Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:00 PM UTC

PDB ID	:	2JLB / pdb_00002jlb
Title	:	Xanthomonas campestris putative OGT (XCC0866), complex with UDP- GlcNAc phosphonate analogue
Authors	:	Schuettelkopf, A.W.; Clarke, A.J.; van Aalten, D.M.F.
Deposited on	:	2008-09-07
Resolution	:	2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

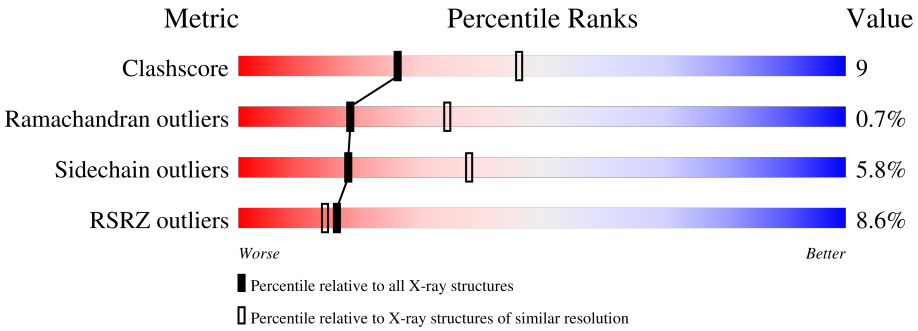
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	568	14% 79% 15%
1	B	568	3% 81% 14%

2 Entry composition

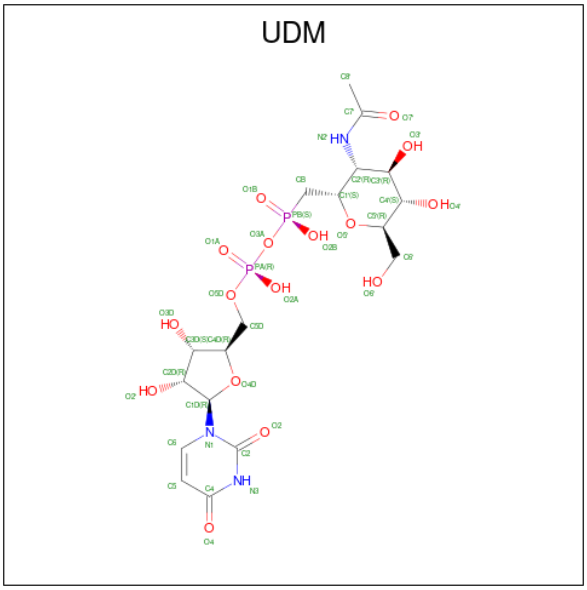
There are 5 unique types of molecules in this entry. The entry contains 8605 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 XCC0866.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	548	Total	C	N	O	S	0	0	0
			4171	2635	771	749	16			
1	B	548	Total	C	N	O	S	0	1	0
			4179	2639	772	752	16			

- Molecule 2 is URIDINE-DIPHOSPHATE-METHYLENE-N-ACETYL-GLUCOSAMINE (CCD ID: UDM) (formula: $C_{18}H_{29}N_3O_{16}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	1
			64	28	5	27	4		
2	B	1	Total	C	N	O	P	0	0
			39	18	3	16	2		

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mn 1 1	0	0
3	B	1	Total Mn 1 1	0	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0

- Molecule 5 is water.

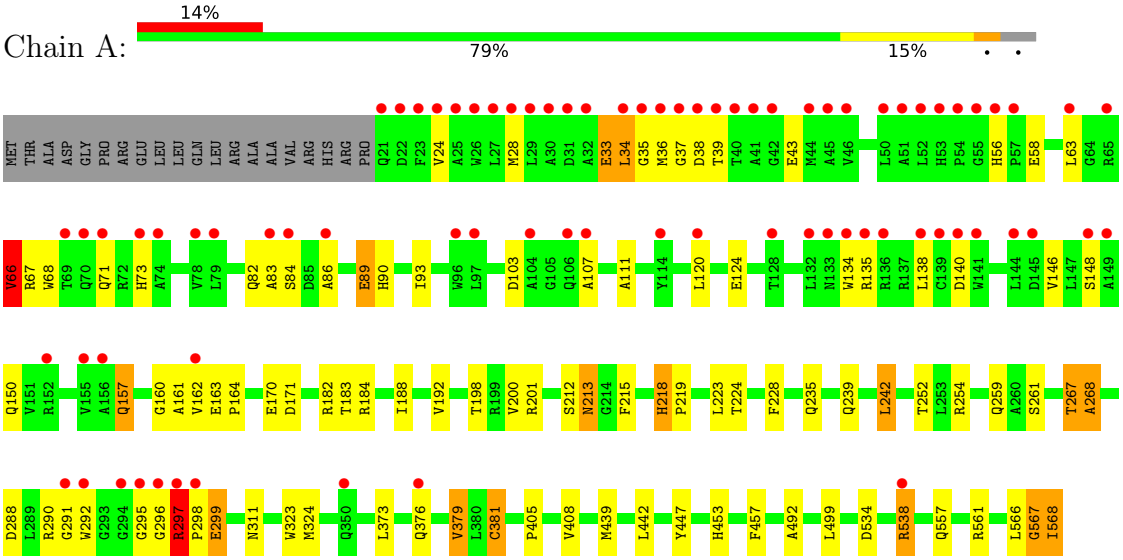
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	79	Total O 79 79	0	0
5	B	70	Total O 70 70	0	0

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.

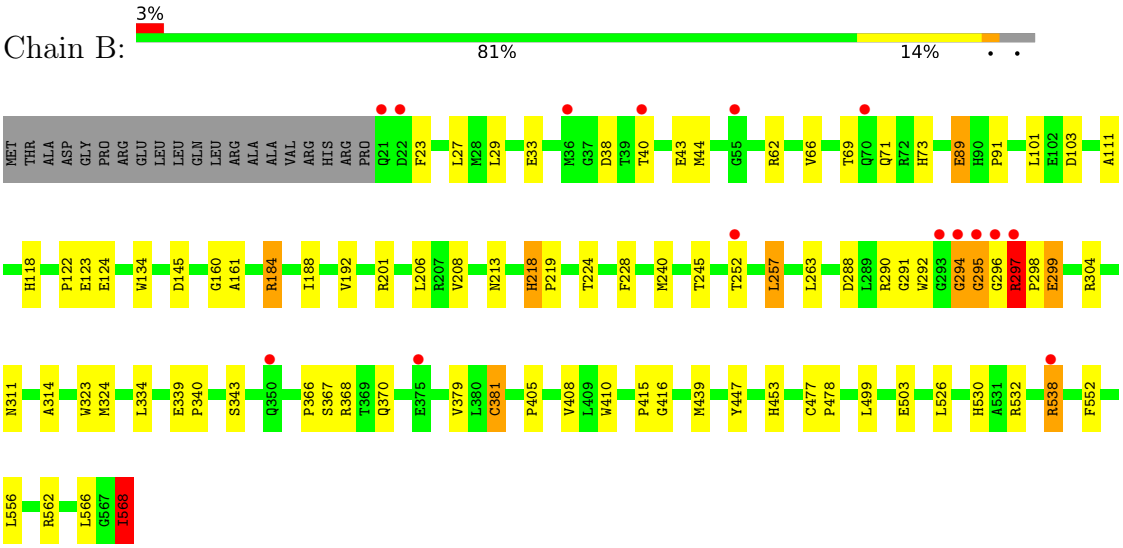
• Molecule 1: XCC0866

Chain A:



