Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 04:29 PM BST

PDB ID	:	4AN4
Title	:	Crystal structure of the glycosyltransferase SnogD from Streptomyces nogalater
Authors	:	Claesson, M.; Siitonen, V.; Dobritzsch, D.; Metsa-Ketela, M.; Schneider, G.
Deposited on	:	2012-03-15
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 ⓘ symbol.

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

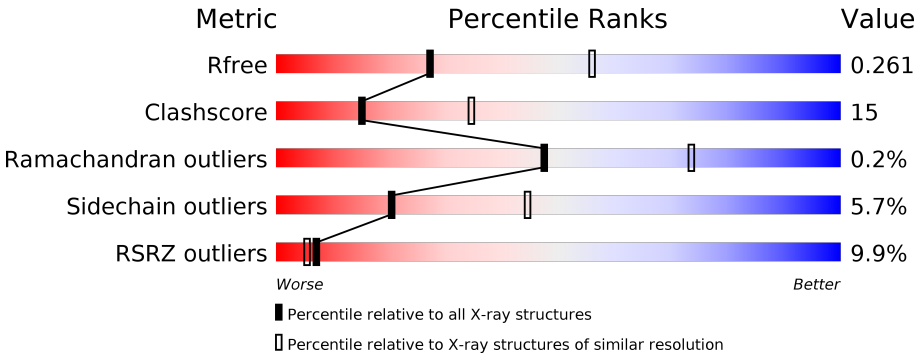
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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)
RSRZ outliers	127900	2737 (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 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	400	2% 68% 19% • 11%
1	B	400	9% 70% 19% • 10%
1	C	400	14% 60% 20% • 18%
1	D	400	9% 67% 18% • 13%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10329 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 GLYCOSYL TRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	0	0
			2623	1655	466	491	11			
1	B	359	Total	C	N	O	S	0	2	0
			2644	1671	472	490	11			
1	C	328	Total	C	N	O	S	0	0	0
			2418	1540	430	437	11			
1	D	348	Total	C	N	O	S	0	0	0
			2548	1610	455	472	11			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	expression tag	UNP Q9RN61
A	-8	HIS	-	expression tag	UNP Q9RN61
A	-7	HIS	-	expression tag	UNP Q9RN61
A	-6	HIS	-	expression tag	UNP Q9RN61
A	-5	HIS	-	expression tag	UNP Q9RN61
A	-4	HIS	-	expression tag	UNP Q9RN61
A	-3	HIS	-	expression tag	UNP Q9RN61
A	-2	SER	-	expression tag	UNP Q9RN61
A	-1	SER	-	expression tag	UNP Q9RN61
A	0	GLY	-	expression tag	UNP Q9RN61
A	1	VAL	-	expression tag	UNP Q9RN61
A	2	ASP	-	expression tag	UNP Q9RN61
A	3	LEU	-	expression tag	UNP Q9RN61
A	4	GLY	-	expression tag	UNP Q9RN61
A	5	THR	-	expression tag	UNP Q9RN61
A	6	GLU	-	expression tag	UNP Q9RN61
A	7	ASN	-	expression tag	UNP Q9RN61
A	8	LEU	-	expression tag	UNP Q9RN61
A	9	TYR	-	expression tag	UNP Q9RN61
A	10	PHE	-	expression tag	UNP Q9RN61
A	11	GLN	-	expression tag	UNP Q9RN61

Continued on next page...

Continued from previous page...

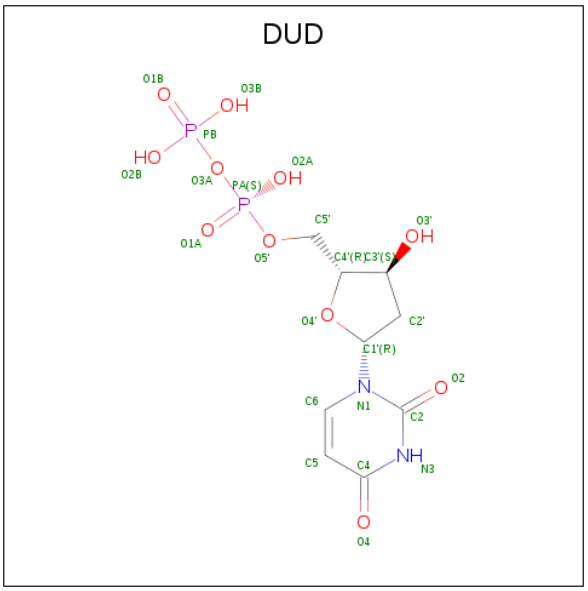
Chain	Residue	Modelled	Actual	Comment	Reference
A	12	SER	-	expression tag	UNP Q9RN61
B	-9	MET	-	expression tag	UNP Q9RN61
B	-8	HIS	-	expression tag	UNP Q9RN61
B	-7	HIS	-	expression tag	UNP Q9RN61
B	-6	HIS	-	expression tag	UNP Q9RN61
B	-5	HIS	-	expression tag	UNP Q9RN61
B	-4	HIS	-	expression tag	UNP Q9RN61
B	-3	HIS	-	expression tag	UNP Q9RN61
B	-2	SER	-	expression tag	UNP Q9RN61
B	-1	SER	-	expression tag	UNP Q9RN61
B	0	GLY	-	expression tag	UNP Q9RN61
B	1	VAL	-	expression tag	UNP Q9RN61
B	2	ASP	-	expression tag	UNP Q9RN61
B	3	LEU	-	expression tag	UNP Q9RN61
B	4	GLY	-	expression tag	UNP Q9RN61
B	5	THR	-	expression tag	UNP Q9RN61
B	6	GLU	-	expression tag	UNP Q9RN61
B	7	ASN	-	expression tag	UNP Q9RN61
B	8	LEU	-	expression tag	UNP Q9RN61
B	9	TYR	-	expression tag	UNP Q9RN61
B	10	PHE	-	expression tag	UNP Q9RN61
B	11	GLN	-	expression tag	UNP Q9RN61
B	12	SER	-	expression tag	UNP Q9RN61
C	-9	MET	-	expression tag	UNP Q9RN61
C	-8	HIS	-	expression tag	UNP Q9RN61
C	-7	HIS	-	expression tag	UNP Q9RN61
C	-6	HIS	-	expression tag	UNP Q9RN61
C	-5	HIS	-	expression tag	UNP Q9RN61
C	-4	HIS	-	expression tag	UNP Q9RN61
C	-3	HIS	-	expression tag	UNP Q9RN61
C	-2	SER	-	expression tag	UNP Q9RN61
C	-1	SER	-	expression tag	UNP Q9RN61
C	0	GLY	-	expression tag	UNP Q9RN61
C	1	VAL	-	expression tag	UNP Q9RN61
C	2	ASP	-	expression tag	UNP Q9RN61
C	3	LEU	-	expression tag	UNP Q9RN61
C	4	GLY	-	expression tag	UNP Q9RN61
C	5	THR	-	expression tag	UNP Q9RN61
C	6	GLU	-	expression tag	UNP Q9RN61
C	7	ASN	-	expression tag	UNP Q9RN61
C	8	LEU	-	expression tag	UNP Q9RN61
C	9	TYR	-	expression tag	UNP Q9RN61

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	10	PHE	-	expression tag	UNP Q9RN61
C	11	GLN	-	expression tag	UNP Q9RN61
C	12	SER	-	expression tag	UNP Q9RN61
D	-9	MET	-	expression tag	UNP Q9RN61
D	-8	HIS	-	expression tag	UNP Q9RN61
D	-7	HIS	-	expression tag	UNP Q9RN61
D	-6	HIS	-	expression tag	UNP Q9RN61
D	-5	HIS	-	expression tag	UNP Q9RN61
D	-4	HIS	-	expression tag	UNP Q9RN61
D	-3	HIS	-	expression tag	UNP Q9RN61
D	-2	SER	-	expression tag	UNP Q9RN61
D	-1	SER	-	expression tag	UNP Q9RN61
D	0	GLY	-	expression tag	UNP Q9RN61
D	1	VAL	-	expression tag	UNP Q9RN61
D	2	ASP	-	expression tag	UNP Q9RN61
D	3	LEU	-	expression tag	UNP Q9RN61
D	4	GLY	-	expression tag	UNP Q9RN61
D	5	THR	-	expression tag	UNP Q9RN61
D	6	GLU	-	expression tag	UNP Q9RN61
D	7	ASN	-	expression tag	UNP Q9RN61
D	8	LEU	-	expression tag	UNP Q9RN61
D	9	TYR	-	expression tag	UNP Q9RN61
D	10	PHE	-	expression tag	UNP Q9RN61
D	11	GLN	-	expression tag	UNP Q9RN61
D	12	SER	-	expression tag	UNP Q9RN61

- Molecule 2 is DEOXYURIDINE-5'-DIPHOSPHATE (three-letter code: DUD) (formula: $C_9H_{14}N_2O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			24	9	2	11	2		
2	D	1	Total	C	N	O	P	0	0
			24	9	2	11	2		

- Molecule 3 is water.

