Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 01:26 AM EDT

PDB ID	:	1JVD
Title	:	CRYSTAL STRUCTURE OF HUMAN AGX2 COMPLEXED WITH UDPGLCNAC
Authors	:	Peneff, C.; Bourne, Y.
Deposited on	:	2001-08-29
Resolution	:	2.40 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:

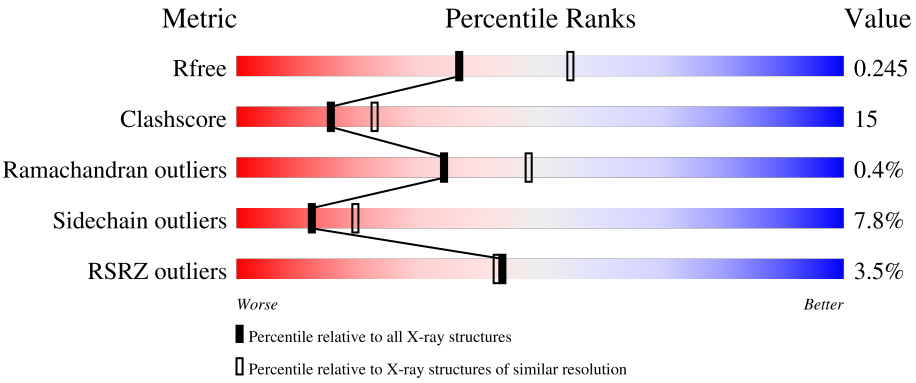
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	522	3% 68% 21% · 8%
1	B	522	3% 63% 24% 6% 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8055 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.

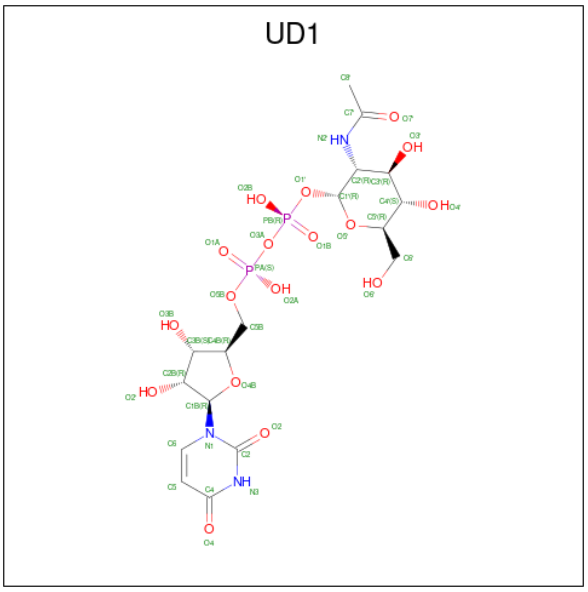
- Molecule 1 is a protein called UDPGLCNAC PYROPHOSPHORYLASE (AGX2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	480	Total	C	N	O	S	0	0	0
			3816	2446	646	706	18			
1	B	486	Total	C	N	O	S	0	0	0
			3851	2466	652	715	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	445	GLY	SER	SEE REMARK 999	UNP Q16222
A	454	SER	GLN	SEE REMARK 999	UNP Q16222
B	445	GLY	SER	SEE REMARK 999	UNP Q16222
B	454	SER	GLN	SEE REMARK 999	UNP Q16222

- Molecule 2 is URIDINE-DIPHOSPHATE-N-ACETYLGLUCOSAMINE (three-letter code: UD1) (formula: $C_{17}H_{27}N_3O_{17}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
2	B	1	Total	C	N	O	P	0	0
			39	17	3	17	2		

- Molecule 3 is water.

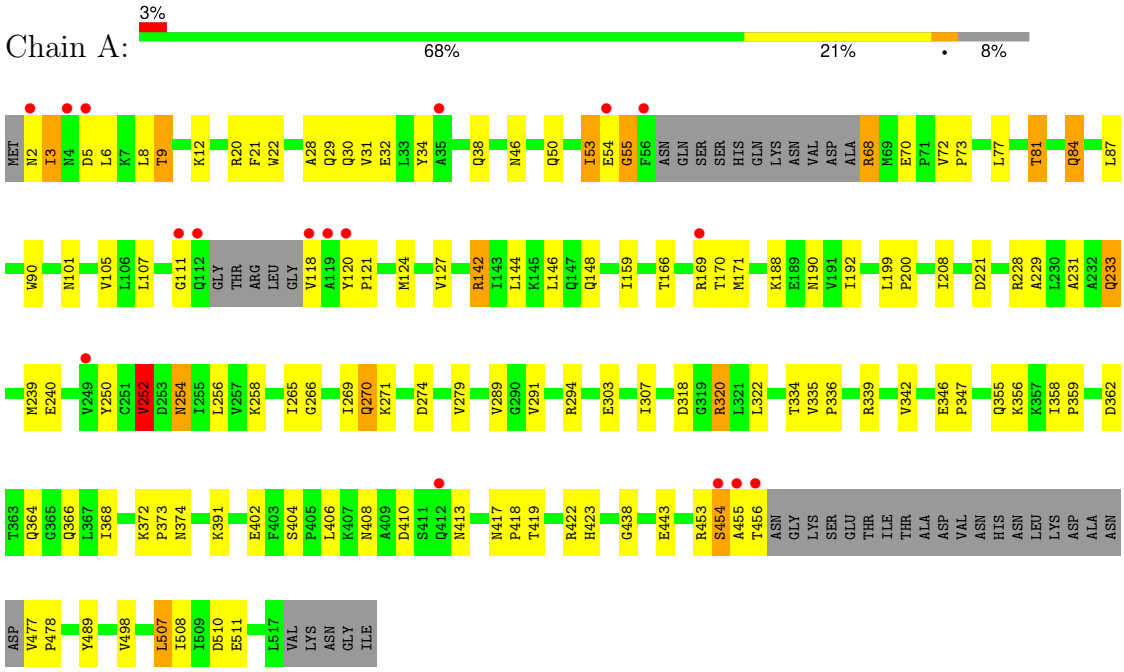
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	185	Total	O	0	0
			185	185		
3	B	125	Total	O	0	0
			125	125		

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.

