Full wwPDB X-ray Structure Validation Report (i)

Oct 18, 2023 – 02:55 PM EDT

PDB ID	:	1JVG
Title	:	CRYSTAL STRUCTURE OF HUMAN AGX2 COMPLEXED WITH UDP-GALNAC
Authors	:	Peneff, C.; Bourne, Y.
Deposited on	:	2001-08-30
Resolution	:	2.30 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
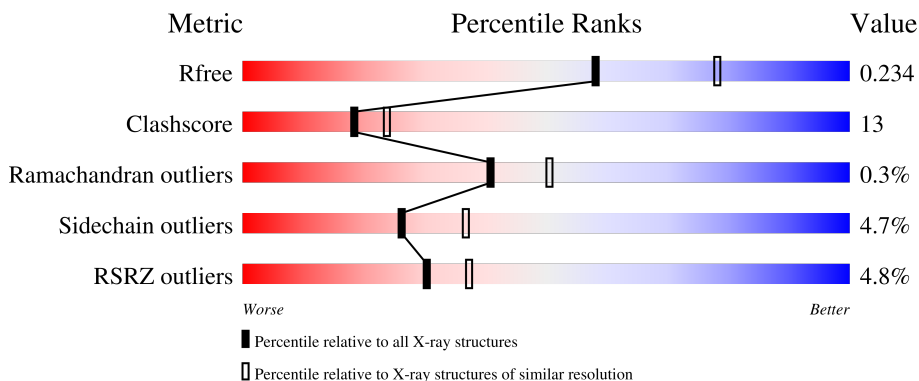http://www.wwpdb.org/validation/2017/FAQs#types.

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1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.30 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	Percentile Ranks	Value
Rfree		0.234
Clashscore		13
Ramachandran outliers		0.3%
Sidechain outliers		4.7%
RSRZ outliers		4.8%

Worse — *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	2% / 71% / 19% / • / 7%
1	B	522	7% / 64% / 24% / • / 8%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 8040 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 GLCNAC1P URIDYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total 3851	C 2467	N 654	O 712	S 18	0	1	0
1	B	480	Total 3803	C 2439	N 643	O 703	S 18	0	0	0

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-ACETYLGALACTOSAMINE (three-letter code: UD2) (formula: $C_{17}H_{27}N_3O_{17}P_2$).
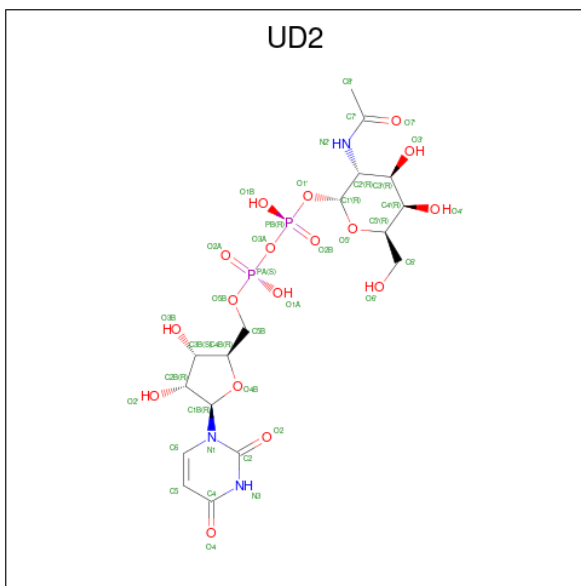
| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
2	B	1	Total	C	N	O	P	0	0
			39	17	3	17	2		

- Molecule 3 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	183	Total	O	0	0
			183	183		
3	B	125	Total	O	0	0
			125	125		

3 Residue-property plots ⓘ

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: GLCNAC1P URIDYLTRANSFERASE
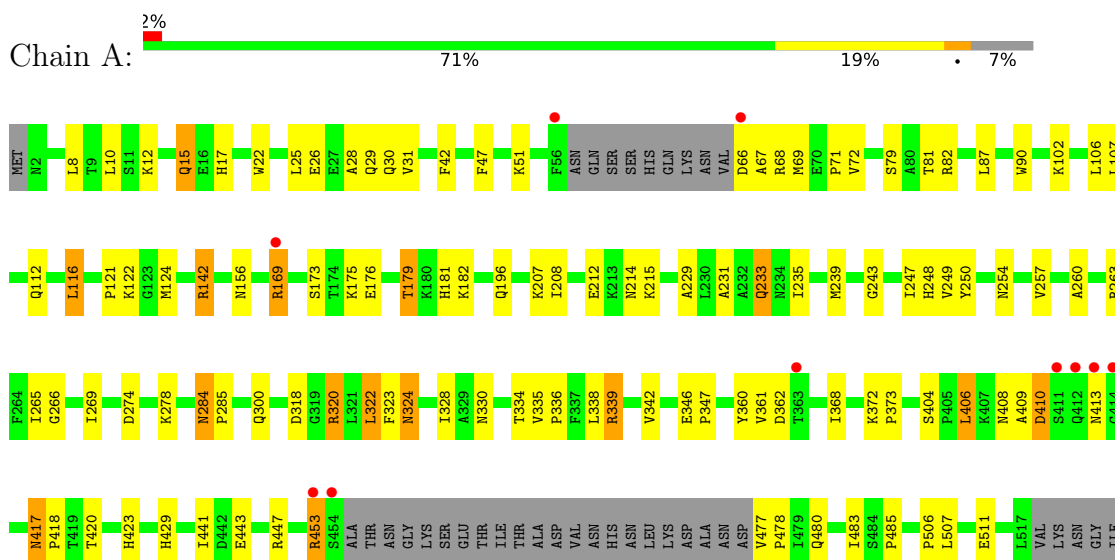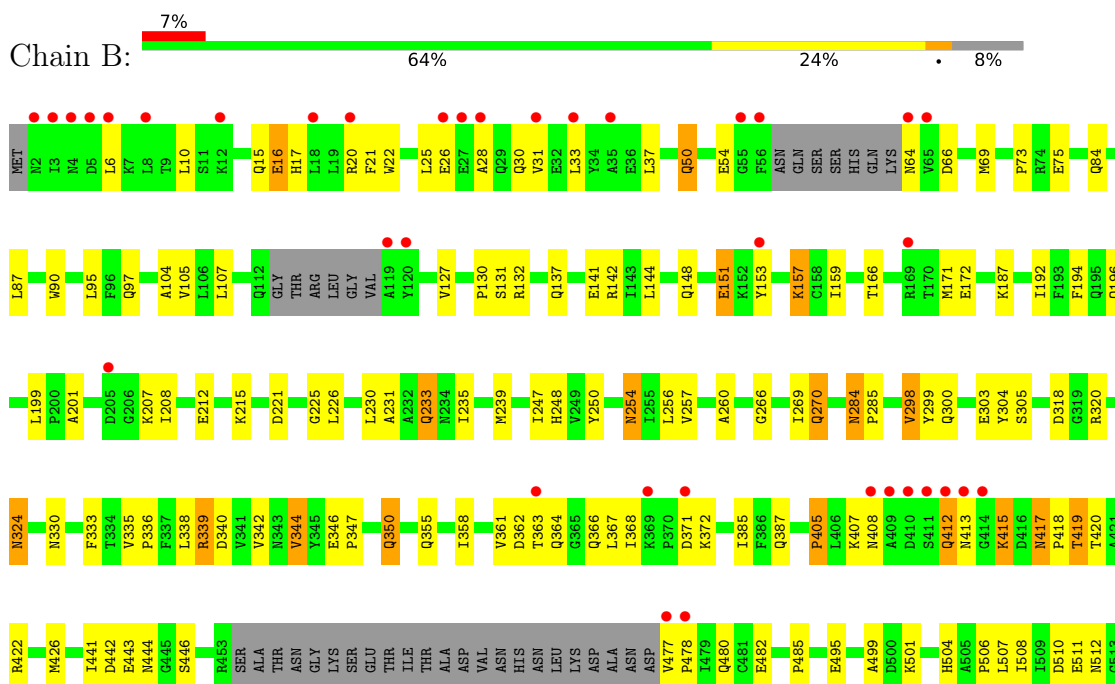
- Molecule 1: GLCNAC1P URIDYLTRANSFERASE

