Full wwPDB X-ray Structure Validation Report (i)

Dec 17, 2023 – 11:44 AM EST

PDB ID	:	4W6Q
Title	:	Glycosyltransferase C from Streptococcus agalactiae
Authors	:	Zhu, F.; Zhang, H.; Wu, H.
Deposited on	:	2014-08-20
Resolution	:	2.70 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:

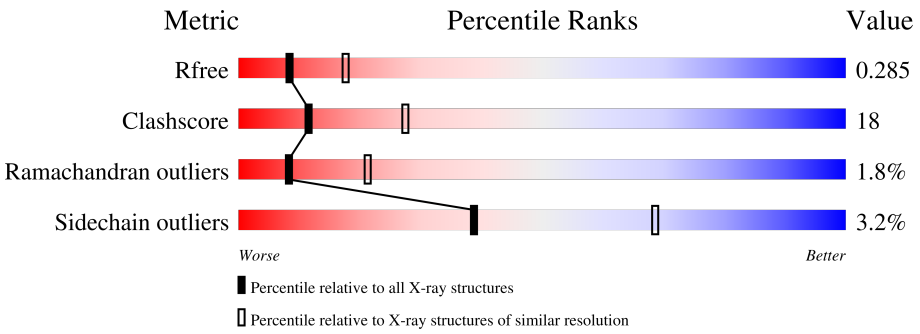
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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%

Mol	Chain	Length	Quality of chain
1	A	333	61% 37% •••
1	B	333	66% 31% •
1	C	333	62% 34% •
1	D	333	56% 41% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11158 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.

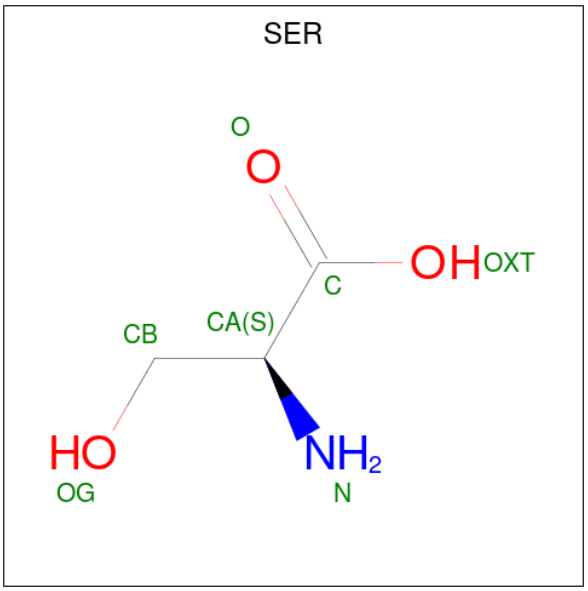
- Molecule 1 is a protein called glucosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	331	2668	1713	443	497	15	0	0	0
1	B	332	2674	1716	444	499	15	0	0	0
1	C	332	2674	1716	444	499	15	0	0	0
1	D	332	2674	1716	444	499	15	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

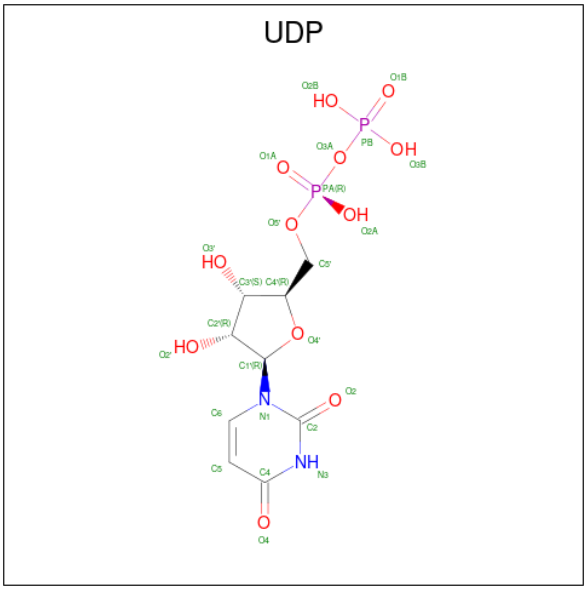
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	-	expression tag	UNP Q3D9X5
A	0	CYS	-	expression tag	UNP Q3D9X5
B	-1	ALA	-	expression tag	UNP Q3D9X5
B	0	CYS	-	expression tag	UNP Q3D9X5
C	-1	ALA	-	expression tag	UNP Q3D9X5
C	0	CYS	-	expression tag	UNP Q3D9X5
D	-1	ALA	-	expression tag	UNP Q3D9X5
D	0	CYS	-	expression tag	UNP Q3D9X5

- Molecule 2 is SERINE (three-letter code: SER) (formula: $C_3H_7NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	6	3	1	2	0	0

- Molecule 3 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



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

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

- Molecule 4 is water.

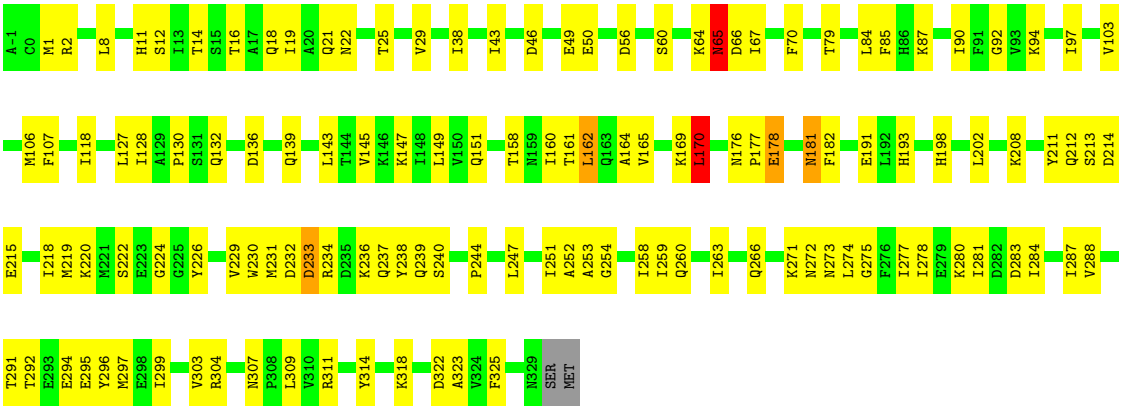
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	96	96	96	0	0
			Total	O		
4	B	94	94	94	0	0
			Total	O		
4	C	102	102	102	0	0
			Total	O		
4	D	70	70	70	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

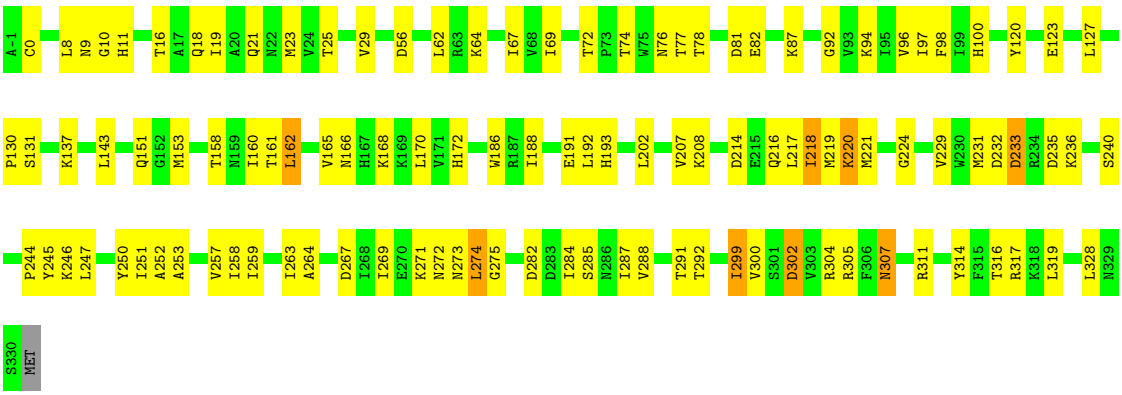
• Molecule 1: glucosyltransferase

Chain A:



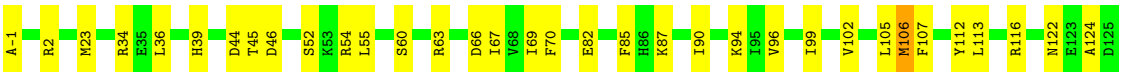
• Molecule 1: glucosyltransferase

Chain B:



• Molecule 1: glucosyltransferase

Chain C:



V126 L127 I128 M134 K137 L138 Q139 L143 T144 K147 I148 L149 D155 H156 P157 T158 N159 I160 T161 L162 V165 N166 H167 P174 P177 E178 R179 F180 N181 F182 I183 K184 N185 W186 R187 I188 P189 T190 E191 L192 H198 N199 T205 K208 Y211 Q212 S213 D214