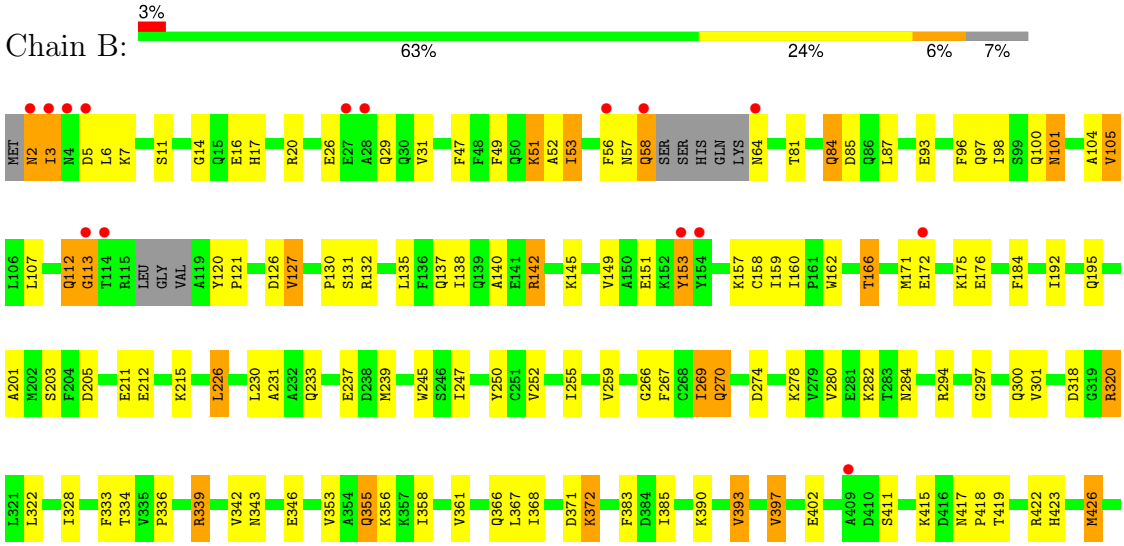
• Molecule 1: UDPGLCNAC PYROPHOSPHORYLASE (AGX2)

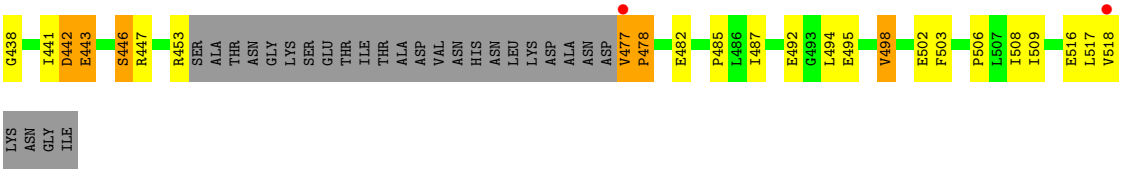
Chain A:



• Molecule 1: UDPGLCNAC PYROPHOSPHORYLASE (AGX2)

Chain B:




G438
I441
D442
E443
S446
R447
R453
SER
ALA
THR
ASN
GLY
LYS
SER
GLU
THR
ILE
THR
ALA
ASP
VAL
ASN
HIS
ASN
LEU
LYS
ASP
ALA
ASN
ASP
V477
P478
E482
P485
L486
I487
E492
G493
L494
E495
V498
E502
F503
P506
L507
I508
I509
E516
L517
V518
LYS
ASN
GLY
ILE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	86.54Å 71.28Å 91.39Å 90.00° 92.82° 90.00°	Depositor
Resolution (Å)	19.97 – 2.40 29.33 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.97-2.40) 99.8 (29.33-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	3.79 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.193 , 0.251 0.187 , 0.245	Depositor DCC
R_{free} test set	2182 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	34.4	Xtriage
Anisotropy	0.658	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 50.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8055	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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: UD1

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	0.75	0/3900	0.88	3/5269 (0.1%)
1	B	0.69	0/3935	0.91	6/5320 (0.1%)
All	All	0.72	0/7835	0.89	9/10589 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	477	VAL	C-N-CD	-20.50	75.50	120.60
1	B	477	VAL	C-N-CA	11.24	169.21	122.00
1	A	142	ARG	NE-CZ-NH2	-9.39	115.61	120.30
1	A	142	ARG	NE-CZ-NH1	8.71	124.66	120.30
1	A	252	VAL	CB-CA-C	-8.45	95.34	111.40
1	B	142	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	B	478	PRO	CA-N-CD	-5.63	103.62	111.50
1	B	478	PRO	N-CA-C	-5.46	97.90	112.10
1	B	113	GLY	N-CA-C	-5.06	100.46	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3816	0	3771	99	0
1	B	3851	0	3787	140	0
2	A	39	0	25	0	0
2	B	39	0	25	0	0
3	A	185	0	0	7	0
3	B	125	0	0	5	0
All	All	8055	0	7608	227	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 15.