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	85.58Å 71.78Å 93.56Å 90.00° 94.01° 90.00°	Depositor
Resolution (Å)	19.94 – 2.30 19.94 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.4 (19.94-2.30) 97.6 (19.94-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 1.90Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.201 , 0.240 0.195 , 0.234	Depositor DCC
R_{free} test set	3469 reflections (3.99%)	wwPDB-VP
Wilson B-factor (Å^2)	27.0	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 53.7	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8040	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: UD2

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	0.60	0/3940	0.70	3/5324 (0.1%)
1	B	0.54	0/3887	0.63	0/5254
All	All	0.57	0/7827	0.67	3/10578 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	142	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	A	453[A]	ARG	CB-CA-C	5.42	121.25	110.40
1	A	453[B]	ARG	CB-CA-C	5.42	121.25	110.40

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	3851	0	3800	93	0
1	B	3803	0	3743	117	0
2	A	39	0	24	0	0
2	B	39	0	25	1	0
3	A	183	0	0	4	0
3	B	125	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8040	0	7592	203	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 13.

All (203) 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:15:GLN:NE2	1:A:208:ILE:H	1.66	0.93
1:B:20:ARG:HH21	1:B:363:THR:HA	1.36	0.91
1:A:239:MET:HE3	1:A:335:VAL:HG22	1.54	0.89
1:A:26:GLU:H	1:A:29:GLN:HE21	1.16	0.88
1:A:239:MET:CE	1:A:335:VAL:HG22	2.06	0.85
1:B:15:GLN:HE22	1:B:207:LYS:HA	1.45	0.82
1:A:443:GLU:HB3	1:B:372:LYS:HD2	1.63	0.79
1:A:453[B]:ARG:HH11	1:A:453[B]:ARG:HB2	1.47	0.79
1:B:64:ASN:ND2	1:B:66:ASP:HB2	1.98	0.79
1:B:212:GLU:HB2	1:B:215:LYS:HB3	1.65	0.79
1:B:15:GLN:NE2	1:B:208:ILE:H	1.81	0.78
1:A:175:LYS:O	1:A:179:THR:HG22	1.85	0.76
1:A:47:PHE:CE1	1:A:51:LYS:HE2	2.22	0.75
1:A:284:ASN:HD22	1:A:285:PRO:HD2	1.54	0.72
1:A:72:VAL:HG22	3:A:1930:HOH:O	1.88	0.72
1:B:20:ARG:NH2	1:B:363:THR:HA	2.04	0.72
1:B:417:ASN:ND2	1:B:420:THR:H	1.87	0.72
1:A:28:ALA:O	1:A:31:VAL:HG12	1.89	0.71
1:A:429:HIS:CD2	1:A:483:ILE:H	2.08	0.71
1:B:15:GLN:HG2	1:B:208:ILE:HD12	1.71	0.71
1:A:112:GLN:HB2	1:A:169:ARG:NH1	2.06	0.71
1:A:116:LEU:HD11	1:A:406:LEU:HD22	1.71	0.70
1:A:15:GLN:HE22	1:A:208:ILE:H	1.40	0.69
1:A:248:HIS:HD1	1:A:260:ALA:H	1.39	0.68
1:A:87:LEU:HD22	1:A:263:ARG:HD3	1.75	0.68
1:A:284:ASN:HD22	1:A:285:PRO:CD	2.06	0.68
1:A:8:LEU:HG	1:A:12:LYS:HE3	1.75	0.67
1:A:423:HIS:CD2	1:B:413:ASN:HB3	2.30	0.67
1:B:417:ASN:ND2	1:B:419:THR:HG23	2.09	0.67
1:A:124:MET:HE1	1:A:173:SER:HB3	1.77	0.66
1:B:64:ASN:HD22	1:B:66:ASP:HB2	1.61	0.65
1:B:417:ASN:HD22	1:B:417:ASN:C	2.00	0.64
1:B:248:HIS:HD1	1:B:260:ALA:H	1.44	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:PRO:HB2	1:B:508:ILE:HD11	1.80	0.64
1:A:408:ASN:HB3	1:A:413:ASN:HD22	1.63	0.64
1:B:442:ASP:OD2	1:B:446:SER:HB2	1.98	0.63
1:B:15:GLN:HE21	1:B:17:HIS:HE1	1.46	0.63
1:A:429:HIS:HD2	1:A:483:ILE:H	1.45	0.62
1:B:84:GLN:HA	1:B:87:LEU:HG	1.81	0.62
1:A:409:ALA:O	1:A:410:ASP:HB2	2.00	0.62
1:A:26:GLU:O	1:A:30:GLN:HG2	2.00	0.62
1:B:235:ILE:HG22	1:B:239:MET:HE3	1.83	0.60
1:B:26:GLU:O	1:B:30:GLN:HG3	2.00	0.60
1:B:340:ASP:O	1:B:344:VAL:HB	2.01	0.60
1:A:66:ASP:HA	1:A:69:MET:HE2	1.83	0.59
1:A:346:GLU:HB3	1:A:347:PRO:HD3	1.84	0.59
1:A:121:PRO:HD2	1:A:124:MET:HE1	1.84	0.59
1:B:97:GLN:HG3	1:B:269:ILE:CD1	2.32	0.59
1:B:324:ASN:H	1:B:324:ASN:HD22	1.50	0.59
