Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 01:26 PM EDT

PDB ID	:	1NKH
Title	:	Crystal structure of Lactose synthase complex with UDP and Manganese
Authors	:	Ramakrishnan, B.; Qasba, P.K.
Deposited on	:	2003-01-03
Resolution	:	2.00 Å(reported)

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

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

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

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

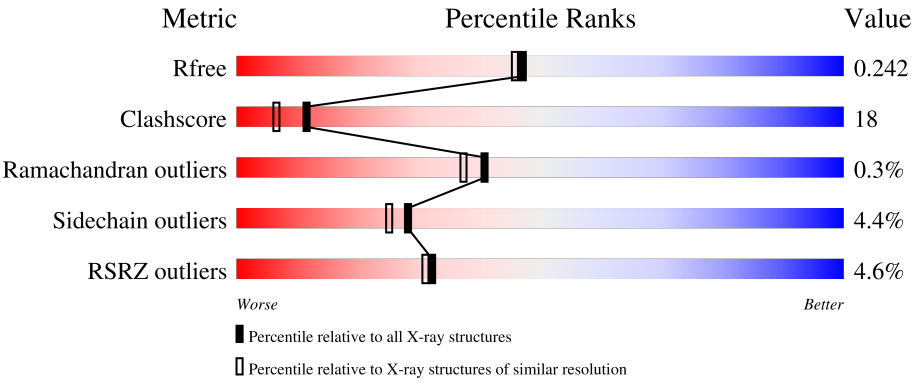
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	123	7% 78% 20% ·
1	C	123	7% 74% 26%
2	B	286	3% 70% 22% · 5%
2	D	286	3% 67% 24% · 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PG4	B	817	-	-	X	-
5	PG4	D	816	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 7183 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

Continued on next page...

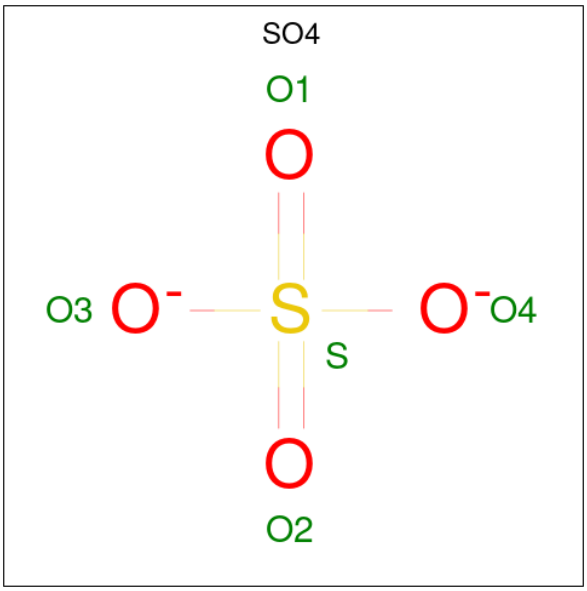
Continued from previous page...

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).

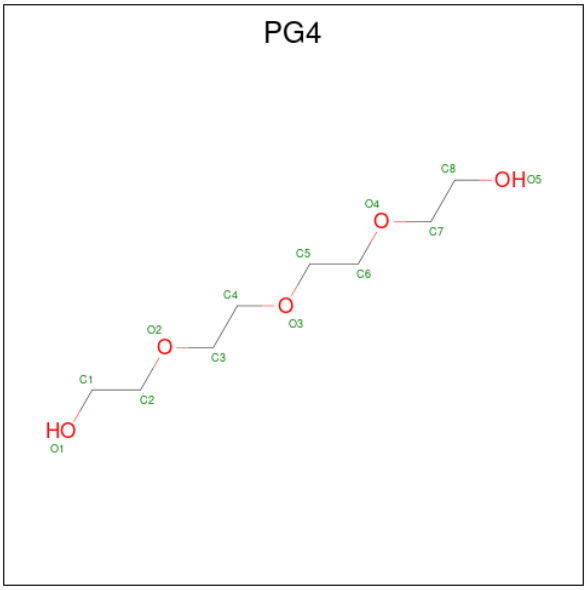
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).

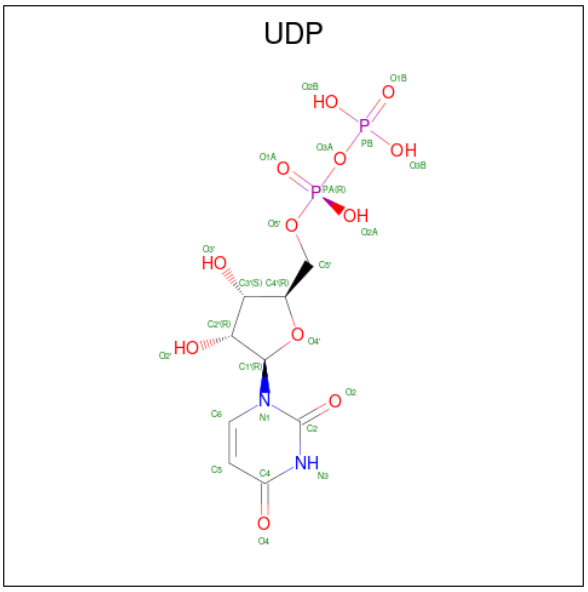


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 13 8 5	0	0
5	B	1	Total C O 13 8 5	0	0
5	B	1	Total C O 13 8 5	0	0
5	C	1	Total C O 13 8 5	0	0
5	D	1	Total C O 13 8 5	0	0

- Molecule 6 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 7 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C N O P 25 9 2 12 2	0	0
7	B	1	Total C N O P 25 9 2 12 2	0	0
7	D	1	Total C N O P 25 9 2 12 2	0	0
7	D	1	Total C N O P 25 9 2 12 2	0	0

- Molecule 8 is water.

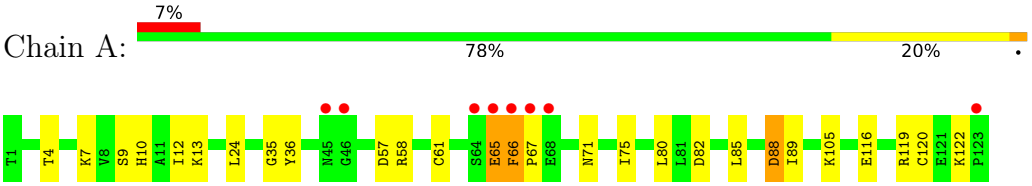
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	110	Total O 110 110	0	0
8	B	204	Total O 204 204	0	0
8	C	111	Total O 111 111	0	0
8	D	183	Total O 183 183	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

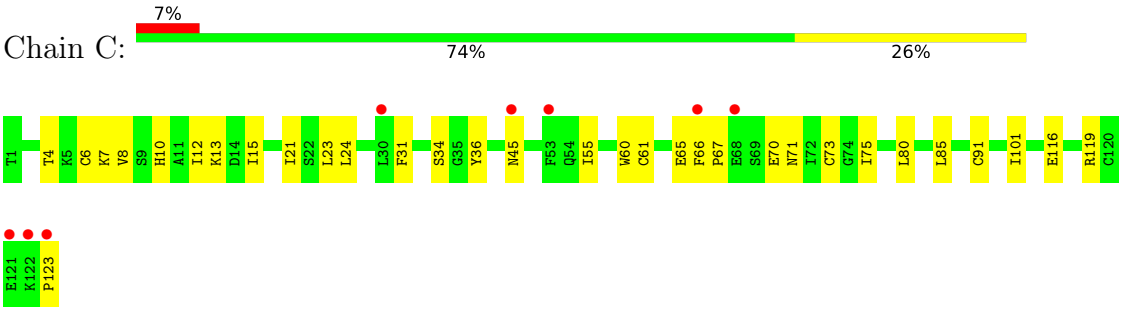
• Molecule 1: ALPHA-LACTALBUMIN

Chain A:



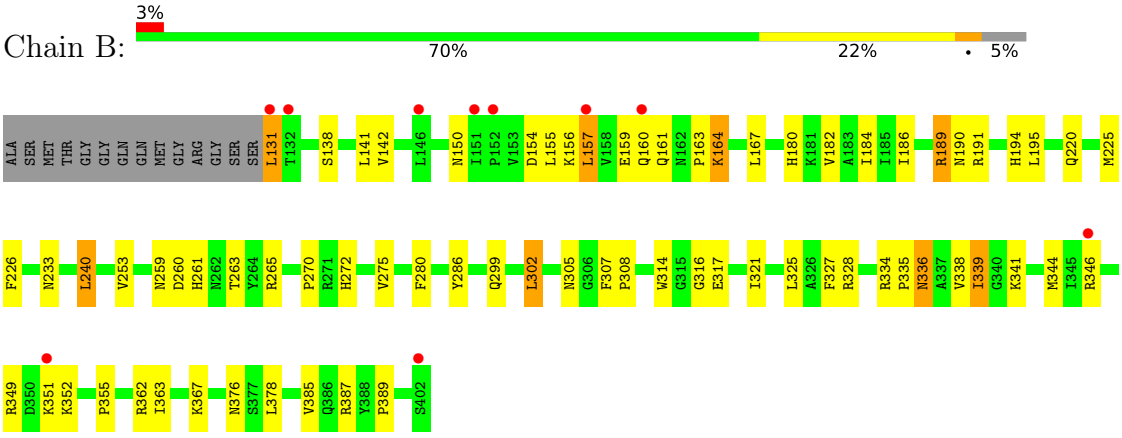
• Molecule 1: ALPHA-LACTALBUMIN

Chain C:



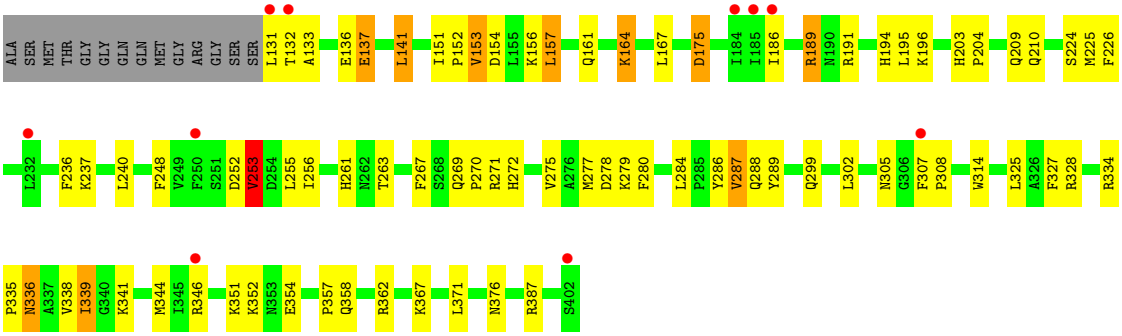
• Molecule 2: BETA-1,4-GALACTOSYLTRANSFERASE

Chain B:



• Molecule 2: BETA-1,4-GALACTOSYLTRANSFERASE

Chain D:


ALA SER MET THR GLY GLY GLN GLN MET GLY ARG GLY SER SER L131 T132 A133 E136 E137 L141 I151 P152 V153 D154 L155 K156 L157 Q161 K164 L167 D175 I184 I185 I186 R189 N190 R191 H194 L195 K196 H203 P204 Q209 Q210 S224 M225 F226
L232 F236 K237 L240 F248 V249 P250 S251 D252 V253 D254 L255 I256 H261 N262 T263 F267 S268 Q269 P270 R271 H272 V275 A276 M277 D278 K279 F280 L284 P285 Y286 V287 Q288 Y289 Q299 L302 M305 G306 F307 P308 W314 L325 A326 F327 R328 R334
P335 N336 A337 V338 I339 G340 K341 M344 I345 R346 K351 K352 N353 E354 P357 Q358 R362 K367 L371 N376 R387 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	55.47Å 99.14Å 102.26Å 90.00° 104.14° 90.00°	Depositor
Resolution (Å)	24.71 – 2.00 24.71 – 2.00	Depositor EDS
% Data completeness (in resolution range)	79.5 (24.71-2.00) 79.6 (24.71-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 2.01Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.196 , 0.251 0.187 , 0.242	Depositor DCC
R_{free} test set	5840 reflections (10.16%)	wwPDB-VP
Wilson B-factor (Å^2)	29.8	Xtriage
Anisotropy	0.528	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 47.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7183	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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: UDP, MN, SO4, PG4, CA

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	0.48	0/1001	0.74	0/1350
1	C	0.53	0/1001	0.75	0/1350
2	B	0.52	0/2278	0.73	0/3085
2	D	0.51	0/2278	0.78	3/3085 (0.1%)
All	All	0.51	0/6558	0.75	3/8870 (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})
2	D	253	VAL	CB-CA-C	-6.42	99.19	111.40
2	D	278	ASP	CB-CG-OD1	5.34	123.10	118.30
2	D	284	LEU	CA-CB-CG	5.02	126.85	115.30

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	23	0
1	C	980	0	936	27	0
2	B	2218	0	2185	83	0
2	D	2218	0	2185	87	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	5	0	0	0	0
4	D	5	0	0	0	0
5	A	13	0	18	1	0
5	B	26	0	36	18	0
5	C	13	0	18	6	0
5	D	13	0	18	9	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
7	B	50	0	22	3	0
7	D	50	0	22	3	0
8	A	110	0	0	2	0
8	B	204	0	0	11	0
8	C	111	0	0	4	0
8	D	183	0	0	6	0
All	All	7183	0	6376	228	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 18.