• Molecule 1: XCC0866

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	83.86Å 100.53Å 154.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.83 – 2.50 19.83 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.4 (19.83-2.50) 95.1 (19.83-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.13 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, R_{free}	0.210 , 0.247 0.211 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	30.5	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 38.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	8605	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, MN, UDM

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	0.77	1/4280 (0.0%)	0.99	15/5840 (0.3%)
1	B	0.71	1/4288 (0.0%)	0.97	10/5851 (0.2%)
All	All	0.74	2/8568 (0.0%)	0.98	25/11691 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	162	VAL	CA-CB	-5.50	1.48	1.54
1	B	257	LEU	CG-CD2	-5.14	1.35	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	295	GLY	N-CA-C	-8.96	101.30	112.77
1	B	568	ILE	CA-CB-CG1	-6.50	99.35	110.40
1	B	304	ARG	NE-CZ-NH2	5.92	124.53	119.20
1	B	257	LEU	CD1-CG-CD2	-5.89	97.84	110.80
1	A	218	HIS	CA-C-N	5.71	125.18	119.24
1	A	218	HIS	C-N-CA	5.71	125.18	119.24
1	A	405	PRO	CA-C-N	-5.58	113.75	122.73
1	A	405	PRO	C-N-CA	-5.58	113.75	122.73
1	A	373	LEU	CA-C-N	-5.49	114.59	120.03
1	A	373	LEU	C-N-CA	-5.49	114.59	120.03
1	A	267	THR	N-CA-C	-5.29	102.44	110.28
1	A	492	ALA	N-CA-C	-5.29	105.52	111.28
1	B	218	HIS	CA-C-N	5.27	124.72	119.24
1	B	218	HIS	C-N-CA	5.27	124.72	119.24
1	A	212	SER	N-CA-C	5.21	116.99	108.76
1	A	235	GLN	CA-C-N	5.16	124.95	119.28
1	A	235	GLN	C-N-CA	5.16	124.95	119.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	568	ILE	CB-CG1-CD1	-5.15	102.98	113.80
1	B	405	PRO	CA-C-N	-5.11	114.50	122.73
1	B	405	PRO	C-N-CA	-5.11	114.50	122.73
1	A	534	ASP	N-CA-C	5.10	116.83	111.28
1	B	568	ILE	CG1-CB-CG2	-5.04	95.57	110.70
1	B	343	SER	N-CA-C	-5.03	106.40	112.54
1	A	567	GLY	CA-C-N	-5.00	112.70	121.70
1	A	567	GLY	C-N-CA	-5.00	112.70	121.70

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	4171	0	4093	80	0
1	B	4179	0	4096	71	0
2	A	64	0	39	3	0
2	B	39	0	27	7	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	B	1	0	0	0	0
5	A	79	0	0	0	0
5	B	70	0	0	1	0
All	All	8605	0	8255	157	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 9.

All (157) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:GLU:HG3	1:A:38:ASP:OD2	1.32	1.24
2:B:1569:UDM:H8'2	2:B:1569:UDM:O3'	1.49	1.10
1:B:538:ARG:HH21	1:B:538:ARG:HG3	1.19	1.04

