Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 10:55 pm BST

PDB ID	:	1OQM
Title	:	A 1:1 complex between alpha-lactalbumin and beta1,4-galactosyltransferase in the presence of UDP-N-acetyl-galactosamine
Authors	:	Ramakrishnan, B.; Qasba, P.K.
Deposited on	:	2003-03-10
Resolution	:	2.10 Å(reported)

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

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

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

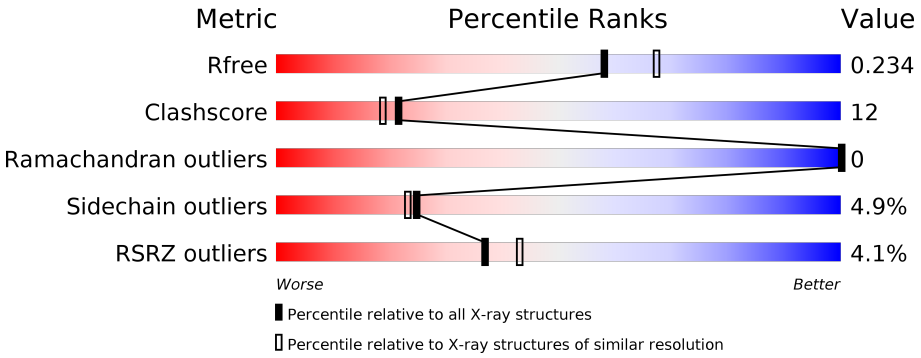
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	123	7% 79% 21%
1	C	123	3% 76% 24%
2	B	286	3% 74% 17% 5%
2	D	286	3% 73% 19% 5%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7121 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 Alpha-lactalbumin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	123	Total	C	N	O	S	0	0	0
			980	620	156	195	9			
1	C	123	Total	C	N	O	S	0	0	0
			980	620	156	195	9			

- Molecule 2 is a protein called beta-1,4-galactosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	272	Total	C	N	O	S	0	0	0
			2218	1424	382	398	14			
2	D	272	Total	C	N	O	S	0	0	0
			2218	1424	382	398	14			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	117	ALA	-	SEE REMARK 999	UNP P08037
B	118	SER	-	SEE REMARK 999	UNP P08037
B	119	MET	-	SEE REMARK 999	UNP P08037
B	120	THR	-	SEE REMARK 999	UNP P08037
B	121	GLY	-	SEE REMARK 999	UNP P08037
B	122	GLY	-	SEE REMARK 999	UNP P08037
B	123	GLN	-	SEE REMARK 999	UNP P08037
B	124	GLN	-	SEE REMARK 999	UNP P08037
B	125	MET	-	SEE REMARK 999	UNP P08037
B	126	GLY	-	SEE REMARK 999	UNP P08037
B	127	ARG	-	SEE REMARK 999	UNP P08037
B	128	GLY	-	SEE REMARK 999	UNP P08037
B	129	SER	-	SEE REMARK 999	UNP P08037
D	117	ALA	-	SEE REMARK 999	UNP P08037
D	118	SER	-	SEE REMARK 999	UNP P08037
D	119	MET	-	SEE REMARK 999	UNP P08037

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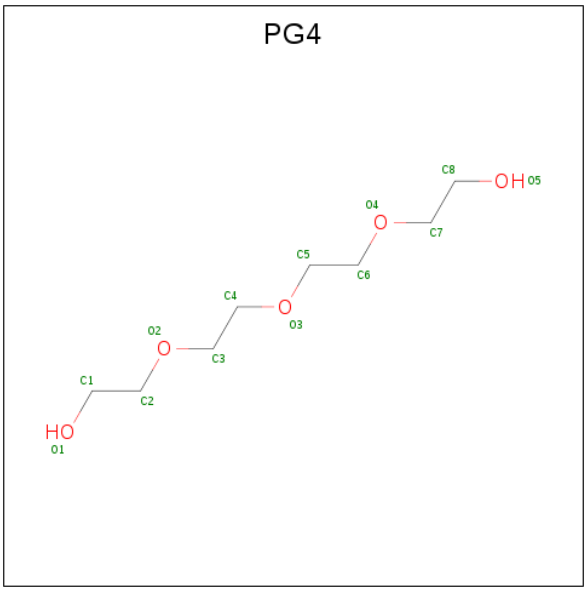
Chain	Residue	Modelled	Actual	Comment	Reference
D	120	THR	-	SEE REMARK 999	UNP P08037
D	121	GLY	-	SEE REMARK 999	UNP P08037
D	122	GLY	-	SEE REMARK 999	UNP P08037
D	123	GLN	-	SEE REMARK 999	UNP P08037
D	124	GLN	-	SEE REMARK 999	UNP P08037
D	125	MET	-	SEE REMARK 999	UNP P08037
D	126	GLY	-	SEE REMARK 999	UNP P08037
D	127	ARG	-	SEE REMARK 999	UNP P08037
D	128	GLY	-	SEE REMARK 999	UNP P08037
D	129	SER	-	SEE REMARK 999	UNP P08037

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).

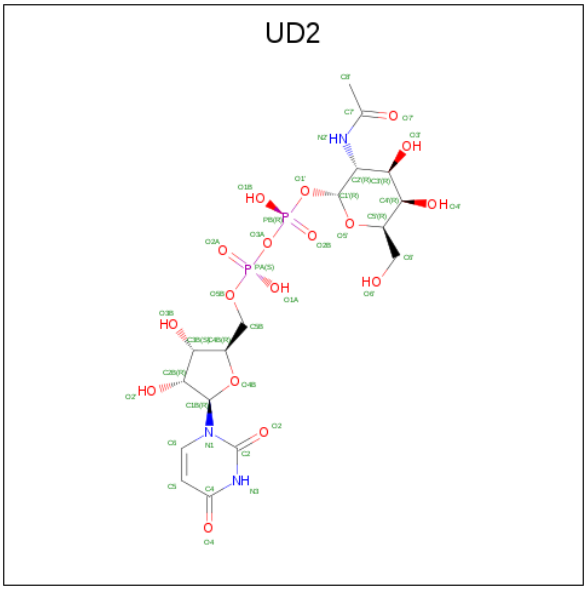


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Mn 1 1	0	0
5	D	1	Total Mn 1 1	0	0

- Molecule 6 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
6	B	1	Total C N O P 39 17 3 17 2	0	0
6	D	1	Total C N O P 39 17 3 17 2	0	0

- Molecule 7 is water.