E215 Q216 L217 I218 M219 K220 M221 S222 V229 W230 M231 D232 D233 R234 D235 K236 Q239 S240 L241 Y242 C243 P244 Y245 K246 L247 Y250 I255 P256 V257 I258 I259 I263 K271 G275 F276 I277 I278 E279 K280 I281 D282 D283 I284 T291 T292 E293 E294 E295 Y296 I299 V300

S301 D302 R305 F306 N307 R311 Q312 F315 T316 R317 A323 S326 S330 MET

- Molecule 1: glucosyltransferase

Chain D: 56% 41% •

A-1 R2 T3 Y4 L8 I13 T14 S15 I19 A20 Q21 N22 M23 I27 A28 F33 R34 E35 L36 H39 S40 Y41 P42 I43 D44 T45 D46 S47 P48 E49 K53 R54 L55 I58 C59 S60 K64 N65 D66 I67 V68 I69 P73 T74 W75 N76 T77 T78 T79

E82 F85 K89 I90 F91 G92 V93 K94 I95 V96 I97 F98 D101 V102 V103 P104 F107 N110 F111 Y112 L113 M114 D115 R116 T117 N122 E123 L127 I128 A129 P130 M134 V135 Q139 L143 I148 L149 D155 T158 N159 I160 T161 L162 V165

K168 K169 L170 F173 N176 P177 F182 I183 I188 E191 L192 H193 V194 D197 H198 N199 L202 P203 T204 T205 V206 V207 K208 S213 D214 E215 Q216 L217 I218 M221 G224 G225 Y226 V229 W230 K236 Q239 S240 L241 Y242 C243 P244 Y245 K246 L247 G248 A249

Y250 I251 G254 I255 P256 V257 I258 I259 Q260 I263 Q266 N273 L274 G275 F276 I277 I278 E279 K280 I281 D282 D283 I284 S285 T291 E295 I299 V300 S301 D302 V303 R304 N307 P308 L309 Y314 F315 T316 R317 D322 L328 N329 S330 MET

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	77.20Å 99.27Å 188.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.91 – 2.70 29.91 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.91-2.70) 98.0 (29.91-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.74 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.184 , 0.284 0.186 , 0.285	Depositor DCC
R_{free} test set	2000 reflections (2.38%)	wwPDB-VP
Wilson B-factor (Å^2)	33.9	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 67.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11158	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.77% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: UDP

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	0/2728	0.70	2/3701 (0.1%)
1	B	0.52	0/2734	0.65	3/3709 (0.1%)
1	C	0.48	0/2734	0.66	1/3709 (0.0%)
1	D	0.46	0/2734	0.67	1/3709 (0.0%)
All	All	0.48	0/10930	0.67	7/14828 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	2
All	All	0	3

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	162	LEU	CA-CB-CG	7.21	131.87	115.30
1	A	170	LEU	CA-CB-CG	6.78	130.89	115.30
1	B	274	LEU	CA-CB-CG	-6.07	101.35	115.30
1	D	162	LEU	CA-CB-CG	5.58	128.12	115.30
1	B	218	ILE	CG1-CB-CG2	-5.37	99.58	111.40
1	C	162	LEU	CA-CB-CG	5.35	127.61	115.30
1	B	162	LEU	CA-CB-CG	5.28	127.44	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	65	ASN	Peptide
1	C	165	VAL	Peptide
1	C	166	ASN	Peptide