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:GLY:O	1:A:297:ARG:HB2	1.58	1.02
1:A:33:GLU:HB3	1:A:38:ASP:HB3	1.42	1.02
1:B:294:GLY:HA2	1:B:296:GLY:N	1.83	0.93
1:B:294:GLY:HA2	1:B:295:GLY:C	1.97	0.90
1:B:290:ARG:HB2	1:B:291:GLY:HA2	1.53	0.89
1:A:568:ILE:HG22	1:A:568:ILE:O	1.72	0.87
1:A:267:THR:O	1:A:268:ALA:HB3	1.72	0.87
1:A:33:GLU:CB	1:A:38:ASP:HB3	2.05	0.85
1:A:33:GLU:CG	1:A:38:ASP:OD2	2.22	0.85
2:B:1569:UDM:O3'	2:B:1569:UDM:C8'	2.24	0.85
1:A:290:ARG:HB2	1:A:291:GLY:HA2	1.59	0.83
1:B:296:GLY:O	1:B:297:ARG:HB2	1.79	0.83
1:A:267:THR:O	1:A:268:ALA:CB	2.27	0.82
1:B:298:PRO:HG2	1:B:299:GLU:OE1	1.84	0.77
1:A:568:ILE:O	1:A:568:ILE:CG2	2.33	0.77
1:A:111:ALA:HB2	1:A:134:TRP:HD1	1.51	0.76
1:A:297:ARG:N	1:A:298:PRO:HD3	2.01	0.76
1:B:298:PRO:HD2	1:B:299:GLU:OE1	1.85	0.75
1:B:290:ARG:NE	1:B:296:GLY:O	2.18	0.74
1:B:379:VAL:HG11	1:B:453:HIS:O	1.86	0.74
1:A:439:MET:HE1	1:A:447:TYR:HD1	1.53	0.73
1:B:538:ARG:HH21	1:B:538:ARG:CG	1.98	0.71
1:A:538:ARG:HG2	1:A:538:ARG:HH21	1.56	0.70
2:B:1569:UDM:O7'	5:B:2069:HOH:O	2.09	0.70
1:B:290:ARG:CB	1:B:291:GLY:HA2	2.22	0.70
1:B:188:ILE:HD12	1:B:292:TRP:HH2	1.55	0.69
1:A:33:GLU:HG3	1:A:38:ASP:CG	2.17	0.69
1:A:297:ARG:N	1:A:298:PRO:CD	2.56	0.68
1:A:290:ARG:NE	1:A:296:GLY:O	2.23	0.67
1:A:439:MET:HE1	1:A:447:TYR:CD1	2.30	0.67
1:B:379:VAL:CG1	1:B:453:HIS:O	2.42	0.67
1:B:33:GLU:HB3	1:B:38:ASP:HB3	1.77	0.66
1:A:213:ASN:HD22	1:A:213:ASN:H	1.43	0.66
1:B:145[B]:ASP:N	1:B:145[B]:ASP:OD1	2.29	0.66
2:B:1569:UDM:H8'2	2:B:1569:UDM:H4	1.60	0.65
1:B:294:GLY:CA	1:B:296:GLY:N	2.58	0.64
1:B:297:ARG:N	1:B:298:PRO:HD3	2.12	0.64
1:B:367:SER:OG	1:B:370:GLN:HG3	1.97	0.64
1:A:33:GLU:O	1:A:34:LEU:O	2.16	0.63
1:A:73:HIS:ND1	1:A:103:ASP:HB3	2.13	0.63
1:A:379:VAL:HG11	1:A:453:HIS:O	1.98	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:ASN:HD22	1:B:213:ASN:H	1.47	0.63
1:A:213:ASN:H	1:A:213:ASN:ND2	1.98	0.62
1:B:288:ASP:OD1	1:B:290:ARG:HB2	2.01	0.60
1:A:379:VAL:CG1	1:A:453:HIS:O	2.49	0.60
1:B:298:PRO:CD	1:B:299:GLU:OE1	2.50	0.60
1:B:23:PHE:CZ	1:B:27:LEU:HD11	2.37	0.59
1:B:298:PRO:CG	1:B:299:GLU:OE1	2.50	0.59
1:B:43:GLU:HG3	1:B:66:VAL:HG11	1.83	0.59
1:A:148:SER:OG	1:A:170:GLU:OE1	2.16	0.59
1:A:146:VAL:O	1:A:150:GLN:HG3	2.04	0.58
1:B:184:ARG:HA	1:B:184:ARG:NH1	2.18	0.58
1:B:62:ARG:O	1:B:66:VAL:HG23	2.04	0.58
1:A:439:MET:CE	1:A:447:TYR:HD1	2.17	0.58
1:B:73:HIS:ND1	1:B:103:ASP:HB3	2.18	0.57
1:A:43:GLU:CD	1:A:67:ARG:HH12	2.13	0.57
1:A:298:PRO:HD2	1:A:299:GLU:OE1	2.03	0.57
1:B:538:ARG:HG3	1:B:538:ARG:NH2	2.00	0.56
1:A:288:ASP:OD2	1:A:290:ARG:NH2	2.39	0.55
1:A:297:ARG:H	1:A:298:PRO:HD3	1.71	0.55
1:B:297:ARG:N	1:B:298:PRO:CD	2.69	0.55
1:A:290:ARG:CB	1:A:291:GLY:HA2	2.33	0.55
1:A:43:GLU:OE1	1:A:67:ARG:NH1	2.41	0.54
1:A:218:HIS:HB3	1:A:219:PRO:HD2	1.89	0.54
1:A:24:VAL:O	1:A:28:MET:HG3	2.08	0.54
1:A:557:GLN:O	1:A:561:ARG:HG3	2.08	0.54
1:A:66:VAL:O	1:A:67:ARG:C	2.51	0.53
1:B:213:ASN:H	1:B:213:ASN:ND2	2.05	0.53
1:A:38:ASP:O	1:A:39:THR:C	2.51	0.53
1:B:294:GLY:CA	1:B:295:GLY:C	2.70	0.53
1:B:323:TRP:CD1	1:B:324:MET:HE2	2.44	0.53
1:A:71:GLN:C	1:A:73:HIS:HD2	2.16	0.52
1:B:208:VAL:HB	1:B:240:MET:CE	2.39	0.52
1:A:34:LEU:O	1:A:36:MET:N	2.43	0.52
1:A:188:ILE:HD12	1:A:292:TRP:HH2	1.75	0.52
1:A:43:GLU:CD	1:A:67:ARG:NH1	2.68	0.51
1:A:439:MET:HE3	1:A:442:LEU:HD12	1.91	0.51
1:A:538:ARG:HH21	1:A:538:ARG:CG	2.23	0.51
1:A:567:GLY:O	1:A:568:ILE:C	2.50	0.51
1:B:245:THR:HG21	1:B:297:ARG:HG2	1.93	0.51
1:B:366:PRO:HB3	1:B:370:GLN:HE21	1.75	0.51
1:B:111:ALA:HB2	1:B:134:TRP:HD1	1.76	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:TRP:CD1	1:A:324:MET:HE2	2.46	0.51
1:A:34:LEU:O	1:A:37:GLY:N	2.34	0.51
1:A:82:GLN:O	1:A:83:ALA:C	2.55	0.50
1:A:223:LEU:HD12	2:A:1569[A]:UDM:H8'1	1.93	0.50
1:B:219:PRO:HB2	2:B:1569:UDM:H3'	1.94	0.49
1:B:29:LEU:O	1:B:33:GLU:HG2	2.12	0.49
1:B:339:GLU:N	1:B:340:PRO:CD	2.77	0.48
1:A:288:ASP:CG	1:A:290:ARG:HH21	2.21	0.48
1:B:69:THR:C	1:B:71:GLN:H	2.21	0.48
1:A:224:THR:HB	1:A:228:PHE:CE2	2.48	0.48
1:A:538:ARG:HD3	1:A:538:ARG:O	2.14	0.48
1:B:89:GLU:O	1:B:91:PRO:HD3	2.14	0.48
1:B:224:THR:HB	1:B:228:PHE:CE2	2.48	0.48
1:A:56:HIS:CD2	1:A:58:GLU:HB2	2.49	0.47
1:B:294:GLY:C	1:B:296:GLY:N	2.72	0.47
1:B:314:ALA:HA	2:B:1569:UDM:H8'3	1.96	0.47
1:B:218:HIS:HB3	1:B:219:PRO:HD2	1.96	0.47
2:B:1569:UDM:O1A	2:B:1569:UDM:HB1	2.14	0.47
1:B:184:ARG:HA	1:B:184:ARG:HH11	1.78	0.46
1:B:23:PHE:CE1	1:B:27:LEU:HD11	2.50	0.46
1:B:188:ILE:CD1	1:B:292:TRP:HH2	2.25	0.46
1:A:242:LEU:HD22	1:A:261:SER:OG	2.15	0.46
1:A:298:PRO:HG2	1:A:299:GLU:OE1	2.17	0.45
1:B:290:ARG:NH1	1:B:298:PRO:CA	2.80	0.45
1:A:83:ALA:O	1:A:84:SER:C	2.59	0.45
1:A:107:ALA:HB1	1:A:138:LEU:HD21	1.99	0.45
1:A:182:ARG:HD2	1:A:182:ARG:C	2.42	0.45
1:A:201:ARG:HB3	1:A:201:ARG:CZ	2.47	0.45
1:A:290:ARG:HE	1:A:297:ARG:HB2	1.82	0.45
1:A:323:TRP:HD1	1:A:324:MET:HE2	1.82	0.45
1:A:90:HIS:CG	1:A:93:ILE:HG13	2.52	0.44
1:A:252:THR:HG22	1:B:252:THR:HA	1.98	0.44
1:A:63:LEU:HA	1:A:66:VAL:HG23	1.99	0.44
1:B:208:VAL:HB	1:B:240:MET:HE2	1.99	0.44
1:A:290:ARG:NH1	1:A:298:PRO:CA	2.81	0.44
1:B:290:ARG:CB	1:B:291:GLY:CA	2.94	0.44
1:B:323:TRP:HD1	1:B:324:MET:HE2	1.81	0.44
1:A:33:GLU:CA	1:A:38:ASP:HB3	2.47	0.44
1:B:415:PRO:O	1:B:416:GLY:C	2.60	0.43
1:B:552:PHE:CE2	1:B:556:LEU:HD11	2.53	0.43
1:A:290:ARG:HB2	1:A:291:GLY:CA	2.39	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:GLN:O	1:B:73:HIS:CD2	2.70	0.43
1:B:201:ARG:HB3	1:B:201:ARG:CZ	2.47	0.43
1:B:188:ILE:HD12	1:B:292:TRP:CH2	2.45	0.43
1:B:297:ARG:H	1:B:298:PRO:HD3	1.83	0.43
1:A:66:VAL:O	1:A:68:TRP:N	2.51	0.43
1:B:184:ARG:HG2	1:B:292:TRP:CH2	2.54	0.43
1:A:83:ALA:O	1:A:86:ALA:N	2.52	0.43
1:A:163:GLU:HA	1:A:164:PRO:HD3	1.76	0.42
1:A:200:VAL:O	1:A:201:ARG:C	2.61	0.42
1:A:157:GLN:HE21	1:A:157:GLN:HB2	1.62	0.42
1:B:296:GLY:O	1:B:297:ARG:CB	2.54	0.42
1:A:215:PHE:O	1:A:254:ARG:HD3	2.19	0.42
1:B:368:ARG:HG3	1:B:453:HIS:CE1	2.55	0.42
1:B:477:CYS:HA	1:B:478:PRO:HD3	1.91	0.42
1:A:381:CYS:O	1:A:457:PHE:HA	2.20	0.42
1:B:118:HIS:O	1:B:122:PRO:HA	2.19	0.42
1:B:568:ILE:HD13	1:B:568:ILE:HA	1.16	0.42
1:A:135:ARG:HB3	1:A:140:ASP:O	2.19	0.42
1:B:160:GLY:O	1:B:161:ALA:C	2.61	0.41
1:A:160:GLY:O	1:A:161:ALA:C	2.60	0.41
2:A:1569[A]:UDM:C7'	2:A:1569[A]:UDM:O1B	2.69	0.41
1:A:568:ILE:HG23	1:A:568:ILE:HD13	1.64	0.41
1:A:89:GLU:O	1:A:120:LEU:HD13	2.21	0.41
1:B:381:CYS:HB2	1:B:410:TRP:HB3	2.02	0.41
1:B:526:LEU:O	1:B:530:HIS:HD2	2.04	0.41
1:A:538:ARG:HD3	1:A:538:ARG:C	2.46	0.41
1:B:188:ILE:CD1	1:B:292:TRP:CH2	3.04	0.41
1:B:263:LEU:C	1:B:263:LEU:HD23	2.45	0.41
1:B:503:GLU:OE1	1:B:532:ARG:NH1	2.46	0.41
2:A:1569[A]:UDM:O1B	2:A:1569[A]:UDM:N2'	2.54	0.41
1:A:73:HIS:CD2	1:A:73:HIS:H	2.39	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	546/568 (96%)	519 (95%)	22 (4%)	5 (1%)	14	27
1	B	547/568 (96%)	531 (97%)	13 (2%)	3 (0%)	24	43
All	All	1093/1136 (96%)	1050 (96%)	35 (3%)	8 (1%)	18	34