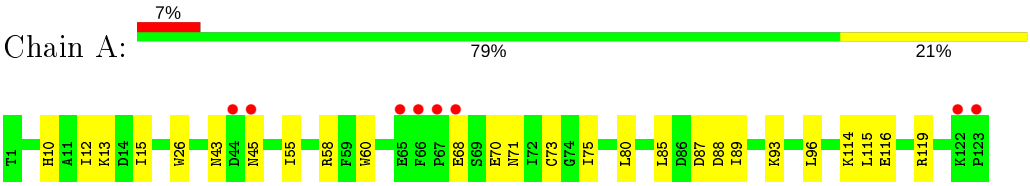
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	114	Total O 114 114	0	0
7	B	191	Total O 191 191	0	0
7	C	134	Total O 134 134	0	0
7	D	190	Total O 190 190	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

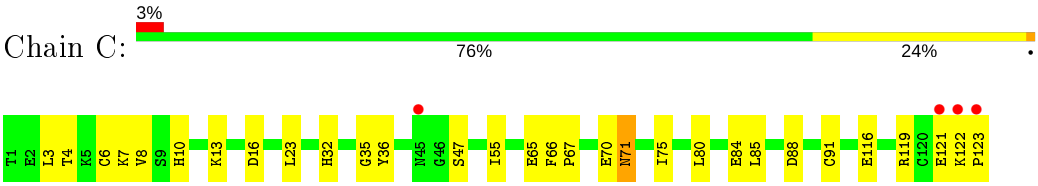
- Molecule 1: Alpha-lactalbumin

Chain A:



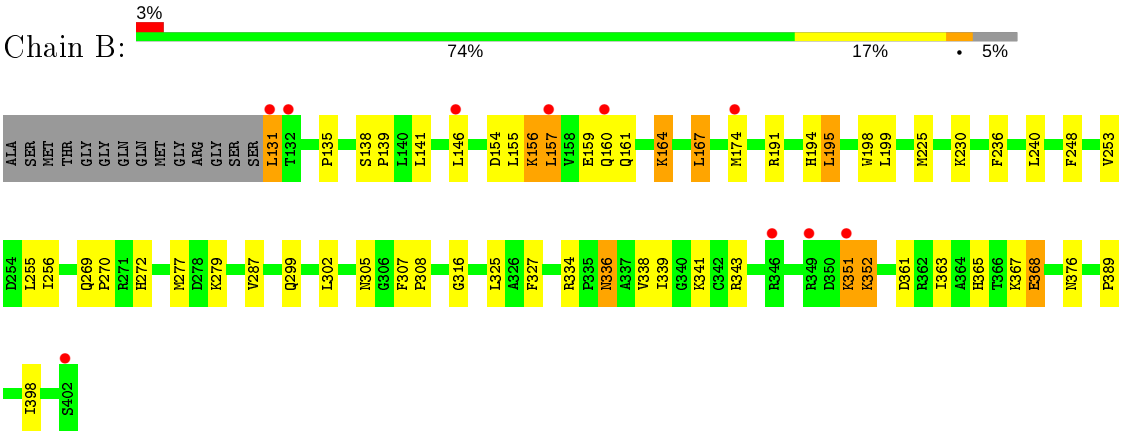
- Molecule 1: Alpha-lactalbumin

Chain C:



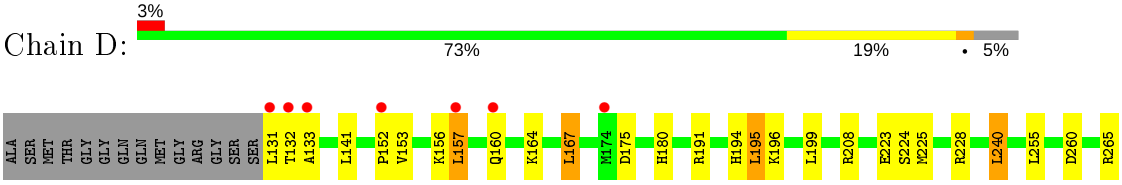
- Molecule 2: beta-1,4-galactosyltransferase

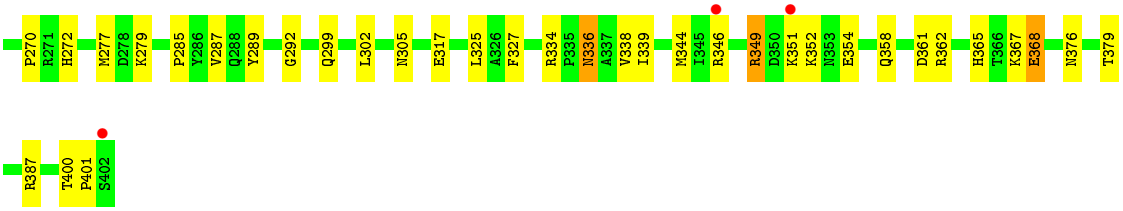
Chain B:



- Molecule 2: beta-1,4-galactosyltransferase

Chain D:




P270
R271
H272
M277
D278
K279
P285
Y286
V287
Q288
Y289
G292
Q299
L302
N305
E317
L325
A326
F327
R334
P335
N336
A337
V338
I339
M344
I345
R346
R349
D350
K351
K352
N353
E354
Q358
D361
R362
H365
T366
K367
E368
N376
T379