1:B:22:TRP:CH2	1:B:30:GLN:HB3	2.37	0.59
1:B:166:THR:HG21	1:B:171:MET:SD	2.43	0.59
1:A:15:GLN:HE22	1:A:207:LYS:HA	1.67	0.59
1:B:408:ASN:O	1:B:412:GLN:HG3	2.03	0.58
1:A:453[A]:ARG:HG3	1:B:305:SER:HB3	1.85	0.58
1:A:408:ASN:HB3	1:A:413:ASN:HB2	1.84	0.58
1:A:22:TRP:CH2	1:A:30:GLN:HB2	2.39	0.57
1:B:159:ILE:HD11	3:B:1993:HOH:O	2.03	0.57
1:A:278:LYS:HG2	1:A:328:ILE:HD11	1.86	0.57
1:B:284:ASN:HD22	1:B:285:PRO:HD2	1.69	0.57
1:B:335:VAL:HB	1:B:336:PRO:HD3	1.86	0.57
1:A:121:PRO:HD2	1:A:124:MET:CE	2.35	0.56
1:A:107:LEU:HD13	1:A:250:TYR:CE1	2.41	0.56
1:B:415:LYS:H	1:B:415:LYS:HD3	1.70	0.56
1:B:318:ASP:CG	1:B:320:ARG:HD2	2.25	0.56
1:A:26:GLU:HG3	1:A:29:GLN:NE2	2.21	0.56
1:B:506:PRO:HG2	1:B:517:LEU:HB2	1.88	0.56
1:B:235:ILE:HG22	1:B:239:MET:CE	2.36	0.55
1:A:373:PRO:HD2	1:B:444:ASN:ND2	2.22	0.55
1:B:284:ASN:HD22	1:B:285:PRO:CD	2.19	0.55
1:B:33:LEU:O	1:B:37:LEU:HG	2.06	0.55
1:A:362:ASP:OD1	1:A:368:ILE:HD11	2.07	0.55
1:A:408:ASN:HB3	1:A:413:ASN:ND2	2.21	0.55
1:B:142:ARG:HG2	1:B:485:PRO:HB3	1.88	0.55
1:B:362:ASP:OD2	1:B:366:GLN:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:PRO:HB2	1:B:75:GLU:HG2	1.90	0.54
1:B:144:LEU:O	1:B:148:GLN:HG3	2.08	0.54
1:B:50:GLN:O	1:B:54:GLU:HG3	2.08	0.53
1:B:417:ASN:HD21	1:B:420:THR:HG23	1.73	0.53
1:B:151:GLU:HG3	1:B:157:LYS:HA	1.90	0.53
1:A:233:GLN:HB2	1:A:235:ILE:HG12	1.91	0.52
1:B:21:PHE:O	1:B:25:LEU:HG	2.08	0.52
1:B:66:ASP:HA	1:B:69:MET:CE	2.39	0.52
1:B:318:ASP:OD2	1:B:320:ARG:HD2	2.10	0.52
1:B:127:VAL:HG13	1:B:418:PRO:O	2.08	0.52
1:A:417:ASN:HB2	1:A:418:PRO:CD	2.40	0.52
1:B:441:ILE:HG13	1:B:504:HIS:CD2	2.45	0.52
1:B:417:ASN:HD21	1:B:419:THR:HG23	1.72	0.52
1:A:318:ASP:OD1	1:A:320:ARG:HG2	2.09	0.51
1:A:112:GLN:HB2	1:A:169:ARG:CZ	2.40	0.51
1:A:254:ASN:ND2	1:A:404:SER:H	2.07	0.51
1:B:132:ARG:HG2	1:B:132:ARG:HH11	1.76	0.51
1:B:127:VAL:HG12	1:B:422:ARG:HB2	1.91	0.51
1:A:453[A]:ARG:HG2	1:B:304:TYR:CE1	2.45	0.51
1:A:10:LEU:HD21	1:A:42:PHE:CZ	2.45	0.51
1:A:15:GLN:NE2	1:A:17:HIS:HE1	2.09	0.51
1:B:231:ALA:HB2	1:B:342:VAL:HG13	1.93	0.51
1:A:410:ASP:HA	1:A:417:ASN:HB2	1.93	0.51
1:A:477:VAL:N	1:A:478:PRO:HA	2.26	0.51
1:B:28:ALA:O	1:B:31:VAL:HG12	2.11	0.50
1:B:196:GLN:HE22	2:B:1902:UD2:HN3	1.60	0.50
1:B:257:VAL:HG23	1:B:330:ASN:HD21	1.77	0.50
1:B:362:ASP:OD1	1:B:364:GLN:N	2.44	0.49
1:B:417:ASN:HD22	1:B:420:THR:H	1.60	0.49
1:B:495:GLU:H	1:B:495:GLU:CD	2.14	0.49
1:A:324:ASN:C	1:A:324:ASN:HD22	2.16	0.49
1:A:231:ALA:HB2	1:A:342:VAL:HG13	1.94	0.49
1:B:15:GLN:NE2	1:B:207:LYS:HA	2.22	0.49
1:A:417:ASN:C	1:A:417:ASN:HD22	2.16	0.48
1:A:71:PRO:HG3	1:A:322:LEU:HD22	1.95	0.48
1:B:367:LEU:C	1:B:368:ILE:HD12	2.32	0.48
1:A:212:GLU:HB2	1:A:215:LYS:HB3	1.95	0.48
1:A:284:ASN:ND2	1:A:285:PRO:HD2	2.26	0.48
1:A:417:ASN:ND2	1:A:420:THR:H	2.12	0.48
1:B:405:PRO:HB2	1:B:407:LYS:HE2	1.94	0.48
1:A:453[B]:ARG:HH11	1:A:453[B]:ARG:CB	2.23	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:ASN:HD22	1:B:285:PRO:N	2.12	0.48
1:B:127:VAL:HG12	1:B:127:VAL:O	2.14	0.47
1:A:102:LYS:HE3	1:A:243:GLY:O	2.14	0.47
1:A:480:GLN:O	1:A:506:PRO:HA	2.14	0.47
1:B:270:GLN:HG2	3:B:2004:HOH:O	2.15	0.47
1:B:107:LEU:HD13	1:B:250:TYR:CE1	2.50	0.47
1:B:415:LYS:HD3	1:B:415:LYS:N	2.30	0.46
1:B:194:PHE:HB2	1:B:233:GLN:HG3	1.97	0.46
1:B:339:ARG:HG2	1:B:339:ARG:HH11	1.79	0.46
1:A:239:MET:HE1	1:A:338:LEU:HD12	1.97	0.46
1:A:408:ASN:CB	1:A:413:ASN:HB2	2.45	0.46
1:B:127:VAL:CG1	1:B:422:ARG:HB2	2.46	0.46
1:B:346:GLU:HB3	1:B:347:PRO:HD3	1.96	0.46
1:A:336:PRO:O	1:A:339:ARG:HB3	2.16	0.46