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	35	GLY
1	A	297	ARG
1	B	295	GLY
1	B	297	ARG
1	A	268	ALA
1	A	66	VAL
1	B	294	GLY

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	413/429 (96%)	388 (94%)	25 (6%)	17	35
1	B	414/429 (96%)	391 (94%)	23 (6%)	19	39
All	All	827/858 (96%)	779 (94%)	48 (6%)	18	38

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	GLU
1	A	66	VAL
1	A	89	GLU
1	A	124	GLU
1	A	157	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	171	ASP
1	A	183	THR
1	A	184	ARG
1	A	192	VAL
1	A	198	THR
1	A	213	ASN
1	A	239	GLN
1	A	242	LEU
1	A	259	GLN
1	A	297	ARG
1	A	299	GLU
1	A	311	ASN
1	A	376	GLN
1	A	379	VAL
1	A	381	CYS
1	A	408	VAL
1	A	499	LEU
1	A	538	ARG
1	A	566	LEU
1	A	568	ILE
1	B	40	THR
1	B	44	MET
1	B	89	GLU
1	B	101	LEU
1	B	123	GLU
1	B	124	GLU
1	B	184	ARG
1	B	192	VAL
1	B	206	LEU
1	B	257	LEU
1	B	297	ARG
1	B	299	GLU
1	B	311	ASN
1	B	334	LEU
1	B	381	CYS
1	B	408	VAL
1	B	439	MET
1	B	447	TYR
1	B	499	LEU
1	B	538	ARG
1	B	562	ARG
1	B	566	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	568	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	56	HIS
1	A	73	HIS
1	A	150	GLN
1	A	157	GLN
1	A	177	GLN
1	A	213	ASN
1	A	235	GLN
1	A	259	GLN
1	A	370	GLN
1	A	392	GLN
1	A	429	GLN
1	B	47	GLN
1	B	56	HIS
1	B	150	GLN
1	B	213	ASN
1	B	235	GLN
1	B	370	GLN
1	B	392	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
2	UDM	A	1569[B]	-	26,26,41	2.13	8 (30%)	36,40,62	2.04	10 (27%)
2	UDM	B	1569	-	41,41,41	1.26	6 (14%)	53,62,62	1.89	13 (24%)
2	UDM	A	1569[A]	-	41,41,41	1.24	5 (12%)	53,62,62	1.95	14 (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
2	UDM	A	1569[B]	-	-	5/13/32/63	0/2/2/3
2	UDM	B	1569	-	-	10/24/63/63	0/3/3/3
2	UDM	A	1569[A]	-	-	12/24/63/63	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1569[B]	UDM	PB-O3A	5.27	1.64	1.58
2	A	1569[B]	UDM	C2-N1	-4.33	1.31	1.38
2	A	1569[B]	UDM	C5-C4	-3.32	1.36	1.43
2	B	1569	UDM	PB-O3A	3.21	1.62	1.58
2	A	1569[A]	UDM	PB-O2B	-3.15	1.48	1.56
2	B	1569	UDM	PB-O2B	-3.06	1.48	1.56
2	A	1569[B]	UDM	PA-O3A	2.96	1.62	1.59
2	A	1569[B]	UDM	C3D-C2D	-2.67	1.46	1.53
2	A	1569[B]	UDM	PB-O2B	-2.67	1.47	1.54
2	A	1569[B]	UDM	O2'-C2D	-2.53	1.36	1.43
2	A	1569[A]	UDM	C2-N1	-2.42	1.34	1.38
2	A	1569[A]	UDM	PB-O3A	2.35	1.61	1.58
2	B	1569	UDM	O4D-C1D	2.34	1.47	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1569	UDM	C2-N1	-2.31	1.34	1.38
2	B	1569	UDM	PA-O3A	2.24	1.61	1.59
2	B	1569	UDM	C6-C5	2.17	1.40	1.35
2	A	1569[A]	UDM	C6-C5	2.15	1.40	1.35
2	A	1569[B]	UDM	O4D-C1D	-2.09	1.37	1.42
2	A	1569[A]	UDM	C5-C4	-2.03	1.39	1.43