R387
T400
P401
S402

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	57.47Å 95.68Å 100.58Å 90.00° 101.40° 90.00°	Depositor
Resolution (Å)	19.56 – 2.10 19.56 – 2.09	Depositor EDS
% Data completeness (in resolution range)	90.1 (19.56-2.10) 89.6 (19.56-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.99 (at 2.09Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.194 , 0.244 0.184 , 0.234	Depositor DCC
R_{free} test set	5711 reflections (10.17%)	wwPDB-VP
Wilson B-factor (Å^2)	29.3	Xtriage
Anisotropy	0.526	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 53.1	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	0.95	EDS
Total number of atoms	7121	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.37% 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: UD2, CA, MN, PG4

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	0.49	0/1001	0.67	0/1350
1	C	0.52	0/1001	0.72	0/1350
2	B	0.48	0/2278	0.71	0/3085
2	D	0.49	0/2278	0.71	0/3085
All	All	0.49	0/6558	0.71	0/8870

There are no bond length outliers.

There are no bond angle outliers.

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	980	0	936	18	0
1	C	980	0	936	23	0
2	B	2218	0	2185	51	0
2	D	2218	0	2185	60	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	7	0	9	3	0
4	B	7	0	9	0	0
5	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	1	0	0	0	0
6	B	39	0	25	5	0
6	D	39	0	25	6	0
7	A	114	0	0	4	0
7	B	191	0	0	4	0
7	C	134	0	0	2	0
7	D	190	0	0	8	0
All	All	7121	0	6310	152	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 12.