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	2668	0	2662	103	0
1	B	2674	0	2667	86	0
1	C	2674	0	2667	99	0
1	D	2674	0	2667	104	0
2	A	6	0	4	1	0
3	A	25	0	11	0	0
3	B	25	0	11	0	0
3	C	25	0	11	1	0
3	D	25	0	11	0	0
4	A	96	0	0	9	0
4	B	94	0	0	5	0
4	C	102	0	0	9	0
4	D	70	0	0	3	0
All	All	11158	0	10711	379	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 (379) 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:C:233:ASP:HA	1:C:236:LYS:HD3	1.25	1.11
1:B:56:ASP:OD1	1:B:87:LYS:NZ	1.96	0.97
1:B:165:VAL:HG11	1:B:300:VAL:HG11	1.50	0.92
1:C:292:THR:HG22	1:C:294:GLU:H	1.38	0.89
1:C:166:ASN:HA	1:C:296:TYR:HE1	1.40	0.85
1:B:273:ASN:HD21	1:B:299:ILE:HA	1.42	0.84
1:D:229:VAL:HB	1:D:259:ILE:HG22	1.58	0.83
1:A:128:ILE:HD11	1:A:323:ALA:HB2	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ILE:O	1:A:311:ARG:NH2	2.14	0.80
1:B:282:ASP:OD2	4:B:578:HOH:O	1.98	0.80
1:C:128:ILE:HD11	1:C:323:ALA:HB2	1.64	0.80
1:D:98:PHE:HA	1:D:128:ILE:HG23	1.62	0.79
1:B:252:ALA:O	1:B:311:ARG:NH1	2.16	0.79
1:C:259:ILE:HD11	1:C:277:ILE:HG12	1.65	0.78
1:D:239:GLN:NE2	1:D:263:ILE:HG13	1.99	0.78
1:C:229:VAL:HB	1:C:259:ILE:HG22	1.66	0.77
1:A:191:GLU:N	1:A:191:GLU:OE1	2.15	0.77
1:B:273:ASN:HD22	1:B:302:ASP:HB2	1.49	0.77
1:A:181:ASN:H	1:A:233:ASP:HB3	1.48	0.77
1:A:237:GLN:OE1	1:A:260:GLN:NE2	2.18	0.77
1:D:85:PHE:HE2	1:D:123:GLU:HB2	1.49	0.76
1:B:0:CYS:SG	4:C:588:HOH:O	2.44	0.75
1:D:67:ILE:HD11	1:D:328:LEU:HD21	1.69	0.74
1:A:149:LEU:HD21	1:A:322:ASP:HB3	1.69	0.74
1:D:139:GLN:HG2	1:D:143:LEU:HD23	1.70	0.74
1:D:47:SER:O	1:D:49:GLU:N	2.21	0.73
1:C:191:GLU:OE1	1:C:191:GLU:N	2.17	0.73
1:D:160:ILE:HG12	1:D:215:GLU:HG3	1.71	0.73
1:C:198:HIS:O	1:C:208:LYS:NZ	2.21	0.72
1:D:273:ASN:ND2	1:D:302:ASP:OD2	2.22	0.72
1:A:229:VAL:HB	1:A:259:ILE:HG22	1.70	0.72
1:C:326:SER:OG	4:C:570:HOH:O	2.06	0.72
1:B:160:ILE:HG13	1:B:311:ARG:HH22	1.53	0.72
1:D:258:ILE:HG21	1:D:284:ILE:HG23	1.72	0.71
1:B:160:ILE:HG21	1:B:218:ILE:HB	1.72	0.71
1:C:177:PRO:O	1:C:181:ASN:ND2	2.23	0.71
1:B:302:ASP:HA	1:B:305:ARG:HB2	1.74	0.70
1:C:317:ARG:NH1	4:C:596:HOH:O	2.24	0.70
1:B:23:MET:HE1	1:B:245:TYR:HE1	1.54	0.70
1:A:266:GLN:NE2	1:A:277:ILE:HG21	2.08	0.69
1:A:251:ILE:HG23	1:A:303:VAL:HG13	1.75	0.69
1:D:168:LYS:HB3	1:D:170:LEU:HD13	1.74	0.68
1:C:160:ILE:O	1:C:311:ARG:NH2	2.27	0.68
1:B:165:VAL:HG23	1:B:224:GLY:HA2	1.75	0.68
1:A:292:THR:HG22	1:A:295:GLU:H	1.59	0.68
1:D:85:PHE:CE2	1:D:123:GLU:HB2	2.29	0.67
1:C:330:SER:OG	4:C:545:HOH:O	2.13	0.67
1:D:260:GLN:OE1	4:D:547:HOH:O	2.12	0.67
1:A:165:VAL:HG13	1:A:224:GLY:HA2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:ASP:HB3	1:A:236:LYS:HB2	1.77	0.67
1:C:280:LYS:HG3	1:C:282:ASP:H	1.60	0.67
1:B:214:ASP:O	1:B:218:ILE:HG13	1.95	0.66
1:D:165:VAL:HG23	1:D:304:ARG:NH2	2.11	0.66
1:B:21:GLN:HG2	1:B:100:HIS:CE1	2.30	0.65
1:C:236:LYS:HD2	1:C:236:LYS:N	2.11	0.65
1:D:165:VAL:HG13	1:D:224:GLY:HA2	1.78	0.65
1:D:183:ILE:HD12	1:D:192:LEU:HD21	1.78	0.65
1:D:110:ASN:HA	1:D:112:TYR:HD2	1.61	0.65
1:B:202:LEU:HD12	1:B:208:LYS:HB2	1.79	0.65
1:A:11:HIS:HB2	1:A:18:GLN:OE1	1.98	0.64
4:A:516:HOH:O	1:B:9:ASN:HB3	1.96	0.64
1:D:199:ASN:OD1	1:D:199:ASN:N	2.31	0.64
1:B:273:ASN:ND2	1:B:302:ASP:OD2	2.30	0.64
1:A:176:ASN:ND2	1:A:178:GLU:OE2	2.31	0.63
1:C:139:GLN:NE2	4:C:508:HOH:O	2.30	0.63
1:C:67:ILE:HD12	1:C:94:LYS:HB2	1.80	0.63
1:A:294:GLU:HA	1:A:297:MET:HB2	1.81	0.63
1:C:301:SER:O	1:C:305:ARG:HG3	1.99	0.63
1:D:149:LEU:HD11	1:D:322:ASP:HB3	1.80	0.63
1:D:244:PRO:HG2	1:D:247:LEU:HB3	1.79	0.63
1:B:160:ILE:O	1:B:311:ARG:NH2	2.32	0.63
1:A:281:ILE:H	1:A:281:ILE:HD12	1.63	0.62
1:A:160:ILE:HG21	1:A:218:ILE:HB	1.82	0.62
1:D:2:ARG:NH2	1:D:66:ASP:OD2	2.32	0.62
1:D:110:ASN:HA	1:D:112:TYR:CD2	2.35	0.62
1:A:160:ILE:HG13	1:A:311:ARG:HH22	1.64	0.62
1:A:56:ASP:OD1	1:A:87:LYS:NZ	2.23	0.62
1:A:97:ILE:HG22	1:A:127:LEU:HG	1.82	0.62
1:D:127:LEU:HD21	1:D:143:LEU:HD21	1.82	0.61
1:B:160:ILE:HD12	1:B:161:THR:O	2.01	0.61
1:A:309:LEU:HG	1:D:328:LEU:HD12	1.82	0.61
1:B:233:ASP:HA	1:B:236:LYS:HD2	1.82	0.61
1:A:318:LYS:NZ	4:A:566:HOH:O	2.32	0.60
1:C:312:GLN:NE2	4:C:588:HOH:O	2.34	0.60
1:C:-1:ALA:N	4:C:578:HOH:O	2.28	0.60
1:D:55:LEU:HD23	1:D:58:ILE:HD12	1.84	0.60
1:D:191:GLU:OE1	1:D:191:GLU:N	2.32	0.60
1:C:216:GLN:HG2	1:C:220:LYS:HE3	1.84	0.60
1:B:273:ASN:ND2	1:B:302:ASP:HB2	2.17	0.59
1:A:130:PRO:HA	1:A:151:GLN:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:TRP:CZ3	1:A:260:GLN:HB2	2.36	0.59
1:A:287:ILE:O	1:A:291:THR:HB	2.02	0.59
1:D:78:THR:O	1:D:82:GLU:HG2	2.02	0.59
1:B:231:MET:HE3	1:B:263:ILE:HG22	1.82	0.59
1:A:127:LEU:HD22	1:A:143:LEU:HD21	1.85	0.59
1:A:158:THR:OG1	1:A:160:ILE:HG23	2.03	0.58
1:C:166:ASN:HA	1:C:296:TYR:CE1	2.29	0.58
1:B:217:LEU:O	1:B:221:MET:HG3	2.03	0.58
1:B:127:LEU:HD22	1:B:143:LEU:HD11	1.86	0.58
1:D:8:LEU:HG	1:D:21:GLN:OE1	2.04	0.58
1:D:160:ILE:HD13	1:D:218:ILE:HB	1.86	0.58
1:A:275:GLY:HA2	1:A:299:ILE:HD11	1.86	0.58
1:D:263:ILE:HG22	1:D:266:GLN:HB3	1.86	0.58
1:B:9:ASN:OD1	1:B:10:GLY:N	2.37	0.58
1:B:160:ILE:HG13	1:B:311:ARG:NH2	2.19	0.57
1:D:198:HIS:O	1:D:208:LYS:NZ	2.36	0.57
1:A:8:LEU:HD11	1:A:18:GLN:HB2	1.87	0.57
1:A:160:ILE:HG13	1:A:311:ARG:NH2	2.20	0.57
1:D:259:ILE:HD12	1:D:263:ILE:HG21	1.87	0.56
1:D:173:PHE:O	1:D:194:VAL:HA	2.05	0.56
1:A:214:ASP:O	1:A:218:ILE:HG12	2.05	0.56
1:C:85:PHE:HZ	1:C:124:ALA:HB2	1.70	0.55
1:D:177:PRO:HD2	1:D:198:HIS:CD2	2.41	0.55
1:B:11:HIS:HB2	1:B:18:GLN:OE1	2.05	0.55
1:C:122:ASN:CG	1:C:144:THR:HG22	2.26	0.55
1:C:167:HIS:CE1	1:C:291:THR:HG23	2.41	0.55
1:A:230:TRP:CH2	1:A:260:GLN:HB2	2.42	0.55
1:C:233:ASP:HA	1:C:236:LYS:CD	2.17	0.55
1:D:177:PRO:HD2	1:D:198:HIS:HD2	1.72	0.55
1:A:64:LYS:HD3	1:A:92:GLY:H	1.72	0.54
1:B:67:ILE:HD11	1:B:328:LEU:HD21	1.89	0.54
1:C:45:THR:O	1:D:53:LYS:NZ	2.41	0.54