All (227) 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:68:ARG:HE	1:A:68:ARG:HA	1.11	1.07
1:A:107:LEU:HD11	1:A:252:VAL:HG13	1.51	0.93
1:B:506:PRO:HG2	1:B:517:LEU:HB2	1.51	0.90
1:B:130:PRO:HB2	1:B:508:ILE:HD11	1.53	0.89
1:B:278:LYS:HG2	1:B:328:ILE:HD11	1.56	0.87
1:A:68:ARG:HA	1:A:68:ARG:NE	1.92	0.84
1:A:443:GLU:HB3	1:B:372:LYS:HD2	1.60	0.83
1:B:166:THR:HG21	1:B:171:MET:SD	2.20	0.82
1:A:373:PRO:HD3	1:B:443:GLU:HG2	1.63	0.81
1:B:3:ILE:O	1:B:7:LYS:HB2	1.81	0.80
1:B:49:PHE:CZ	1:B:53:ILE:HG13	2.17	0.79
1:A:453:ARG:HD3	1:A:456:THR:HG22	1.65	0.79
1:A:28:ALA:O	1:A:31:VAL:HG12	1.84	0.77
1:A:118:VAL:HG13	1:A:120:TYR:CD2	2.20	0.77
1:B:171:MET:HB2	1:B:195:GLN:HE21	1.50	0.77
1:A:169:ARG:HG3	1:A:170:THR:HG23	1.67	0.77
1:B:318:ASP:OD2	1:B:320:ARG:HD3	1.83	0.77
1:A:231:ALA:HB2	1:A:342:VAL:HG13	1.68	0.75
1:A:372:LYS:HA	1:B:443:GLU:HG3	1.69	0.75
1:B:132:ARG:HH11	1:B:132:ARG:HG2	1.51	0.74
1:B:336:PRO:O	1:B:339:ARG:HB2	1.87	0.73
1:B:2:ASN:HD22	1:B:3:ILE:H	1.33	0.73
1:B:17:HIS:HB2	1:B:20:ARG:NH1	2.03	0.73
1:A:438:GLY:HA3	1:A:498:VAL:HG13	1.71	0.73
1:A:454:SER:HB3	1:B:411:SER:OG	1.88	0.73
1:B:97:GLN:HG3	1:B:269:ILE:HD12	1.72	0.71
1:B:267:PHE:HE2	1:B:393:VAL:HG13	1.55	0.71
1:B:127:VAL:HG13	1:B:422:ARG:HB2	1.71	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:GLU:H	1:B:29:GLN:HE21	1.37	0.71
1:B:160:ILE:O	3:B:945:HOH:O	2.09	0.70
1:A:29:GLN:HA	1:A:32:GLU:OE1	1.92	0.70
1:A:362:ASP:OD2	1:A:364:GLN:N	2.24	0.69
1:B:361:VAL:HG22	1:B:367:LEU:HD23	1.74	0.69
1:B:361:VAL:HG22	1:B:367:LEU:CD2	2.22	0.69
1:B:84:GLN:HA	1:B:87:LEU:HG	1.74	0.68
1:B:231:ALA:HB2	1:B:342:VAL:HG13	1.76	0.68
1:B:171:MET:SD	1:B:175:LYS:HE3	2.33	0.68
1:A:362:ASP:HB3	1:A:368:ILE:CD1	2.24	0.68
1:B:151:GLU:OE1	1:B:157:LYS:HD3	1.94	0.68
1:B:442:ASP:HB2	1:B:446:SER:H	1.59	0.67
1:A:453:ARG:O	1:A:455:ALA:N	2.28	0.67
1:B:104:ALA:HB3	1:B:247:ILE:CD1	2.25	0.66
1:A:239:MET:HE2	1:A:335:VAL:HG22	1.76	0.66
1:B:158:CYS:O	1:B:159:ILE:HD13	1.96	0.65
1:A:373:PRO:HD3	1:B:443:GLU:CG	2.25	0.65
1:B:203:SER:OG	1:B:205:ASP:OD1	2.14	0.65
1:A:254:ASN:HD21	1:A:256:LEU:HB2	1.61	0.65
1:B:132:ARG:HG2	1:B:132:ARG:NH1	2.08	0.64
1:A:410:ASP:HB3	1:A:413:ASN:ND2	2.13	0.64
1:B:516:GLU:C	1:B:518:VAL:H	2.00	0.63
1:A:239:MET:CE	1:A:335:VAL:HG22	2.29	0.62
1:A:2:ASN:HD22	1:A:5:ASP:HB2	1.64	0.62
1:B:56:PHE:HE1	1:B:355:GLN:OE1	1.82	0.61
1:B:201:ALA:HB1	1:B:358:ILE:HD13	1.81	0.61
1:A:362:ASP:HB3	1:A:368:ILE:HD13	1.82	0.61
1:B:2:ASN:HB2	1:B:5:ASP:OD2	2.01	0.61
1:B:267:PHE:CE2	1:B:393:VAL:HG13	2.35	0.60
1:A:22:TRP:CZ3	1:A:30:GLN:HB2	2.35	0.60
1:B:142:ARG:HG2	1:B:485:PRO:HB3	1.83	0.60
1:B:442:ASP:HB2	1:B:446:SER:N	2.17	0.60
1:A:373:PRO:CD	1:B:443:GLU:HG2	2.32	0.60
1:A:81:THR:HG23	3:A:1076:HOH:O	2.00	0.59
1:B:274:ASP:OD2	1:B:390:LYS:N	2.31	0.59
1:B:372:LYS:HZ3	1:B:372:LYS:HB3	1.66	0.59
1:A:254:ASN:ND2	1:A:256:LEU:H	2.00	0.59
1:B:294:ARG:HD3	1:B:297:GLY:HA2	1.84	0.59
1:B:104:ALA:HB3	1:B:247:ILE:HD13	1.85	0.59
1:B:372:LYS:NZ	1:B:372:LYS:CB	2.66	0.58
1:A:456:THR:CG2	1:B:356:LYS:HZ1	2.16	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:494:LEU:N	1:B:495:GLU:OE1	2.36	0.57
1:B:57:ASN:C	1:B:58:GLN:HG3	2.25	0.57
1:B:477:VAL:HG12	1:B:477:VAL:O	2.05	0.57
1:B:166:THR:CG2	1:B:195:GLN:HG3	2.35	0.57
1:A:50:GLN:O	1:A:54:GLU:HB2	2.04	0.57
1:A:271:LYS:NZ	3:A:995:HOH:O	2.36	0.57
1:B:171:MET:CB	1:B:195:GLN:HE21	2.16	0.56
1:A:356:LYS:HB3	1:A:358:ILE:HD11	1.88	0.56
1:A:336:PRO:O	1:A:339:ARG:HB3	2.06	0.56
1:B:226:LEU:HD22	1:B:230:LEU:HG	1.87	0.56
1:B:96:PHE:CE1	1:B:100:GLN:NE2	2.74	0.55
1:B:112:GLN:CG	1:B:113:GLY:H	2.19	0.55
1:B:137:GLN:HG3	1:B:184:PHE:CD2	2.41	0.55
1:A:438:GLY:CA	1:A:498:VAL:HG13	2.37	0.55
1:B:138:ILE:O	1:B:142:ARG:HG3	2.06	0.55
1:A:54:GLU:O	1:A:55:GLY:O	2.25	0.55
1:A:372:LYS:HG2	1:B:443:GLU:HB2	1.88	0.55
1:B:231:ALA:HB2	1:B:342:VAL:CG1	2.36	0.55
1:A:346:GLU:HB3	1:A:347:PRO:HD3	1.89	0.55
1:A:127:VAL:HG13	1:A:422:ARG:HB2	1.89	0.54
1:A:228:ARG:HD3	3:A:969:HOH:O	2.08	0.54
1:B:415:LYS:HE3	3:B:999:HOH:O	2.08	0.54
1:B:518:VAL:HG12	1:B:518:VAL:O	2.08	0.53
1:B:274:ASP:OD1	1:B:274:ASP:N	2.38	0.53
1:A:366:GLN:O	1:A:368:ILE:HD12	2.09	0.53
1:B:149:VAL:O	1:B:153:TYR:HB2	2.08	0.53
1:A:240:GLU:OE2	1:A:339:ARG:HD3	2.08	0.53
1:B:14:GLY:HA2	1:B:16:GLU:OE2	2.09	0.52
1:B:397:VAL:HG21	1:B:402:GLU:OE2	2.10	0.52
1:B:151:GLU:OE1	1:B:157:LYS:CD	2.57	0.52
1:B:402:GLU:HB3	3:B:919:HOH:O	2.10	0.52
1:A:362:ASP:HB3	1:A:368:ILE:HD11	1.91	0.52
1:B:17:HIS:HB2	1:B:20:ARG:HH11	1.70	0.52
1:A:368:ILE:HD12	1:A:368:ILE:N	2.25	0.52
1:A:229:ALA:O	1:A:233:GLN:HG2	2.09	0.52
1:B:85:ASP:N	1:B:85:ASP:OD1	2.42	0.51
1:A:2:ASN:N	1:A:34:TYR:HH	2.09	0.51
1:B:301:VAL:HB	1:B:383:PHE:CD1	2.45	0.51
1:B:237:GLU:OE2	1:B:339:ARG:NH2	2.43	0.51
1:B:517:LEU:O	1:B:518:VAL:HB	2.10	0.51
1:A:192:ILE:HD12	1:A:192:ILE:N	2.27	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:VAL:HG13	1:B:250:TYR:HE2	1.77	0.50
1:B:120:TYR:HB2	1:B:121:PRO:HD2	1.94	0.50
1:B:127:VAL:CG1	1:B:422:ARG:HB2	2.40	0.50
1:A:20:ARG:HG3	1:A:20:ARG:HH11	1.77	0.49
1:B:266:GLY:O	1:B:270:GLN:HB2	2.12	0.49
1:B:441:ILE:HG22	1:B:447:ARG:HA	1.94	0.49
1:B:498:VAL:HG22	1:B:503:PHE:CE1	2.48	0.49
1:B:192:ILE:HD12	1:B:192:ILE:H	1.77	0.49