All (152) 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:114:LYS:HA	4:A:814:PG4:H22	1.23	1.11
2:D:277:MET:SD	6:D:528:UD2:H8'1	1.93	1.08
2:D:255:LEU:HD11	6:D:528:UD2:H8'3	1.36	1.04
1:A:10:HIS:HA	1:A:13:LYS:HE2	1.49	0.94
2:D:349:ARG:HG2	2:D:349:ARG:HH11	1.33	0.92
1:A:45:ASN:HA	7:A:1167:HOH:O	1.77	0.84
1:A:71:ASN:HD21	1:A:75:ILE:H	1.24	0.84
1:A:89:ILE:HG22	7:A:1418:HOH:O	1.76	0.83
1:C:71:ASN:HD21	1:C:75:ILE:H	1.23	0.82
2:B:154:ASP:HB3	2:B:157:LEU:HB2	1.62	0.82
2:D:336:ASN:HD22	2:D:338:VAL:H	1.26	0.82
2:B:336:ASN:HD22	2:B:338:VAL:H	1.28	0.80
2:B:327:PHE:CZ	2:B:367:LYS:HB2	2.16	0.80
2:D:132:THR:HG22	2:D:133:ALA:H	1.46	0.78
2:D:305:ASN:HD21	2:D:376:ASN:H	1.32	0.78
2:B:240:LEU:HD11	2:B:248:PHE:CZ	2.21	0.75
2:B:351:LYS:O	2:B:352:LYS:HB2	1.86	0.75
1:C:65:GLU:O	1:C:67:PRO:HD3	1.87	0.74
2:B:191:ARG:HH11	2:B:194:HIS:HD2	1.36	0.73
2:D:336:ASN:HD21	2:D:338:VAL:HB	1.53	0.72
2:B:240:LEU:HD11	2:B:248:PHE:HZ	1.53	0.72
2:D:132:THR:HG22	2:D:133:ALA:N	2.06	0.70
2:B:156:LYS:HE3	2:B:156:LYS:O	1.92	0.69
2:B:365:HIS:O	2:B:368:GLU:HG2	1.92	0.69
2:B:277:MET:CE	6:B:404:UD2:H8'1	2.24	0.68
1:A:26:TRP:HZ2	1:A:96:LEU:HD11	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:255:LEU:HD11	6:B:404:UD2:H8'3	1.77	0.67
1:C:65:GLU:C	1:C:67:PRO:HD3	2.14	0.67
2:B:305:ASN:HD21	2:B:376:ASN:H	1.41	0.66
2:D:225:MET:HE2	2:D:352:LYS:HA	1.77	0.66
1:A:12:ILE:O	1:A:15:ILE:HG22	1.96	0.66
1:C:122:LYS:HD3	1:C:123:PRO:HD2	1.78	0.65
1:C:4:THR:H	1:C:7:LYS:HE2	1.61	0.65
1:C:10:HIS:HB2	7:C:1432:HOH:O	1.97	0.64
2:B:191:ARG:NH1	2:B:194:HIS:HD2	1.95	0.63
2:D:344:MET:CE	6:D:528:UD2:H8'2	2.27	0.63
2:D:336:ASN:ND2	2:D:338:VAL:H	1.95	0.62
2:B:138:SER:HB3	2:B:141:LEU:HD13	1.83	0.61
2:D:349:ARG:CG	2:D:349:ARG:HH11	2.12	0.60
2:B:272:HIS:HB3	2:B:334:ARG:HG2	1.84	0.60
2:B:299:GLN:HG3	7:B:1129:HOH:O	2.02	0.59
2:B:338:VAL:O	2:B:341:LYS:HG3	2.01	0.59
2:B:336:ASN:ND2	2:B:338:VAL:H	1.98	0.59
2:B:155:LEU:O	2:B:159:GLU:HG3	2.03	0.59
2:B:157:LEU:HD12	2:B:161:GLN:OE1	2.03	0.59
2:B:255:LEU:HD11	6:B:404:UD2:C8'	2.31	0.59
2:D:327:PHE:CE2	2:D:367:LYS:HD2	2.38	0.59
2:D:224:SER:HB2	7:D:980:HOH:O	2.01	0.58
2:D:191:ARG:HH11	2:D:194:HIS:HD2	1.51	0.58
2:D:361:ASP:HB3	7:D:1433:HOH:O	2.07	0.55
2:D:379:THR:HA	7:D:1295:HOH:O	2.06	0.55
2:B:236:PHE:O	2:B:240:LEU:HD13	2.07	0.54
2:D:225:MET:HE2	2:D:352:LYS:HE3	1.89	0.54
2:D:255:LEU:HD11	6:D:528:UD2:C8'	2.23	0.54
2:D:344:MET:HE2	6:D:528:UD2:H8'2	1.87	0.54
1:A:116:GLU:HB3	4:A:814:PG4:H11	1.91	0.53
2:B:287:VAL:HB	7:C:1417:HOH:O	2.07	0.53
1:C:32:HIS:HD2	7:D:1156:HOH:O	1.92	0.52
2:D:270:PRO:HG2	2:D:325:LEU:HD22	1.92	0.52
1:A:58:ARG:HB3	7:A:1296:HOH:O	2.10	0.52
1:A:68:GLU:O	1:A:68:GLU:HG2	2.08	0.52
1:C:4:THR:OG1	1:C:7:LYS:HG3	2.09	0.52
2:D:131:LEU:HD22	2:D:175:ASP:O	2.10	0.52
2:D:191:ARG:HD2	2:D:194:HIS:CD2	2.44	0.52
2:B:277:MET:HE1	6:B:404:UD2:H8'1	1.92	0.51
2:D:152:PRO:HA	7:D:1458:HOH:O	2.09	0.51
2:D:228:ARG:HD3	2:D:317:GLU:OE1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:352:LYS:HD2	2:B:352:LYS:N	2.24	0.51
1:A:93:LYS:HD3	7:A:1418:HOH:O	2.11	0.50
1:C:10:HIS:O	1:C:13:LYS:HG3	2.11	0.50
2:D:351:LYS:O	2:D:352:LYS:HB2	2.12	0.50
2:D:336:ASN:HD22	2:D:338:VAL:N	2.03	0.50
2:D:339:ILE:HD11	7:D:1077:HOH:O	2.11	0.50
1:C:116:GLU:OE2	1:C:119:ARG:NH2	2.45	0.49
1:C:70:GLU:N	1:C:70:GLU:OE1	2.45	0.49
1:A:119:ARG:HH21	1:A:119:ARG:HG3	1.77	0.49
1:C:121:GLU:O	1:C:122:LYS:C	2.50	0.49
2:D:153:VAL:HG22	2:D:196:LYS:HB3	1.93	0.49
2:D:132:THR:CG2	2:D:133:ALA:H	2.22	0.49
1:C:16:ASP:HB2	1:C:23:LEU:HD21	1.95	0.49
2:D:365:HIS:O	2:D:368:GLU:HG3	2.13	0.49
1:A:55:ILE:HB	1:A:80:LEU:HD13	1.94	0.48