All (228) 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)
2:B:387:ARG:HH21	5:B:815:PG4:H62	1.31	0.95
1:C:10:HIS:HA	1:C:13:LYS:HE2	1.49	0.95
2:B:275:VAL:HG11	8:B:951:HOH:O	1.70	0.88
2:D:336:ASN:ND2	2:D:338:VAL:HG12	1.92	0.84
2:D:336:ASN:ND2	2:D:339:ILE:H	1.77	0.83
2:D:225:MET:HE1	2:D:352:LYS:HA	1.60	0.82
2:D:336:ASN:HD21	2:D:339:ILE:H	1.29	0.81
2:D:151:ILE:HD12	2:D:152:PRO:HD2	1.64	0.79
2:B:385:VAL:HG21	5:B:815:PG4:H71	1.66	0.77
2:B:336:ASN:HD22	2:B:338:VAL:H	1.30	0.77
2:B:191:ARG:HH11	2:B:194:HIS:HD2	1.33	0.76
2:B:186:ILE:HG21	2:B:253:VAL:HG12	1.65	0.76
2:D:225:MET:HE2	2:D:352:LYS:HE3	1.66	0.76
2:D:314:TRP:HZ2	5:D:816:PG4:H81	1.51	0.75
2:D:151:ILE:HD12	2:D:152:PRO:CD	2.16	0.74
2:B:190:ASN:HB3	8:B:970:HOH:O	1.89	0.72
2:D:336:ASN:HD21	2:D:338:VAL:HG12	1.54	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:280:PHE:HZ	5:B:817:PG4:H11	1.54	0.71
2:B:349:ARG:HG2	2:B:349:ARG:HH11	1.56	0.71
1:A:116:GLU:OE2	1:A:119:ARG:NH2	2.24	0.70
2:B:225:MET:HE2	2:B:352:LYS:HE3	1.73	0.70
2:D:336:ASN:HD22	2:D:338:VAL:H	1.38	0.70
2:D:314:TRP:CZ2	5:D:816:PG4:H81	2.26	0.70
2:D:336:ASN:HD22	2:D:336:ASN:C	1.94	0.69
2:D:225:MET:CE	2:D:352:LYS:HA	2.21	0.69
2:B:154:ASP:OD1	2:B:156:LYS:HB2	1.93	0.69
2:D:191:ARG:HH11	2:D:194:HIS:HD2	1.41	0.69
2:D:336:ASN:HD21	2:D:338:VAL:CG1	2.05	0.69
2:D:157:LEU:O	2:D:161:GLN:HG3	1.93	0.68
2:B:160:GLN:O	2:B:163:PRO:HD3	1.93	0.68
2:B:387:ARG:NH2	5:B:815:PG4:H62	2.06	0.68
1:C:71:ASN:HD21	1:C:75:ILE:H	1.38	0.68
2:B:155:LEU:O	2:B:159:GLU:HG3	1.93	0.68
2:B:138:SER:HB3	2:B:141:LEU:HD13	1.75	0.67
2:D:236:PHE:O	2:D:240:LEU:HD23	1.93	0.67
2:D:286:TYR:HE2	5:D:816:PG4:H52	1.59	0.67
2:B:186:ILE:CG2	2:B:253:VAL:HG12	2.24	0.67
2:B:336:ASN:ND2	2:B:338:VAL:H	1.92	0.67
2:B:349:ARG:NH1	2:B:355:PRO:HD3	2.11	0.66
1:C:21:ILE:HG13	1:C:101:ILE:HD13	1.77	0.65
2:D:336:ASN:ND2	2:D:338:VAL:H	1.93	0.65
1:A:66:PHE:O	1:A:66:PHE:CD2	2.49	0.65
2:D:358:GLN:OE1	2:D:362:ARG:NH1	2.29	0.65
2:D:191:ARG:NH1	2:D:194:HIS:HD2	1.95	0.64
1:A:71:ASN:HD21	1:A:75:ILE:H	1.44	0.64
2:B:286:TYR:HE2	5:B:817:PG4:H31	1.63	0.64
2:D:267:PHE:CE1	2:D:271:ARG:HD2	2.33	0.64
1:A:58:ARG:HA	1:A:66:PHE:CZ	2.33	0.64
2:B:280:PHE:CZ	5:B:817:PG4:H11	2.34	0.63
2:B:336:ASN:HD22	2:B:336:ASN:C	2.02	0.63
1:A:57:ASP:O	1:A:66:PHE:HE2	1.81	0.62
2:D:270:PRO:HG2	2:D:325:LEU:HD22	1.83	0.61
2:B:259:ASN:OD1	2:B:261:HIS:HB2	2.01	0.61
2:D:153:VAL:HG22	2:D:196:LYS:HB3	1.83	0.61
2:D:186:ILE:HG21	2:D:253:VAL:HG13	1.82	0.60
5:C:814:PG4:H51	2:D:314:TRP:CH2	2.35	0.60
2:B:194:HIS:HE1	8:B:955:HOH:O	1.85	0.60
2:B:154:ASP:HB3	2:B:157:LEU:HB2	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:305:ASN:HD21	2:B:376:ASN:H	1.49	0.60
1:A:61:CYS:HA	1:A:71:ASN:ND2	2.16	0.60
2:B:314:TRP:CE2	5:B:817:PG4:H82	2.37	0.59
1:C:34:SER:HA	5:C:814:PG4:H32	1.84	0.59
5:B:817:PG4:H12	8:B:1026:HOH:O	2.02	0.58
2:D:336:ASN:HD22	2:D:338:VAL:N	2.01	0.58
2:D:236:PHE:O	2:D:240:LEU:CD2	2.52	0.58
2:D:338:VAL:O	2:D:341:LYS:HG3	2.02	0.58
1:C:119:ARG:HE	1:C:123:PRO:HD3	1.68	0.58
1:C:10:HIS:O	1:C:13:LYS:HG2	2.03	0.58
2:D:305:ASN:HD21	2:D:376:ASN:H	1.51	0.58
5:C:814:PG4:H51	2:D:314:TRP:HH2	1.69	0.58
1:A:65:GLU:O	1:A:67:PRO:HD3	2.04	0.57
2:D:151:ILE:HG13	2:D:152:PRO:O	2.05	0.57
1:C:4:THR:OG1	1:C:7:LYS:HG3	2.04	0.57
2:D:191:ARG:HH11	2:D:194:HIS:CD2	2.22	0.57
1:C:55:ILE:HB	1:C:80:LEU:HD13	1.86	0.56
1:A:4:THR:HG23	1:A:7:LYS:HZ3	1.71	0.56
2:B:385:VAL:HG21	5:B:815:PG4:C7	2.36	0.56
1:C:65:GLU:C	1:C:67:PRO:HD3	2.26	0.55
2:B:167:LEU:CD1	2:B:387:ARG:HB3	2.37	0.55
2:B:225:MET:CE	2:B:352:LYS:HE3	2.36	0.55
1:C:61:CYS:HA	1:C:71:ASN:ND2	2.21	0.55
2:B:189:ARG:HG3	2:B:220:GLN:HB3	1.90	0.54
2:D:153:VAL:HA	8:D:1443:HOH:O	2.06	0.54
2:B:314:TRP:CH2	5:B:817:PG4:H51	2.43	0.54
2:D:225:MET:HE1	2:D:352:LYS:CA	2.37	0.54
2:B:191:ARG:HD2	2:B:194:HIS:CD2	2.42	0.53
1:C:60:TRP:O	1:C:73:CYS:HB2	2.09	0.53
1:A:4:THR:HG23	1:A:7:LYS:NZ	2.22	0.53
2:D:137:GLU:CD	2:D:137:GLU:N	2.62	0.53
2:D:189:ARG:HB2	2:D:226:PHE:HE1	1.74	0.53
2:B:233:ASN:HB3	2:B:378:LEU:HD22	1.89	0.53
2:D:132:THR:HG22	2:D:133:ALA:H	1.74	0.53
2:D:137:GLU:CD	2:D:137:GLU:H	2.12	0.53
2:B:191:ARG:NH1	2:B:194:HIS:HD2	2.03	0.53
2:D:167:LEU:CD1	2:D:387:ARG:HB3	2.39	0.53
2:D:191:ARG:NH1	2:D:194:HIS:CD2	2.77	0.53
2:D:289:TYR:HE1	5:D:816:PG4:H21	1.73	0.53
2:B:316:GLY:H	5:B:817:PG4:H61	1.75	0.52
2:B:191:ARG:HH11	2:B:194:HIS:CD2	2.22	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:CYS:HA	1:C:71:ASN:HD22	1.75	0.52
2:D:253:VAL:HG22	7:D:810:UDP:O2'	2.09	0.52
2:B:272:HIS:HB3	2:B:334:ARG:HG2	1.92	0.52
1:C:66:PHE:HB2	8:C:1311:HOH:O	2.08	0.52
2:D:277:MET:HE2	2:D:279:LYS:HD2	1.92	0.52
2:D:336:ASN:ND2	2:D:336:ASN:C	2.61	0.52
2:B:335:PRO:HB2	2:B:339:ILE:HG13	1.91	0.52
1:A:12:ILE:HD13	1:A:89:ILE:HD11	1.91	0.51
2:B:225:MET:CE	2:B:352:LYS:HA	2.41	0.51
2:B:307:PHE:HB3	2:B:308:PRO:HD2	1.92	0.51
1:C:8:VAL:HG21	1:C:36:TYR:CD1	2.45	0.51
2:B:182:VAL:HG12	2:B:184:ILE:HD12	1.91	0.51
1:C:116:GLU:OE1	1:C:119:ARG:NH2	2.45	0.50
2:B:131:LEU:HD23	2:B:131:LEU:N	2.26	0.50
2:B:186:ILE:CG2	2:B:253:VAL:CG1	2.89	0.50
1:C:119:ARG:HE	1:C:123:PRO:CD	2.24	0.50
2:B:184:ILE:HD12	2:B:184:ILE:N	2.26	0.50
1:C:6:CYS:O	1:C:10:HIS:CD2	2.65	0.50