1:B:145:LYS:HD3	1:B:485:PRO:O	2.12	0.49
1:B:81:THR:O	1:B:84:GLN:HG2	2.13	0.48
1:B:2:ASN:CB	1:B:5:ASP:OD2	2.62	0.48
1:A:105:VAL:CG1	1:A:250:TYR:HE2	2.26	0.48
1:B:49:PHE:CZ	1:B:53:ILE:CG1	2.94	0.48
1:B:422:ARG:O	1:B:426:MET:HG2	2.13	0.48
1:B:26:GLU:H	1:B:29:GLN:NE2	2.07	0.48
1:B:212:GLU:HB2	1:B:215:LYS:HB3	1.95	0.48
1:A:166:THR:HG21	1:A:171:MET:HA	1.95	0.48
1:B:397:VAL:HG21	1:B:402:GLU:CD	2.34	0.48
1:B:166:THR:HG23	1:B:195:GLN:HG3	1.95	0.47
1:A:199:LEU:HG	1:A:221:ASP:HB3	1.96	0.47
1:B:105:VAL:HG21	1:B:259:VAL:HG12	1.97	0.47
1:B:131:SER:HB3	1:B:482:GLU:OE1	2.15	0.47
1:B:367:LEU:C	1:B:368:ILE:HD12	2.35	0.47
1:A:270:GLN:HE21	1:A:270:GLN:HB3	1.49	0.47
1:A:362:ASP:OD1	1:A:366:GLN:HB2	2.15	0.47
1:B:372:LYS:HZ3	1:B:372:LYS:CB	2.24	0.47
1:A:274:ASP:HA	1:A:334:THR:HG23	1.95	0.47
1:A:20:ARG:HD2	1:A:21:PHE:CZ	2.49	0.47
1:A:144:LEU:O	1:A:148:GLN:HG3	2.14	0.47
1:B:239:MET:HB2	1:B:239:MET:HE2	1.78	0.47
1:B:517:LEU:O	1:B:518:VAL:CB	2.63	0.46
1:A:423:HIS:HB3	3:A:963:HOH:O	2.14	0.46
1:A:303:GLU:HG2	1:B:453:ARG:HH12	1.81	0.46
1:A:53:ILE:HD13	1:A:53:ILE:HA	1.68	0.46
1:A:453:ARG:CD	1:A:456:THR:HG22	2.42	0.46
1:A:443:GLU:CB	1:B:372:LYS:HD2	2.41	0.46
1:B:47:PHE:CE2	1:B:51:LYS:HE3	2.51	0.46
1:B:371:ASP:OD1	1:B:372:LYS:HG2	2.16	0.46
1:B:47:PHE:CZ	1:B:51:LYS:HE3	2.51	0.46
1:A:84:GLN:HA	1:A:87:LEU:HG	1.98	0.46
1:A:454:SER:O	1:A:455:ALA:C	2.55	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:ARG:NH1	3:A:1044:HOH:O	2.48	0.46
1:B:120:TYR:HB2	1:B:121:PRO:CD	2.46	0.45
1:A:456:THR:OG1	1:B:356:LYS:NZ	2.46	0.45
1:A:507:LEU:HD23	1:A:508:ILE:N	2.31	0.45
1:A:121:PRO:HB2	1:A:124:MET:HE3	1.99	0.45
1:A:358:ILE:O	1:A:374:ASN:ND2	2.50	0.45
1:B:2:ASN:ND2	1:B:3:ILE:H	2.09	0.45
1:A:3:ILE:HD12	1:A:22:TRP:CE2	2.52	0.44
1:B:107:LEU:HD13	1:B:250:TYR:CE1	2.51	0.44
1:B:107:LEU:HD11	1:B:252:VAL:HB	1.98	0.44
1:B:245:TRP:CZ3	1:B:336:PRO:HG2	2.52	0.44
1:A:200:PRO:HB2	1:A:208:ILE:HG23	1.99	0.44
1:A:265:ILE:O	1:A:269:ILE:HG12	2.16	0.44
1:B:278:LYS:CG	1:B:328:ILE:HD11	2.38	0.44
1:B:333:PHE:CE2	1:B:385:ILE:HD11	2.52	0.44
1:B:2:ASN:ND2	3:B:1005:HOH:O	2.47	0.44
1:A:362:ASP:OD1	1:A:368:ILE:HD11	2.16	0.44
1:A:417:ASN:HB2	1:A:418:PRO:CD	2.48	0.44
1:A:510:ASP:HB2	1:A:511:GLU:OE1	2.17	0.44
1:B:267:PHE:CE2	1:B:393:VAL:CG1	3.01	0.44
1:A:254:ASN:ND2	1:A:404:SER:H	2.16	0.44
1:B:132:ARG:NH1	1:B:132:ARG:CG	2.75	0.44
1:A:90:TRP:O	1:A:266:GLY:HA3	2.18	0.44
1:A:142:ARG:HD3	3:A:956:HOH:O	2.17	0.43
1:B:52:ALA:HB1	1:B:353:VAL:CG2	2.48	0.43
1:B:57:ASN:C	1:B:58:GLN:CG	2.86	0.43
1:B:140:ALA:HB2	1:B:162:TRP:CZ3	2.52	0.43
1:B:172:GLU:HG2	1:B:176:GLU:OE2	2.18	0.43
1:A:46:ASN:O	1:A:50:GLN:HG3	2.18	0.43
1:B:142:ARG:HD3	3:B:914:HOH:O	2.18	0.43
1:A:355:GLN:HE21	1:A:355:GLN:HB2	1.67	0.43
1:B:135:LEU:HD21	1:B:255:ILE:HD12	2.01	0.43
1:A:3:ILE:HD12	1:A:22:TRP:CZ2	2.54	0.43
1:A:454:SER:C	1:A:456:THR:N	2.72	0.43
1:B:11:SER:HA	1:B:16:GLU:HG3	2.01	0.43
1:B:101:ASN:OD1	1:B:158:CYS:HA	2.19	0.43
1:B:516:GLU:C	1:B:518:VAL:N	2.71	0.43
1:A:72:VAL:HB	1:A:73:PRO:HD2	1.99	0.43
1:B:127:VAL:HG13	1:B:127:VAL:O	2.19	0.42
1:B:282:LYS:HE2	1:B:284:ASN:O	2.19	0.42
1:A:159:ILE:HD12	1:A:190:ASN:ND2	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:GLU:CG	1:B:176:GLU:OE2	2.68	0.42
1:B:17:HIS:HB2	1:B:20:ARG:HH12	1.83	0.42
1:A:121:PRO:HD2	1:A:124:MET:HE1	2.00	0.42
1:B:57:ASN:O	1:B:58:GLN:CB	2.67	0.42
1:B:274:ASP:HA	1:B:334:THR:HG23	2.01	0.42
1:A:5:ASP:O	1:A:9:THR:CG2	2.68	0.42
1:A:70:GLU:OE2	1:A:294:ARG:NH2	2.53	0.42
1:A:188:LYS:HD3	1:A:188:LYS:C	2.40	0.42
1:B:93:GLU:OE1	1:B:270:GLN:NE2	2.53	0.42
1:A:121:PRO:HG3	1:A:170:THR:HB	2.02	0.42
1:B:64:ASN:CG	1:B:64:ASN:O	2.59	0.42
1:B:96:PHE:HE1	1:B:100:GLN:NE2	2.18	0.42
1:B:487:ILE:HG13	1:B:509:ILE:HG22	2.02	0.42
1:A:8:LEU:O	1:A:12:LYS:HG3	2.19	0.41
1:A:358:ILE:HB	1:A:374:ASN:HD22	1.85	0.41
1:B:100:GLN:O	1:B:101:ASN:HB2	2.21	0.41
1:B:366:GLN:O	1:B:368:ILE:HD13	2.20	0.41
1:A:258:LYS:HD3	1:A:402:GLU:CD	2.41	0.41
1:B:438:GLY:HA3	1:B:498:VAL:HG13	2.02	0.41
1:A:146:LEU:HD23	1:A:146:LEU:HA	1.96	0.41
1:A:318:ASP:OD1	1:A:320:ARG:HG2	2.21	0.41
1:A:477:VAL:HB	1:A:478:PRO:O	2.20	0.41
1:B:417:ASN:HB2	1:B:418:PRO:CD	2.50	0.41
1:A:101:ASN:HB3	3:A:945:HOH:O	2.21	0.41
1:A:410:ASP:HB3	1:A:413:ASN:HD21	1.86	0.41
1:B:96:PHE:HE1	1:B:100:GLN:HE21	1.63	0.41
1:B:107:LEU:HD11	1:B:252:VAL:CB	2.51	0.41
1:B:151:GLU:CD	1:B:157:LYS:HD3	2.40	0.41
1:B:171:MET:CB	1:B:195:GLN:NE2	2.84	0.41
1:B:98:ILE:HD13	1:B:160:ILE:HD11	2.02	0.41
1:A:454:SER:HB3	1:B:411:SER:CB	2.50	0.40
1:A:121:PRO:HD2	1:A:124:MET:CE	2.52	0.40
1:A:146:LEU:HD11	1:A:489:TYR:CZ	2.56	0.40
1:A:6:LEU:HA	1:A:9:THR:HG23	2.01	0.40
1:B:135:LEU:CD2	1:B:255:ILE:HD12	2.51	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	472/522 (90%)	452 (96%)	17 (4%)	3 (1%)	25 36
1	B	478/522 (92%)	442 (92%)	35 (7%)	1 (0%)	47 62
All	All	950/1044 (91%)	894 (94%)	52 (6%)	4 (0%)	34 48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	478	PRO
1	A	55	GLY
1	A	111	GLY
1	A	454	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	410/447 (92%)	386 (94%)	24 (6%)	19 32
1	B	412/447 (92%)	372 (90%)	40 (10%)	8 12
All	All	822/894 (92%)	758 (92%)	64 (8%)	12 19

