP-CAQ
2	A	600	4UW	CAR-O2P-P-O5'
2	B	600	4UW	CAR-O2P-P-O3P
2	A	600	4UW	CAJ-CAK-CAP-CAQ

There are no ring outliers.

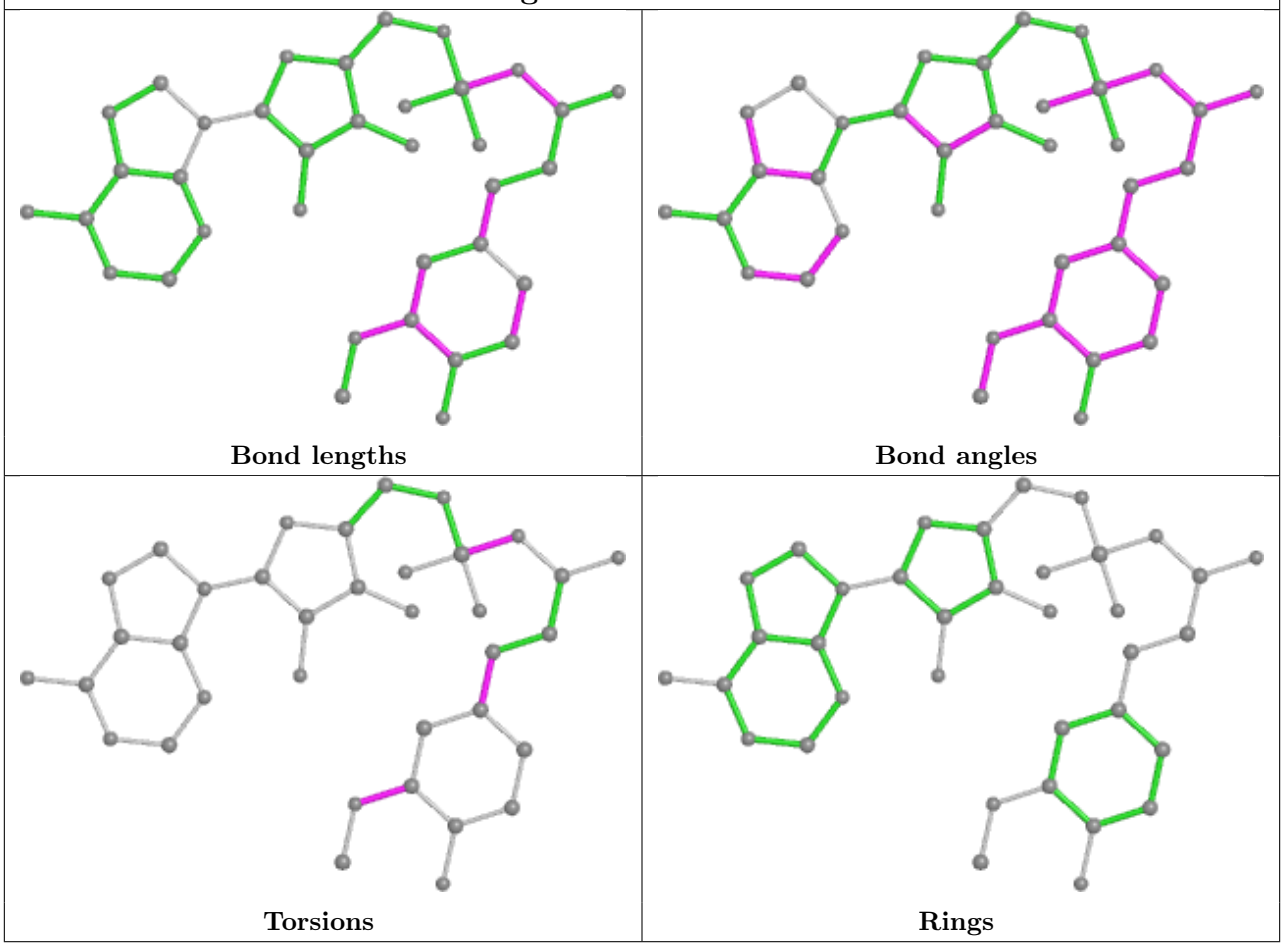
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	4UW	1	0
2	B	600	4UW	2	0