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1569[A]	UDM	C4'-C3'-C2'	-5.44	102.47	110.40
2	B	1569	UDM	C4-N3-C2	-5.43	119.88	126.61
2	B	1569	UDM	N3-C2-N1	5.24	121.71	114.89
2	A	1569[B]	UDM	C4-N3-C2	-5.18	120.18	126.61
2	A	1569[A]	UDM	C4-N3-C2	-5.14	120.23	126.61
2	A	1569[B]	UDM	O4D-C1D-N1	-5.11	96.78	108.36
2	A	1569[B]	UDM	N3-C2-N1	5.08	121.51	114.89
2	B	1569	UDM	O4D-C1D-N1	-4.76	97.57	108.36
2	A	1569[A]	UDM	O4D-C1D-N1	-4.32	98.56	108.36
2	A	1569[A]	UDM	N3-C2-N1	4.26	120.44	114.89
2	A	1569[B]	UDM	O2-C2-N1	-3.39	118.38	122.80
2	A	1569[A]	UDM	C5-C4-N3	3.38	119.53	114.80
2	A	1569[A]	UDM	O2B-PB-O1B	3.16	120.24	109.95
2	A	1569[B]	UDM	O2B-PB-O1B	3.03	118.96	111.58
2	B	1569	UDM	O2-C2-N1	-2.99	118.90	122.80
2	B	1569	UDM	O4D-C4D-C5D	2.90	118.63	109.33
2	A	1569[A]	UDM	O2'-C2D-C3D	-2.89	102.55	111.82
2	A	1569[A]	UDM	O5'-C5'-C6'	-2.86	99.35	106.44
2	B	1569	UDM	C5-C4-N3	2.86	118.80	114.80
2	B	1569	UDM	O2B-PB-O1B	2.81	119.10	109.95
2	A	1569[A]	UDM	C1'-C2'-N2'	-2.73	105.03	110.77
2	B	1569	UDM	PB-O3A-PA	-2.71	123.52	132.37
2	A	1569[B]	UDM	O4-C4-C5	-2.59	120.69	125.16
2	A	1569[B]	UDM	C5-C4-N3	2.52	118.33	114.80
2	A	1569[A]	UDM	O3D-C3D-C2D	-2.51	103.78	111.82
2	A	1569[B]	UDM	O2'-C2D-C3D	-2.39	104.16	111.82
2	A	1569[A]	UDM	O4-C4-C5	-2.38	121.05	125.16
2	B	1569	UDM	C5'-O5'-C1'	-2.35	109.08	113.19
2	A	1569[B]	UDM	O1B-PB-CB	-2.34	104.93	113.94
2	B	1569	UDM	C2D-C3D-C4D	2.28	107.01	102.61
2	B	1569	UDM	O4-C4-C5	-2.27	121.25	125.16
2	A	1569[A]	UDM	PB-O3A-PA	-2.23	125.09	132.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1569[B]	UDM	C5D-C4D-C3D	-2.20	107.28	115.21
2	B	1569	UDM	C4'-C3'-C2'	-2.20	107.19	110.40
2	A	1569[A]	UDM	O2-C2-N1	-2.20	119.93	122.80
2	B	1569	UDM	C3'-C2'-N2'	2.16	114.59	110.62
2	A	1569[A]	UDM	C3'-C2'-N2'	2.01	114.32	110.62

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1569[A]	UDM	C3'-C2'-N2'-C7'
2	A	1569[A]	UDM	C5D-O5D-PA-O1A
2	A	1569[A]	UDM	C5D-O5D-PA-O3A
2	B	1569	UDM	C2'-C1'-CB-PB
2	B	1569	UDM	C5D-O5D-PA-O2A
2	B	1569	UDM	C5D-O5D-PA-O3A
2	A	1569[A]	UDM	O4D-C4D-C5D-O5D
2	A	1569[A]	UDM	C8'-C7'-N2'-C2'
2	A	1569[A]	UDM	O7'-C7'-N2'-C2'
2	B	1569	UDM	C8'-C7'-N2'-C2'
2	B	1569	UDM	O7'-C7'-N2'-C2'
2	A	1569[A]	UDM	O5'-C5'-C6'-O6'
2	A	1569[A]	UDM	C3D-C4D-C5D-O5D
2	B	1569	UDM	O4D-C4D-C5D-O5D
2	A	1569[A]	UDM	C4'-C5'-C6'-O6'
2	B	1569	UDM	C1'-C2'-N2'-C7'
2	A	1569[B]	UDM	O4D-C4D-C5D-O5D
2	B	1569	UDM	C3D-C4D-C5D-O5D
2	B	1569	UDM	C3'-C2'-N2'-C7'
2	A	1569[B]	UDM	PB-O3A-PA-O5D
2	A	1569[A]	UDM	C5D-O5D-PA-O2A
2	A	1569[B]	UDM	C5D-O5D-PA-O1A
2	A	1569[B]	UDM	C5D-O5D-PA-O2A
2	A	1569[B]	UDM	C5D-O5D-PA-O3A
2	A	1569[A]	UDM	C2'-C1'-CB-PB
2	A	1569[A]	UDM	O5'-C1'-CB-PB
2	B	1569	UDM	O5'-C1'-CB-PB