1:A:441:ILE:HG22	1:A:447:ARG:HA	1.97	0.46
1:B:333:PHE:CE2	1:B:385:ILE:HD11	2.50	0.46
1:A:274:ASP:HA	1:A:334:THR:HG23	1.97	0.46
1:A:26:GLU:HG3	1:A:29:GLN:HE21	1.79	0.46
1:A:66:ASP:C	1:A:68:ARG:H	2.20	0.46
1:B:226:LEU:O	1:B:230:LEU:HG	2.16	0.46
1:A:372:LYS:HG2	1:B:443:GLU:CG	2.46	0.45
1:B:507:LEU:HD11	1:B:514:VAL:HG13	1.99	0.45
1:B:199:LEU:HG	1:B:221:ASP:HB3	1.98	0.45
1:B:192:ILE:N	1:B:192:ILE:HD12	2.31	0.45
1:A:25:LEU:HD22	1:A:214:ASN:HB3	1.99	0.45
1:A:300:GLN:HB2	3:A:1989:HOH:O	2.16	0.45
1:A:372:LYS:HG2	1:B:443:GLU:HG3	1.99	0.45
1:A:176:GLU:HA	1:A:179:THR:CG2	2.46	0.45
1:A:511:GLU:H	1:A:511:GLU:CD	2.20	0.45
1:A:322:LEU:HD13	1:A:323:PHE:CE1	2.52	0.45
1:B:298:VAL:HG22	1:B:387:GLN:HA	1.98	0.45
1:B:477:VAL:N	1:B:478:PRO:CA	2.80	0.45
1:B:201:ALA:HB1	1:B:358:ILE:HD13	1.98	0.45
1:B:15:GLN:NE2	1:B:17:HIS:HE1	2.14	0.44
1:B:105:VAL:CG1	1:B:250:TYR:HE2	2.30	0.44
1:B:142:ARG:HD3	3:B:1912:HOH:O	2.17	0.44
1:A:116:LEU:HD22	1:A:122:LYS:HG2	1.99	0.44
1:A:239:MET:HE1	1:A:247:ILE:HG13	2.00	0.44
1:A:142:ARG:HG2	1:A:485:PRO:HB3	1.98	0.44
1:B:284:ASN:HD22	1:B:284:ASN:C	2.20	0.44
1:B:499:ALA:O	1:B:501:LYS:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:ARG:HG2	1:B:132:ARG:NH1	2.33	0.44
1:B:137:GLN:O	1:B:141:GLU:HG3	2.17	0.44
1:B:303:GLU:OE1	1:B:303:GLU:HA	2.18	0.44
1:A:142:ARG:HD3	3:A:1944:HOH:O	2.18	0.43
1:A:265:ILE:O	1:A:269:ILE:HG12	2.18	0.43
1:B:412:GLN:O	1:B:415:LYS:HD3	2.19	0.43
1:B:417:ASN:HB2	1:B:418:PRO:HD2	2.00	0.43
1:A:66:ASP:O	1:A:67:ALA:HB3	2.18	0.43
1:B:10:LEU:HB3	1:B:16:GLU:HA	2.00	0.43
1:B:97:GLN:HG3	1:B:269:ILE:HD13	2.01	0.43
1:B:480:GLN:HB2	1:B:506:PRO:HB3	2.00	0.43
1:A:79:SER:HB3	1:A:82:ARG:HB2	2.00	0.43
1:B:131:SER:HB3	1:B:482:GLU:OE1	2.18	0.43
1:B:417:ASN:ND2	1:B:420:THR:HG23	2.33	0.43
1:B:212:GLU:C	1:B:361:VAL:HG21	2.40	0.43
1:B:221:ASP:OD1	1:B:225:GLY:HA3	2.19	0.43
1:A:360:TYR:HB2	3:A:2012:HOH:O	2.19	0.42
1:B:20:ARG:CB	1:B:20:ARG:HH11	2.31	0.42
1:B:443:GLU:H	1:B:443:GLU:CD	2.17	0.42
1:B:426:MET:HE1	1:B:480:GLN:HB3	2.00	0.42
1:B:338:LEU:O	1:B:342:VAL:HG23	2.18	0.42
1:B:350:GLN:HE21	1:B:350:GLN:HB2	1.56	0.42
1:A:181:HIS:O	1:A:182:LYS:HB2	2.20	0.42
1:A:106:LEU:HB3	1:A:249:VAL:HG22	2.00	0.42
1:A:284:ASN:HD22	1:A:285:PRO:N	2.17	0.42
1:A:284:ASN:HD22	1:A:284:ASN:C	2.23	0.42
1:B:299:TYR:C	1:B:300:GLN:HG2	2.39	0.42
1:A:196:GLN:HA	1:A:229:ALA:HB2	2.00	0.42
1:B:324:ASN:HD22	1:B:324:ASN:N	2.13	0.41
1:A:257:VAL:HG23	1:A:330:ASN:HD21	1.85	0.41
1:B:90:TRP:O	1:B:266:GLY:HA3	2.20	0.41
1:B:417:ASN:HB2	1:B:418:PRO:CD	2.50	0.41
1:A:25:LEU:HB3	1:A:29:GLN:HB2	2.03	0.41
1:A:409:ALA:O	1:A:410:ASP:CB	2.67	0.41
1:A:417:ASN:HB2	1:A:418:PRO:HD2	2.02	0.41
1:A:116:LEU:HA	1:A:116:LEU:HD12	1.87	0.41
1:A:408:ASN:HB3	1:A:413:ASN:CB	2.50	0.41
1:B:187:LYS:HA	1:B:187:LYS:HD3	1.90	0.41
1:B:417:ASN:ND2	1:B:417:ASN:C	2.72	0.41
1:B:510:ASP:C	1:B:512:ASN:H	2.24	0.41
1:B:415:LYS:HA	1:B:420:THR:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:510:ASP:HB2	1:B:511:GLU:OE1	2.20	0.41
1:A:90:TRP:O	1:A:266:GLY:HA3	2.20	0.40
1:B:254:ASN:ND2	1:B:256:LEU:H	2.19	0.40
1:B:15:GLN:NE2	1:B:208:ILE:N	2.60	0.40
1:B:104:ALA:HB3	1:B:247:ILE:CD1	2.52	0.40
1:B:254:ASN:ND2	1:B:254:ASN:C	2.75	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	480/522 (92%)	462 (96%)	17 (4%)	1 (0%)	47	58
1	B	472/522 (90%)	451 (96%)	19 (4%)	2 (0%)	34	42
All	All	952/1044 (91%)	913 (96%)	36 (4%)	3 (0%)	41	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	410	ASP
1	B	344	VAL
1	B	412	GLN