1:A:127:LEU:HD13	1:A:145:VAL:HG21	1.90	0.54
1:D:135:VAL:HG11	1:D:148:ILE:HD12	1.89	0.54
1:C:149:LEU:HD11	4:C:519:HOH:O	2.08	0.54
1:B:257:VAL:HG23	1:B:259:ILE:HD11	1.89	0.54
1:C:128:ILE:HD11	1:C:323:ALA:CB	2.36	0.54
1:C:239:GLN:HG3	1:C:263:ILE:HG13	1.89	0.54
1:D:130:PRO:HD2	1:D:134:MET:HG2	1.90	0.54
1:D:46:ASP:OD2	1:D:54:ARG:NH1	2.41	0.53
1:B:218:ILE:HG22	1:B:253:ALA:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:317:ARG:NH2	4:D:532:HOH:O	2.40	0.53
1:B:170:LEU:HD22	1:B:193:HIS:NE2	2.23	0.53
1:D:40:SER:HA	1:D:76:ASN:OD1	2.09	0.53
1:D:64:LYS:O	1:D:93:VAL:HG12	2.08	0.53
1:A:147:LYS:HZ1	2:A:401:SER:N	2.07	0.53
1:D:192:LEU:HD23	1:D:206:VAL:HG22	1.91	0.53
1:C:23:MET:CE	1:C:156:HIS:HA	2.39	0.53
1:C:186:TRP:CZ2	1:C:192:LEU:HD13	2.44	0.53
1:B:258:ILE:HD13	1:B:284:ILE:HG23	1.91	0.53
1:C:155:ASP:OD1	1:C:315:PHE:HB2	2.09	0.53
1:C:160:ILE:HG12	1:C:218:ILE:HD12	1.91	0.53
1:B:244:PRO:HG2	1:B:247:LEU:HB3	1.91	0.52
1:B:316:THR:O	1:B:319:LEU:HG	2.09	0.52
1:A:296:TYR:O	1:A:299:ILE:HG22	2.10	0.52
1:C:216:GLN:O	1:C:220:LYS:HG3	2.10	0.52
1:C:214:ASP:O	1:C:218:ILE:HG12	2.08	0.52
1:D:242:TYR:HE1	1:D:244:PRO:HB3	1.75	0.52
1:A:266:GLN:HE21	1:A:277:ILE:HG21	1.74	0.52
1:A:272:ASN:O	1:A:273:ASN:HB3	2.10	0.52
1:B:120:TYR:HA	1:B:123:GLU:HG3	1.91	0.52
1:A:178:GLU:OE2	1:A:198:HIS:ND1	2.43	0.52
1:B:69:ILE:HG12	1:B:96:VAL:HB	1.91	0.52
1:B:166:ASN:OD1	1:B:168:LYS:HG3	2.10	0.52
1:C:234:ARG:NH1	1:C:235:ASP:OD2	2.42	0.52
1:A:161:THR:HG21	1:C:213:SER:HB2	1.92	0.52
1:A:278:ILE:HG12	1:A:284:ILE:HG12	1.90	0.52
1:C:23:MET:HE3	1:C:156:HIS:HA	1.91	0.52
1:D:280:LYS:HE2	1:D:282:ASP:HB2	1.92	0.52
1:C:54:ARG:HA	1:D:54:ARG:HA	1.92	0.52
1:D:244:PRO:HG2	1:D:247:LEU:CB	2.39	0.52
1:A:8:LEU:HD23	1:A:21:GLN:NE2	2.25	0.52
1:D:229:VAL:HB	1:D:259:ILE:CG2	2.36	0.51
1:A:244:PRO:HG2	1:A:247:LEU:HB3	1.92	0.51
1:C:258:ILE:HD13	1:C:284:ILE:HG23	1.92	0.51
1:A:65:ASN:ND2	4:A:574:HOH:O	2.25	0.51
1:C:281:ILE:HA	1:C:284:ILE:HD12	1.92	0.51
1:D:127:LEU:CD2	1:D:143:LEU:HD21	2.41	0.51
1:B:25:THR:O	1:B:29:VAL:HG23	2.11	0.51
1:C:69:ILE:HG12	1:C:96:VAL:HB	1.92	0.51
1:D:15:SER:O	1:D:19:ILE:HG23	2.10	0.51
1:A:165:VAL:HG22	1:A:222:SER:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:LYS:NZ	4:B:548:HOH:O	2.43	0.51
1:B:188:ILE:HG21	1:B:285:SER:OG	2.11	0.51
1:A:164:ALA:N	4:A:554:HOH:O	2.12	0.50
1:B:231:MET:CE	1:B:263:ILE:HG22	2.40	0.50
1:A:97:ILE:CG2	1:A:127:LEU:HG	2.41	0.50
1:C:162:LEU:HD21	1:C:307:ASN:HD21	1.76	0.50
1:D:160:ILE:HD11	1:D:215:GLU:HA	1.91	0.50
1:D:113:LEU:HD22	1:D:116:ARG:HD3	1.93	0.50
1:A:202:LEU:HD12	1:A:208:LYS:HB2	1.93	0.50
1:A:236:LYS:N	1:A:236:LYS:HD2	2.26	0.50
1:C:99:ILE:HD11	1:C:127:LEU:HD11	1.93	0.50
1:C:99:ILE:HD12	1:C:127:LEU:HD21	1.94	0.50
1:B:232:ASP:O	1:B:233:ASP:HB2	2.10	0.50
1:B:272:ASN:O	1:B:273:ASN:HB3	2.11	0.50
1:D:254:GLY:HA3	1:D:304:ARG:HE	1.75	0.50
1:B:16:THR:O	1:B:19:ILE:HG22	2.12	0.50
1:A:65:ASN:HB3	1:A:66:ASP:OD1	2.12	0.50
1:B:131:SER:HB3	1:B:264:ALA:HB1	1.95	0.49
1:B:8:LEU:HD23	1:B:18:GLN:HA	1.92	0.49
1:C:180:PHE:O	1:C:183:ILE:HG22	2.12	0.49
1:D:155:ASP:OD1	1:D:315:PHE:HB2	2.12	0.49
1:A:258:ILE:HG21	1:A:284:ILE:HG23	1.95	0.49
1:B:263:ILE:HD12	1:B:264:ALA:O	2.12	0.49
1:D:251:ILE:HG23	1:D:303:VAL:HG13	1.95	0.49
1:A:299:ILE:O	1:A:303:VAL:HG23	2.12	0.48
1:D:230:TRP:CZ3	1:D:284:ILE:HD11	2.47	0.48
1:D:257:VAL:O	1:D:275:GLY:HA3	2.13	0.48
1:C:126:VAL:HG22	1:C:147:LYS:HB2	1.94	0.48
1:D:188:ILE:HG21	1:D:285:SER:OG	2.13	0.48
1:D:236:LYS:O	1:D:239:GLN:HB3	2.14	0.48
1:A:49:GLU:HG3	1:A:50:GLU:N	2.28	0.48
1:A:181:ASN:N	1:A:233:ASP:HB3	2.23	0.48
1:A:87:LYS:O	1:A:90:ILE:HG13	2.14	0.48
1:A:181:ASN:OD1	1:A:182:PHE:N	2.47	0.48
1:B:172:HIS:HA	1:B:193:HIS:HB2	1.95	0.48
1:B:267:ASP:HB2	1:B:271:LYS:HE2	1.95	0.47
1:B:273:ASN:O	1:B:273:ASN:CG	2.52	0.47
1:B:257:VAL:O	1:B:275:GLY:HA3	2.13	0.47
1:D:102:VAL:HG12	1:D:104:PRO:HD2	1.95	0.47
1:D:256:PRO:HB3	1:D:299:ILE:HG21	1.95	0.47
1:D:259:ILE:HG13	1:D:277:ILE:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:MET:O	1:C:236:LYS:NZ	2.43	0.47
1:A:2:ARG:HE	1:A:2:ARG:HB2	1.44	0.47
1:A:232:ASP:CB	1:A:236:LYS:HB2	2.45	0.47
1:C:183:ILE:CD1	1:C:192:LEU:HD23	2.44	0.47
1:D:191:GLU:H	1:D:191:GLU:CD	2.15	0.47
1:B:191:GLU:OE2	1:B:207:VAL:HG21	2.15	0.47
1:A:325:PHE:CD1	1:D:309:LEU:HD11	2.49	0.47
1:D:92:GLY:HA3	4:D:549:HOH:O	2.15	0.47
1:A:107:PHE:HB3	1:A:236:LYS:NZ	2.30	0.47
1:B:231:MET:SD	1:B:236:LYS:HG2	2.55	0.47
1:C:155:ASP:OD2	1:C:316:THR:N	2.35	0.46
1:B:162:LEU:HD22	1:B:304:ARG:HD3	1.97	0.46
1:C:221:MET:HE2	1:C:255:ILE:HD11	1.97	0.46
1:C:158:THR:OG1	1:C:160:ILE:HG23	2.16	0.46
1:D:113:LEU:HD23	1:D:113:LEU:HA	1.75	0.46
1:A:218:ILE:HG22	1:A:253:ALA:HA	1.96	0.46
1:D:236:LYS:C	1:D:239:GLN:HB3	2.36	0.46
1:A:79:THR:HG21	4:A:533:HOH:O	2.16	0.46
1:D:77:THR:HG23	1:D:79:THR:H	1.80	0.46
1:D:221:MET:O	1:D:255:ILE:HG21	2.16	0.46
1:A:139:GLN:NE2	4:A:559:HOH:O	2.30	0.45
1:C:39:HIS:HB2	1:D:60:SER:HB2	1.97	0.45
1:C:134:MET:HA	1:C:241:LEU:HD22	1.98	0.45
1:C:292:THR:HG22	1:C:294:GLU:N	2.19	0.45
1:D:246:LYS:HA	1:D:249:ALA:HB3	1.97	0.45
1:B:216:GLN:HE21	1:B:220:LYS:NZ	2.14	0.45
1:A:292:THR:HB	1:A:295:GLU:CG	2.47	0.45
1:C:178:GLU:OE2	1:C:184:LYS:NZ	2.49	0.45
1:A:230:TRP:CZ2	1:A:281:ILE:HG13	2.52	0.45
1:B:269:ILE:HG23	1:B:274:LEU:HB2	1.98	0.45
1:C:148:ILE:HG13	4:C:585:HOH:O	2.17	0.45
1:C:188:ILE:CG2	1:C:189:PRO:HD2	2.47	0.45
1:C:278:ILE:HG12	1:C:284:ILE:HG12	1.98	0.45
1:D:85:PHE:CE1	1:D:95:ILE:HG21	2.52	0.45
1:B:161:THR:HG21	1:D:213:SER:HB2	1.99	0.45
1:B:216:GLN:HE21	1:B:220:LYS:HZ1	1.63	0.45
1:A:1:MET:HG2	1:A:2:ARG:N	2.32	0.45
1:A:212:GLN:NE2	1:A:220:LYS:HE3	2.32	0.45
1:C:60:SER:HB2	1:D:39:HIS:HB2	1.98	0.45
1:A:191:GLU:H	1:A:191:GLU:CD	2.09	0.45