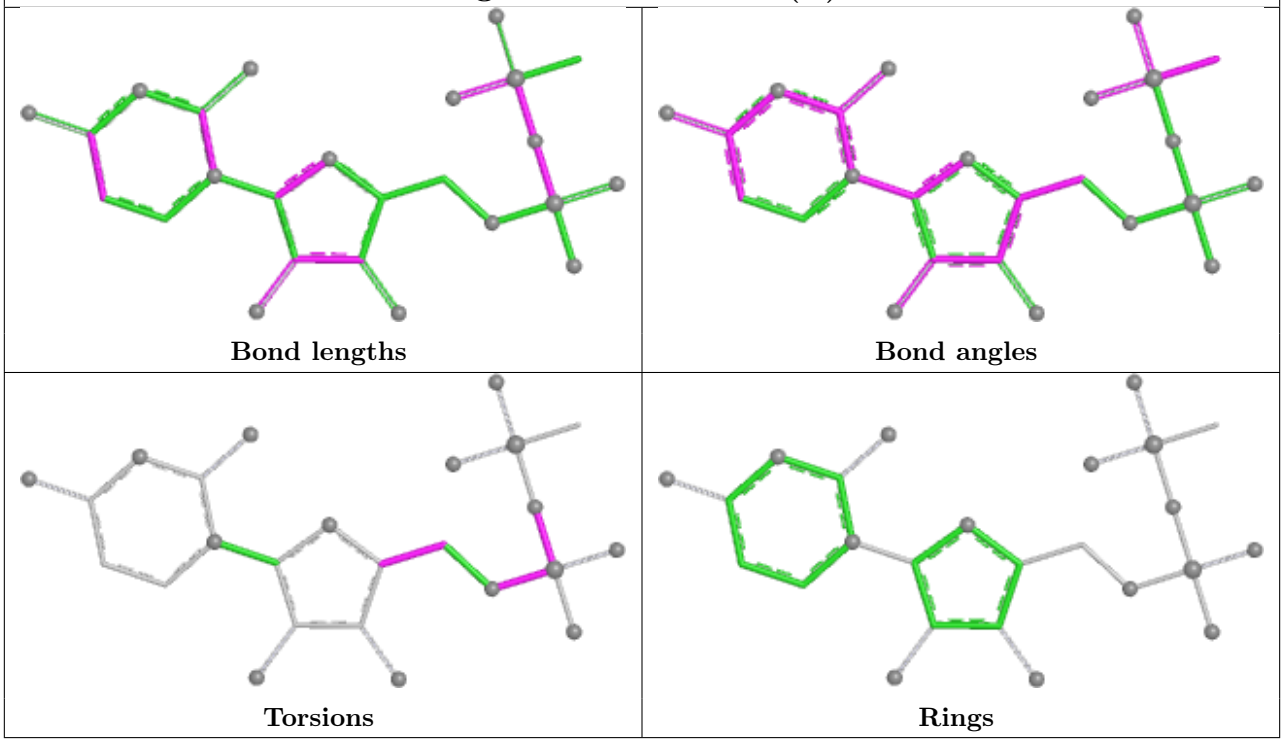
There are no ring outliers.

2 monomers are involved in 10 short contacts:

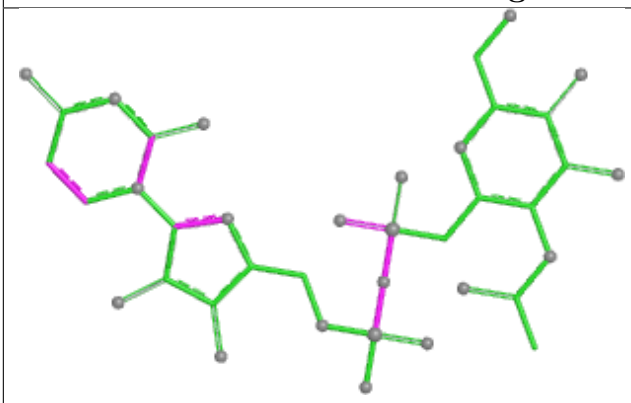
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1569	UDM	7	0
2	A	1569[A]	UDM	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

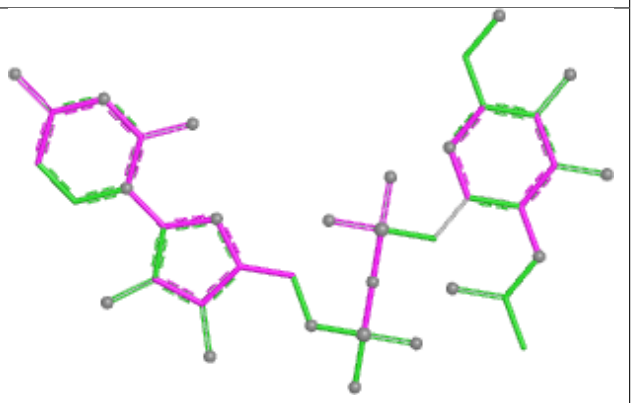
Ligand UDM A 1569 (B)