2:D:253:VAL:CG2	7:D:810:UDP:H2'	2.41	0.50
1:C:10:HIS:CA	1:C:13:LYS:HE2	2.33	0.50
2:D:131:LEU:HD21	2:D:175:ASP:O	2.11	0.50
2:D:327:PHE:CE1	2:D:367:LYS:HB2	2.47	0.50
1:C:45:ASN:HB3	8:C:1502:HOH:O	2.13	0.49
2:B:142:VAL:HG12	2:B:142:VAL:O	2.12	0.49
1:C:12:ILE:O	1:C:15:ILE:HG22	2.12	0.49
2:D:153:VAL:CG2	2:D:196:LYS:HB3	2.43	0.49
2:B:225:MET:HE2	2:B:352:LYS:HA	1.94	0.49
2:D:132:THR:HG22	2:D:133:ALA:N	2.27	0.49
2:B:346:ARG:HG3	8:B:973:HOH:O	2.13	0.49
1:A:12:ILE:O	1:A:12:ILE:HG22	2.12	0.49
1:A:58:ARG:HA	1:A:66:PHE:HZ	1.75	0.49
2:D:280:PHE:HZ	5:D:816:PG4:H71	1.78	0.49
2:D:289:TYR:HE1	5:D:816:PG4:C2	2.25	0.49
5:C:814:PG4:H12	8:C:967:HOH:O	2.12	0.48
1:A:24:LEU:HD21	1:A:119:ARG:HB2	1.95	0.48
2:B:351:LYS:O	2:B:352:LYS:HB2	2.14	0.48
2:B:167:LEU:HD13	2:B:387:ARG:HB3	1.94	0.48
2:B:336:ASN:ND2	2:B:339:ILE:H	2.12	0.48
2:D:252:ASP:HB3	7:D:810:UDP:O3'	2.13	0.48
2:B:389:PRO:HG2	7:B:811:UDP:O4	2.14	0.48
2:D:328:ARG:HH22	2:D:371:LEU:HD21	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:286:TYR:CE2	5:B:817:PG4:H31	2.47	0.48
2:B:131:LEU:N	8:B:1255:HOH:O	2.47	0.47
2:B:141:LEU:HD23	2:B:261:HIS:CD2	2.49	0.47
2:B:316:GLY:HA2	2:B:363:ILE:HD11	1.96	0.47
2:D:154:ASP:HB3	2:D:157:LEU:HB2	1.95	0.47
2:D:327:PHE:CZ	2:D:367:LYS:HB2	2.49	0.47
2:B:314:TRP:HZ2	5:B:817:PG4:H22	1.79	0.47
2:D:131:LEU:CD2	2:D:175:ASP:O	2.63	0.47
2:D:269:GLN:HE21	2:D:270:PRO:HD2	1.78	0.47
5:D:816:PG4:H21	5:D:816:PG4:H41	1.49	0.47
2:B:327:PHE:CZ	2:B:367:LYS:HB2	2.50	0.47
2:D:336:ASN:HD21	2:D:339:ILE:N	2.05	0.47
2:D:279:LYS:HE3	8:D:1181:HOH:O	2.15	0.47
2:B:189:ARG:HB2	2:B:226:PHE:HE1	1.80	0.47
2:D:209:GLN:NE2	2:D:263:THR:HA	2.29	0.47
5:A:813:PG4:H31	5:B:817:PG4:H22	1.97	0.46
2:B:154:ASP:O	2:B:157:LEU:N	2.47	0.46
2:B:253:VAL:HG22	7:B:809:UDP:H2'	1.96	0.46
2:D:307:PHE:HB3	2:D:308:PRO:HD2	1.97	0.46
2:D:336:ASN:ND2	2:D:338:VAL:N	2.61	0.46
2:B:156:LYS:HE3	7:B:811:UDP:O2	2.15	0.46
1:C:13:LYS:HD3	1:C:23:LEU:HD11	1.98	0.46
2:D:286:TYR:CE2	5:D:816:PG4:H52	2.45	0.46
1:C:55:ILE:HD13	1:C:91:CYS:SG	2.56	0.46
2:B:180:HIS:CE1	2:B:265:ARG:HD2	2.51	0.46
1:C:70:GLU:O	1:C:71:ASN:C	2.55	0.45
8:B:1466:HOH:O	2:D:167:LEU:HD23	2.15	0.45
2:B:336:ASN:HD22	2:B:338:VAL:N	2.08	0.45
2:D:154:ASP:OD2	2:D:156:LYS:HB2	2.17	0.45
2:B:314:TRP:CZ2	5:B:817:PG4:H82	2.52	0.45
1:C:65:GLU:O	1:C:67:PRO:HD3	2.17	0.45
5:C:814:PG4:H81	8:C:967:HOH:O	2.16	0.45
2:D:351:LYS:O	2:D:352:LYS:HB2	2.16	0.45
1:C:24:LEU:HD11	1:C:119:ARG:NH2	2.31	0.45
2:D:167:LEU:HD13	2:D:387:ARG:HB3	1.98	0.45
2:D:327:PHE:CD2	2:D:367:LYS:HD3	2.52	0.45
2:B:344:MET:HE2	8:B:908:HOH:O	2.16	0.44
2:B:336:ASN:ND2	2:B:336:ASN:C	2.70	0.44
2:B:270:PRO:HG2	2:B:325:LEU:HD22	2.00	0.44
5:B:817:PG4:H81	8:B:1026:HOH:O	2.17	0.44
2:D:141:LEU:HD23	2:D:261:HIS:CD2	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ILE:O	1:A:12:ILE:CG2	2.65	0.44
1:A:61:CYS:HA	1:A:71:ASN:HD22	1.81	0.44
2:B:157:LEU:O	2:B:161:GLN:HG3	2.17	0.44
2:D:287:VAL:HG12	2:D:288:GLN:OE1	2.18	0.44
2:D:299:GLN:CD	2:D:299:GLN:H	2.21	0.44
5:D:816:PG4:H71	8:D:1181:HOH:O	2.17	0.44
2:B:339:ILE:O	2:B:339:ILE:HD12	2.17	0.43
2:D:210:GLN:NE2	8:D:1353:HOH:O	2.51	0.43
1:A:80:LEU:CD2	1:A:88:ASP:HA	2.48	0.43
2:B:164:LYS:HE3	8:B:961:HOH:O	2.18	0.43
2:B:335:PRO:HB2	2:B:339:ILE:CG1	2.47	0.43
2:D:164:LYS:HB2	8:D:1073:HOH:O	2.19	0.43
2:D:224:SER:HA	2:D:352:LYS:HE2	1.99	0.43
2:B:184:ILE:N	2:B:184:ILE:CD1	2.80	0.43
2:B:385:VAL:HG11	5:B:815:PG4:H61	1.99	0.43
2:B:349:ARG:HG2	2:B:349:ARG:NH1	2.29	0.43
1:C:8:VAL:O	1:C:12:ILE:HG12	2.18	0.43
1:A:122:LYS:HG3	8:A:1288:HOH:O	2.17	0.43
2:D:275:VAL:HG21	2:D:335:PRO:HD2	2.00	0.43
2:D:277:MET:HE1	2:D:344:MET:HE3	1.99	0.43
2:B:338:VAL:O	2:B:341:LYS:HG3	2.19	0.43
2:B:349:ARG:HH11	2:B:349:ARG:CG	2.28	0.43
2:D:255:LEU:C	2:D:256:ILE:HD12	2.39	0.43
2:D:225:MET:HE1	2:D:354:GLU:OE1	2.18	0.43
2:D:240:LEU:HD21	2:D:248:PHE:CZ	2.55	0.42
2:B:191:ARG:NH1	2:B:194:HIS:CD2	2.84	0.42
1:A:10:HIS:O	1:A:13:LYS:HG2	2.19	0.42
5:B:817:PG4:H32	5:B:817:PG4:O4	2.20	0.42
1:A:9:SER:O	1:A:13:LYS:HE2	2.20	0.42
2:D:237:LYS:HE2	2:D:237:LYS:HB3	1.83	0.42
2:B:240:LEU:HD12	2:B:240:LEU:HA	1.92	0.41
2:D:358:GLN:O	2:D:362:ARG:HG3	2.20	0.41
2:B:362:ARG:NH2	8:B:1290:HOH:O	2.53	0.41
2:D:186:ILE:CG2	2:D:253:VAL:HG13	2.49	0.41
1:A:120:CYS:HB3	8:A:1080:HOH:O	2.20	0.41
2:B:336:ASN:HD21	2:B:339:ILE:H	1.67	0.41
1:C:31:PHE:O	5:C:814:PG4:H62	2.20	0.41
2:D:203:HIS:HB2	2:D:204:PRO:HD3	2.03	0.41
2:D:272:HIS:HB3	2:D:334:ARG:HG2	2.01	0.41
1:A:35:GLY:O	1:A:36:TYR:HB2	2.21	0.41
1:A:82:ASP:OD1	1:A:82:ASP:C	2.59	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:LYS:HB2	1:A:105:LYS:HE3	1.86	0.41
2:B:142:VAL:H	2:B:260:ASP:CG	2.23	0.41
2:D:131:LEU:HD23	2:D:131:LEU:HA	1.77	0.41
2:D:357:PRO:HD2	8:D:1393:HOH:O	2.20	0.41
2:B:317:GLU:O	2:B:321:ILE:HG13	2.22	0.40
2:B:302:LEU:HD12	2:B:302:LEU:HA	1.96	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%)	6 (5%)	1 (1%)	19 13
1	C	121/123 (98%)	112 (93%)	9 (7%)	0	100 100
2	B	270/286 (94%)	261 (97%)	9 (3%)	0	100 100
2	D	270/286 (94%)	259 (96%)	10 (4%)	1 (0%)	34 30
All	All	782/818 (96%)	746 (95%)	34 (4%)	2 (0%)	41 37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	GLU
2	D	189	ARG