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	9	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	38	GLN
1	A	53	ILE
1	A	68	ARG
1	A	77	LEU
1	A	81	THR
1	A	84	GLN
1	A	233	GLN
1	A	252	VAL
1	A	254	ASN
1	A	270	GLN
1	A	279	VAL
1	A	289	VAL
1	A	291	VAL
1	A	307	ILE
1	A	320	ARG
1	A	322	LEU
1	A	359	PRO
1	A	391	LYS
1	A	406	LEU
1	A	408	ASN
1	A	419	THR
1	A	507	LEU
1	B	2	ASN
1	B	3	ILE
1	B	6	LEU
1	B	31	VAL
1	B	51	LYS
1	B	53	ILE
1	B	58	GLN
1	B	84	GLN
1	B	101	ASN
1	B	105	VAL
1	B	112	GLN
1	B	126	ASP
1	B	127	VAL
1	B	153	TYR
1	B	166	THR
1	B	211	GLU
1	B	226	LEU
1	B	233	GLN
1	B	269	ILE
1	B	270	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	280	VAL
1	B	300	GLN
1	B	320	ARG
1	B	322	LEU
1	B	339	ARG
1	B	343	ASN
1	B	346	GLU
1	B	355	GLN
1	B	372	LYS
1	B	393	VAL
1	B	397	VAL
1	B	419	THR
1	B	423	HIS
1	B	426	MET
1	B	442	ASP
1	B	443	GLU
1	B	446	SER
1	B	492	GLU
1	B	498	VAL
1	B	502	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	30	GLN
1	A	38	GLN
1	A	50	GLN
1	A	84	GLN
1	A	148	GLN
1	A	254	ASN
1	A	270	GLN
1	A	355	GLN
1	A	374	ASN
1	A	413	ASN
1	A	504	HIS
1	B	2	ASN
1	B	29	GLN
1	B	38	GLN
1	B	58	GLN
1	B	64	ASN
1	B	84	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	195	GLN
1	B	233	GLN
1	B	300	GLN
1	B	412	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 monosaccharides in this entry.