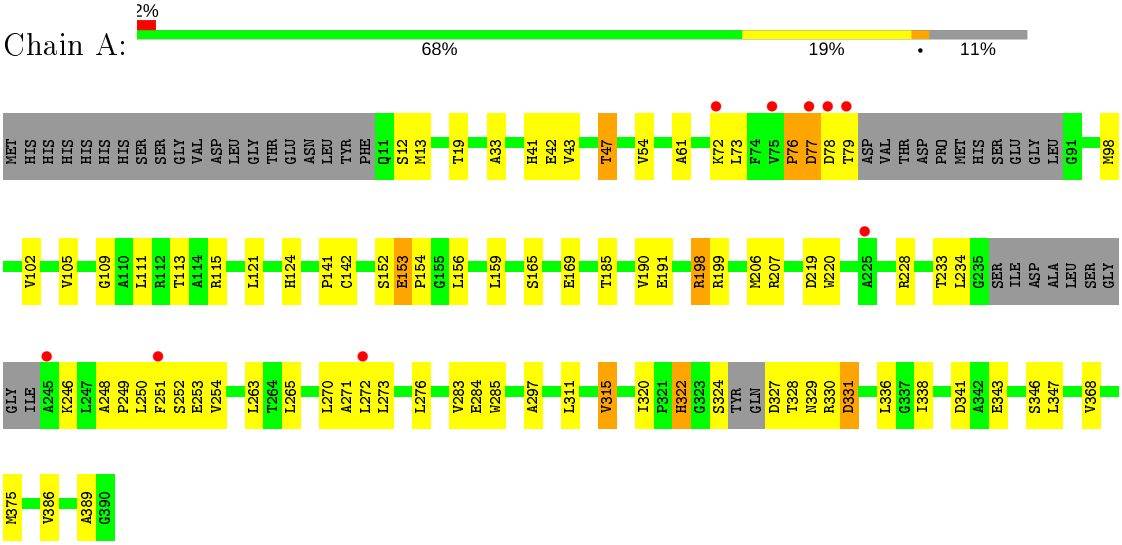
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	34	Total	O	0	0
			34	34		
3	B	9	Total	O	0	0
			9	9		
3	C	4	Total	O	0	0
			4	4		
3	D	1	Total	O	0	0
			1	1		

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.

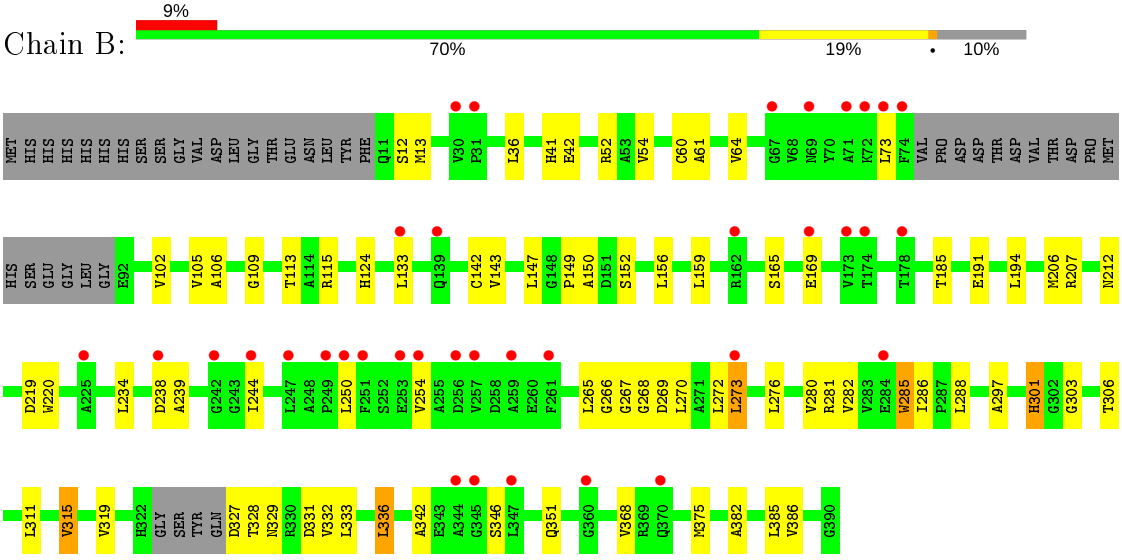
- Molecule 1: GLYCOSYL TRANSFERASE

Chain A:



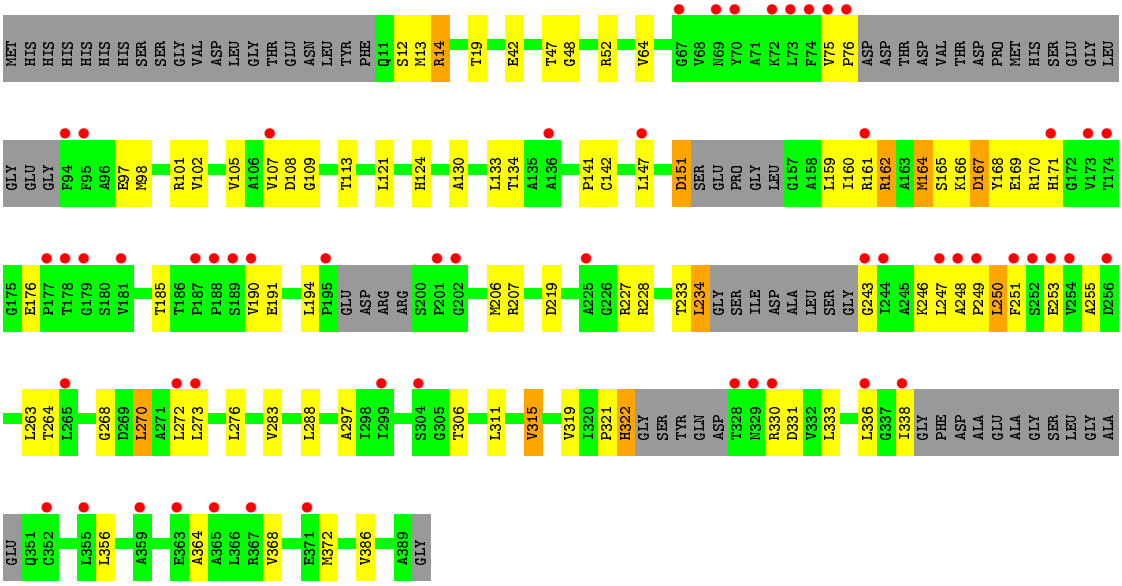
- Molecule 1: GLYCOSYL TRANSFERASE

Chain B:



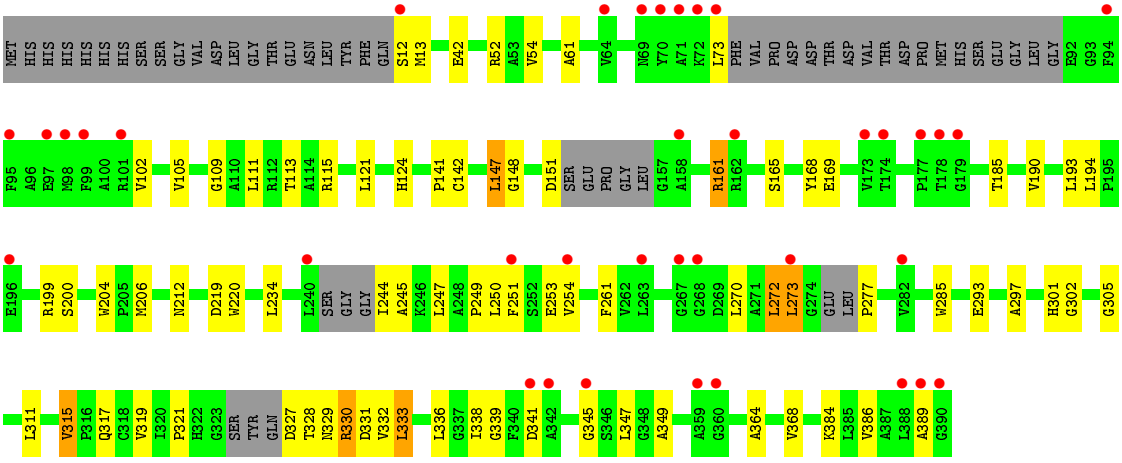
- Molecule 1: GLYCOSYL TRANSFERASE

Chain C:



- Molecule 1: GLYCOSYL TRANSFERASE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	64.64Å 70.08Å 176.03Å 90.00° 91.71° 90.00°	Depositor
Resolution (Å)	60.00 – 2.70 42.80 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.2 (60.00-2.70) 98.3 (42.80-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.6.0119	Depositor
R, R_{free}	0.227 , 0.266 0.228 , 0.261	Depositor DCC
R_{free} test set	2158 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	70.2	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 69.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.045 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10329	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.20% 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: MLY, DUD

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	0.61	0/2666	0.80	0/3641
1	B	0.58	2/2694 (0.1%)	0.77	0/3678
1	C	0.56	0/2456	0.78	2/3355 (0.1%)
1	D	0.55	1/2586 (0.0%)	0.74	0/3527
All	All	0.58	3/10402 (0.0%)	0.78	2/14201 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	220	TRP	CD2-CE2	5.53	1.48	1.41
1	B	220	TRP	CD2-CE2	5.01	1.47	1.41
1	B	285	TRP	CD2-CE2	5.00	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	14	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	C	14	ARG	NE-CZ-NH2	-5.10	117.75	120.30