2:D:153:VAL:CG2	2:D:196:LYS:HB3	2.43	0.48
2:B:154:ASP:N	7:B:1408:HOH:O	2.45	0.48
2:D:349:ARG:NH1	2:D:349:ARG:HG2	2.13	0.48
2:B:225:MET:HE3	2:B:352:LYS:O	2.14	0.47
2:B:279:LYS:HE2	7:B:1297:HOH:O	2.13	0.47
2:B:198:TRP:HA	2:B:256:ILE:HD11	1.97	0.47
2:B:164:LYS:HD2	2:B:174:MET:HE1	1.97	0.47
1:C:4:THR:N	1:C:7:LYS:HE2	2.30	0.47
2:B:191:ARG:NH1	2:B:194:HIS:CD2	2.79	0.46
1:A:115:LEU:H	4:A:814:PG4:H32	1.80	0.46
2:B:327:PHE:CE1	2:B:367:LYS:HB2	2.50	0.46
2:D:167:LEU:HD22	2:D:387:ARG:HB3	1.98	0.46
2:B:191:ARG:HD2	2:B:194:HIS:CD2	2.51	0.46
2:D:156:LYS:O	2:D:160:GLN:HG2	2.16	0.46
2:D:327:PHE:CZ	2:D:367:LYS:HB2	2.50	0.46
2:D:358:GLN:OE1	2:D:362:ARG:NH1	2.49	0.46
2:D:180:HIS:CE1	2:D:265:ARG:HD2	2.51	0.45
2:D:164:LYS:HE2	7:D:1342:HOH:O	2.16	0.45
1:C:4:THR:H	1:C:7:LYS:CE	2.26	0.45
2:D:358:GLN:O	2:D:362:ARG:HG3	2.16	0.45
2:B:270:PRO:CG	2:B:325:LEU:HD22	2.46	0.45
2:D:164:LYS:H	2:D:164:LYS:HD3	1.81	0.45
2:B:195:LEU:HD22	2:B:199:LEU:CD1	2.47	0.45
2:B:174:MET:HE3	7:B:1163:HOH:O	2.16	0.44
1:A:60:TRP:O	1:A:73:CYS:HB2	2.17	0.44
2:B:157:LEU:O	2:B:160:GLN:HB3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:157:LEU:CD1	2:B:161:GLN:OE1	2.66	0.44
2:B:270:PRO:HG2	2:B:325:LEU:HD22	1.99	0.44
1:C:116:GLU:OE1	1:C:119:ARG:NH2	2.51	0.44
2:B:253:VAL:HG12	6:B:404:UD2:H2B	1.98	0.44
1:C:35:GLY:O	1:C:36:TYR:HB2	2.17	0.44
1:C:122:LYS:HD3	1:C:123:PRO:CD	2.44	0.44
2:D:191:ARG:NH1	2:D:194:HIS:HD2	2.14	0.44
2:D:272:HIS:HB3	2:D:334:ARG:HG2	2.00	0.43
2:D:336:ASN:ND2	2:D:338:VAL:N	2.62	0.43
1:C:55:ILE:HD13	1:C:91:CYS:SG	2.57	0.43
2:B:336:ASN:ND2	2:B:339:ILE:H	2.16	0.43
2:B:307:PHE:HB3	2:B:308:PRO:HD2	2.01	0.43
2:B:336:ASN:HD22	2:B:338:VAL:N	2.06	0.43
2:D:195:LEU:HD22	2:D:199:LEU:HG	2.00	0.43
2:D:400:THR:HB	2:D:401:PRO:HD2	2.00	0.43
2:B:343:ARG:HG2	2:B:343:ARG:HH11	1.84	0.43
2:B:316:GLY:HA2	2:B:363:ILE:HD11	2.00	0.42
2:D:336:ASN:ND2	2:D:338:VAL:HB	2.29	0.42
1:C:55:ILE:HB	1:C:80:LEU:HD13	2.01	0.42
2:D:362:ARG:HB3	7:D:1239:HOH:O	2.19	0.42
1:C:6:CYS:SG	1:C:122:LYS:HB2	2.59	0.42
1:C:3:LEU:HA	1:C:7:LYS:HE3	2.02	0.42
2:D:365:HIS:HD2	2:D:368:GLU:OE1	2.02	0.42
1:A:116:GLU:OE2	1:A:119:ARG:NE	2.42	0.42
2:B:167:LEU:HA	2:B:389:PRO:HA	2.01	0.42
2:D:292:GLY:HA2	6:D:528:UD2:H8'3	2.02	0.42
2:B:230:LYS:HD3	2:B:398:ILE:HB	2.02	0.42
2:D:157:LEU:HA	2:D:157:LEU:HD22	1.86	0.42
1:A:75:ILE:CD1	1:A:87:ASP:HB2	2.50	0.42
2:D:225:MET:HE1	2:D:354:GLU:OE2	2.19	0.42
1:C:8:VAL:HG21	1:C:36:TYR:CD1	2.55	0.41
2:B:131:LEU:N	2:B:131:LEU:CD2	2.83	0.41
2:D:285:PRO:HG2	2:D:289:TYR:CG	2.55	0.41
2:D:279:LYS:CD	2:D:346:ARG:HH12	2.33	0.41
1:A:119:ARG:HG3	1:A:119:ARG:NH2	2.35	0.41
2:D:228:ARG:NH1	2:D:317:GLU:OE1	2.52	0.41
2:D:208:ARG:NH2	2:D:260:ASP:OD1	2.50	0.41
2:B:195:LEU:HD22	2:B:199:LEU:HG	2.02	0.41
2:D:240:LEU:HD12	2:D:240:LEU:HA	1.83	0.41
2:B:135:PRO:HG3	2:B:139:PRO:HD3	2.03	0.40
2:D:132:THR:CG2	2:D:133:ALA:N	2.77	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:164:LYS:HD3	2:D:164:LYS:N	2.36	0.40
2:D:400:THR:HB	2:D:401:PRO:CD	2.51	0.40
2:B:269:GLN:O	2:B:270:PRO:C	2.60	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	121/123 (98%)	114 (94%)	7 (6%)	0	100	100
1	C	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
2	B	270/286 (94%)	262 (97%)	8 (3%)	0	100	100
2	D	270/286 (94%)	261 (97%)	9 (3%)	0	100	100
All	All	782/818 (96%)	754 (96%)	28 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	109/109 (100%)	105 (96%)	4 (4%)	34	35
1	C	109/109 (100%)	103 (94%)	6 (6%)	21	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	245/254 (96%)	232 (95%)	13 (5%)	22 20
2	D	245/254 (96%)	233 (95%)	12 (5%)	25 23
All	All	708/726 (98%)	673 (95%)	35 (5%)	25 23