1:C:302:ASP:HA	1:C:305:ARG:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:LYS:HA	1:D:64:LYS:HD3	1.68	0.45
1:D:104:PRO:HG3	1:D:114:MET:HA	1.99	0.44
1:A:215:GLU:OE2	4:A:569:HOH:O	2.21	0.44
1:B:314:TYR:HA	1:B:317:ARG:HB2	1.99	0.44
1:A:181:ASN:H	1:A:233:ASP:CB	2.23	0.44
1:B:23:MET:HE2	1:B:23:MET:HB2	1.83	0.44
1:B:186:TRP:CE3	1:B:192:LEU:HD22	2.52	0.44
1:C:2:ARG:HD2	1:C:34:ARG:NH1	2.33	0.44
1:D:256:PRO:HB3	1:D:299:ILE:CG2	2.46	0.44
1:A:162:LEU:HB3	1:A:304:ARG:NH2	2.33	0.44
1:B:137:LYS:HB2	4:B:531:HOH:O	2.16	0.44
1:C:165:VAL:HG23	1:C:222:SER:O	2.17	0.44
1:A:325:PHE:CE1	1:D:309:LEU:HD21	2.53	0.44
1:A:263:ILE:HD12	1:A:263:ILE:HA	1.76	0.44
1:D:295:GLU:O	1:D:299:ILE:HG13	2.18	0.44
1:B:273:ASN:ND2	1:B:273:ASN:O	2.51	0.44
1:B:64:LYS:HG3	1:B:92:GLY:H	1.83	0.44
1:C:106:MET:C	1:C:107:PHE:HD1	2.21	0.44
1:A:170:LEU:HD13	1:A:193:HIS:CE1	2.52	0.43
1:A:176:ASN:HA	1:A:177:PRO:HD3	1.80	0.43
1:D:160:ILE:HG21	1:D:218:ILE:HG22	2.00	0.43
1:B:158:THR:OG1	1:B:160:ILE:HG23	2.17	0.43
1:C:67:ILE:CD1	1:C:94:LYS:HB2	2.47	0.43
1:D:28:ALA:HB1	1:D:33:PHE:HB2	2.00	0.43
1:A:162:LEU:HD23	1:A:254:GLY:HA3	2.01	0.43
1:A:280:LYS:HG3	1:A:283:ASP:H	1.83	0.43
1:B:72:THR:HG21	1:B:97:ILE:HD11	1.99	0.43
1:D:8:LEU:HD21	1:D:74:THR:HA	2.00	0.43
1:D:13:ILE:H	1:D:13:ILE:HG13	1.53	0.43
1:D:176:ASN:HA	1:D:177:PRO:HD3	1.82	0.43
1:B:246:LYS:NZ	4:B:513:HOH:O	2.26	0.43
1:C:82:GLU:OE2	1:C:116:ARG:HB3	2.18	0.43
1:D:23:MET:O	1:D:27:ILE:HG12	2.18	0.43
1:B:168:LYS:HB3	1:B:170:LEU:HG	2.00	0.43
1:C:87:LYS:O	1:C:90:ILE:HG12	2.18	0.43
1:A:238:TYR:C	1:A:240:SER:H	2.21	0.43
1:C:217:LEU:O	1:C:221:MET:HG3	2.19	0.43
1:C:233:ASP:CA	1:C:236:LYS:HD3	2.19	0.43
1:D:226:TYR:OH	1:D:291:THR:HG21	2.19	0.43
1:A:118:ILE:HD13	1:A:118:ILE:HA	1.83	0.43
1:C:102:VAL:HG11	1:C:105:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:256:PRO:HB3	1:C:299:ILE:HG23	2.00	0.43
1:A:103:VAL:HA	1:A:106:MET:HG3	2.00	0.43
1:C:63:ARG:NH2	1:D:22:ASN:OD1	2.43	0.43
1:B:62:LEU:HA	1:B:62:LEU:HD12	1.63	0.43
1:B:78:THR:O	1:B:82:GLU:HG3	2.19	0.43
1:C:66:ASP:O	1:C:67:ILE:HD13	2.18	0.43
1:D:229:VAL:HG21	1:D:247:LEU:HB2	2.01	0.43
1:D:41:TYR:CZ	1:D:43:ILE:HG22	2.54	0.42
1:B:257:VAL:CG2	1:B:259:ILE:HD11	2.49	0.42
1:D:114:MET:O	1:D:117:THR:HB	2.19	0.42
1:A:25:THR:O	1:A:29:VAL:HG23	2.18	0.42
1:A:43:ILE:O	1:A:46:ASP:HB2	2.19	0.42
1:B:251:ILE:HG22	1:B:307:ASN:HB3	2.01	0.42
1:C:244:PRO:HG2	1:C:247:LEU:CB	2.50	0.42
1:B:221:MET:HE1	1:B:250:TYR:CE1	2.55	0.42
1:A:160:ILE:HB	1:A:219:MET:HE2	2.02	0.42
1:A:271:LYS:HA	1:A:271:LYS:HD3	1.87	0.42
1:B:76:ASN:O	1:B:77:THR:OG1	2.36	0.42
1:C:127:LEU:HD13	1:C:143:LEU:HD11	2.01	0.42
1:C:188:ILE:HG22	1:C:189:PRO:HD2	2.02	0.42
1:D:4:TYR:HB3	1:D:36:LEU:HG	2.01	0.42
1:D:158:THR:OG1	1:D:159:ASN:N	2.52	0.42
1:D:314:TYR:HA	1:D:317:ARG:HB2	2.00	0.42
1:A:18:GLN:O	1:A:22:ASN:ND2	2.52	0.42
1:A:219:MET:HE1	1:C:215:GLU:HG2	2.02	0.42
1:B:218:ILE:HD13	1:B:218:ILE:HG21	1.64	0.42
1:A:160:ILE:HD12	1:A:161:THR:O	2.20	0.42
1:C:271:LYS:HB3	1:C:271:LYS:HE2	1.51	0.42
1:B:74:THR:OG1	1:B:81:ASP:OD1	2.23	0.42
1:B:162:LEU:HD21	1:B:307:ASN:HD21	1.84	0.42
1:C:177:PRO:HD2	1:C:198:HIS:CD2	2.55	0.42
1:C:82:GLU:OE1	1:C:116:ARG:NH2	2.53	0.42
1:A:132:GLN:NE2	1:A:136:ASP:OD1	2.51	0.41
1:B:130:PRO:HA	1:B:151:GLN:HB3	2.02	0.41
1:B:269:ILE:HA	1:B:274:LEU:HD12	2.02	0.41
1:C:137:LYS:HA	1:C:137:LYS:HD2	1.69	0.41
1:C:221:MET:HE1	1:C:250:TYR:CE1	2.55	0.41
1:D:91:PHE:HB3	1:D:93:VAL:HG13	2.01	0.41
1:A:226:TYR:HH	1:A:296:TYR:HD2	1.67	0.41
1:A:309:LEU:HD11	1:D:328:LEU:HB2	2.02	0.41
1:D:73:PRO:HD3	1:D:101:ASP:H	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:ILE:HD11	1:A:323:ALA:CB	2.42	0.41
1:B:219:MET:HE1	1:D:216:GLN:HB2	2.03	0.41
1:C:55:LEU:HD23	1:C:55:LEU:HA	1.82	0.41
1:C:236:LYS:HA	1:C:239:GLN:HB3	2.02	0.41
1:D:4:TYR:HA	1:D:34:ARG:O	2.19	0.41
1:C:2:ARG:NH2	1:C:66:ASP:OD2	2.53	0.41
1:C:183:ILE:HG23	1:C:184:LYS:HG3	2.02	0.41
1:C:281:ILE:H	1:C:281:ILE:HG13	1.69	0.41
1:A:252:ALA:O	1:A:311:ARG:NH1	2.53	0.41
1:C:112:TYR:CE2	1:C:113:LEU:HG	2.55	0.41
1:C:235:ASP:C	1:C:236:LYS:HD2	2.40	0.41
1:D:69:ILE:HG12	1:D:96:VAL:HB	2.01	0.41
1:D:134:MET:HA	1:D:241:LEU:HD22	2.02	0.41
1:C:165:VAL:HG12	1:C:166:ASN:HA	2.02	0.41
1:A:8:LEU:HA	1:A:38:ILE:O	2.21	0.41
1:A:12:SER:C	1:A:14:THR:H	2.23	0.41
1:A:170:LEU:HD11	4:A:563:HOH:O	2.19	0.41
1:B:288:VAL:O	1:B:291:THR:HG22	2.20	0.41
1:D:47:SER:HA	1:D:48:PRO:HD2	1.87	0.41
1:A:16:THR:HA	1:A:19:ILE:HG22	2.02	0.41
1:A:79:THR:HG21	4:A:521:HOH:O	2.21	0.41
1:A:294:GLU:H	1:A:294:GLU:HG2	1.69	0.41
1:B:153:MET:HA	4:B:576:HOH:O	2.20	0.41
1:B:229:VAL:HB	1:B:259:ILE:HG23	2.02	0.41
1:B:240:SER:O	1:B:240:SER:OG	2.34	0.41
1:C:36:LEU:HA	1:C:36:LEU:HD23	1.84	0.41
1:C:257:VAL:O	1:C:275:GLY:HA3	2.21	0.41
1:A:70:PHE:CZ	1:A:84:LEU:HD23	2.55	0.41
1:A:169:LYS:HD3	1:A:288:VAL:O	2.21	0.41
1:A:230:TRP:CZ3	1:A:284:ILE:HD11	2.55	0.41
1:A:314:TYR:O	1:A:318:LYS:HB2	2.20	0.41
1:B:97:ILE:O	1:B:127:LEU:HD12	2.21	0.41
1:C:44:ASP:C	1:C:46:ASP:H	2.22	0.41
1:C:246:LYS:N	3:C:401:UDP:O1B	2.53	0.40
1:C:165:VAL:HG12	1:C:166:ASN:N	2.37	0.40
1:D:122:ASN:OD1	1:D:143:LEU:HA	2.20	0.40
1:D:182:PHE:CZ	1:D:230:TRP:HB3	2.57	0.40
1:A:67:ILE:CD1	1:A:94:LYS:HB2	2.51	0.40
1:C:23:MET:HE1	1:C:245:TYR:CE1	2.57	0.40
1:C:236:LYS:N	1:C:236:LYS:CD	2.79	0.40
1:B:250:TYR:O	1:B:253:ALA:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:HIS:NE2	1:C:291:THR:HG23	2.36	0.40
1:D:89:LYS:HD2	1:D:89:LYS:HA	1.78	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	329/333 (99%)	304 (92%)	17 (5%)	8 (2%)	6 15
1	B	330/333 (99%)	300 (91%)	28 (8%)	2 (1%)	25 50
1	C	330/333 (99%)	303 (92%)	21 (6%)	6 (2%)	8 21
1	D	330/333 (99%)	302 (92%)	20 (6%)	8 (2%)	6 15
All	All	1319/1332 (99%)	1209 (92%)	86 (6%)	24 (2%)	8 21