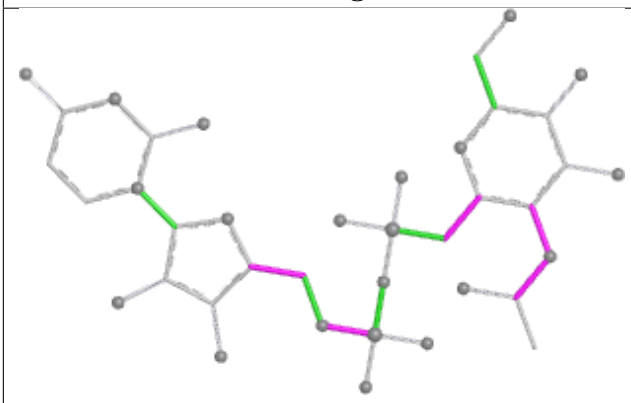
Ligand UDM B 1569



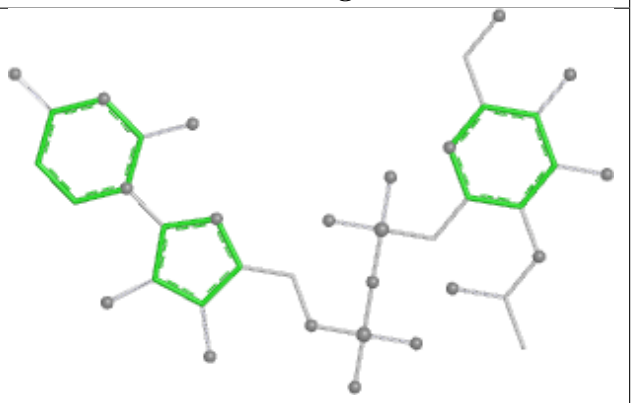
Bond lengths



Bond angles

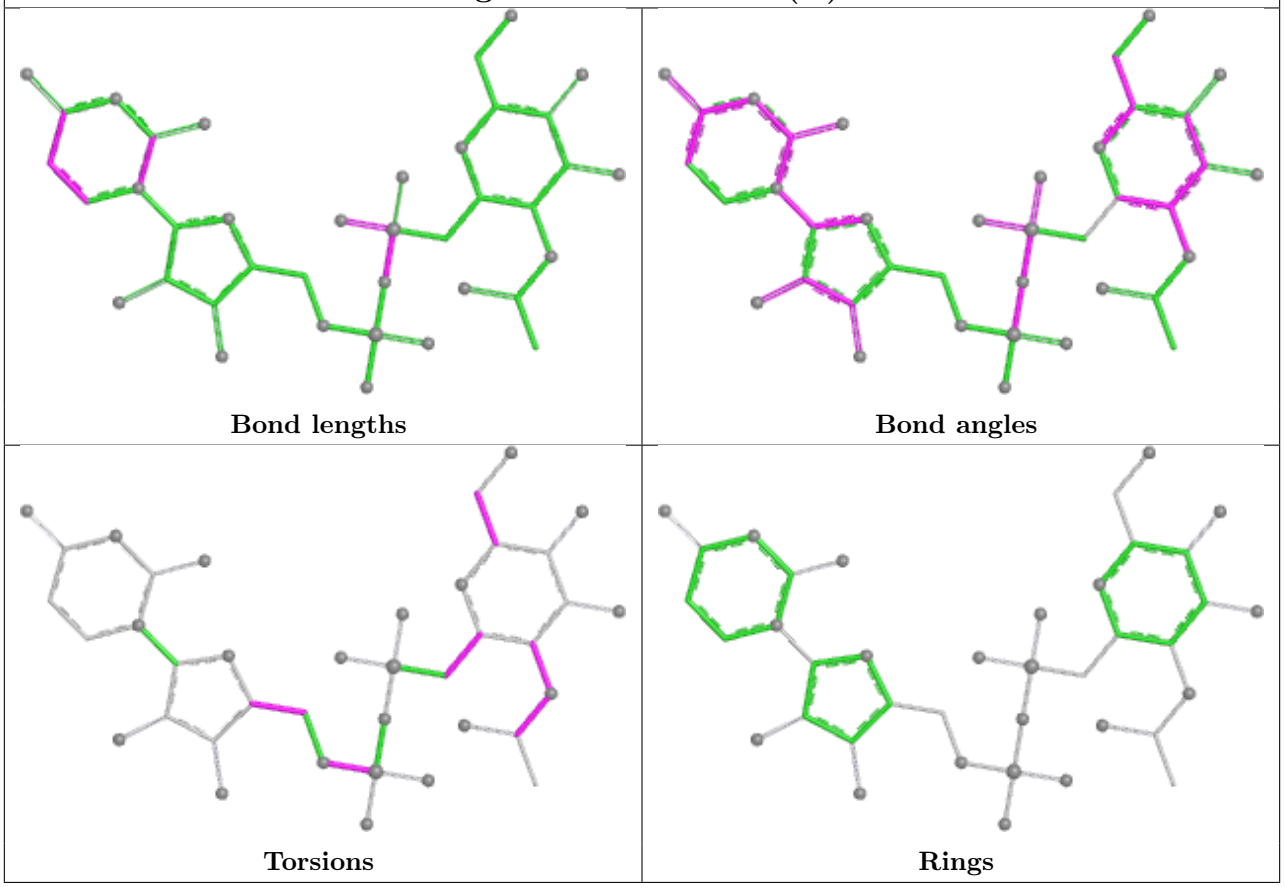


Torsions



Rings

Ligand UDM A 1569 (A)



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	548/568 (96%)	0.48	79 (14%) 6 5	7, 23, 62, 86	2 (0%)
1	B	548/568 (96%)	0.09	15 (2%) 56 51	11, 23, 43, 58	3 (0%)
All	All	1096/1136 (96%)	0.29	94 (8%) 16 14	7, 23, 52, 86	5 (0%)

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	21	GLN	9.0
1	B	70	GLN	8.4
1	A	70	GLN	6.8
1	A	22	ASP	6.7
1	A	34	LEU	6.5
1	A	26	TRP	5.2
1	A	24	VAL	5.0
1	A	25	ALA	4.9
1	A	139	CYS	4.8
1	A	35	GLY	4.7
1	A	36	MET	4.5
1	A	141	TRP	4.4
1	A	23	PHE	4.4
1	A	39	THR	4.3
1	A	29	LEU	4.3
1	A	134	TRP	4.1
1	A	55	GLY	3.9
1	A	30	ALA	3.9
1	A	38	ASP	3.9
1	A	136	ARG	3.8
1	A	297	ARG	3.8
1	A	65	ARG	3.8
1	A	40	THR	3.7
1	A	152	ARG	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	36	MET	3.6
1	A	155	VAL	3.5
1	A	53	HIS	3.5
1	A	71	GLN	3.5
1	A	50	LEU	3.4
1	B	295	GLY	3.3
1	A	132	LEU	3.3
1	A	56	HIS	3.3
1	A	292	TRP	3.3
1	A	69	THR	3.2
1	A	63	LEU	3.2
1	A	148	SER	3.2
1	A	52	LEU	3.2
1	B	21	GLN	3.2
1	B	297	ARG	3.2
1	A	83	ALA	3.1
1	A	74	ALA	3.1
1	A	54	PRO	3.1
1	B	252	THR	3.0
1	A	291	GLY	3.0
1	A	28	MET	3.0
1	B	538	ARG	2.9
1	A	162	VAL	2.9
1	A	79	LEU	2.8
1	A	96	TRP	2.8
1	A	294	GLY	2.8
1	A	27	LEU	2.8
1	A	295	GLY	2.7
1	A	57	PRO	2.7
1	A	114	TYR	2.7
1	B	294	GLY	2.6
1	B	350	GLN	2.6
1	A	31	ASP	2.6
1	A	51	ALA	2.6
1	A	156	ALA	2.6
1	A	73	HIS	2.5
1	A	350	GLN	2.5
1	A	78	VAL	2.5
1	A	296	GLY	2.5
1	A	145	ASP	2.5
1	A	37	GLY	2.4
1	A	144	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	149	ALA	2.4
1	A	42	GLY	2.3
1	A	138	LEU	2.3
1	B	55	GLY	2.3
1	A	376	GLN	2.3
1	A	84	SER	2.2
1	B	22	ASP	2.2
1	B	375	GLU	2.2
1	A	135	ARG	2.2
1	A	32	ALA	2.2
1	A	45	ALA	2.2
1	A	86	ALA	2.2
1	A	104	ALA	2.1
1	B	40	THR	2.1
1	B	293	GLY	2.1
1	A	140	ASP	2.1
1	A	46	VAL	2.1
1	A	97	LEU	2.1
1	A	298	PRO	2.1
1	A	106	GLN	2.0
1	A	41	ALA	2.0
1	B	296	GLY	2.0
1	A	128	THR	2.0
1	A	538	ARG	2.0
1	A	107	ALA	2.0
1	A	120	LEU	2.0
1	A	133	ASN	2.0
1	A	44	MET	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

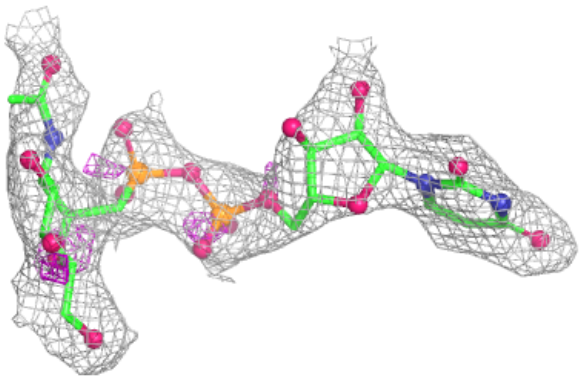
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