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	2623	0	2638	90	0
1	B	2644	0	2675	74	0
1	C	2418	0	2471	80	0
1	D	2548	0	2579	72	0
2	B	24	0	11	5	0
2	D	24	0	11	2	0
3	A	34	0	0	1	0
3	B	9	0	0	1	0
3	C	4	0	0	0	0
3	D	1	0	0	0	0
All	All	10329	0	10385	309	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (309) 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:153:GLU:HG2	1:A:198:ARG:NH1	1.22	1.51
1:A:250:LEU:HD13	1:A:347:LEU:CG	1.54	1.34
1:A:250:LEU:HD13	1:A:347:LEU:CD2	1.57	1.33
1:A:250:LEU:CD1	1:A:347:LEU:HG	1.78	1.12
1:A:153:GLU:CG	1:A:198:ARG:HH12	1.60	1.12
1:A:327:ASP:O	1:A:330:ARG:HG2	1.50	1.11
1:A:153:GLU:CG	1:A:198:ARG:NH1	2.17	1.05
1:A:250:LEU:HD13	1:A:347:LEU:HG	1.11	1.04
1:C:47:THR:HG22	1:C:48:GLY:H	1.26	0.99
1:A:250:LEU:CD1	1:A:347:LEU:CD2	2.41	0.98
1:D:327:ASP:HB3	1:D:330:ARG:CG	1.96	0.95
1:B:244:ILE:CG2	1:B:273:LEU:HD21	2.03	0.88
1:B:244:ILE:HG22	1:B:273:LEU:HD21	1.55	0.86
1:D:245:ALA:HB2	1:D:272:LEU:HD21	1.57	0.85
1:A:153:GLU:HG2	1:A:198:ARG:HH11	1.37	0.85
1:A:220:TRP:CZ2	1:A:283:VAL:HG21	2.11	0.85
1:D:327:ASP:HB3	1:D:330:ARG:HG2	1.59	0.84
1:A:250:LEU:HD22	1:A:347:LEU:HD21	1.63	0.81
1:D:147:LEU:CD1	1:D:151:ASP:HB2	2.11	0.81
1:C:98:MET:O	1:C:102:VAL:HG23	1.80	0.81
1:A:250:LEU:CD1	1:A:347:LEU:HD21	2.11	0.80
1:A:250:LEU:HD13	1:A:347:LEU:HD21	1.59	0.80
1:C:160:ILE:O	1:C:164:MET:HG3	1.82	0.80
1:A:250:LEU:CD1	1:A:347:LEU:CG	2.44	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301[B]:HIS:CE1	1:B:303:GLY:HA3	2.17	0.79
1:A:250:LEU:CD2	1:A:347:LEU:HD21	2.12	0.79
1:D:319:VAL:HG23	1:D:333:LEU:CD1	2.14	0.78
1:A:250:LEU:HD22	1:A:347:LEU:CD2	2.14	0.78
1:C:47:THR:HG22	1:C:48:GLY:N	2.00	0.77
1:A:78:ASP:O	1:A:79:THR:OG1	2.03	0.76
1:C:108:ASP:OD1	1:C:170:ARG:NH2	2.19	0.75
1:D:73:LEU:HD11	1:D:105:VAL:HG11	1.68	0.74
1:C:162:ARG:HH11	1:C:162:ARG:HG2	1.52	0.74
1:A:297:ALA:HA	1:A:315:VAL:HG13	1.69	0.73
1:D:317:GLN:HB2	1:D:333:LEU:HD21	1.69	0.73
1:C:102:VAL:O	1:C:105:VAL:HG22	1.89	0.72
1:D:212:ASN:O	1:D:285:TRP:HZ2	1.73	0.72
1:A:19:THR:OG1	1:A:47:THR:HG21	1.89	0.71
1:C:247:LEU:O	1:C:247:LEU:HD23	1.90	0.71
1:C:130:ALA:O	1:C:134:THR:HG23	1.90	0.70
1:B:281[B]:ARG:CG	1:B:281[B]:ARG:HH11	2.05	0.70
1:D:319:VAL:HG23	1:D:333:LEU:HD12	1.72	0.70
1:B:297:ALA:HA	1:B:315:VAL:HG13	1.74	0.70
1:C:161:ARG:NH2	1:C:176:GLU:HG3	2.06	0.69
1:C:247:LEU:HD11	1:C:263:LEU:HD22	1.72	0.69
1:B:301[B]:HIS:CE1	1:B:303:GLY:H	2.09	0.69
1:A:251:PHE:HZ	1:A:263:LEU:HD22	1.57	0.69
1:B:212:ASN:O	1:B:285:TRP:HZ2	1.75	0.69
1:C:319:VAL:CG2	1:C:333:LEU:HD11	2.22	0.69
1:D:319:VAL:CG2	1:D:333:LEU:HD12	2.23	0.69
1:D:193:LEU:HD12	1:D:336:LEU:HG	1.72	0.69
1:A:250:LEU:O	1:A:254:VAL:HG13	1.93	0.68
1:A:19:THR:O	1:A:47:THR:CG2	2.42	0.68
1:B:250:LEU:O	1:B:254:VAL:HG13	1.93	0.68
1:D:147:LEU:HD12	1:D:151:ASP:HB2	1.74	0.68
1:D:147:LEU:HD11	1:D:151:ASP:HB2	1.74	0.68
1:A:320:ILE:HD11	1:A:347:LEU:HD22	1.74	0.67
1:C:319:VAL:HG23	1:C:333:LEU:HD11	1.76	0.67
1:C:207:ARG:HD3	1:C:372:MET:O	1.95	0.67
1:D:161:ARG:HG3	1:D:168:TYR:CZ	2.29	0.67
1:D:338:ILE:HG22	1:D:364:ALA:CB	2.24	0.67
1:C:47:THR:CG2	1:C:48:GLY:H	2.06	0.67
1:A:109:GLY:O	1:A:113:THR:HG23	1.95	0.66
1:C:297:ALA:HA	1:C:315:VAL:HG13	1.75	0.66
1:D:327:ASP:HB3	1:D:330:ARG:CD	2.26	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:SER:O	1:A:154:PRO:HD3	1.96	0.66
1:D:328:THR:O	1:D:332:VAL:HG23	1.95	0.66
1:C:75:VAL:HG13	1:C:76:PRO:HD2	1.77	0.66
1:B:269:ASP:CG	1:B:272:LEU:HD13	2.15	0.66
1:B:109:GLY:O	1:B:113:THR:HG23	1.96	0.65
1:D:297:ALA:HA	1:D:315:VAL:HG13	1.79	0.65
1:B:327:ASP:OD1	1:B:328:THR:N	2.27	0.65
1:C:160:ILE:O	1:C:164:MET:CG	2.44	0.65
1:B:64:VAL:HG13	1:B:109:GLY:HA3	1.78	0.65
1:A:250:LEU:HD13	1:A:347:LEU:HD23	1.68	0.64
1:D:111:LEU:HD22	1:D:115:ARG:NH1	2.13	0.63
1:A:54:VAL:HG11	1:A:61:ALA:HB2	1.81	0.63
1:D:333:LEU:HD22	1:D:339:GLY:HA3	1.81	0.63
1:B:13:MET:HE2	1:B:386:VAL:HG22	1.80	0.62
1:D:199:ARG:HB3	1:D:199:ARG:NH1	2.14	0.62
1:B:269:ASP:OD1	1:B:272:LEU:N	2.30	0.62
1:B:301[A]:HIS:CD2	1:B:303:GLY:H	2.16	0.62
1:C:19:THR:O	1:C:47:THR:HG23	2.00	0.62
1:C:98:MET:O	1:C:101:ARG:HG2	2.00	0.61
1:D:244:ILE:O	1:D:244:ILE:HG12	2.00	0.61
1:B:301[B]:HIS:CE1	1:B:303:GLY:CA	2.83	0.61
1:B:265:LEU:HD12	1:B:266:GLY:N	2.15	0.61
1:B:346:SER:O	1:B:351:GLN:NE2	2.28	0.61
1:D:13:MET:HE3	1:D:386:VAL:HA	1.82	0.61
1:C:164:MET:HB3	1:C:167:ASP:OD1	2.00	0.61
1:D:199:ARG:HB3	1:D:199:ARG:CZ	2.29	0.61
1:D:272:LEU:HD12	1:D:272:LEU:O	2.01	0.60
1:A:153:GLU:HG2	1:A:198:ARG:HH12	0.78	0.60
1:B:319:VAL:HG23	1:B:333:LEU:HD11	1.83	0.60
1:A:251:PHE:HA	1:A:254:VAL:HG22	1.84	0.60
1:C:133:LEU:HD23	1:C:133:LEU:C	2.22	0.60
1:B:286:ILE:O	2:B:401:DUD:N3	2.25	0.59
1:D:319:VAL:HG23	1:D:333:LEU:HD11	1.84	0.59
1:C:228:ARG:HE	1:C:356:LEU:HD22	1.66	0.59
1:A:248:ALA:N	1:A:249:PRO:HD3	2.18	0.59
1:D:102:VAL:O	1:D:105:VAL:HG22	2.02	0.59
1:B:301[B]:HIS:CE1	1:B:303:GLY:N	2.71	0.58
1:D:272:LEU:HD12	1:D:272:LEU:C	2.22	0.58
1:A:272:LEU:HD23	1:C:272:LEU:HD13	1.84	0.58
1:D:194:LEU:O	1:D:199:ARG:NH2	2.36	0.58
1:B:303:GLY:HA3	2:B:401:DUD:O1A	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:LEU:CD2	1:A:347:LEU:CD2	2.80	0.58
1:D:54:VAL:HG11	1:D:61:ALA:HB2	1.86	0.58
1:C:147:LEU:HG	1:C:151:ASP:OD2	2.03	0.58
1:C:233:THR:O	1:C:234:LEU:HD23	2.03	0.57
1:A:265:LEU:HB2	1:A:284:GLU:O	2.04	0.57
1:C:13:MET:HE2	1:C:386:VAL:HG22	1.86	0.57
1:A:19:THR:OG1	1:A:47:THR:CG2	2.53	0.57
1:C:121:LEU:HD12	1:C:141:PRO:HG2	1.86	0.57
1:D:193:LEU:CD1	1:D:336:LEU:HG	2.35	0.57
1:D:109:GLY:O	1:D:113:THR:HG23	2.05	0.57
1:D:147:LEU:HD12	1:D:151:ASP:CB	2.35	0.57
1:D:253:GLU:OE2	1:D:349:ALA:HB2	2.05	0.56
1:A:251:PHE:CD2	1:A:276:LEU:HD22	2.40	0.56
1:D:251:PHE:CD2	1:D:273:LEU:HD11	2.41	0.56
1:C:108:ASP:CG	1:C:170:ARG:HH22	2.09	0.56
1:D:254:VAL:HG22	1:D:261:PHE:CE1	2.41	0.56
1:A:19:THR:O	1:A:47:THR:HG23	2.05	0.56
1:B:102:VAL:O	1:B:105:VAL:HG22	2.06	0.56
1:B:212:ASN:ND2	2:B:401:DUD:H2'2	2.21	0.55
1:A:102:VAL:O	1:A:105:VAL:HG22	2.07	0.55
1:B:212:ASN:HB3	2:B:401:DUD:O2	2.07	0.55
1:A:250:LEU:HB2	1:A:347:LEU:HD23	1.89	0.55
1:C:234:LEU:HD21	1:C:263:LEU:HD11	1.87	0.55
1:D:270:LEU:HD23	1:D:270:LEU:O	2.06	0.55
1:C:162:ARG:NH1	1:C:162:ARG:HG2	2.20	0.55
1:B:115:ARG:HG2	1:B:115:ARG:HH11	1.71	0.55
1:B:60:CYS:SG	3:B:2004:HOH:O	2.58	0.54
3:A:2006:HOH:O	1:B:207:ARG:NE	2.21	0.54
1:D:121:LEU:HD12	1:D:141:PRO:HG2	1.88	0.54
1:A:327:ASP:O	1:A:331:ASP:OD1	2.25	0.54
1:D:338:ILE:HG22	1:D:364:ALA:HB3	1.89	0.54
1:C:190:VAL:HG22	1:C:336:LEU:HD11	1.89	0.53
1:C:248:ALA:N	1:C:249:PRO:CD	2.71	0.53
1:C:109:GLY:O	1:C:113:THR:HG23	2.07	0.53
1:B:276:LEU:HD13	1:B:280:VAL:HB	1.90	0.53
1:B:281[B]:ARG:HG2	1:B:281[B]:ARG:HH11	1.73	0.53
1:A:251:PHE:CZ	1:A:263:LEU:HD22	2.43	0.52
1:A:311:LEU:HD22	1:A:368:VAL:HG11	1.90	0.52
1:A:13:MET:HE2	1:A:386:VAL:HG22	1.91	0.52
1:C:247:LEU:HD11	1:C:263:LEU:CD2	2.39	0.52
1:D:305:GLY:N	2:D:401:DUD:O1A	2.35	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:MET:HE2	1:A:386:VAL:HA	1.92	0.52
1:A:343:GLU:HB2	1:A:346:SER:HB3	1.92	0.52
1:C:13:MET:HE2	1:C:386:VAL:HA	1.92	0.52
1:B:207:ARG:NH1	1:B:375:MET:O	2.43	0.52
1:B:64:VAL:HG11	1:B:106:ALA:O	2.10	0.51
1:C:164:MET:HB2	1:C:168:TYR:CD2	2.46	0.51
1:B:244:ILE:HG22	1:B:273:LEU:CD2	2.33	0.51