5.6 Ligand geometry

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	UD1	B	902	-	40,41,41	2.24	11 (27%)	59,62,62	1.35	9 (15%)
2	UD1	A	901	-	40,41,41	2.04	8 (20%)	59,62,62	1.53	11 (18%)

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	UD1	B	902	-	-	5/26/63/63	0/3/3/3
2	UD1	A	901	-	-	2/26/63/63	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	902	UD1	PA-O3A	-9.54	1.49	1.59
2	A	901	UD1	PA-O3A	-7.00	1.51	1.59
2	A	901	UD1	PB-O3A	-6.38	1.52	1.59
2	B	902	UD1	PB-O3A	-5.13	1.54	1.59
2	B	902	UD1	C6-N1	4.65	1.49	1.38
2	A	901	UD1	C6-N1	4.14	1.48	1.38
2	B	902	UD1	C4-N3	-2.76	1.33	1.38
2	A	901	UD1	C2-N3	-2.70	1.33	1.38
2	A	901	UD1	PB-O2B	-2.52	1.43	1.55
2	B	902	UD1	C4'-C5'	2.47	1.58	1.53
2	A	901	UD1	C5-C4	2.46	1.49	1.43
2	A	901	UD1	C4'-C5'	2.43	1.58	1.53
2	A	901	UD1	C4-N3	-2.40	1.34	1.38
2	B	902	UD1	C2-N3	-2.35	1.33	1.38
2	B	902	UD1	PB-O2B	-2.26	1.44	1.55
2	B	902	UD1	C2'-N2'	2.17	1.49	1.45
2	B	902	UD1	PA-O2A	-2.08	1.45	1.55
2	B	902	UD1	C5-C4	2.04	1.48	1.43
2	B	902	UD1	PA-O5B	-2.02	1.51	1.59

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	901	UD1	O5'-C1'-O1'	4.50	117.24	111.36
2	B	902	UD1	O5'-C1'-O1'	4.04	116.64	111.36
2	A	901	UD1	O1'-C1'-C2'	-3.97	101.23	108.40
2	A	901	UD1	C4'-C3'-C2'	-3.30	105.60	110.40
2	A	901	UD1	O2-C2-N3	-2.96	116.04	121.49
2	B	902	UD1	C5-C4-N3	2.83	118.76	114.80
2	B	902	UD1	C4'-C3'-C2'	-2.73	106.42	110.40
2	A	901	UD1	C5-C4-N3	2.66	118.53	114.80
2	A	901	UD1	O2-C2-N1	2.61	126.19	122.80
2	B	902	UD1	C1'-C2'-N2'	-2.53	106.67	110.92
2	A	901	UD1	O2A-PA-O3A	2.48	113.98	107.27
2	A	901	UD1	C2'-N2'-C7'	-2.47	117.33	123.11
2	A	901	UD1	O4-C4-C5	-2.44	120.95	125.16
2	B	902	UD1	O4-C4-C5	-2.43	120.97	125.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	902	UD1	O2-C2-N3	-2.40	117.06	121.49
2	A	901	UD1	C1'-C2'-N2'	-2.38	106.92	110.92
2	B	902	UD1	O1'-C1'-C2'	-2.30	104.23	108.40
2	A	901	UD1	N3-C2-N1	2.21	117.77	114.89
2	B	902	UD1	N3-C2-N1	2.20	117.76	114.89
2	B	902	UD1	C1'-O5'-C5'	2.07	117.75	113.72

There are no chirality outliers.