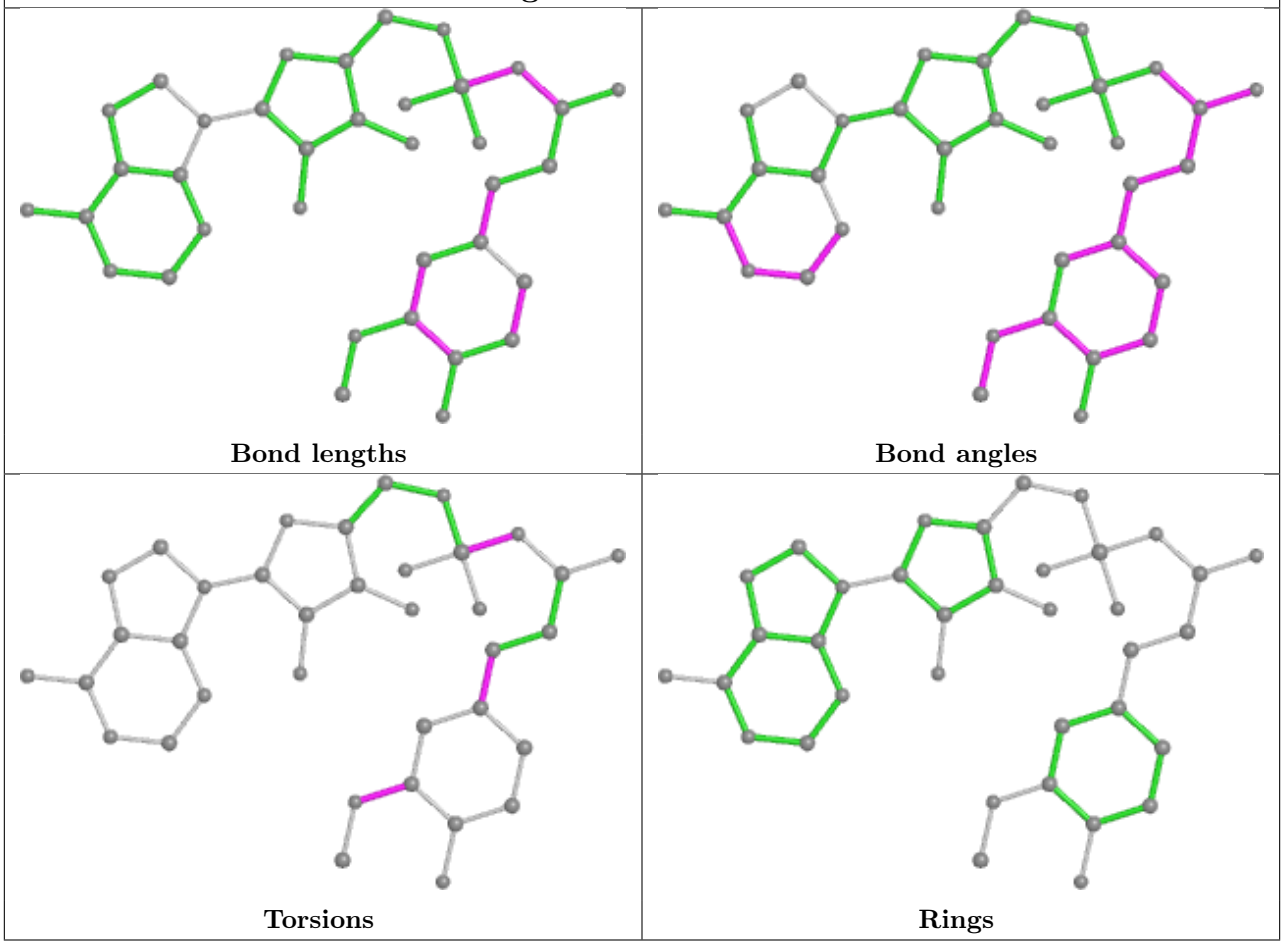
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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 4UW A 600



Ligand 4UW B 600



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	526/541 (97%)	-0.05	18 (3%)	45	51	15, 26, 43, 56	0
1	B	526/541 (97%)	-0.01	20 (3%)	40	46	13, 26, 44, 57	0
All	All	1052/1082 (97%)	-0.03	38 (3%)	42	49	13, 26, 44, 57	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	191	GLY	9.2
1	B	193	THR	8.9
1	B	192	THR	7.2
1	A	193	THR	6.6
1	A	473	GLN	5.5
1	B	190	SER	5.0
1	A	192	THR	5.0
1	B	487	GLY	4.6
1	B	473	GLN	4.3
1	B	486	ASN	4.2
1	A	194	GLY	4.1
1	B	8	VAL	3.9
1	A	472	GLU	3.8
1	A	486	ASN	3.8
1	A	487	GLY	3.6
1	B	194	GLY	3.6
1	B	472	GLU	3.4
1	B	295	ASP	3.4
1	B	293	MET	3.1
1	B	374	LYS	3.1
1	A	295	ASP	3.0
1	B	470	LYS	3.0
1	A	195	LEU	2.9
1	A	190	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	374	LYS	2.7
1	A	191	GLY	2.7
1	A	143	PHE	2.7
1	B	296	ASP	2.7
1	A	292	PRO	2.6
1	A	440	LYS	2.5
1	B	489	THR	2.5
1	B	292	PRO	2.5
1	B	48	ALA	2.5
1	A	529	LYS	2.3
1	A	533	ALA	2.2
1	B	195	LEU	2.2
1	B	264	VAL	2.1
1	A	326	ASN	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