1:B:327:ASP:OD1	1:B:328:THR:HG23	2.12	0.50
1:B:265:LEU:HD12	1:B:266:GLY:H	1.76	0.50
1:D:254:VAL:CG2	1:D:261:PHE:CZ	2.93	0.50
1:C:248:ALA:N	1:C:249:PRO:HD3	2.26	0.50
1:A:270:LEU:HB2	1:C:270:LEU:HD22	1.93	0.50
1:D:327:ASP:O	1:D:331:ASP:HB2	2.11	0.50
1:C:321:PRO:O	1:C:322:HIS:ND1	2.45	0.50
1:A:233:THR:OG1	1:A:233:THR:O	2.27	0.50
1:A:250:LEU:CG	1:A:347:LEU:CD2	2.90	0.49
1:B:149:PRO:HD2	1:B:150:ALA:H	1.77	0.49
1:C:165:SER:O	1:C:169:GLU:HG3	2.13	0.49
1:C:264:THR:HG22	1:C:283:VAL:CG1	2.43	0.49
1:C:161:ARG:HH22	1:C:176:GLU:HG3	1.76	0.49
1:A:76:PRO:HD2	1:A:77:ASP:H	1.78	0.49
1:D:327:ASP:OD1	1:D:328:THR:N	2.45	0.49
1:C:250:LEU:HD12	1:C:250:LEU:O	2.13	0.49
1:A:284:GLU:HG3	1:A:285:TRP:H	1.78	0.49
1:C:247:LEU:HD22	1:C:276:LEU:HD21	1.93	0.49
1:C:319:VAL:HG21	1:C:333:LEU:HD11	1.94	0.49
1:D:254:VAL:HG12	1:D:277:PRO:HG2	1.94	0.49
1:D:199:ARG:NH1	1:D:199:ARG:CB	2.76	0.48
1:A:322:HIS:O	1:A:322:HIS:ND1	2.46	0.48
1:D:185:THR:HA	1:D:206:MET:O	2.13	0.48
1:A:330:ARG:NH2	1:A:341:ASP:OD2	2.47	0.48
1:A:248:ALA:N	1:A:249:PRO:CD	2.76	0.48
1:A:328:THR:O	1:A:331:ASP:N	2.46	0.48
1:B:64:VAL:CG1	1:B:106:ALA:O	2.62	0.48
1:A:207:ARG:NH1	1:A:375:MET:O	2.46	0.48
1:A:311:LEU:HD21	1:A:338:ILE:CD1	2.43	0.48
1:A:165:SER:O	1:A:169:GLU:HG3	2.14	0.48
1:D:204:TRP:CE3	1:D:384:MLY:HE2	2.48	0.48
1:B:270:LEU:HD23	1:B:270:LEU:O	2.14	0.47
1:C:107:VAL:HG11	1:C:171:HIS:CD2	2.49	0.47
1:B:165:SER:O	1:B:169:GLU:HG3	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:VAL:CG1	1:C:171:HIS:CD2	2.97	0.47
1:D:165:SER:O	1:D:169:GLU:HG3	2.14	0.47
1:C:107:VAL:HG12	1:C:171:HIS:NE2	2.30	0.47
1:C:247:LEU:HD22	1:C:276:LEU:CD2	2.45	0.47
1:A:185:THR:HA	1:A:206:MET:O	2.15	0.47
1:C:185:THR:HA	1:C:206:MET:O	2.15	0.47
1:A:154:PRO:C	1:A:156:LEU:H	2.17	0.46
1:B:64:VAL:HG12	1:B:106:ALA:HA	1.96	0.46
1:C:124:HIS:CD2	1:C:142:CYS:HB2	2.50	0.46
1:D:245:ALA:C	1:D:247:LEU:H	2.17	0.46
1:A:270:LEU:HD12	1:C:270:LEU:CD2	2.45	0.46
1:C:75:VAL:CG1	1:C:76:PRO:HD2	2.45	0.46
1:D:254:VAL:CG2	1:D:261:PHE:CE1	2.98	0.46
1:B:319:VAL:CG2	1:B:333:LEU:HD11	2.45	0.46
1:D:338:ILE:HG22	1:D:364:ALA:HB1	1.95	0.46
1:A:190:VAL:CG2	1:A:336:LEU:HD11	2.46	0.46
1:B:54:VAL:HG11	1:B:61:ALA:HB2	1.96	0.46
1:A:248:ALA:H	1:A:249:PRO:HD3	1.80	0.46
1:A:121:LEU:HD12	1:A:141:PRO:HG2	1.97	0.46
1:B:185:THR:HA	1:B:206:MET:O	2.15	0.46
1:D:330:ARG:H	1:D:330:ARG:HG2	1.62	0.46
1:D:333:LEU:HA	1:D:333:LEU:HD23	1.80	0.46
1:B:36:LEU:HD23	1:B:382:ALA:HB1	1.98	0.46
1:C:124:HIS:NE2	1:C:142:CYS:HB2	2.30	0.46
1:B:124:HIS:CD2	1:B:142:CYS:HB2	2.51	0.46
1:A:265:LEU:HB2	1:A:284:GLU:HA	1.98	0.45
1:B:281[B]:ARG:HG3	1:B:281[B]:ARG:HH11	1.81	0.45
1:C:190:VAL:CG2	1:C:336:LEU:HD11	2.46	0.45
1:A:124:HIS:CD2	1:A:142:CYS:HB2	2.51	0.45
1:B:124:HIS:NE2	1:B:142:CYS:HB2	2.32	0.45
1:B:329:ASN:HA	1:B:332:VAL:HG23	1.97	0.45
1:C:133:LEU:CD2	1:C:133:LEU:C	2.85	0.45
1:B:212:ASN:HD22	2:B:401:DUD:H2'2	1.81	0.45
1:B:265:LEU:HD23	1:B:282:VAL:CG1	2.47	0.45
1:B:244:ILE:HG23	1:B:273:LEU:HD21	1.95	0.45
1:B:281[B]:ARG:CG	1:B:281[B]:ARG:NH1	2.69	0.45
1:D:270:LEU:HD23	1:D:270:LEU:C	2.37	0.45
1:D:212:ASN:HB3	2:D:401:DUD:O2	2.17	0.45
1:A:124:HIS:NE2	1:A:142:CYS:HB2	2.32	0.45
1:A:234:LEU:HD12	1:A:234:LEU:HA	1.81	0.45
1:B:281[B]:ARG:HG3	1:B:281[B]:ARG:NH1	2.30	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:ALA:HB2	1:B:351:GLN:HG2	1.98	0.45
1:C:124:HIS:HE2	1:C:142:CYS:CB	2.28	0.45
1:A:154:PRO:C	1:A:156:LEU:N	2.69	0.45
1:A:265:LEU:HD23	1:A:265:LEU:HA	1.74	0.45
1:B:149:PRO:CD	1:B:150:ALA:H	2.30	0.45
1:C:124:HIS:HE2	1:C:142:CYS:HB2	1.82	0.45
1:B:270:LEU:C	1:B:270:LEU:HD23	2.37	0.44
1:B:336:LEU:HD12	1:B:336:LEU:HA	1.84	0.44
1:A:271:ALA:N	1:C:243:GLY:O	2.44	0.44
1:D:338:ILE:CG2	1:D:364:ALA:HB1	2.48	0.44
1:A:33:ALA:HB1	1:A:43:VAL:HG11	1.98	0.44
1:B:191:GLU:HA	1:B:194:LEU:HD12	1.98	0.44
1:C:191:GLU:HA	1:C:194:LEU:HD12	2.00	0.44
1:C:247:LEU:HD21	1:C:251:PHE:CD2	2.52	0.44
1:C:319:VAL:HG23	1:C:333:LEU:CD1	2.47	0.44
1:A:73:LEU:HD11	1:A:105:VAL:HG11	1.99	0.44
1:A:320:ILE:CD1	1:A:347:LEU:HD22	2.46	0.44
1:A:153:GLU:O	1:A:156:LEU:CB	2.66	0.44
1:A:330:ARG:HG3	1:A:331:ASP:OD1	2.18	0.44
1:B:143:VAL:HG21	1:B:385:LEU:HD22	2.00	0.44
1:C:164:MET:HB2	1:C:168:TYR:CE2	2.53	0.44
1:D:161:ARG:HG3	1:D:168:TYR:OH	2.17	0.44
1:A:124:HIS:HE2	1:A:142:CYS:CB	2.30	0.44
1:C:321:PRO:HG3	1:C:330:ARG:HD3	2.00	0.44
1:B:133:LEU:HD23	1:B:133:LEU:C	2.38	0.44
1:B:147:LEU:HD12	1:B:147:LEU:C	2.38	0.44
1:B:124:HIS:HE2	1:B:142:CYS:CB	2.30	0.43
1:A:121:LEU:HD13	1:A:389:ALA:HB2	2.00	0.43
1:B:124:HIS:HE2	1:B:142:CYS:HB2	1.84	0.43
1:D:250:LEU:HB2	1:D:347:LEU:HD23	2.00	0.43
1:D:311:LEU:HD22	1:D:368:VAL:HG11	1.99	0.43
1:B:64:VAL:HG13	1:B:109:GLY:CA	2.45	0.43
1:A:111:LEU:O	1:A:115:ARG:HG3	2.17	0.43
1:C:250:LEU:CD1	1:C:250:LEU:O	2.67	0.43
1:B:311:LEU:HD22	1:B:368:VAL:HG11	2.01	0.43
1:A:124:HIS:HE2	1:A:142:CYS:HB2	1.84	0.43
1:B:234:LEU:HB2	1:B:239:ALA:HB2	2.01	0.43
1:A:153:GLU:O	1:A:156:LEU:HB2	2.19	0.42
1:B:244:ILE:HG12	1:B:268:GLY:HA3	2.01	0.42
1:D:124:HIS:CD2	1:D:142:CYS:HB2	2.54	0.42
1:D:249:PRO:HG2	1:D:345:GLY:HA2	1.99	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:LEU:CB	1:C:270:LEU:HD22	2.49	0.42
1:C:311:LEU:HD22	1:C:368:VAL:HG11	2.00	0.42
1:D:302:GLY:O	1:D:329:ASN:ND2	2.44	0.42
1:A:250:LEU:CG	1:A:347:LEU:HD21	2.49	0.42
1:B:41:HIS:NE2	1:B:386:VAL:HG21	2.34	0.42
1:C:288:LEU:HD21	1:C:306:THR:HG23	2.01	0.42
1:C:14:ARG:NH2	1:D:293:GLU:OE2	2.52	0.42
1:B:13:MET:HE2	1:B:386:VAL:HA	2.02	0.42
1:B:329:ASN:HA	1:B:332:VAL:CG2	2.49	0.42
1:C:364:ALA:O	1:C:368:VAL:HG23	2.20	0.41
1:D:124:HIS:NE2	1:D:142:CYS:HB2	2.36	0.41
1:D:253:GLU:OE2	1:D:349:ALA:CB	2.68	0.41
1:D:147:LEU:CD1	1:D:148:GLY:N	2.84	0.41
1:D:321:PRO:HG3	1:D:341:ASP:CG	2.40	0.41
1:A:190:VAL:HG22	1:A:336:LEU:HD11	2.03	0.41
1:B:288:LEU:HD21	1:B:306:THR:HG23	2.03	0.41
1:C:13:MET:CE	1:C:386:VAL:HA	2.50	0.41
1:C:47:THR:C	1:C:64:VAL:HG22	2.41	0.41
1:D:121:LEU:HD13	1:D:389:ALA:HB2	2.03	0.41
1:A:273:LEU:CD2	1:C:273:LEU:HB2	2.51	0.41
1:A:41:HIS:NE2	1:A:386:VAL:HG21	2.36	0.41
1:A:76:PRO:CD	1:A:77:ASP:H	2.34	0.41
1:C:253:GLU:C	1:C:255:ALA:N	2.74	0.41
1:D:327:ASP:CB	1:D:330:ARG:CD	2.96	0.41
1:B:265:LEU:HD12	1:B:267:GLY:H	1.85	0.41
1:A:328:THR:OG1	1:A:329:ASN:N	2.55	0.40
1:B:156:LEU:O	1:B:156:LEU:HD12	2.22	0.40
1:C:247:LEU:C	1:C:249:PRO:CD	2.89	0.40
1:C:311:LEU:HD21	1:C:338:ILE:CD1	2.51	0.40
1:D:190:VAL:HG13	1:D:332:VAL:HG11	2.03	0.40
1:A:98:MET:O	1:A:102:VAL:HG23	2.21	0.40
1:C:13:MET:CE	1:C:386:VAL:HG22	2.52	0.40
1:D:234:LEU:HD23	1:D:301:HIS:HB3	2.03	0.40
1:D:327:ASP:HB3	1:D:330:ARG:HD3	2.03	0.40
1:A:191:GLU:OE2	1:A:199:ARG:HB2	2.22	0.40
1:A:19:THR:O	1:A:47:THR:HG22	2.20	0.40
1:B:13:MET:CE	1:B:386:VAL:HG22	2.51	0.40
1:C:247:LEU:HD21	1:C:251:PHE:CE2	2.57	0.40
1:C:268:GLY:O	1:C:270:LEU:HD23	2.22	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	349/400 (87%)	330 (95%)	17 (5%)	2 (1%)	25 50
1	B	354/400 (88%)	339 (96%)	14 (4%)	1 (0%)	41 66
1	C	313/400 (78%)	299 (96%)	14 (4%)	0	100 100
1	D	335/400 (84%)	318 (95%)	17 (5%)	0	100 100
All	All	1351/1600 (84%)	1286 (95%)	62 (5%)	3 (0%)	47 73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	152	SER
1	A	76	PRO
1	A	77	ASP