All (7) torsion outliers are listed below:

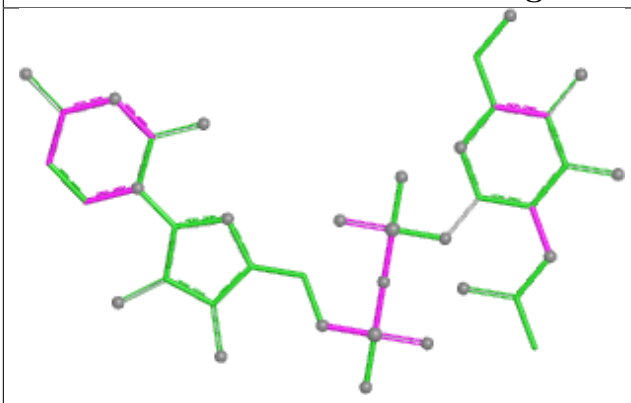
Mol	Chain	Res	Type	Atoms
2	A	901	UD1	C1'-O1'-PB-O3A
2	B	902	UD1	C3B-C4B-C5B-O5B
2	B	902	UD1	O4B-C4B-C5B-O5B
2	B	902	UD1	C5B-O5B-PA-O2A
2	A	901	UD1	C5B-O5B-PA-O1A
2	B	902	UD1	C5B-O5B-PA-O1A
2	B	902	UD1	C5B-O5B-PA-O3A

There are no ring outliers.

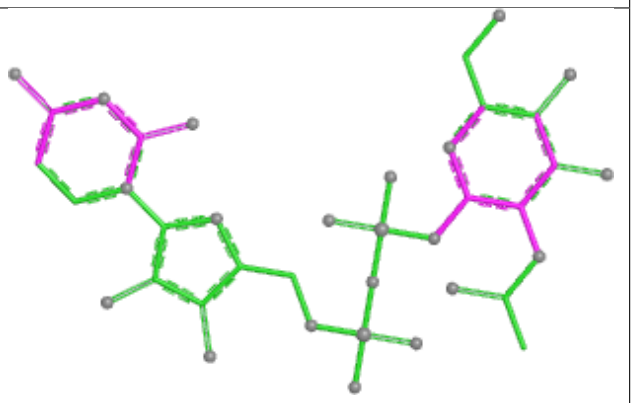
No monomer is involved in short contacts.

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.