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	ASN
1	B	233	ASP
1	C	166	ASN
1	D	48	PRO
1	D	107	PHE
1	D	204	THR
1	C	106	MET
1	D	77	THR
1	D	273	ASN
1	A	211	TYR
1	A	234	ARG
1	B	307	ASN
1	D	49	GLU

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Mol	Chain	Res	Type
1	A	231	MET
1	A	233	ASP
1	A	239	GLN
1	A	274	LEU
1	C	199	ASN
1	C	211	TYR
1	D	279	GLU
1	D	307	ASN
1	A	307	ASN
1	C	174	PRO
1	C	307	ASN

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	298/300 (99%)	292 (98%)	6 (2%)	55	81
1	B	299/300 (100%)	292 (98%)	7 (2%)	50	78
1	C	299/300 (100%)	289 (97%)	10 (3%)	38	67
1	D	299/300 (100%)	284 (95%)	15 (5%)	24	51
All	All	1195/1200 (100%)	1157 (97%)	38 (3%)	39	68

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

Mol	Chain	Res	Type
1	A	60	SER
1	A	85	PHE
1	A	170	LEU
1	A	178	GLU
1	A	181	ASN
1	A	213	SER
1	B	98	PHE
1	B	220	LYS
1	B	235	ASP
1	B	287	ILE

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Mol	Chain	Res	Type
1	B	292	THR
1	B	299	ILE
1	B	302	ASP
1	C	52	SER
1	C	70	PHE
1	C	167	HIS
1	C	180	PHE
1	C	198	HIS
1	C	205	THR
1	C	208	LYS
1	C	218	ILE
1	C	234	ARG
1	C	242	TYR
1	D	13	ILE
1	D	44	ASP
1	D	77	THR
1	D	97	ILE
1	D	127	LEU
1	D	128	ILE
1	D	197	ASP
1	D	199	ASN
1	D	202	LEU
1	D	205	THR
1	D	208	LYS
1	D	277	ILE
1	D	281	ILE
1	D	301	SER
1	D	316	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	266	GLN
1	B	216	GLN
1	B	273	ASN
1	C	181	ASN
1	D	163	GLN
1	D	176	ASN
1	D	198	HIS
1	D	239	GLN

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)

5 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	SER	A	401	-	4,5,6	0.60	0	0,5,7	-	-
3	UDP	B	401	-	24,26,26	0.95	0	37,40,40	1.63	7 (18%)
3	UDP	C	401	-	24,26,26	1.03	0	37,40,40	1.64	8 (21%)
3	UDP	D	401	-	24,26,26	1.00	1 (4%)	37,40,40	1.71	7 (18%)
3	UDP	A	402	-	24,26,26	1.01	1 (4%)	37,40,40	1.69	8 (21%)

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	SER	A	401	-	-	0/2/4/6	-
3	UDP	B	401	-	-	0/16/32/32	0/2/2/2
3	UDP	C	401	-	-	3/16/32/32	0/2/2/2
3	UDP	D	401	-	-	4/16/32/32	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	UDP	A	402	-	-	6/16/32/32	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	UDP	C6-C5	2.02	1.39	1.35
3	D	401	UDP	C6-C5	2.02	1.39	1.35

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	401	UDP	C4-N3-C2	-5.70	119.06	126.58
3	A	402	UDP	C4-N3-C2	-5.41	119.44	126.58
3	B	401	UDP	C4-N3-C2	-5.29	119.60	126.58
3	C	401	UDP	C4-N3-C2	-5.08	119.88	126.58
3	D	401	UDP	N3-C2-N1	4.54	120.92	114.89
3	B	401	UDP	N3-C2-N1	4.21	120.47	114.89
3	A	402	UDP	N3-C2-N1	3.58	119.65	114.89
3	C	401	UDP	O4-C4-C5	-3.57	118.89	125.16
3	D	401	UDP	C5-C4-N3	3.43	119.98	114.84
3	B	401	UDP	C5-C4-N3	3.35	119.85	114.84
3	C	401	UDP	C5-C4-N3	3.30	119.78	114.84
3	A	402	UDP	C5-C6-N1	-3.13	116.58	121.81
3	C	401	UDP	N3-C2-N1	3.07	118.97	114.89
3	A	402	UDP	C5-C4-N3	2.95	119.26	114.84
3	D	401	UDP	O2-C2-N1	-2.86	118.98	122.79
3	D	401	UDP	PA-O3A-PB	-2.74	123.42	132.83
3	A	402	UDP	PA-O3A-PB	-2.71	123.53	132.83
3	B	401	UDP	PA-O3A-PB	-2.65	123.73	132.83
3	A	402	UDP	O4-C4-C5	-2.63	120.54	125.16
3	A	402	UDP	O2-C2-N1	-2.62	119.30	122.79
3	C	401	UDP	O2-C2-N1	-2.59	119.34	122.79
3	C	401	UDP	PA-O3A-PB	-2.56	124.04	132.83
3	C	401	UDP	O2B-PB-O3A	2.35	112.52	104.64
3	C	401	UDP	C2'-C1'-N1	-2.24	106.86	113.22
3	B	401	UDP	O4'-C1'-N1	2.22	113.45	108.36
3	B	401	UDP	O4-C4-C5	-2.22	121.26	125.16
3	D	401	UDP	O4-C4-C5	-2.17	121.34	125.16
3	B	401	UDP	C2'-C1'-N1	-2.14	107.16	113.22
3	A	402	UDP	O3B-PB-O3A	2.09	111.64	104.64
3	D	401	UDP	C5-C6-N1	-2.05	118.38	121.81

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	UDP	C5'-O5'-PA-O1A
3	A	402	UDP	C5'-O5'-PA-O2A
3	A	402	UDP	C5'-O5'-PA-O3A
3	C	401	UDP	C5'-O5'-PA-O3A
3	D	401	UDP	C5'-O5'-PA-O3A
3	D	401	UDP	O4'-C4'-C5'-O5'
3	A	402	UDP	PB-O3A-PA-O1A
3	C	401	UDP	C5'-O5'-PA-O1A
3	D	401	UDP	C5'-O5'-PA-O1A
3	A	402	UDP	PB-O3A-PA-O2A
3	A	402	UDP	O4'-C4'-C5'-O5'
3	D	401	UDP	PB-O3A-PA-O2A
3	C	401	UDP	O4'-C4'-C5'-O5'

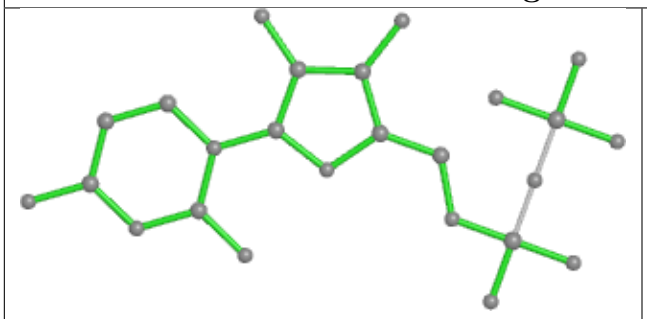
There are no ring outliers.

2 monomers are involved in 2 short contacts:

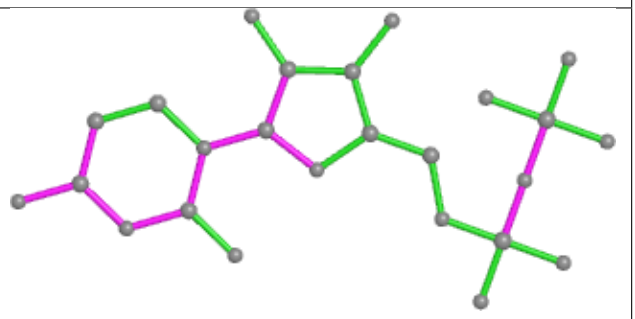
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	SER	1	0
3	C	401	UDP	1	0

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.