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	267/303 (88%)	251 (94%)	16 (6%)	19 42
1	B	269/303 (89%)	256 (95%)	13 (5%)	25 53
1	C	248/303 (82%)	229 (92%)	19 (8%)	13 30
1	D	258/303 (85%)	246 (95%)	12 (5%)	26 54
All	All	1042/1212 (86%)	982 (94%)	60 (6%)	20 43

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	SER
1	A	42	GLU
1	A	47	THR
1	A	72	LYS
1	A	153	GLU
1	A	159	LEU
1	A	198	ARG
1	A	219	ASP
1	A	228	ARG
1	A	246	LYS
1	A	252	SER
1	A	253	GLU
1	A	315	VAL
1	A	322	HIS
1	A	324	SER
1	A	331	ASP
1	B	12	SER
1	B	42	GLU
1	B	52	ARG
1	B	73	LEU
1	B	159	LEU
1	B	219	ASP
1	B	238	ASP
1	B	273	LEU
1	B	301[A]	HIS
1	B	301[B]	HIS
1	B	315	VAL
1	B	331	ASP
1	B	336	LEU
1	C	12	SER
1	C	42	GLU
1	C	52	ARG
1	C	97	GLU
1	C	151	ASP
1	C	159	LEU
1	C	162	ARG
1	C	164	MET
1	C	166	LYS
1	C	167	ASP
1	C	219	ASP
1	C	227	ARG
1	C	234	LEU
1	C	246	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	250	LEU
1	C	270	LEU
1	C	315	VAL
1	C	322	HIS
1	C	331	ASP
1	D	12	SER
1	D	42	GLU
1	D	52	ARG
1	D	147	LEU
1	D	161	ARG
1	D	200	SER
1	D	219	ASP
1	D	272	LEU
1	D	273	LEU
1	D	315	VAL
1	D	330	ARG
1	D	333	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	212	ASN
1	C	34	GLN
1	C	171	HIS
1	C	301	HIS
1	C	351	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)

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	MLY	C	384	1	9,10,11	0.49	0	6,11,13	0.55	0
1	MLY	D	384	1	9,10,11	0.55	0	6,11,13	0.69	0
1	MLY	A	384	1	9,10,11	0.54	0	6,11,13	0.58	0
1	MLY	B	384	1	9,10,11	0.51	0	6,11,13	0.63	0