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%)	106 (97%)	3 (3%)	43 44
1	C	109/109 (100%)	108 (99%)	1 (1%)	78 83
2	B	245/254 (96%)	232 (95%)	13 (5%)	22 18
2	D	245/254 (96%)	231 (94%)	14 (6%)	20 16
All	All	708/726 (98%)	677 (96%)	31 (4%)	28 25

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

Mol	Chain	Res	Type
1	A	66	PHE
1	A	85	LEU
1	A	88	ASP
2	B	131	LEU
2	B	150	ASN
2	B	157	LEU
2	B	164	LYS
2	B	189	ARG
2	B	195	LEU
2	B	240	LEU
2	B	263	THR
2	B	299	GLN
2	B	302	LEU
2	B	328	ARG
2	B	336	ASN
2	B	339	ILE
1	C	85	LEU
2	D	136	GLU
2	D	137	GLU
2	D	141	LEU
2	D	153	VAL
2	D	157	LEU
2	D	164	LYS
2	D	175	ASP
2	D	195	LEU
2	D	253	VAL
2	D	287	VAL
2	D	302	LEU
2	D	336	ASN
2	D	339	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	346	ARG

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	32	HIS
1	A	71	ASN
2	B	160	GLN
2	B	194	HIS
2	B	305	ASN
2	B	310	ASN
2	B	336	ASN
2	B	386	GLN
1	C	10	HIS
1	C	32	HIS
1	C	43	ASN
1	C	71	ASN
2	D	160	GLN
2	D	180	HIS
2	D	190	ASN
2	D	194	HIS
2	D	210	GLN
2	D	261	HIS
2	D	269	GLN
2	D	310	ASN
2	D	336	ASN
2	D	365	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 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	SO4	A	819	-	4,4,4	1.96	1 (25%)	6,6,6	0.97	0
7	UDP	B	811	-	24,26,26	1.26	2 (8%)	37,40,40	1.48	6 (16%)
5	PG4	A	813	-	12,12,12	0.54	0	11,11,11	0.34	0
5	PG4	D	816	-	12,12,12	0.42	0	11,11,11	0.40	0
5	PG4	B	815	-	12,12,12	0.54	0	11,11,11	0.24	0
4	SO4	D	818	-	4,4,4	1.93	2 (50%)	6,6,6	0.87	0
5	PG4	C	814	-	12,12,12	0.62	0	11,11,11	0.13	0
7	UDP	B	809	6	24,26,26	1.32	3 (12%)	37,40,40	1.53	7 (18%)
5	PG4	B	817	-	12,12,12	0.58	0	11,11,11	0.35	0
7	UDP	D	810	6	24,26,26	1.23	2 (8%)	37,40,40	1.47	7 (18%)
7	UDP	D	812	-	24,26,26	1.31	3 (12%)	37,40,40	1.49	7 (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
7	UDP	B	811	-	-	3/16/32/32	0/2/2/2
5	PG4	A	813	-	-	5/10/10/10	-
5	PG4	D	816	-	-	6/10/10/10	-
5	PG4	B	815	-	-	5/10/10/10	-
5	PG4	C	814	-	-	3/10/10/10	-
7	UDP	B	809	6	-	1/16/32/32	0/2/2/2
5	PG4	B	817	-	-	6/10/10/10	-
7	UDP	D	810	6	-	1/16/32/32	0/2/2/2
7	UDP	D	812	-	-	2/16/32/32	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	812	UDP	PB-O1B	3.53	1.61	1.50
7	B	811	UDP	PB-O1B	3.44	1.61	1.50
4	A	819	SO4	O1-S	3.34	1.64	1.46
7	B	809	UDP	PB-O1B	3.23	1.61	1.50
4	D	818	SO4	O1-S	3.21	1.63	1.46
7	D	810	UDP	C2-N1	2.64	1.42	1.38
7	B	811	UDP	C2-N1	2.47	1.42	1.38
7	D	812	UDP	C2-N1	2.44	1.42	1.38
7	D	810	UDP	PB-O1B	2.35	1.58	1.50
7	D	812	UDP	C4-N3	2.31	1.42	1.38
7	B	809	UDP	C3'-C2'	-2.17	1.47	1.53
4	D	818	SO4	O3-S	-2.12	1.30	1.47
7	B	809	UDP	C4-N3	2.04	1.42	1.38

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	810	UDP	O3B-PB-O1B	4.02	126.41	110.68
7	D	812	UDP	O3B-PB-O1B	3.92	126.04	110.68
7	B	811	UDP	O3B-PB-O1B	3.90	125.95	110.68
7	B	809	UDP	O3B-PB-O1B	3.80	125.57	110.68
7	D	810	UDP	O4'-C4'-C3'	-3.62	97.96	105.11
7	B	809	UDP	O2-C2-N1	-3.51	118.13	122.79
7	B	811	UDP	O5'-C5'-C4'	3.19	119.99	108.99
7	B	809	UDP	O4'-C4'-C3'	-3.12	98.94	105.11
7	D	812	UDP	O5'-C5'-C4'	2.95	119.16	108.99
7	B	809	UDP	O2-C2-N3	2.89	126.88	121.50
7	B	811	UDP	C2'-C1'-N1	2.83	121.24	113.22
7	D	812	UDP	O2-C2-N1	-2.81	119.05	122.79
7	D	812	UDP	C2'-C1'-N1	2.78	121.10	113.22
7	D	810	UDP	O2-C2-N1	-2.75	119.13	122.79
7	B	811	UDP	O2-C2-N1	-2.62	119.30	122.79
7	D	812	UDP	O2-C2-N3	2.42	126.01	121.50
7	B	811	UDP	O2-C2-N3	2.41	125.99	121.50
7	B	809	UDP	C2'-C1'-N1	2.39	120.00	113.22
7	B	811	UDP	O3A-PB-O1B	-2.33	98.27	111.19
7	D	810	UDP	O2-C2-N3	2.28	125.75	121.50
7	D	810	UDP	O3A-PB-O1B	-2.28	98.57	111.19
7	B	809	UDP	O3A-PB-O1B	-2.24	98.78	111.19
7	D	810	UDP	C2'-C1'-N1	2.23	119.53	113.22
7	D	812	UDP	O3A-PB-O1B	-2.21	98.94	111.19
7	D	812	UDP	O4'-C4'-C3'	-2.09	100.97	105.11
7	D	810	UDP	O5'-C5'-C4'	2.01	115.93	108.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	809	UDP	O5'-C5'-C4'	2.01	115.92	108.99

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	816	PG4	C4-C3-O2-C2
5	D	816	PG4	O2-C3-C4-O3
5	A	813	PG4	O2-C3-C4-O3
5	A	813	PG4	O1-C1-C2-O2
5	B	817	PG4	O1-C1-C2-O2
5	C	814	PG4	O1-C1-C2-O2
5	B	815	PG4	O4-C7-C8-O5
5	B	815	PG4	O3-C5-C6-O4
5	B	817	PG4	O2-C3-C4-O3
5	C	814	PG4	O4-C7-C8-O5
7	D	810	UDP	PA-O3A-PB-O1B
5	D	816	PG4	C3-C4-O3-C5
5	B	815	PG4	C6-C5-O3-C4
5	B	817	PG4	C8-C7-O4-C6
5	D	816	PG4	C8-C7-O4-C6
5	B	815	PG4	C8-C7-O4-C6
7	B	811	UDP	C5'-O5'-PA-O3A
5	D	816	PG4	C6-C5-O3-C4
5	A	813	PG4	C1-C2-O2-C3
7	B	811	UDP	C5'-O5'-PA-O1A
5	B	815	PG4	C3-C4-O3-C5
5	B	817	PG4	C1-C2-O2-C3
5	C	814	PG4	C1-C2-O2-C3
7	D	812	UDP	O4'-C4'-C5'-O5'
5	D	816	PG4	O1-C1-C2-O2
5	A	813	PG4	C4-C3-O2-C2
5	B	817	PG4	C6-C5-O3-C4
5	B	817	PG4	C5-C6-O4-C7
5	A	813	PG4	O3-C5-C6-O4
7	B	811	UDP	O4'-C4'-C5'-O5'
7	B	809	UDP	C5'-O5'-PA-O1A
7	D	812	UDP	C5'-O5'-PA-O2A

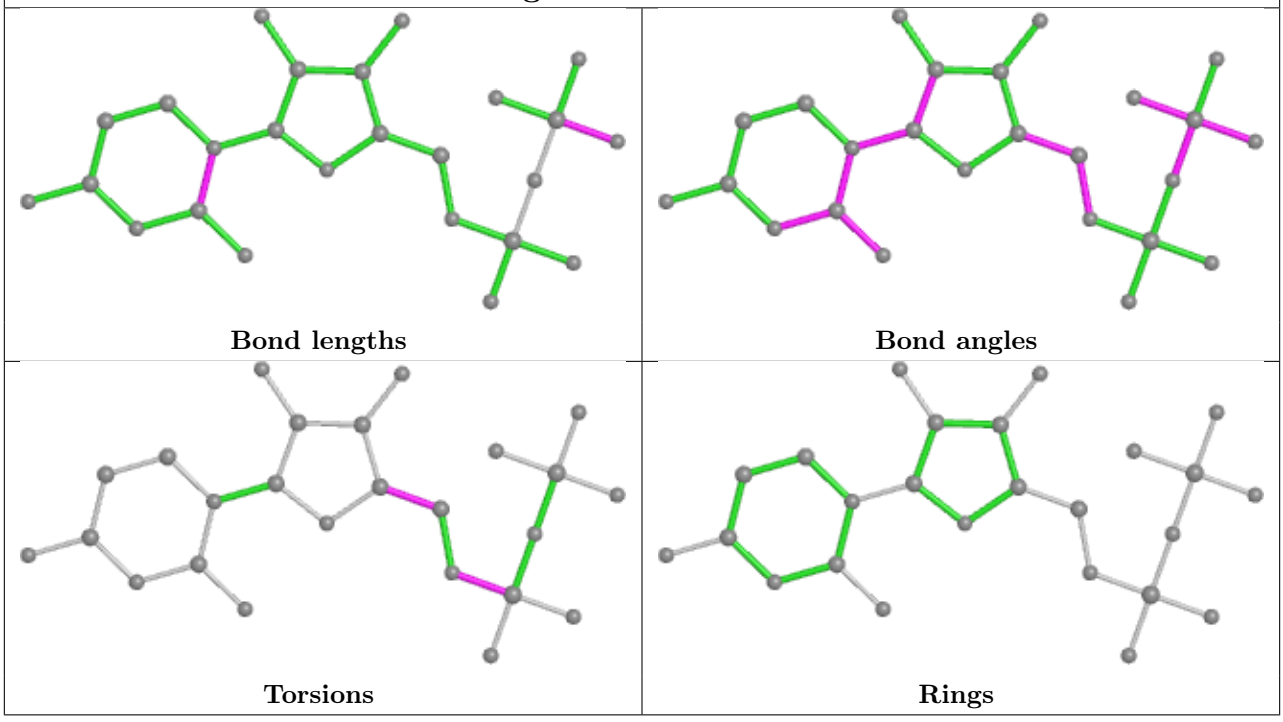
There are no ring outliers.