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	70	GLU
1	A	85	LEU
1	A	88	ASP
2	B	131	LEU
2	B	146	LEU
2	B	156	LYS
2	B	157	LEU
2	B	164	LYS
2	B	167	LEU
2	B	195	LEU
2	B	302	LEU
2	B	336	ASN
2	B	351	LYS
2	B	352	LYS
2	B	361	ASP
2	B	368	GLU
1	C	47	SER
1	C	66	PHE
1	C	71	ASN
1	C	84	GLU
1	C	85	LEU
1	C	88	ASP
2	D	141	LEU
2	D	157	LEU
2	D	167	LEU
2	D	195	LEU
2	D	223	GLU
2	D	240	LEU
2	D	287	VAL
2	D	299	GLN
2	D	302	LEU
2	D	336	ASN
2	D	349	ARG

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Mol	Chain	Res	Type
2	D	368	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	71	ASN
2	B	160	GLN
2	B	194	HIS
2	B	207	GLN
2	B	305	ASN
2	B	310	ASN
2	B	336	ASN
1	C	32	HIS
1	C	71	ASN
2	D	160	GLN
2	D	161	GLN
2	D	194	HIS
2	D	207	GLN
2	D	305	ASN
2	D	336	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
4	PG4	B	813	-	6,6,12	0.64	0	5,5,11	0.15	0
4	PG4	A	814	-	6,6,12	0.45	0	5,5,11	0.33	0
6	UD2	D	528	5	34,41,41	1.93	7 (20%)	45,62,62	1.82	11 (24%)
6	UD2	B	404	5	34,41,41	1.84	6 (17%)	45,62,62	1.80	11 (24%)