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
1	MLY	C	384	1	-	4/8/9/11	-
1	MLY	D	384	1	-	5/8/9/11	-
1	MLY	A	384	1	-	4/8/9/11	-
1	MLY	B	384	1	-	4/8/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	384	MLY	N-CA-CB-CG
1	D	384	MLY	C-CA-CB-CG
1	A	384	MLY	N-CA-CB-CG
1	A	384	MLY	C-CA-CB-CG
1	B	384	MLY	N-CA-CB-CG
1	B	384	MLY	C-CA-CB-CG
1	C	384	MLY	CD-CE-NZ-CH1
1	D	384	MLY	CG-CD-CE-NZ
1	C	384	MLY	CD-CE-NZ-CH2
1	D	384	MLY	CA-CB-CG-CD
1	A	384	MLY	CG-CD-CE-NZ
1	A	384	MLY	CE-CD-CG-CB
1	B	384	MLY	CE-CD-CG-CB
1	C	384	MLY	CA-CB-CG-CD
1	C	384	MLY	CE-CD-CG-CB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	D	384	MLY	CE-CD-CG-CB
1	B	384	MLY	CG-CD-CE-NZ

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	384	MLY	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	DUD	D	401	-	20,25,25	0.76	1 (5%)	25,38,38	0.92	0
2	DUD	B	401	-	20,25,25	0.78	1 (5%)	25,38,38	1.18	1 (4%)

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	DUD	D	401	-	-	9/13/28/28	0/2/2/2
2	DUD	B	401	-	-	5/13/28/28	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	DUD	C2-N3	-2.24	1.33	1.38
2	D	401	DUD	C2-N3	-2.09	1.34	1.38

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	DUD	PA-O3A-PB	-2.98	122.59	132.83

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	DUD	C5'-O5'-PA-O2A
2	D	401	DUD	PB-O3A-PA-O5'
2	D	401	DUD	PA-O3A-PB-O2B
2	D	401	DUD	PA-O3A-PB-O3B
2	B	401	DUD	C5'-O5'-PA-O1A
2	B	401	DUD	C5'-O5'-PA-O3A
2	D	401	DUD	O4'-C4'-C5'-O5'
2	D	401	DUD	C3'-C4'-C5'-O5'
2	D	401	DUD	C5'-O5'-PA-O3A
2	D	401	DUD	C5'-O5'-PA-O1A
2	B	401	DUD	C5'-O5'-PA-O2A
2	B	401	DUD	PA-O3A-PB-O1B
2	B	401	DUD	O4'-C4'-C5'-O5'
2	D	401	DUD	PA-O3A-PB-O1B

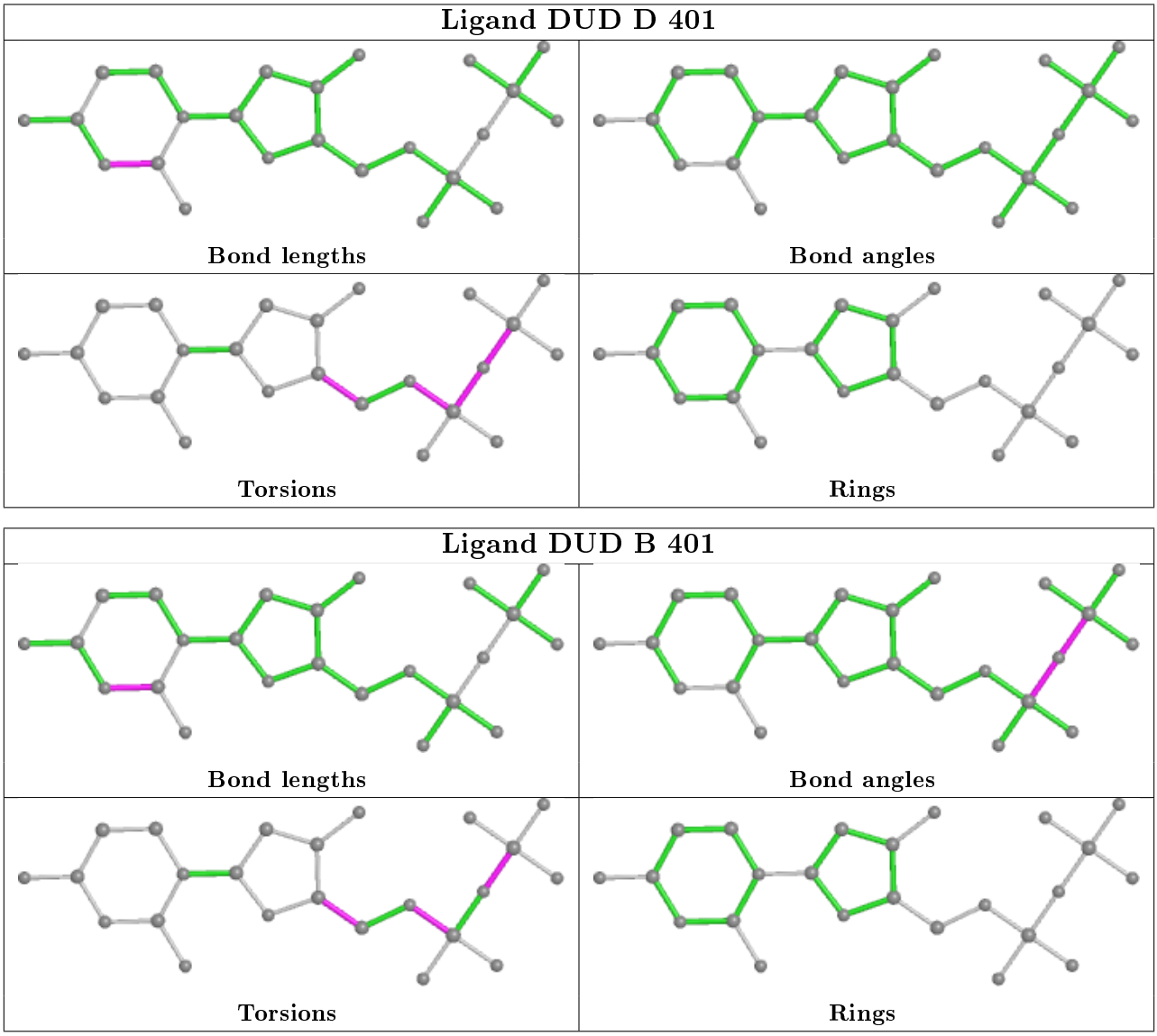
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	DUD	2	0
2	B	401	DUD	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.



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	357/400 (89%)	0.21	9 (2%) 57 59	26, 49, 95, 131	0
1	B	358/400 (89%)	0.62	36 (10%) 7 5	32, 73, 116, 123	0
1	C	327/400 (81%)	1.04	56 (17%) 1 1	58, 98, 136, 152	0
1	D	347/400 (86%)	0.88	37 (10%) 6 4	57, 98, 130, 157	0
All	All	1389/1600 (86%)	0.68	138 (9%) 7 5	26, 83, 128, 157	0