8 monomers are involved in 39 short contacts:

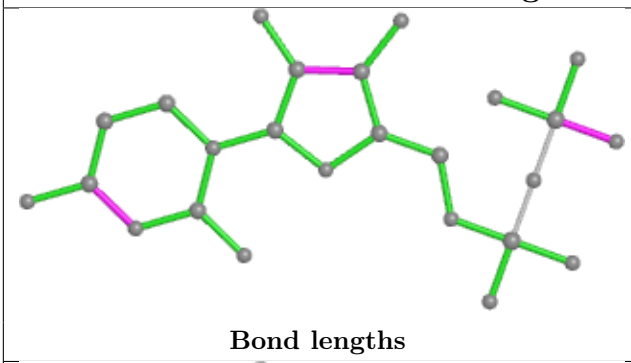
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	811	UDP	2	0
5	A	813	PG4	1	0
5	D	816	PG4	9	0
5	B	815	PG4	5	0
5	C	814	PG4	6	0
7	B	809	UDP	1	0
5	B	817	PG4	13	0
7	D	810	UDP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

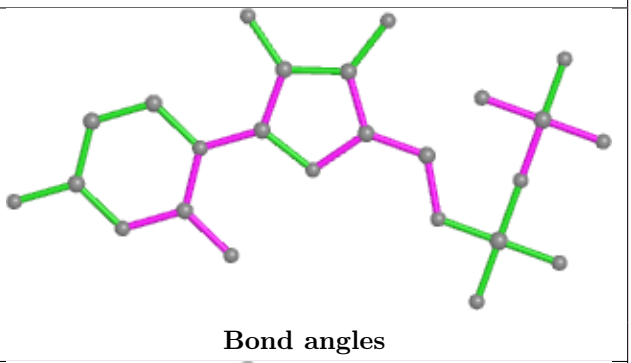
Ligand UDP B 811



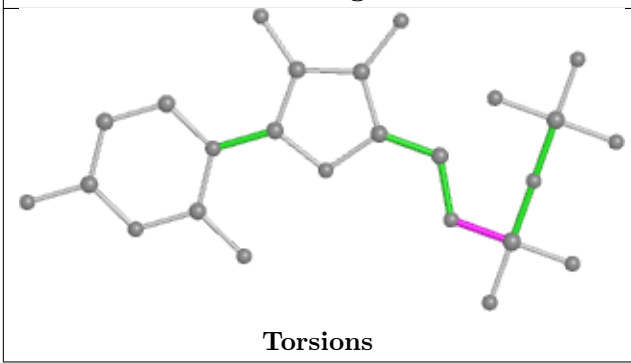
Ligand UDP B 809



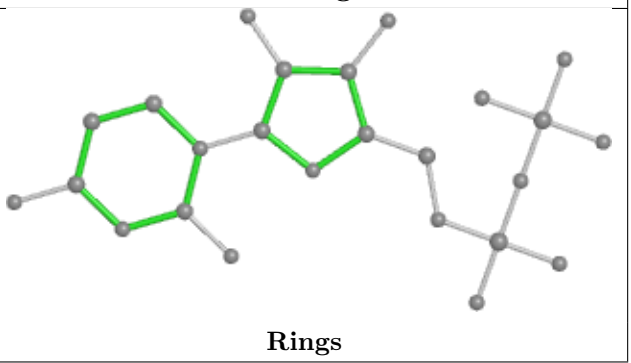
Bond lengths



Bond angles

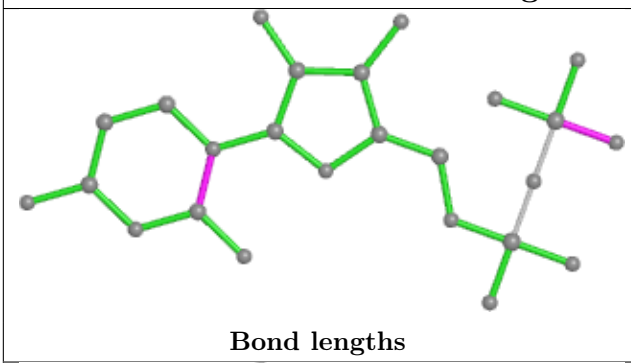


Torsions

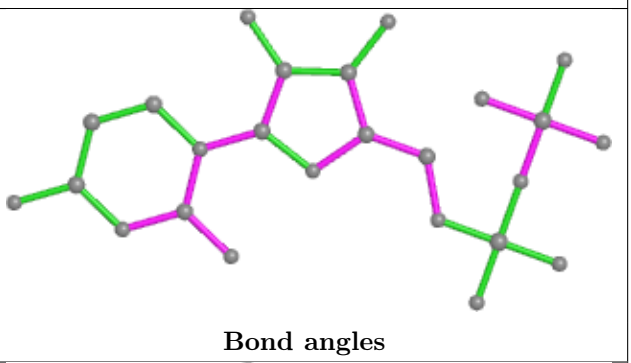


Rings

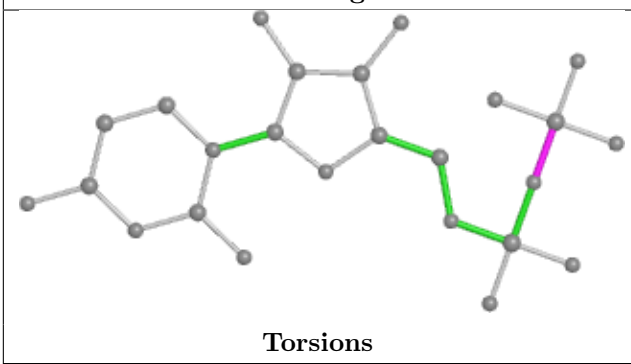
Ligand UDP D 810



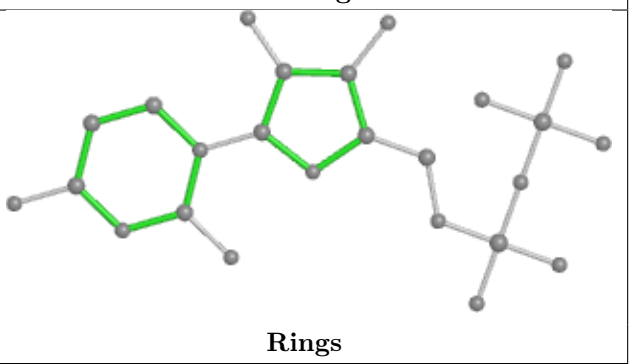
Bond lengths



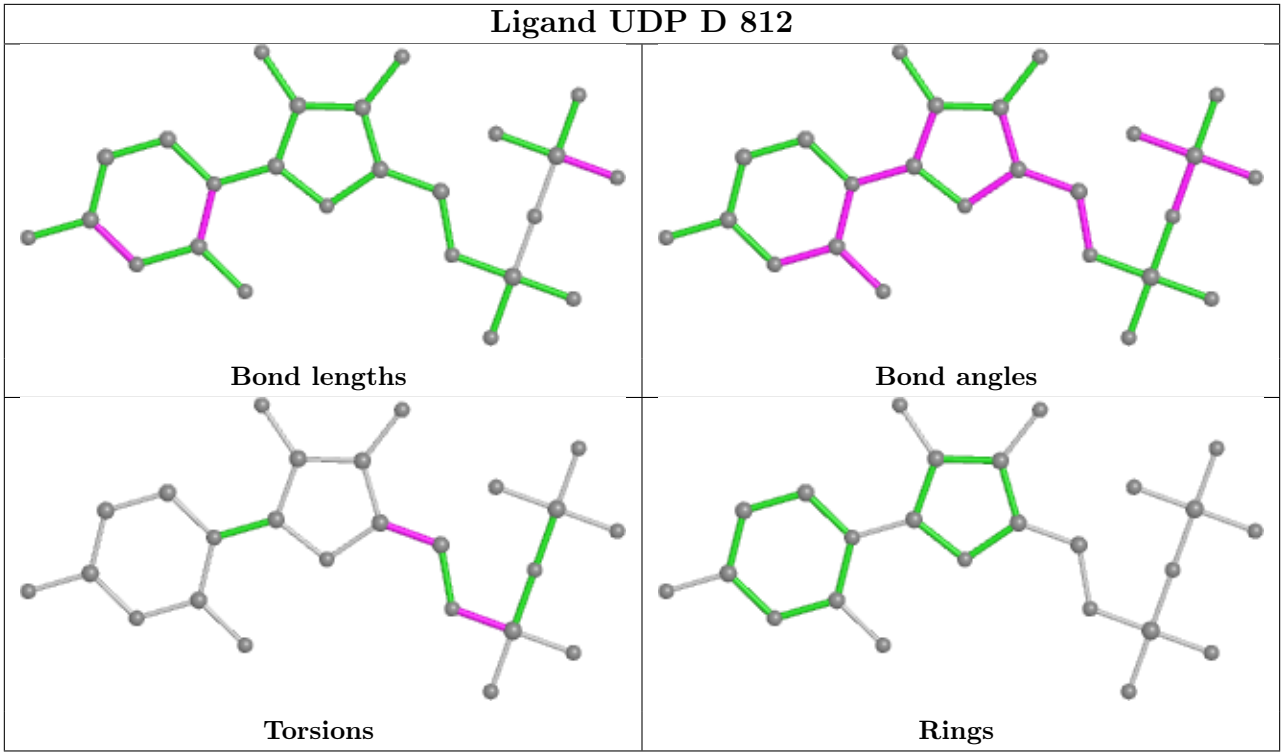
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	123/123 (100%)	-0.14	8 (6%)	18	18	26, 39, 60, 76	0
1	C	123/123 (100%)	-0.00	8 (6%)	18	18	24, 34, 60, 93	0
2	B	272/286 (95%)	-0.20	10 (3%)	41	41	21, 35, 56, 65	0
2	D	272/286 (95%)	-0.16	10 (3%)	41	41	25, 38, 57, 76	0
All	All	790/818 (96%)	-0.15	36 (4%)	32	31	21, 37, 57, 93	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	123	PRO	10.9
1	C	122	LYS	7.9
2	D	402	SER	6.0
2	D	131	LEU	4.5
1	C	68	GLU	4.3
2	B	402	SER	4.1
1	A	68	GLU	3.4
1	C	121	GLU	3.3
2	D	132	THR	3.2