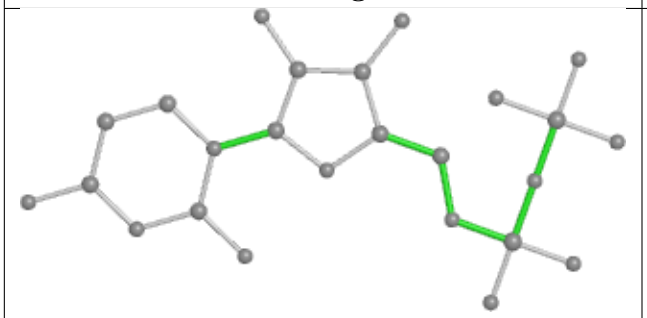
Ligand UDP B 401



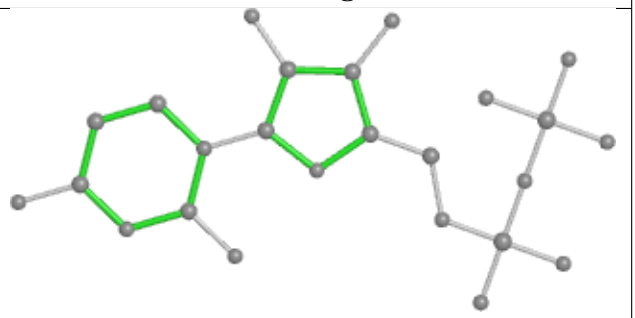
Bond lengths



Bond angles

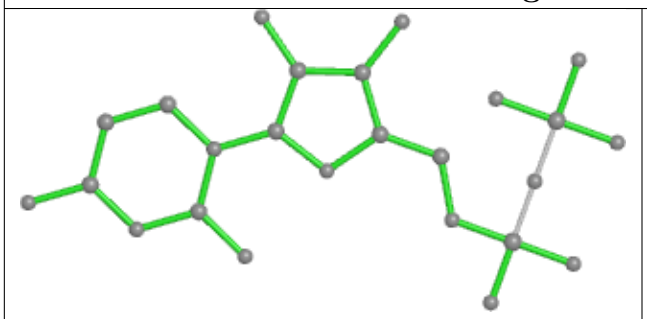


Torsions

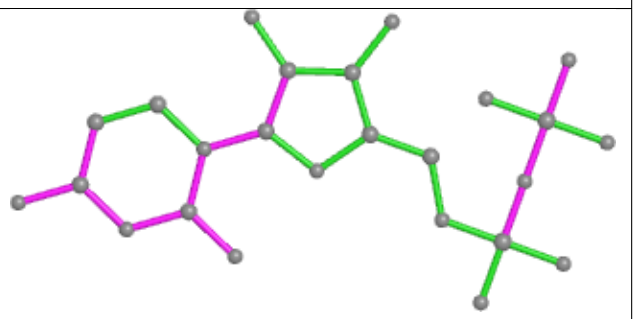


Rings

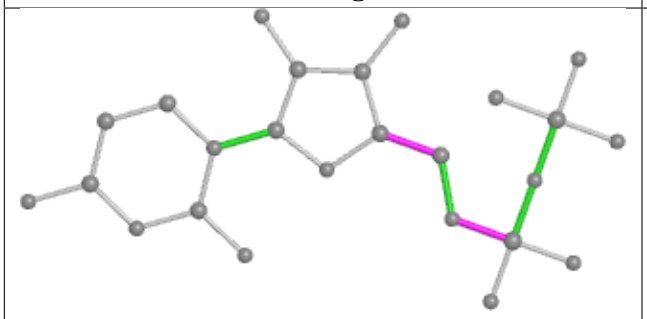
Ligand UDP C 401



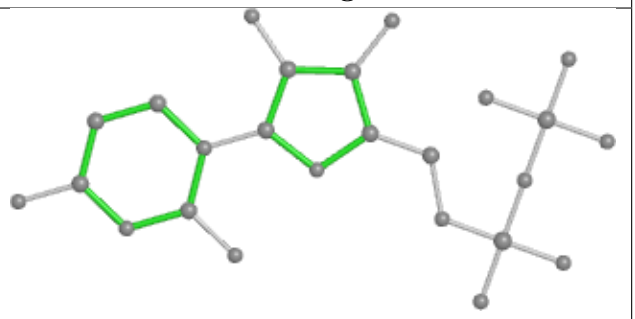
Bond lengths



Bond angles

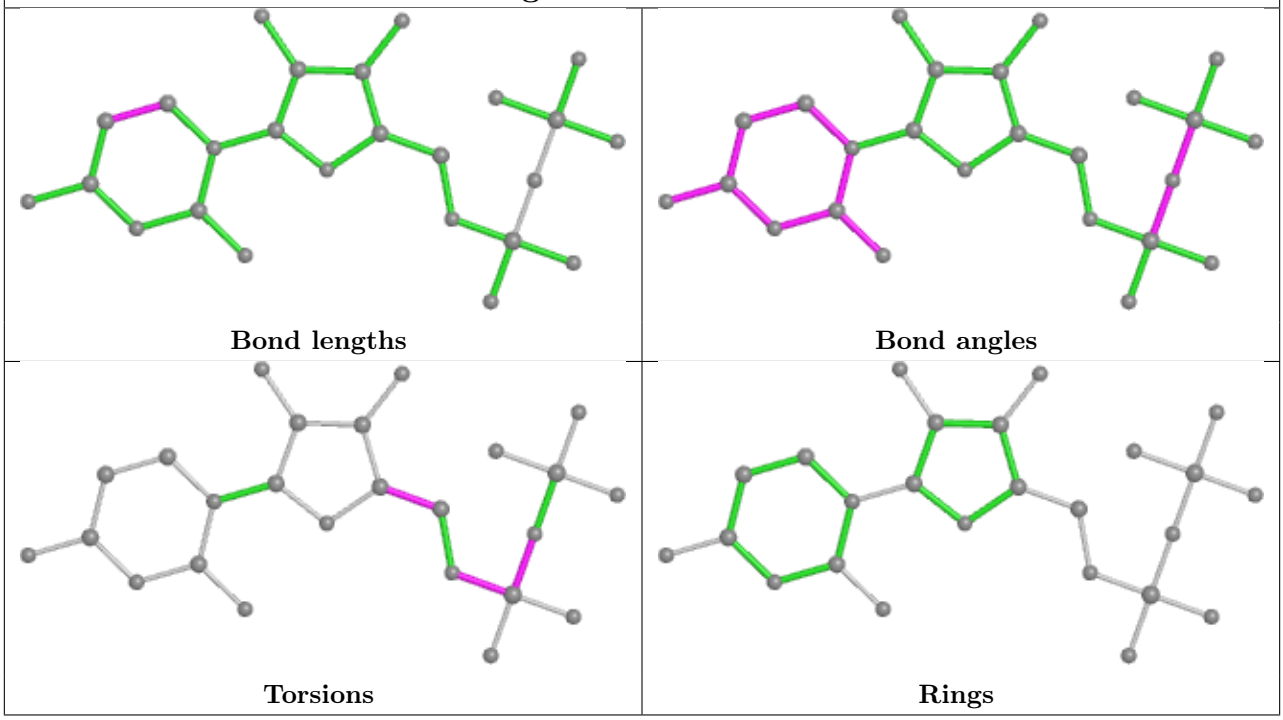


Torsions

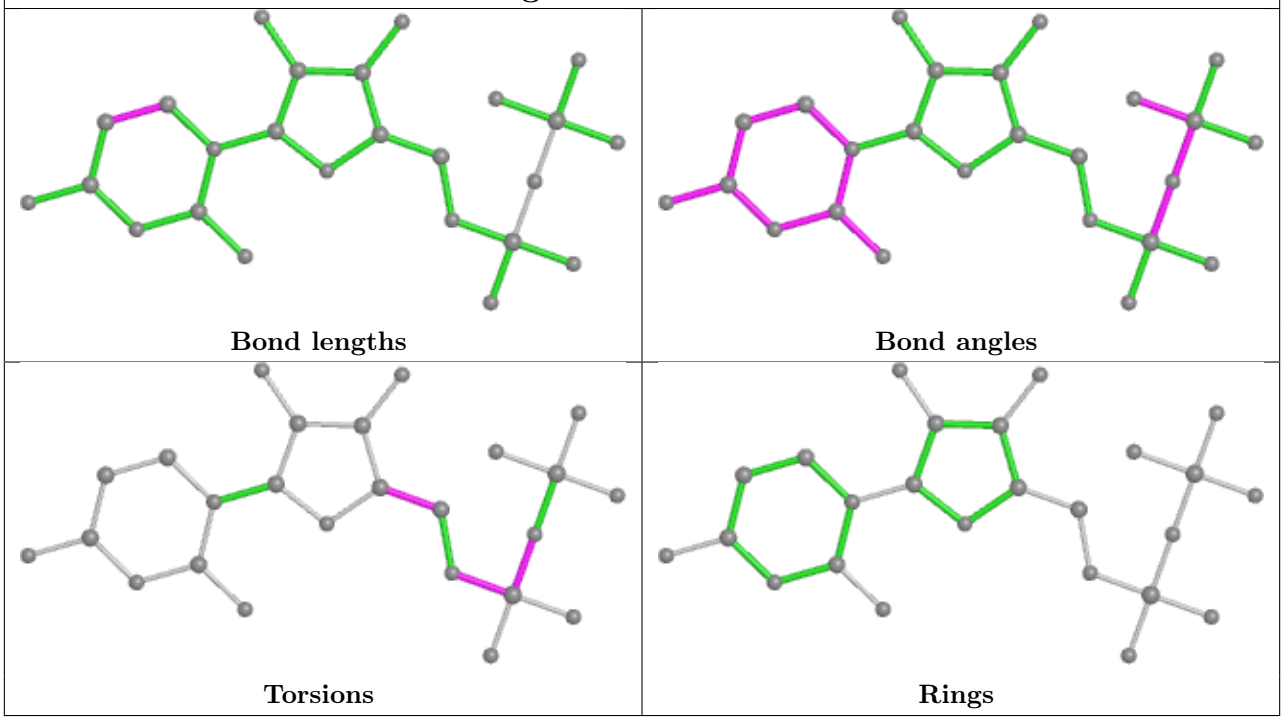


Rings

Ligand UDP D 401



Ligand UDP A 402



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 (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

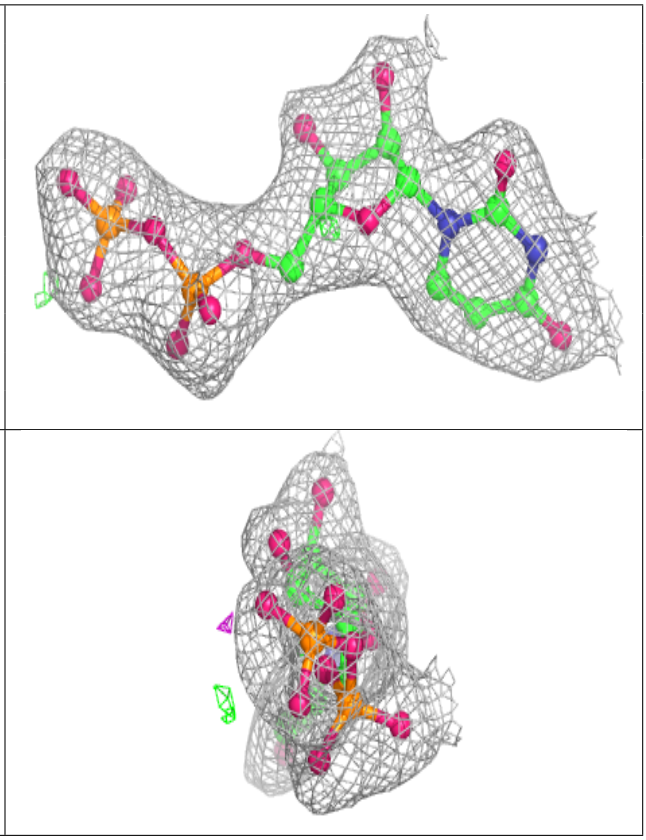