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	94	PHE	10.8
1	D	240	LEU	6.5
1	C	247	LEU	6.2
1	C	253	GLU	5.8
1	C	363	GLU	5.6
1	C	76	PRO	5.5
1	C	338	ILE	5.1
1	A	245	ALA	5.0
1	D	70	TYR	4.9
1	C	251	PHE	4.9
1	D	72	LYS	4.8
1	D	73	LEU	4.8
1	C	329	ASN	4.7
1	C	243	GLY	4.7
1	B	74	PHE	4.6
1	D	273	LEU	4.6
1	C	178	THR	4.6
1	C	336	LEU	4.6
1	A	79	THR	4.5
1	C	352	CYS	4.5
1	D	263	LEU	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	94	PHE	4.4
1	B	347	LEU	4.3
1	C	254	VAL	4.3
1	C	74	PHE	4.1
1	C	173	VAL	4.1
1	B	259	ALA	4.1
1	D	178	THR	4.0
1	D	162	ARG	3.9
1	C	249	PRO	3.8
1	C	201	PRO	3.8
1	B	250	LEU	3.8
1	A	75	VAL	3.7
1	C	225	ALA	3.7
1	B	257	VAL	3.7
1	D	254	VAL	3.6
1	C	136	ALA	3.6
1	A	225	ALA	3.6
1	B	225	ALA	3.6
1	A	72	LYS	3.5
1	C	179	GLY	3.5
1	D	359	ALA	3.5
1	D	251	PHE	3.4
1	C	190	VAL	3.3
1	C	367	ARG	3.3
1	C	147	LEU	3.3
1	C	328	THR	3.3
1	A	77	ASP	3.3
1	C	72	LYS	3.2
1	C	265	LEU	3.2
1	C	273	LEU	3.1
1	C	355	LEU	3.1
1	D	196	GLU	3.1
1	B	174	THR	3.1
1	B	251	PHE	3.1
1	C	248	ALA	3.1
1	A	78	ASP	3.0
1	C	359	ALA	3.0
1	D	268	GLY	3.0
1	A	251	PHE	3.0
1	C	69	ASN	3.0
1	C	171	HIS	3.0
1	B	72	LYS	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	304	SER	2.9
1	C	244	ILE	2.9
1	B	30	VAL	2.9
1	D	390	GLY	2.9
1	C	272	LEU	2.8
1	D	64	VAL	2.8
1	D	99	PHE	2.8
1	D	97	GLU	2.8
1	C	195	PRO	2.8
1	C	75	VAL	2.8
1	D	98	MET	2.8
1	C	330	ARG	2.8
1	C	174	THR	2.7
1	D	389	ALA	2.7
1	D	173	VAL	2.7
1	D	12	SER	2.7
1	B	249	PRO	2.7
1	B	173	VAL	2.6
1	C	371	GLU	2.6
1	B	244	ILE	2.6
1	B	253	GLU	2.6
1	B	256	ASP	2.5
1	B	69	ASN	2.5
1	B	345	GLY	2.5
1	B	284	GLU	2.5
1	D	388	LEU	2.5
1	B	139	GLN	2.4
1	D	177	PRO	2.4
1	B	273	LEU	2.4
1	B	254	VAL	2.4
1	C	188	PRO	2.4
1	A	272	LEU	2.4
1	D	342	ALA	2.4
1	C	189	SER	2.4
1	B	247	LEU	2.4
1	B	67	GLY	2.4
1	C	181	VAL	2.4
1	B	261	PHE	2.3
1	C	95	PHE	2.3
1	D	95	PHE	2.3
1	C	256	ASP	2.3
1	C	73	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	267	GLY	2.3
1	B	344	ALA	2.3
1	C	161	ARG	2.2
1	D	341	ASP	2.2
1	C	67	GLY	2.2
1	C	202	GLY	2.2
1	D	360	GLY	2.2
1	B	71	ALA	2.2
1	B	31	PRO	2.2
1	C	177	PRO	2.2
1	B	242	GLY	2.2
1	B	370	GLN	2.2
1	B	238	ASP	2.2
1	D	158	ALA	2.2
1	D	282	VAL	2.1
1	B	178	THR	2.1
1	D	174	THR	2.1
1	C	107	VAL	2.1
1	B	133	LEU	2.1
1	B	169	GLU	2.1
1	D	71	ALA	2.1
1	C	70	TYR	2.1
1	B	73	LEU	2.1
1	C	299	ILE	2.1
1	D	345	GLY	2.1
1	C	187	PRO	2.1
1	C	252	SER	2.1
1	B	162	ARG	2.1
1	D	101	ARG	2.1
1	B	360	GLY	2.1
1	D	69	ASN	2.0
1	C	365	ALA	2.0
1	D	179	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	MLY	D	384	11/12	0.94	0.29	70,78,83,84	0
1	MLY	B	384	11/12	0.94	0.23	48,52,63,65	0
1	MLY	C	384	11/12	0.95	0.20	75,82,85,90	0
1	MLY	A	384	11/12	0.97	0.18	34,36,39,46	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

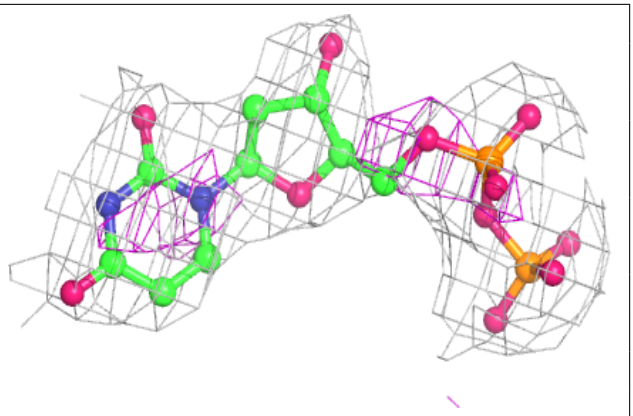
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

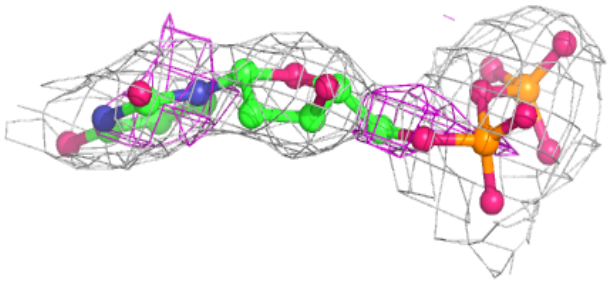
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	DUD	B	401	24/24	0.91	0.17	65,77,90,92	0
2	DUD	D	401	24/24	0.94	0.15	75,85,98,103	0

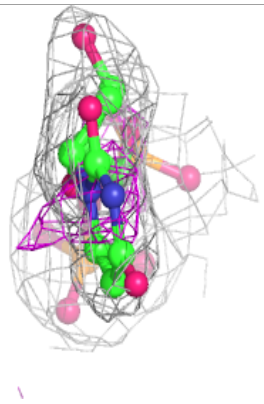
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DUD 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)

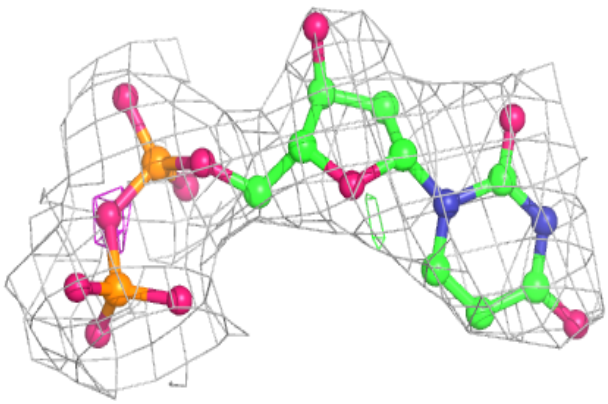


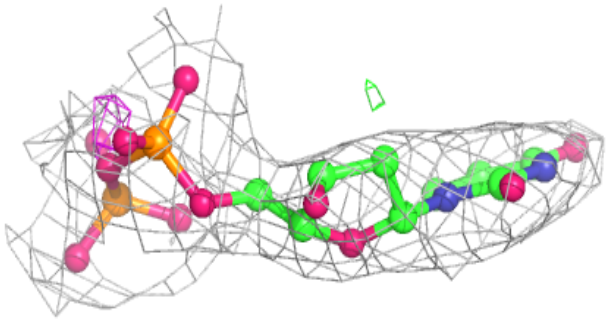


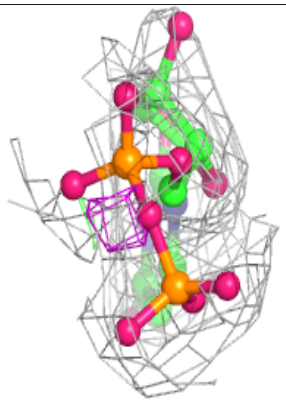


Electron density around DUD D 401:

$2mF_o$-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)

There are no such residues in this entry.