2	B	131	LEU	3.2
1	A	65	GLU	3.1
2	D	232	LEU	3.0
2	D	307	PHE	2.8
2	B	346	ARG	2.7
1	A	66	PHE	2.6
2	B	152	PRO	2.6
2	B	151	ILE	2.6
1	A	46	GLY	2.5
2	B	157	LEU	2.5
2	B	160	GLN	2.5
1	A	67	PRO	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	64	SER	2.5
2	D	185	ILE	2.4
1	C	30	LEU	2.4
1	A	123	PRO	2.4
2	D	184	ILE	2.4
2	B	132	THR	2.4
2	B	146	LEU	2.3
1	C	66	PHE	2.3
2	D	250	PHE	2.3
2	B	351	LYS	2.2
1	A	45	ASN	2.2
1	C	45	ASN	2.1
1	C	53	PHE	2.1
2	D	346	ARG	2.1
2	D	186	ILE	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
7	UDP	D	812	25/25	0.72	0.19	58,76,100,100	0
5	PG4	B	815	13/13	0.78	0.28	64,66,73,75	0
5	PG4	B	817	13/13	0.82	0.31	64,66,73,75	0
7	UDP	B	811	25/25	0.84	0.17	69,82,98,99	0
4	SO4	A	819	5/5	0.84	0.24	88,89,89,89	0
5	PG4	D	816	13/13	0.85	0.22	64,66,70,70	0
5	PG4	C	814	13/13	0.89	0.16	52,55,64,66	0
5	PG4	A	813	13/13	0.89	0.11	46,48,49,50	0

Continued on next page...

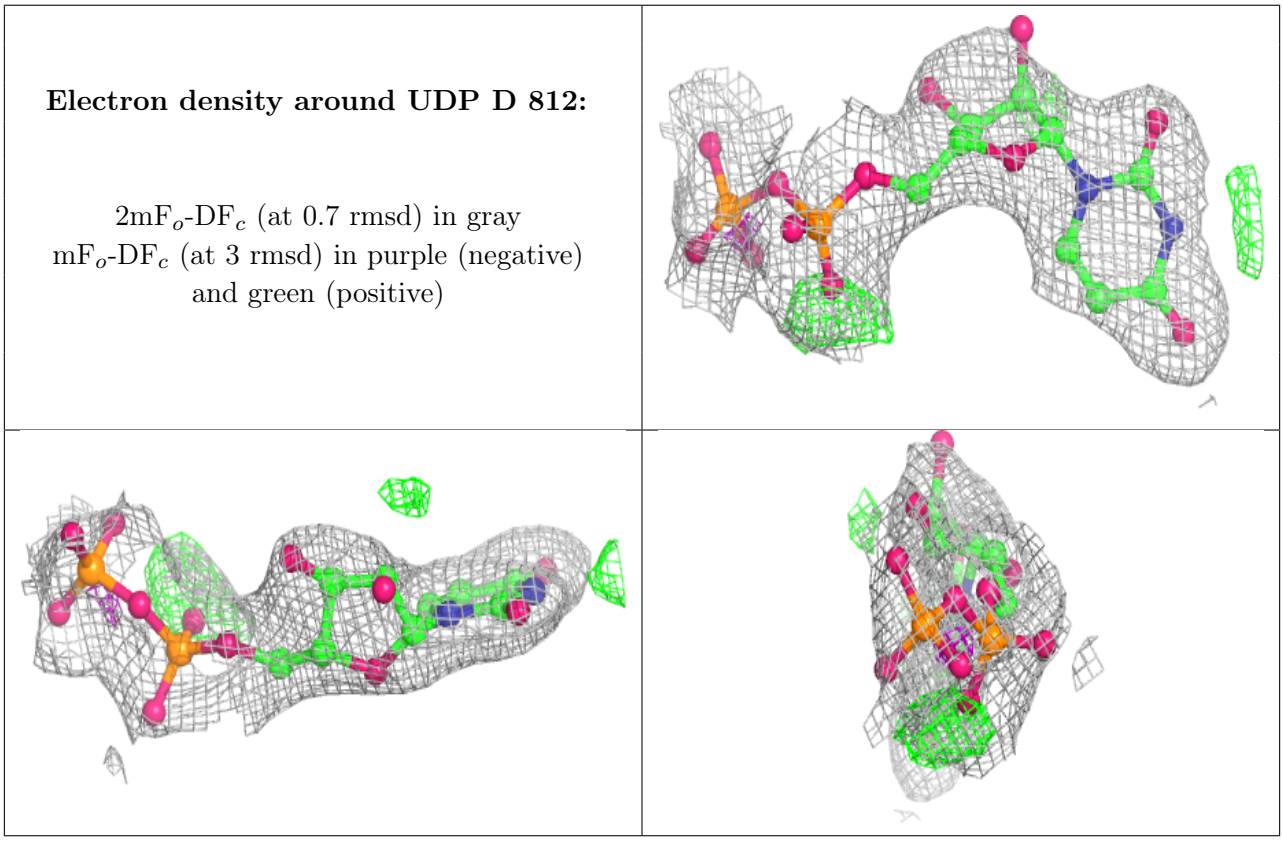
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	D	818	5/5	0.93	0.26	82,83,83,84	0
7	UDP	B	809	25/25	0.97	0.09	30,34,38,40	0
7	UDP	D	810	25/25	0.98	0.08	26,30,34,36	0
3	CA	C	806	1/1	0.99	0.08	33,33,33,33	0
3	CA	A	805	1/1	0.99	0.05	34,34,34,34	0
6	MN	B	807	1/1	1.00	0.05	35,35,35,35	0
6	MN	D	808	1/1	1.00	0.08	35,35,35,35	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.