5.3.2 Protein sidechains ⓘ

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	412/447 (92%)	396 (96%)	16 (4%)	32	46
1	B	406/447 (91%)	384 (95%)	22 (5%)	22	30
All	All	818/894 (92%)	780 (95%)	38 (5%)	26	38

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	81	THR
1	A	116	LEU
1	A	156	ASN
1	A	169	ARG
1	A	179	THR
1	A	233	GLN
1	A	284	ASN
1	A	320	ARG
1	A	322	LEU
1	A	324	ASN
1	A	339	ARG
1	A	361	VAL
1	A	406	LEU
1	A	417	ASN
1	A	507	LEU
1	B	6	LEU
1	B	16	GLU
1	B	50	GLN
1	B	95	LEU
1	B	151	GLU
1	B	153	TYR
1	B	157	LYS
1	B	172	GLU
1	B	233	GLN
1	B	254	ASN
1	B	270	GLN
1	B	284	ASN
1	B	298	VAL
1	B	324	ASN
1	B	339	ARG
1	B	350	GLN
1	B	355	GLN
1	B	371	ASP
1	B	405	PRO

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Mol	Chain	Res	Type
1	B	415	LYS
1	B	417	ASN
1	B	419	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	29	GLN
1	A	38	GLN
1	A	50	GLN
1	A	137	GLN
1	A	139	GLN
1	A	148	GLN
1	A	156	ASN
1	A	233	GLN
1	A	254	ASN
1	A	284	ASN
1	A	300	GLN
1	A	324	ASN
1	A	330	ASN
1	A	343	ASN
1	A	355	GLN
1	A	413	ASN
1	A	417	ASN
1	A	429	HIS
1	A	504	HIS
1	B	15	GLN
1	B	23	ASN
1	B	46	ASN
1	B	50	GLN
1	B	64	ASN
1	B	84	GLN
1	B	137	GLN
1	B	139	GLN
1	B	181	HIS
1	B	195	GLN
1	B	196	GLN
1	B	233	GLN
1	B	254	ASN
1	B	270	GLN
1	B	284	ASN

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Mol	Chain	Res	Type
1	B	313	GLN
1	B	324	ASN
1	B	330	ASN
1	B	350	GLN
1	B	355	GLN
1	B	387	GLN
1	B	412	GLN
1	B	413	ASN
1	B	417	ASN
1	B	439	HIS

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	UD2	B	1902	-	38,41,41	1.57	6 (15%)	57,62,62	2.14	14 (24%)
2	UD2	A	1901	-	38,41,41	1.91	9 (23%)	57,62,62	2.10	17 (29%)

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	UD2	B	1902	-	-	2/26/63/63	0/3/3/3
2	UD2	A	1901	-	-	0/26/63/63	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1901	UD2	C1'-C2'	5.42	1.62	1.53
2	A	1901	UD2	C6-N1	5.32	1.50	1.38
2	B	1902	UD2	C6-N1	5.11	1.50	1.38
2	B	1902	UD2	C3'-C2'	3.33	1.59	1.53
2	A	1901	UD2	O4'-C4'	-3.24	1.35	1.43
2	A	1901	UD2	C3'-C2'	2.99	1.58	1.53
2	A	1901	UD2	C2'-N2'	2.94	1.50	1.45
2	A	1901	UD2	O5'-C1'	2.92	1.49	1.41
2	A	1901	UD2	C4-N3	-2.85	1.33	1.38
2	A	1901	UD2	C5-C4	2.76	1.49	1.43
2	B	1902	UD2	C1'-C2'	2.73	1.57	1.53
2	B	1902	UD2	C5-C4	2.66	1.49	1.43
2	B	1902	UD2	O4'-C4'	-2.57	1.36	1.43
2	A	1901	UD2	O4-C4	-2.30	1.20	1.24
2	B	1902	UD2	C2-N3	-2.02	1.34	1.38