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
4	PG4	B	813	-	-	3/4/4/10	-
4	PG4	A	814	-	-	2/4/4/10	-
6	UD2	D	528	5	-	6/24/63/63	0/3/3/3
6	UD2	B	404	5	-	9/24/63/63	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	404	UD2	C6-N1	5.63	1.42	1.35
6	D	528	UD2	C4-N3	5.47	1.42	1.33
6	D	528	UD2	PB-O1'	-5.46	1.46	1.60
6	D	528	UD2	C6-N1	4.85	1.41	1.35
6	B	404	UD2	C4-N3	4.67	1.41	1.33
6	B	404	UD2	PB-O1'	-4.34	1.49	1.60
6	B	404	UD2	C2B-C1B	-2.95	1.49	1.53
6	D	528	UD2	C6-C5	-2.65	1.32	1.38
6	D	528	UD2	O5'-C1'	2.55	1.48	1.41
6	B	404	UD2	O5'-C5'	2.21	1.49	1.44
6	D	528	UD2	O5'-C5'	2.11	1.49	1.44
6	D	528	UD2	C1'-C2'	2.10	1.56	1.53
6	B	404	UD2	C4'-C5'	2.06	1.57	1.53

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	404	UD2	O5'-C5'-C6'	-4.63	94.92	106.44
6	D	528	UD2	O1B-PB-O1'	4.44	124.32	106.78
6	B	404	UD2	O1B-PB-O1'	4.35	123.93	106.78
6	D	528	UD2	C5-C4-N3	-3.92	114.68	123.31
6	D	528	UD2	O5'-C5'-C6'	-3.91	96.72	106.44
6	D	528	UD2	O5'-C1'-O1'	3.86	116.41	111.36
6	B	404	UD2	C5-C4-N3	-3.80	114.96	123.31
6	B	404	UD2	O3A-PB-O1'	3.47	109.48	102.48
6	D	528	UD2	O3A-PB-O1'	3.42	109.38	102.48
6	D	528	UD2	O5B-C5B-C4B	3.20	120.00	108.99
6	D	528	UD2	C8'-C7'-N2'	-3.15	110.76	116.10
6	B	404	UD2	C8'-C7'-N2'	-3.10	110.85	116.10
6	B	404	UD2	O4B-C4B-C3B	-3.06	99.07	105.11
6	B	404	UD2	O5'-C1'-O1'	2.97	115.25	111.36
6	D	528	UD2	O7'-C7'-N2'	2.97	127.41	121.95
6	B	404	UD2	C3'-C2'-N2'	-2.81	105.30	110.62
6	D	528	UD2	O4B-C4B-C3B	-2.74	99.70	105.11
6	B	404	UD2	O5B-C5B-C4B	2.73	118.40	108.99
6	B	404	UD2	O7'-C7'-N2'	2.62	126.78	121.95
6	D	528	UD2	O3'-C3'-C4'	-2.42	104.76	110.35
6	B	404	UD2	C6'-C5'-C4'	2.30	118.38	113.00
6	D	528	UD2	C6'-C5'-C4'	2.01	117.71	113.00

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	528	UD2	C1'-O1'-PB-O1B
6	B	404	UD2	C1'-C2'-N2'-C7'
6	B	404	UD2	C1'-O1'-PB-O1B
6	B	404	UD2	C1'-O1'-PB-O2B
4	A	814	PG4	O1-C1-C2-O2
4	B	813	PG4	O1-C1-C2-O2
6	B	404	UD2	C1'-O1'-PB-O3A
6	D	528	UD2	C1'-O1'-PB-O3A
6	D	528	UD2	O5'-C5'-C6'-O6'
6	B	404	UD2	O5'-C5'-C6'-O6'
6	D	528	UD2	C4B-C5B-O5B-PA
6	B	404	UD2	C4B-C5B-O5B-PA
6	B	404	UD2	C5B-O5B-PA-O3A
4	A	814	PG4	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
4	B	813	PG4	C4-C3-O2-C2
6	D	528	UD2	PB-O3A-PA-O1A
6	B	404	UD2	PB-O3A-PA-O1A
6	D	528	UD2	PA-O3A-PB-O1B
4	B	813	PG4	O2-C3-C4-O3
6	B	404	UD2	C5B-O5B-PA-O1A

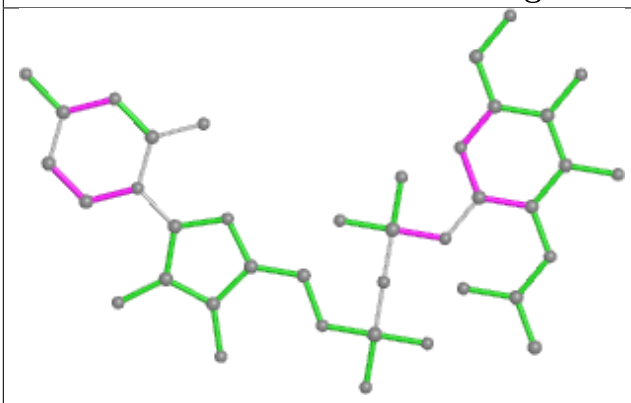
There are no ring outliers.

3 monomers are involved in 14 short contacts:

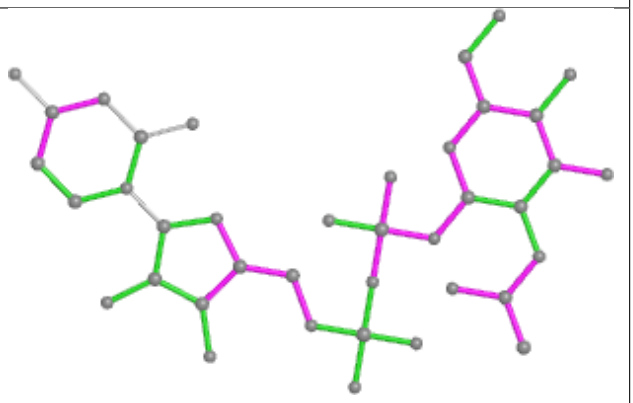
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	814	PG4	3	0
6	D	528	UD2	6	0
6	B	404	UD2	5	0

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.