6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

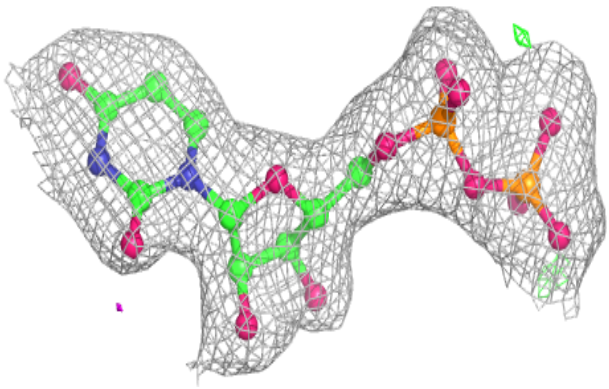
Electron density around UDP A 402:

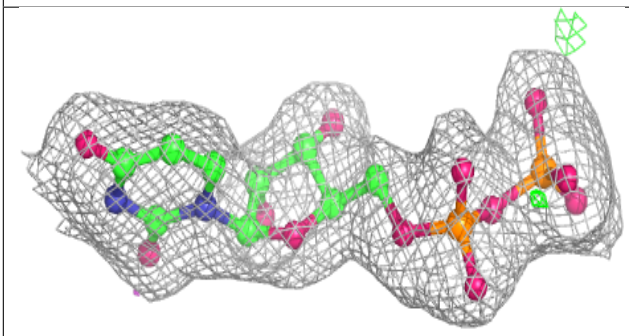
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around UDP B 401:

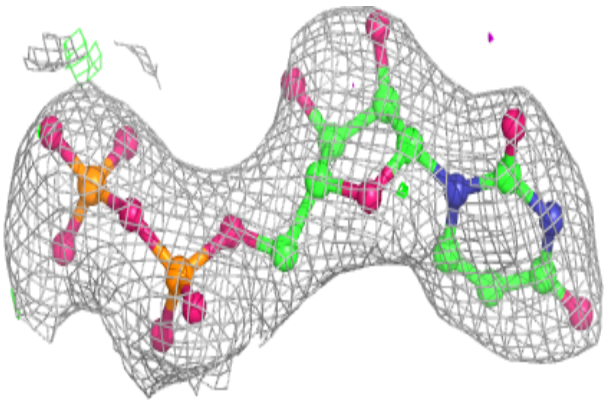
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

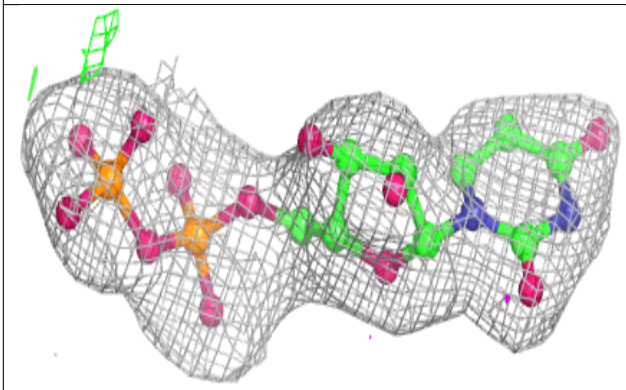


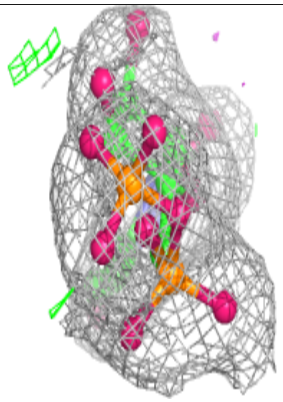


Electron density around UDP C 401:

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

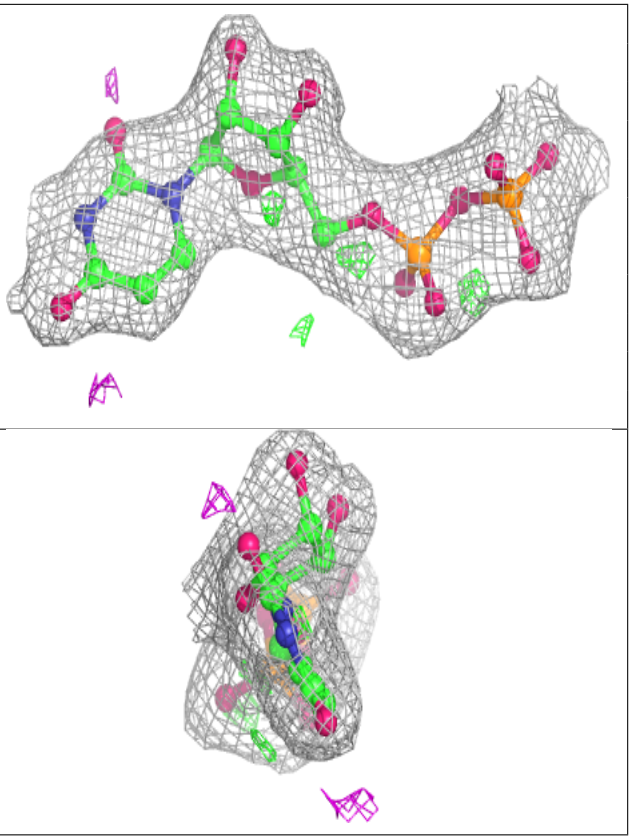






Electron density around UDP D 401:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.