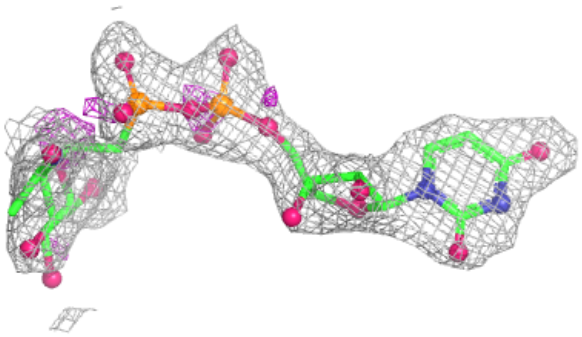
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	UDM	B	1569	39/39	0.88	0.12	40,57,61,61	0
2	UDM	A	1569[B]	25/39	0.92	0.11	81,85,86,86	25
2	UDM	A	1569[A]	39/39	0.92	0.11	13,16,19,21	39
4	CL	B	1571	1/1	0.97	0.06	25,25,25,25	0
3	MN	A	1570	1/1	0.99	0.04	27,27,27,27	0
3	MN	B	1570	1/1	1.00	0.04	14,14,14,14	0

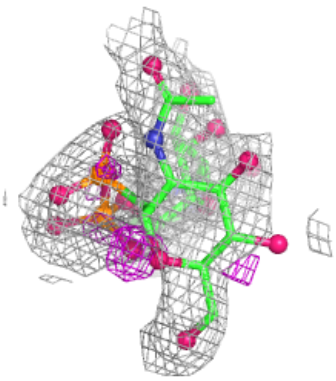
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UDM B 1569:

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

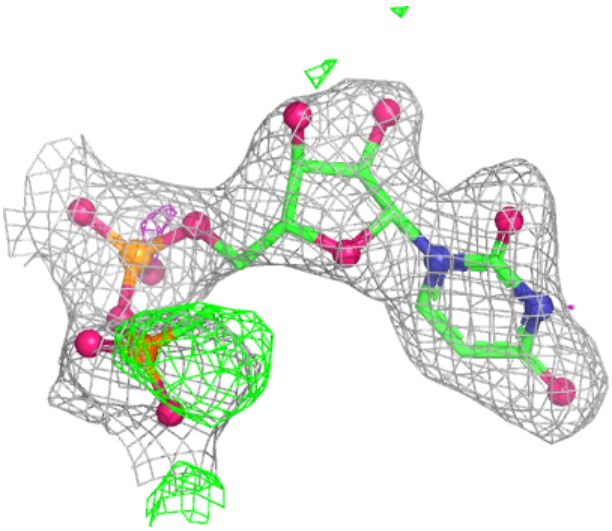


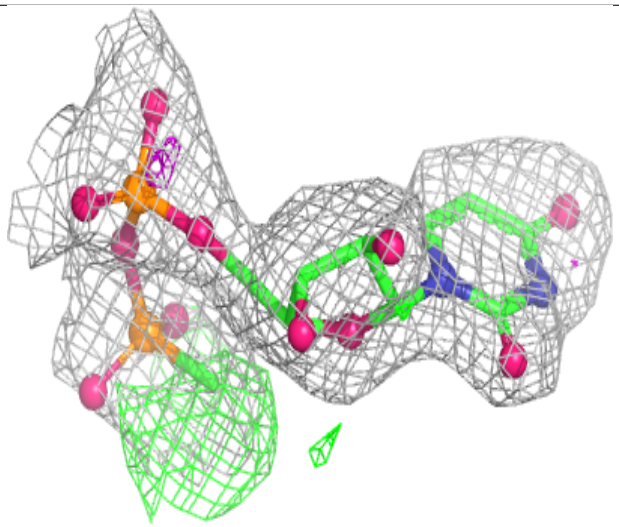


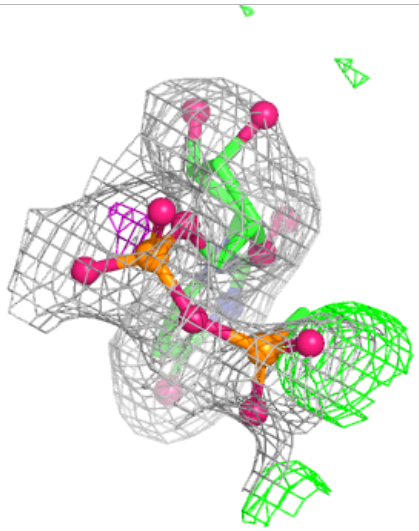


Electron density around UDM A 1569 (B):

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

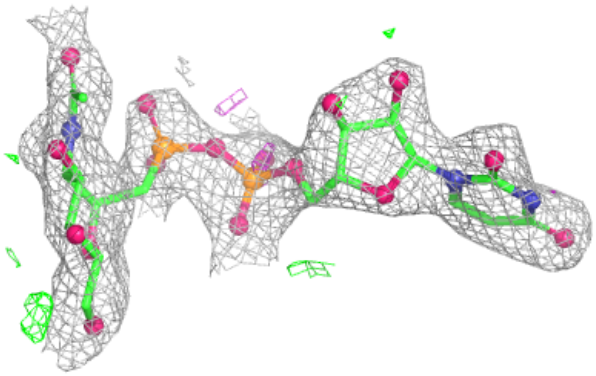


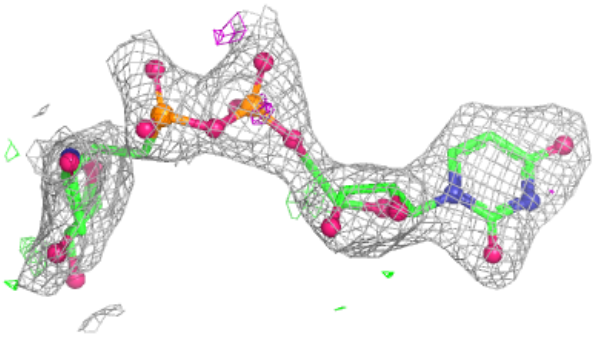


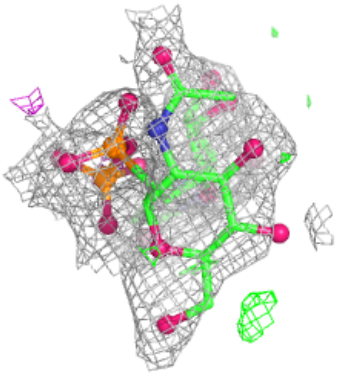


Electron density around UDM A 1569 (A):

$2mF_o$-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

There are no such residues in this entry.