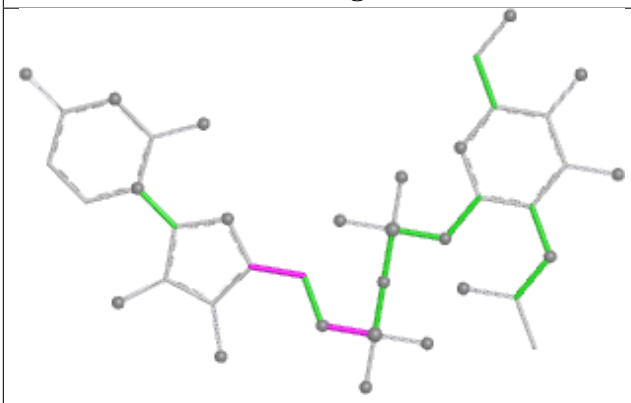
Ligand UD1 B 902



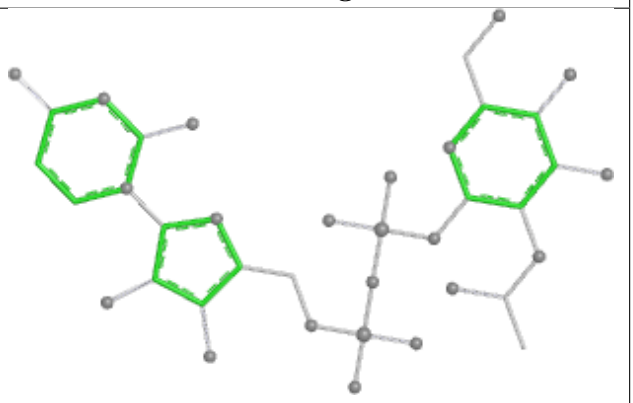
Bond lengths



Bond angles

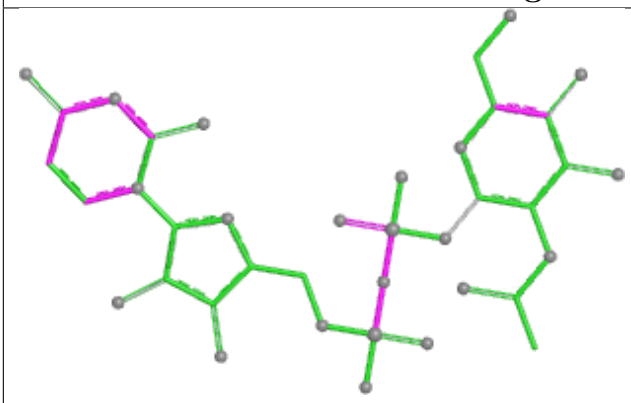


Torsions

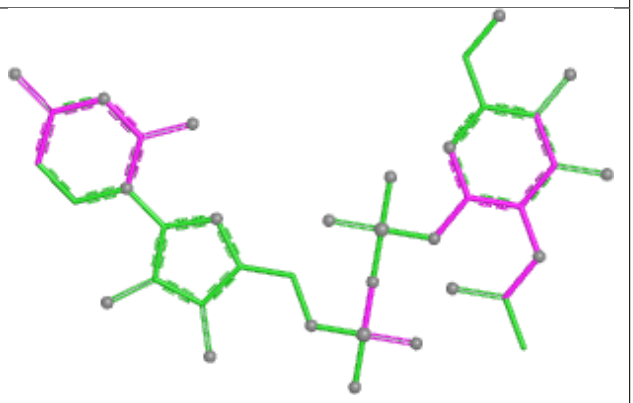


Rings

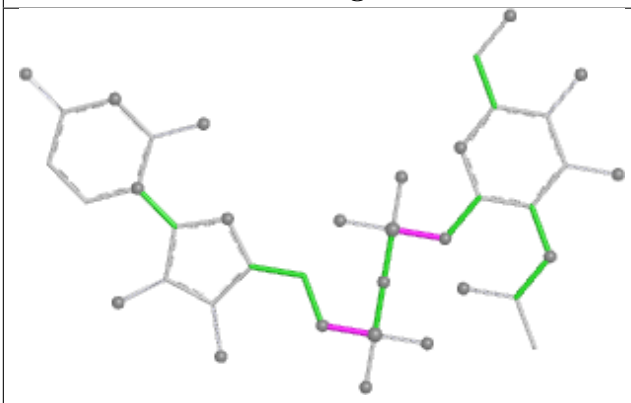
Ligand UD1 A 901



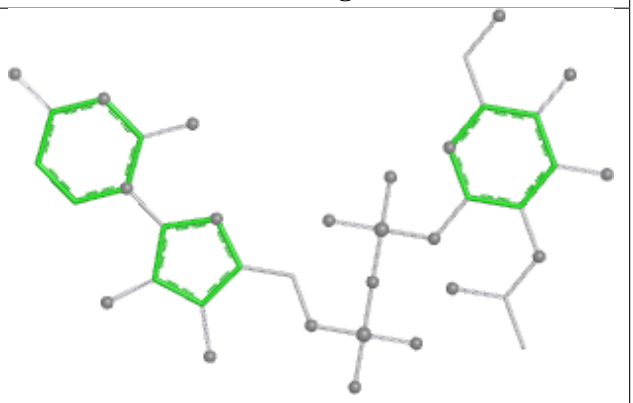
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	480/522 (91%)	-0.14	17 (3%)	44	43	17, 33, 64, 75	0
1	B	486/522 (93%)	-0.08	17 (3%)	44	43	20, 40, 62, 75	0
All	All	966/1044 (92%)	-0.11	34 (3%)	44	43	17, 36, 63, 75	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	456	THR	6.1
1	B	518	VAL	5.4
1	A	455	ALA	5.0
1	A	120	TYR	4.8
1	A	454	SER	4.5
1	B	28	ALA	4.5
1	B	5	ASP	3.7
1	B	64	ASN	3.4
1	B	154	TYR	3.3
1	A	169	ARG	3.2
1	A	119	ALA	3.2
1	B	3	ILE	3.1
1	A	112	GLN	3.1
1	B	2	ASN	3.1
1	A	4	ASN	3.1
1	B	114	THR	3.0
1	B	409	ALA	2.6
1	A	412	GLN	2.6
1	A	54	GLU	2.5
1	B	27	GLU	2.5
1	B	113	GLY	2.5
1	B	58	GLN	2.4
1	A	249	VAL	2.4
1	A	111	GLY	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	5	ASP	2.3
1	B	4	ASN	2.2
1	A	35	ALA	2.2
1	B	153	TYR	2.2
1	B	477	VAL	2.2
1	A	56	PHE	2.2
1	A	2	ASN	2.2
1	B	172	GLU	2.2
1	B	56	PHE	2.1
1	A	118	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

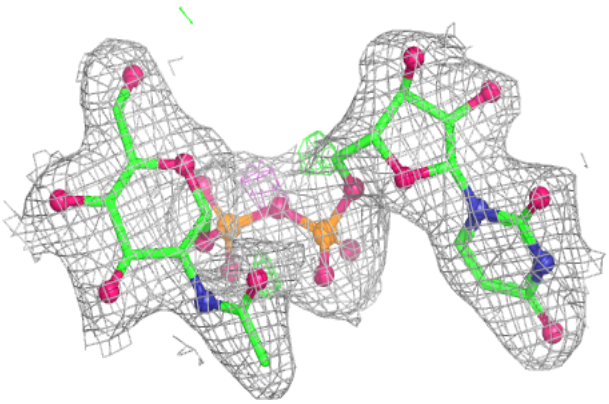
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

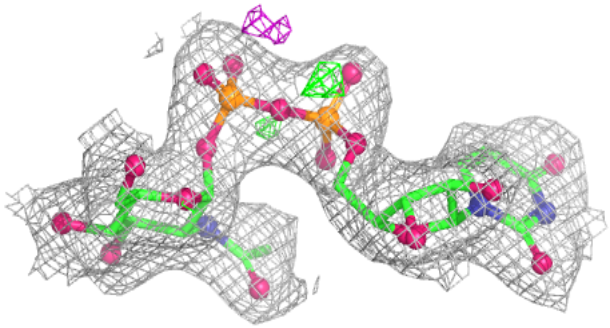
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	UD1	A	901	39/39	0.96	0.13	22,29,44,46	0
2	UD1	B	902	39/39	0.96	0.13	25,35,46,46	0

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 UD1 A 901:

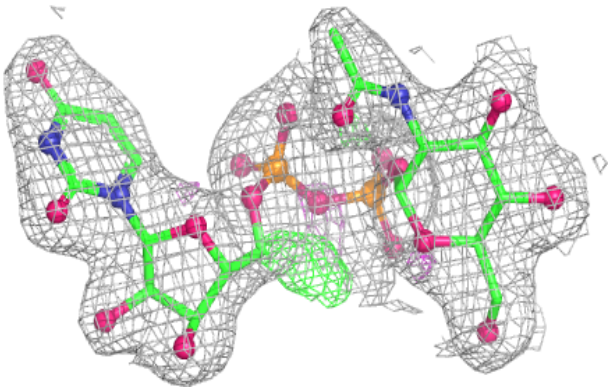
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

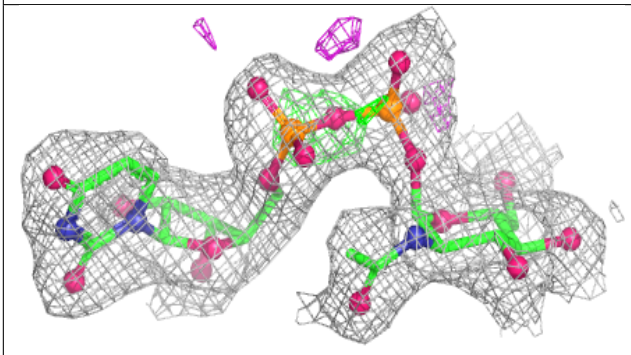


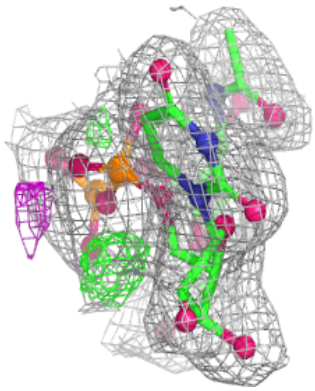


Electron density around UD1 B 902:

$2mF_o$-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.