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1901	UD2	C4'-C3'-C2'	-8.03	98.58	110.34
2	B	1902	UD2	C4'-C3'-C2'	-7.58	99.24	110.34
2	A	1901	UD2	O4'-C4'-C5'	5.85	123.82	109.30
2	B	1902	UD2	O4'-C4'-C5'	5.72	123.50	109.30
2	B	1902	UD2	O4'-C4'-C3'	5.59	123.26	110.35
2	A	1901	UD2	O4'-C4'-C3'	4.81	121.47	110.35
2	B	1902	UD2	C3'-C4'-C5'	-3.97	103.15	110.24
2	B	1902	UD2	O3A-PB-O1'	3.85	110.24	102.48
2	B	1902	UD2	C1'-C2'-N2'	-3.67	104.69	111.00
2	B	1902	UD2	O3'-C3'-C2'	-3.46	102.67	109.66
2	A	1901	UD2	O3'-C3'-C2'	-3.37	102.86	109.66
2	A	1901	UD2	C1'-C2'-N2'	-3.36	105.22	111.00
2	A	1901	UD2	O3A-PB-O1'	3.15	108.83	102.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1901	UD2	C3'-C4'-C5'	-3.06	104.79	110.24
2	A	1901	UD2	O5'-C1'-O1'	3.00	115.28	111.36
2	A	1901	UD2	O1'-C1'-C2'	-2.84	103.27	108.40
2	A	1901	UD2	C5-C4-N3	2.78	119.00	114.84