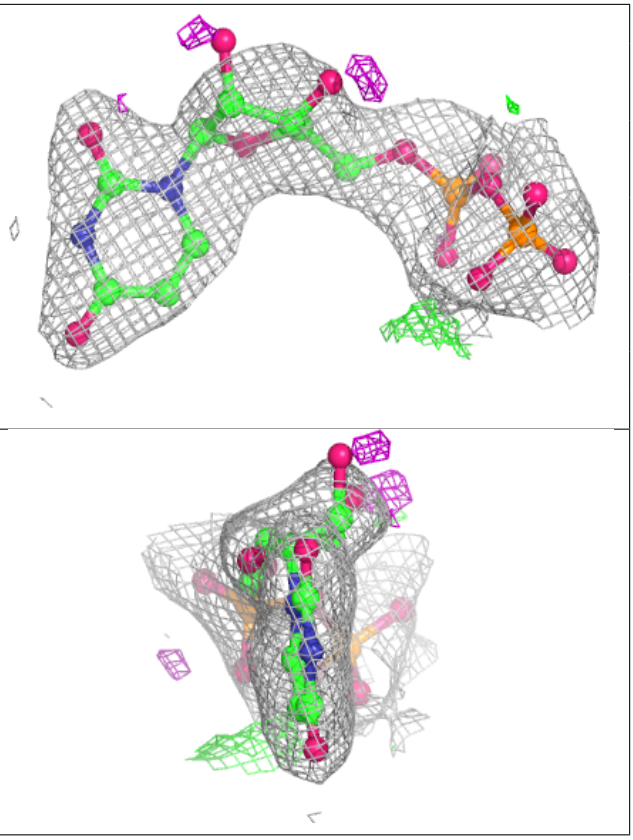
Electron density around UDP D 812:

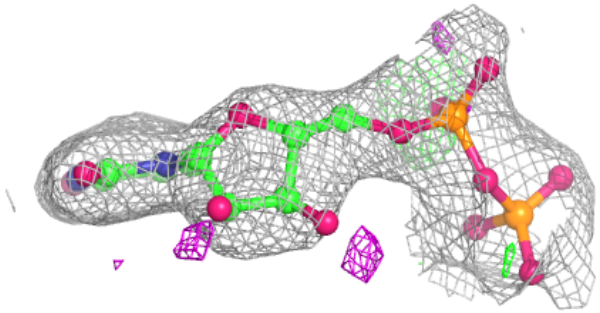
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around UDP B 811:

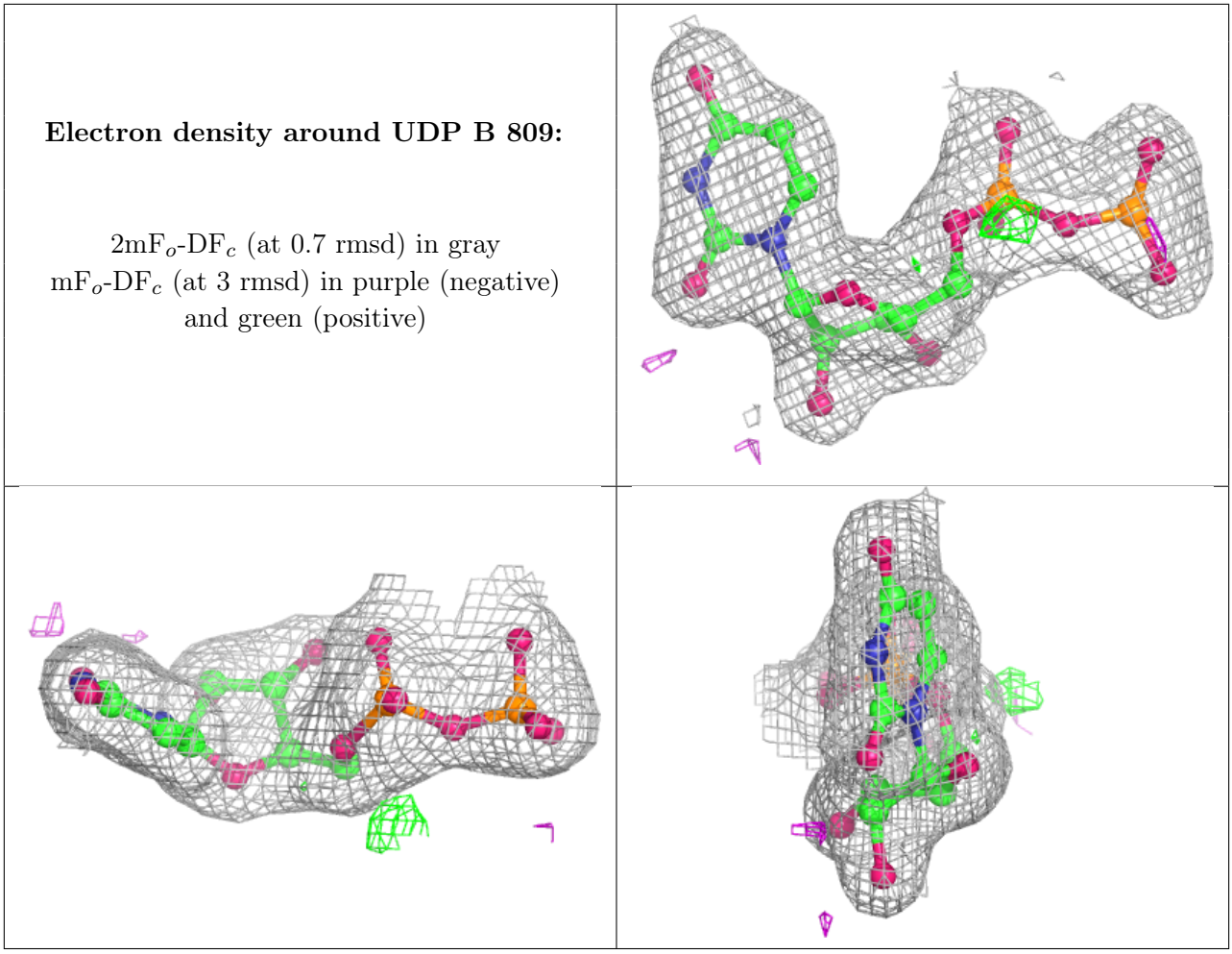
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





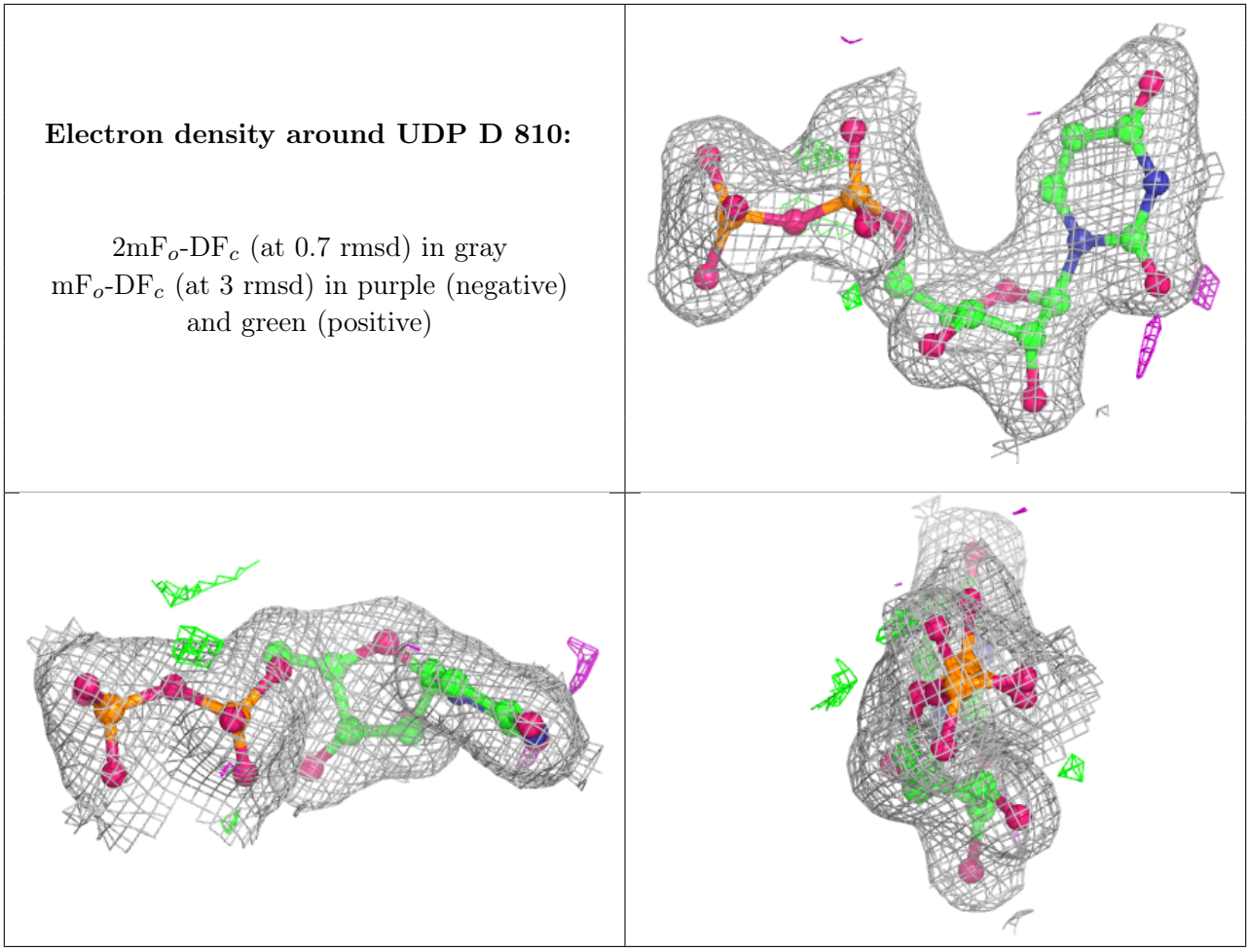
Electron density around UDP B 809:

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



Electron density around UDP D 810:

$2mF_o$-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.