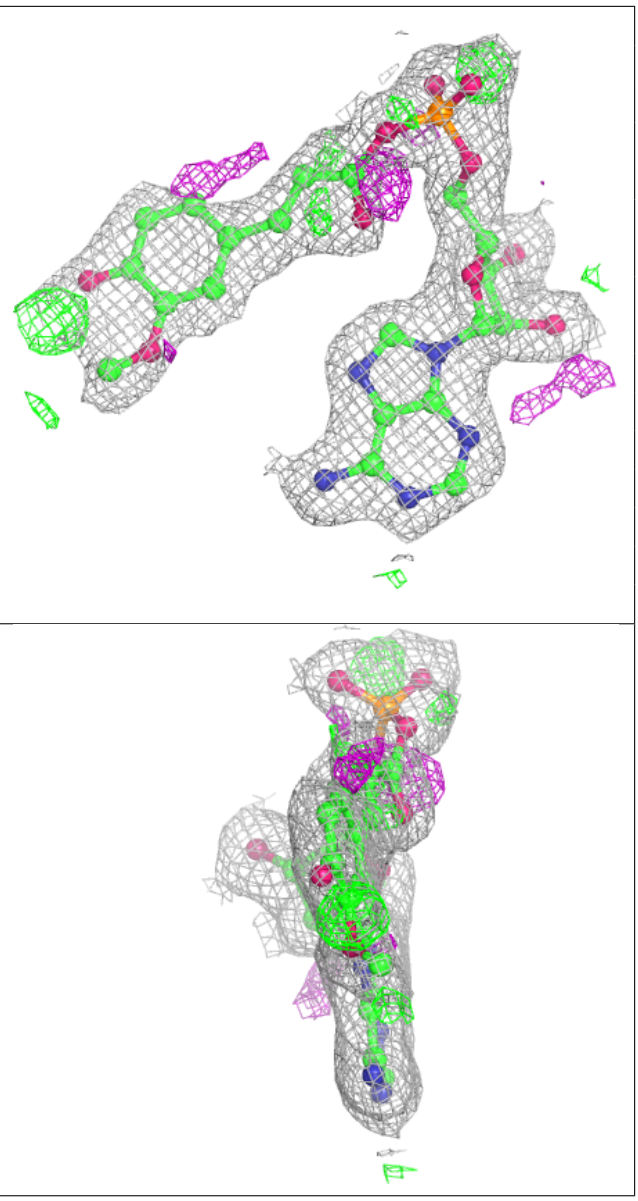
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

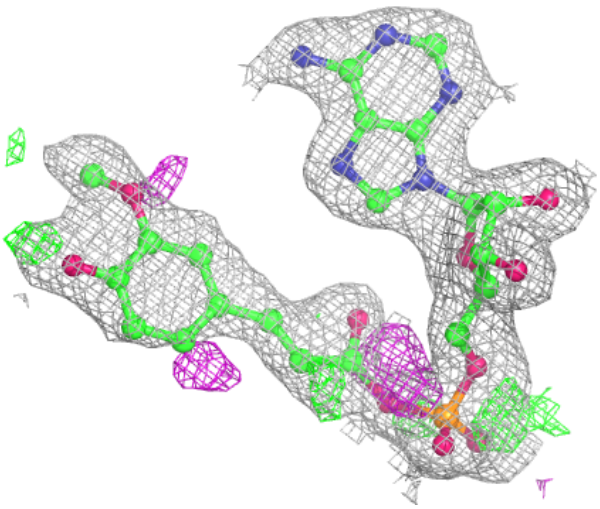
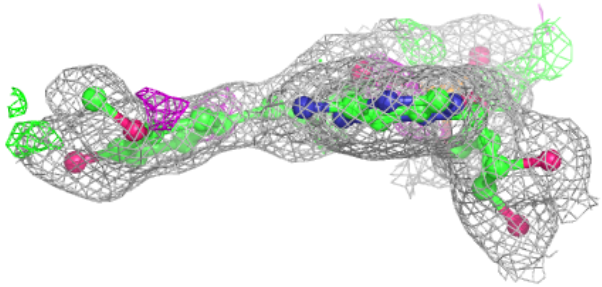
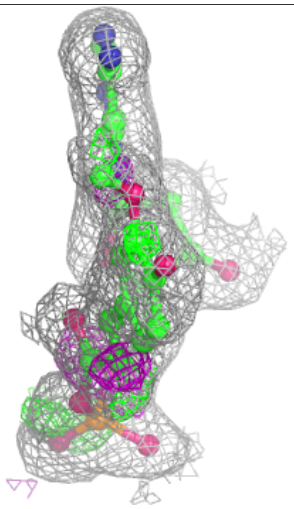
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	4UW	A	600	36/36	0.93	0.14	18,22,39,39	0
2	4UW	B	600	36/36	0.93	0.14	18,21,39,39	0

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 4UW A 600:

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



Electron density around 4UW B 600: 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.