2	B	1902	UD2	O5'-C5'-C4'	-2.71	104.76	109.69
2	B	1902	UD2	C5-C4-N3	2.70	118.88	114.84
2	A	1901	UD2	O4-C4-C5	-2.50	120.76	125.16
2	B	1902	UD2	C3'-C2'-N2'	2.48	115.30	110.62
2	B	1902	UD2	O4-C4-C5	-2.40	120.94	125.16
2	A	1901	UD2	C6'-C5'-C4'	-2.38	107.44	113.00
2	B	1902	UD2	O2-C2-N3	-2.37	117.09	121.50
2	A	1901	UD2	O5'-C5'-C4'	-2.22	105.67	109.69
2	B	1902	UD2	O5'-C1'-O1'	2.20	114.24	111.36
2	A	1901	UD2	C3'-C2'-N2'	2.13	114.64	110.62
2	A	1901	UD2	N3-C2-N1	2.10	117.67	114.89
2	A	1901	UD2	O2-C2-N3	-2.09	117.61	121.50
2	A	1901	UD2	C5-C6-N1	-2.04	118.39	121.81
2	B	1902	UD2	O1'-C1'-C2'	-2.01	104.76	108.40

There are no chirality outliers.

All (2) torsion outliers are listed below:

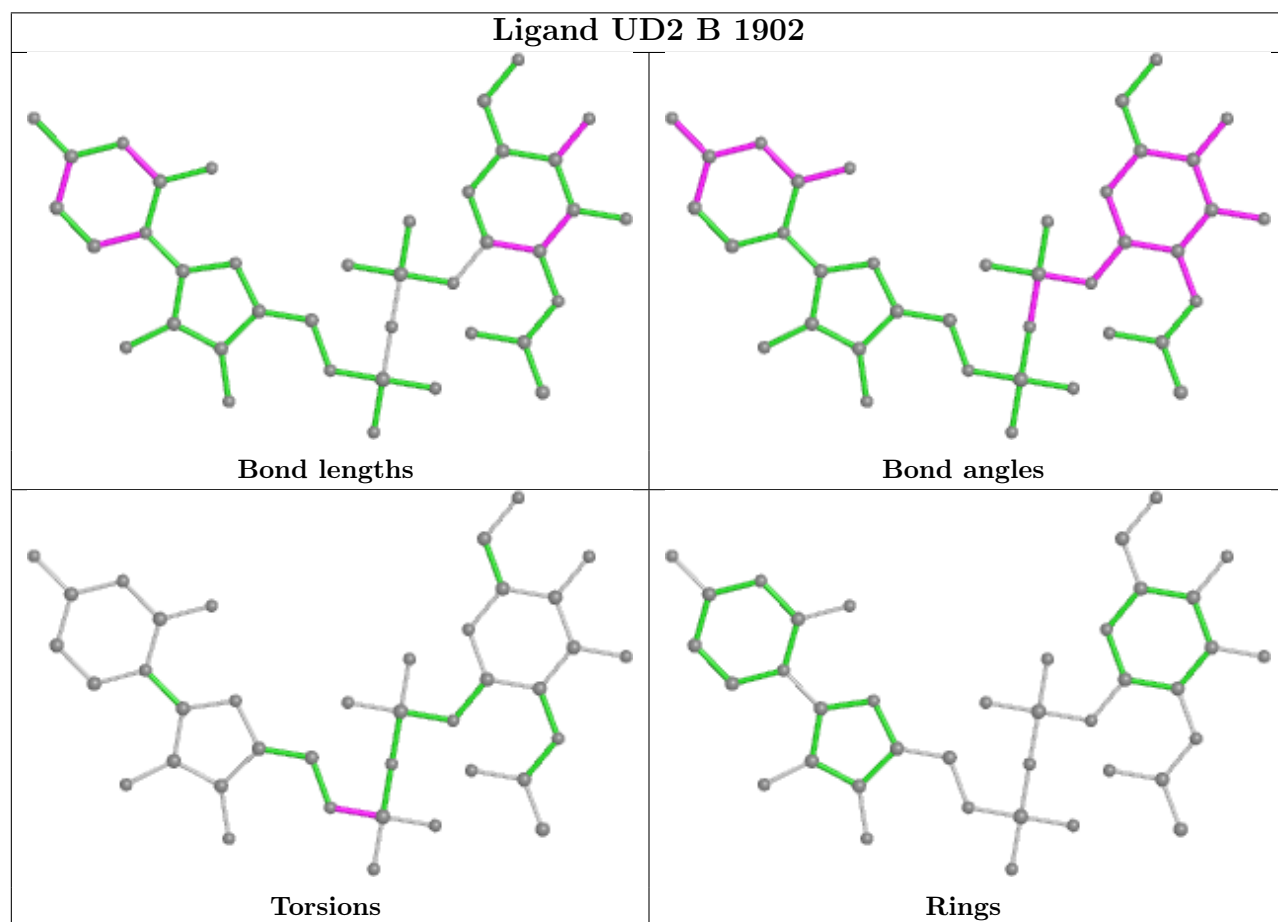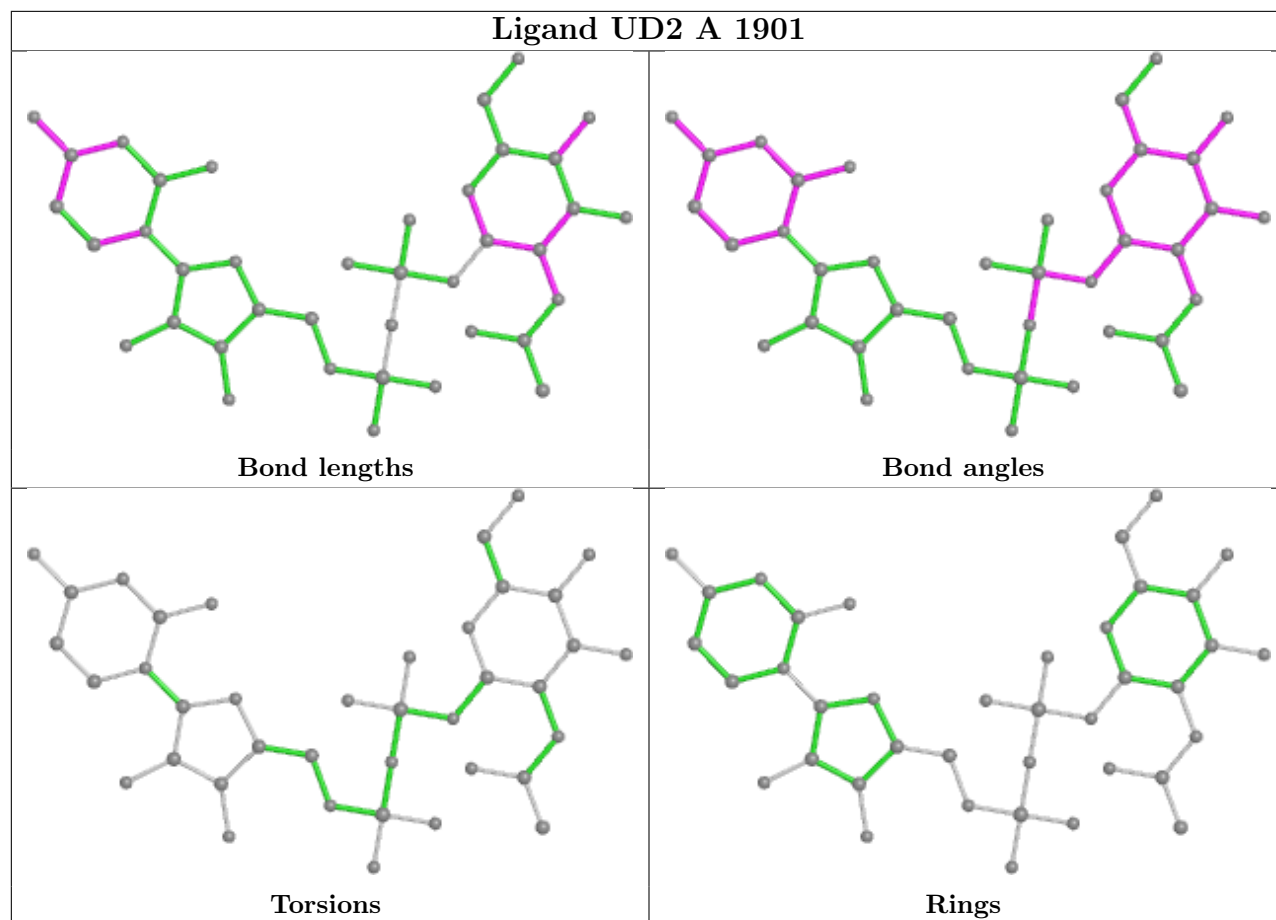| Mol	Chain	Res	Type	Atoms
2	B	1902	UD2	C5B-O5B-PA-O3A
2	B	1902	UD2	C5B-O5B-PA-O1A