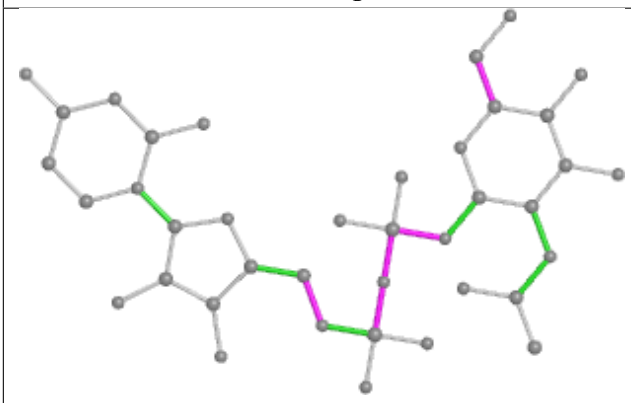
Ligand UD2 D 528



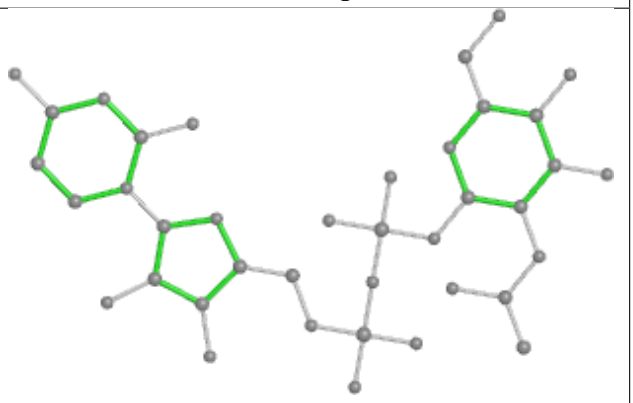
Bond lengths



Bond angles

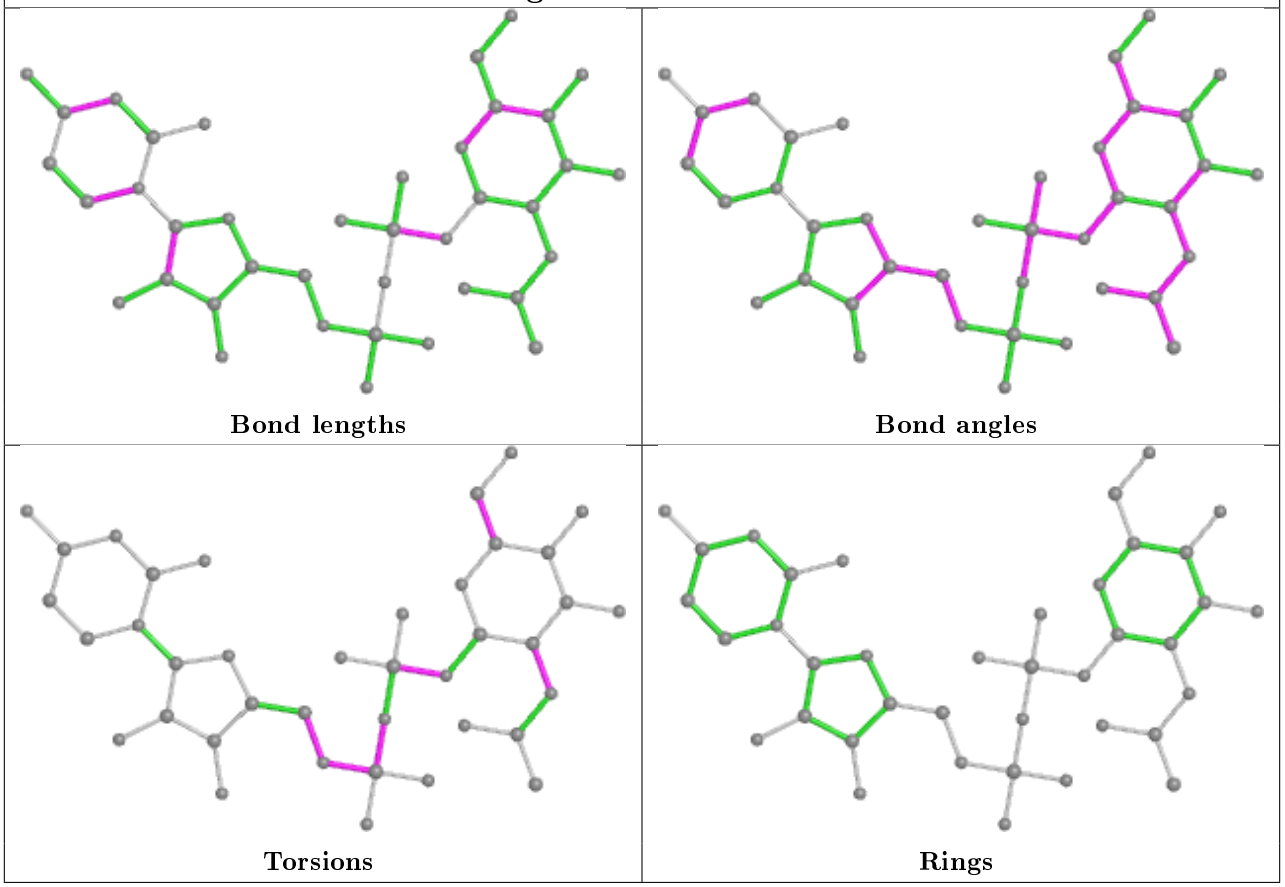


Torsions



Rings

Ligand UD2 B 404



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	123/123 (100%)	-0.11	8 (6%)	18	23	21, 30, 58, 69	0
1	C	123/123 (100%)	-0.18	4 (3%)	46	53	19, 28, 51, 82	0
2	B	272/286 (95%)	-0.12	10 (3%)	41	48	20, 32, 56, 67	0
2	D	272/286 (95%)	-0.21	10 (3%)	41	48	20, 33, 51, 62	0
All	All	790/818 (96%)	-0.16	32 (4%)	37	43	19, 31, 55, 82	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	123	PRO	7.7
2	D	402	SER	5.1
2	B	402	SER	4.7
1	A	123	PRO	4.3
1	C	122	LYS	4.3
1	A	45	ASN	3.8
2	B	346	ARG	3.2
2	B	131	LEU	3.0
2	D	132	THR	2.9
2	D	160	GLN	2.8
2	D	346	ARG	2.8
1	A	66	PHE	2.7
1	A	67	PRO	2.6
2	B	160	GLN	2.6
1	A	65	GLU	2.6
1	A	68	GLU	2.5
2	D	157	LEU	2.5
2	B	174	MET	2.5
2	B	157	LEU	2.3
2	D	133	ALA	2.3
2	B	349	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	122	LYS	2.3
2	D	131	LEU	2.3
2	D	174	MET	2.3
1	C	121	GLU	2.3
2	B	351	LYS	2.2
1	C	45	ASN	2.2
2	B	146	LEU	2.2
2	D	152	PRO	2.1
2	D	351	LYS	2.1
1	A	44	ASP	2.1
2	B	132	THR	2.1

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

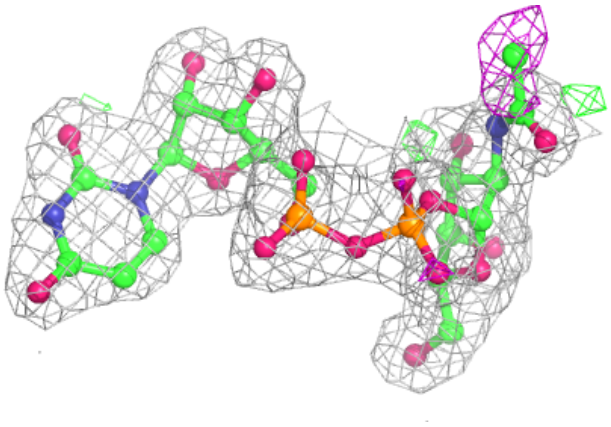
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

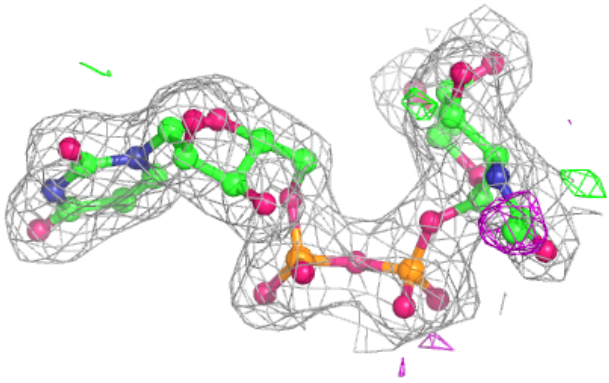
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PG4	B	813	7/13	0.72	0.25	48,50,52,53	0
4	PG4	A	814	7/13	0.82	0.27	47,53,55,58	0
6	UD2	B	404	39/39	0.96	0.10	20,30,38,41	0
6	UD2	D	528	39/39	0.97	0.10	20,24,30,36	0
5	MN	D	403	1/1	0.99	0.04	29,29,29,29	0
3	CA	A	124	1/1	0.99	0.07	24,24,24,24	0
3	CA	C	124	1/1	0.99	0.06	26,26,26,26	0
5	MN	B	403	1/1	1.00	0.04	31,31,31,31	0

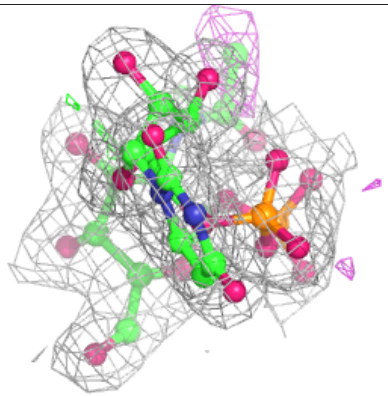
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UD2 B 404:

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

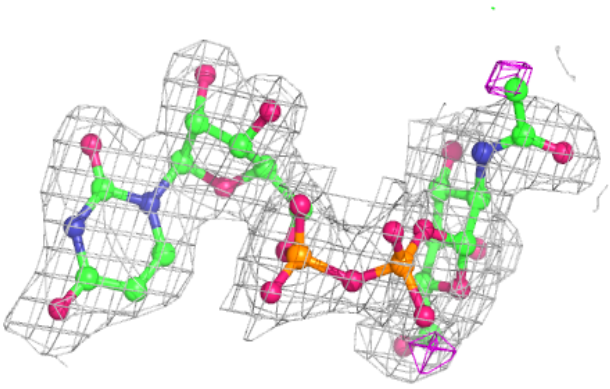


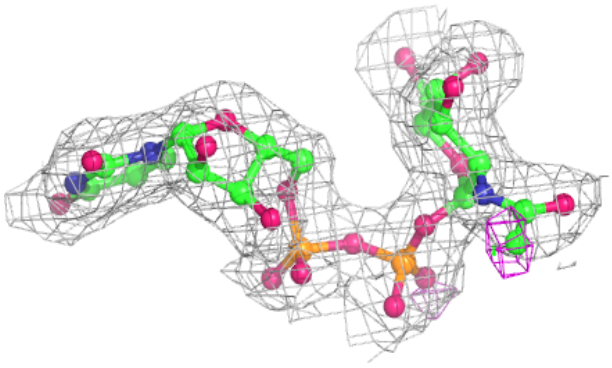


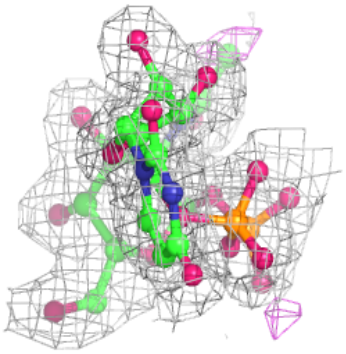


Electron density around UD2 D 528:

$2mF_o$-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.