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1902	UD2	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand UD2 B 1902

Bond lengths

Bond angles

Torsions

Rings

Ligand UD2 A 1901

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, 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	485/522 (92%)	-0.32	10 (2%)	63	70	13, 27, 56, 74	0
1	B	480/522 (91%)	0.13	36 (7%)	14	19	14, 38, 70, 85	0
All	All	965/1044 (92%)	-0.10	46 (4%)	30	37	13, 32, 64, 85	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	409	ALA	10.7
1	B	56	PHE	7.0
1	B	2	ASN	6.9
1	B	412	GLN	6.1
1	B	414	GLY	5.8
1	B	119	ALA	5.7
1	B	411	SER	5.7
1	B	410	ASP	4.8
1	B	477	VAL	4.4
1	A	413	ASN	4.2
1	B	31	VAL	4.2
1	B	65	VAL	4.2
1	B	27	GLU	4.1
1	A	454	SER	4.1
1	B	4	ASN	4.0
1	B	153	TYR	3.9
1	A	169	ARG	3.8
1	B	363	THR	3.8
1	B	120	TYR	3.8
1	B	169	ARG	3.8
1	B	64	ASN	3.7
1	B	413	ASN	3.5
1	A	411	SER	3.5
1	B	55	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	8	LEU	3.4
1	A	453[A]	ARG	3.3
1	B	28	ALA	3.2
1	B	26	GLU	3.1
1	B	3	ILE	3.1
1	B	35	ALA	3.1
1	B	6	LEU	3.0
1	A	414	GLY	2.8
1	A	66	ASP	2.8
1	B	18	LEU	2.7
1	B	478	PRO	2.6
1	B	408	ASN	2.6
1	B	371	ASP	2.6
1	A	412	GLN	2.6
1	B	369	LYS	2.5
1	B	5	ASP	2.4
1	A	363	THR	2.3
1	B	20	ARG	2.2
1	A	56	PHE	2.2
1	B	205	ASP	2.2
1	B	33	LEU	2.0
1	B	12	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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.
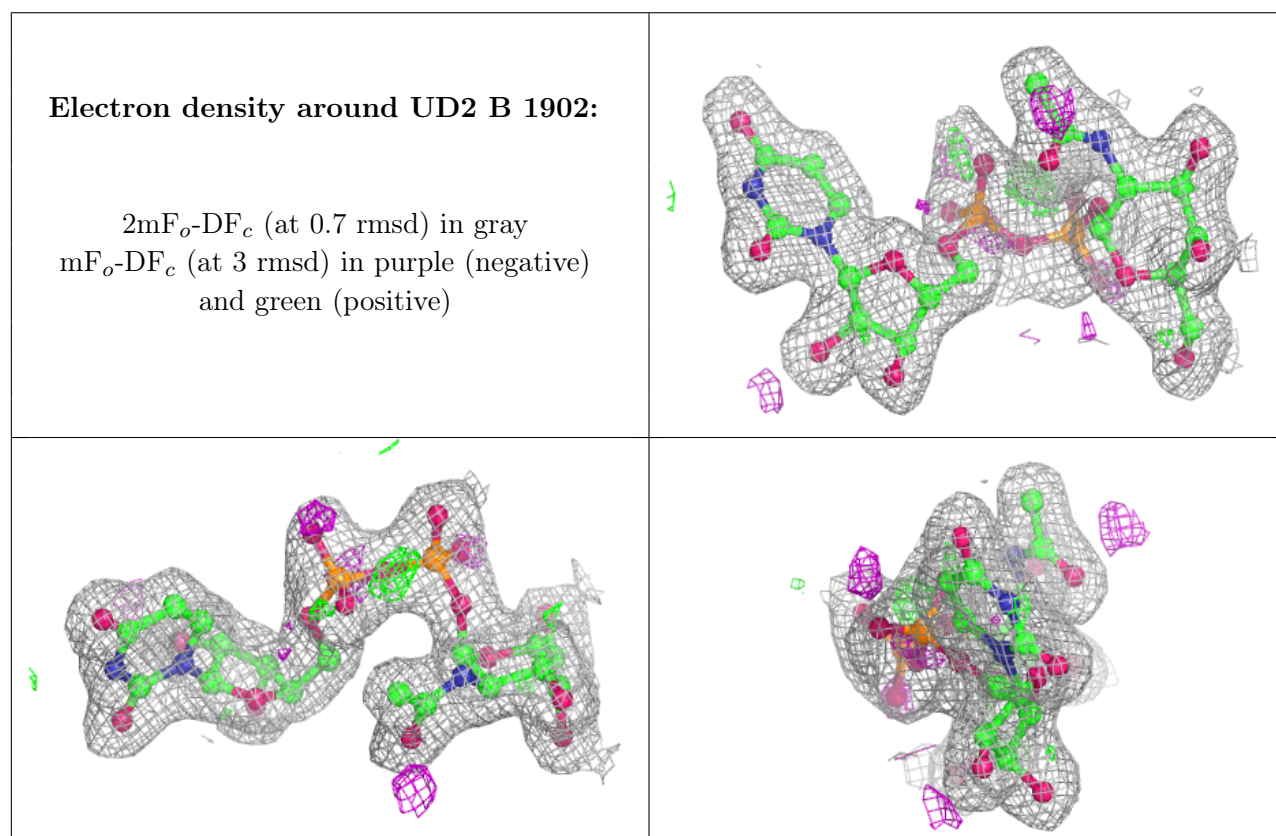
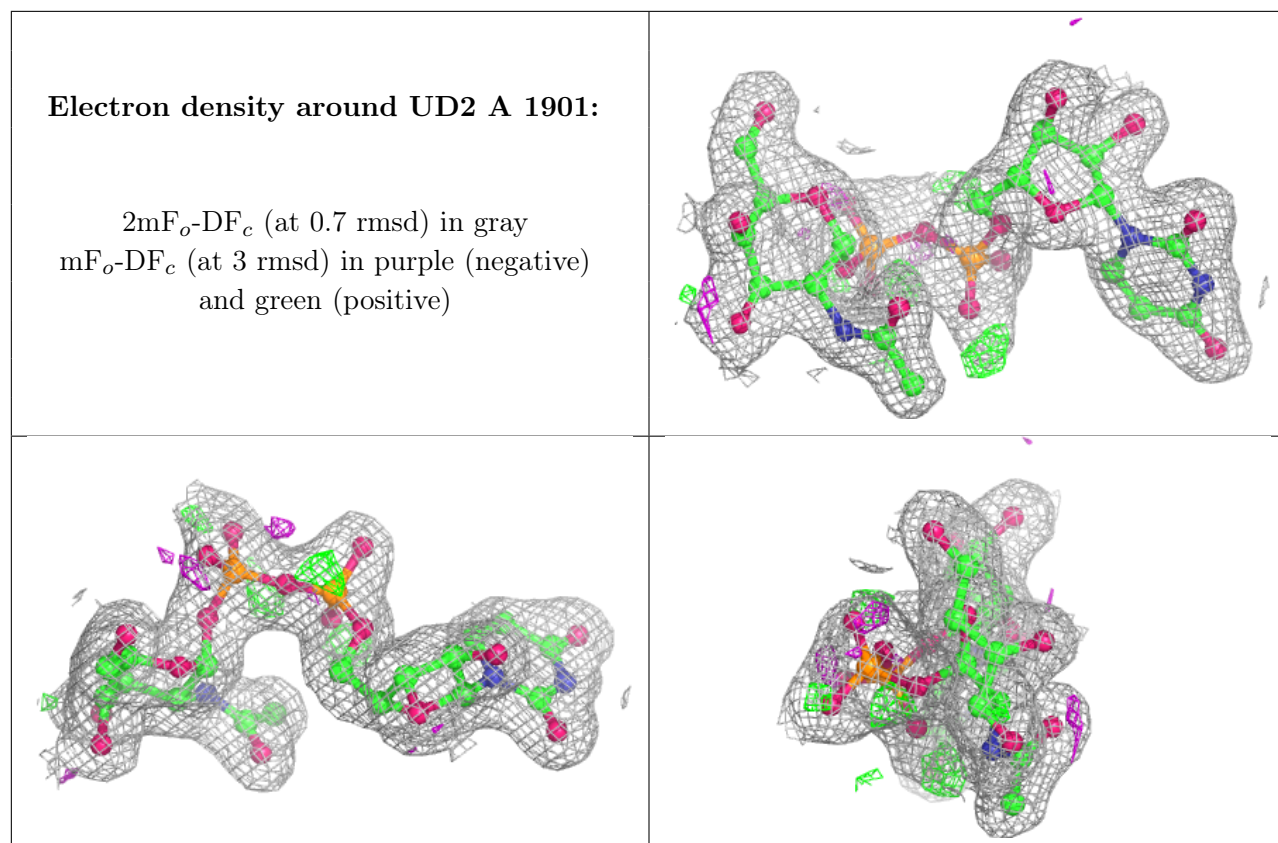| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	UD2	B	1902	39/39	0.92	0.10	16,29,42,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	UD2	A	1901	39/39	0.93	0.10	17,25,38,41	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 UD2 B 1902:

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 UD2 A 1901:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.