



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:17 am GMT

PDB ID : 4AN4  
Title : Crystal structure of the glycosyltransferase SnogD from *Streptomyces nogalater*  
Authors : Claesson, M.; Siitonen, V.; Dobritzsch, D.; Metsä-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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

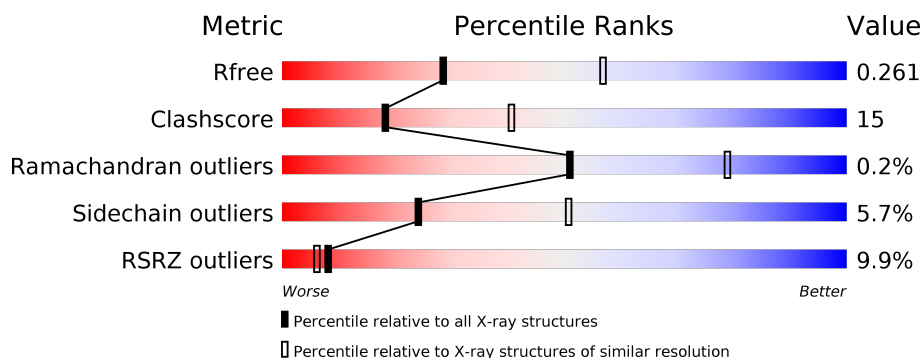
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . 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	<div> <div>2%</div> <div>68% 19% 11%</div> </div>
1	B	400	<div> <div>9%</div> <div>70% 19% 10%</div> </div>
1	C	400	<div> <div>14%</div> <div>60% 20% 18%</div> </div>
1	D	400	<div> <div>9%</div> <div>67% 18% 13%</div> </div>

## 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...*

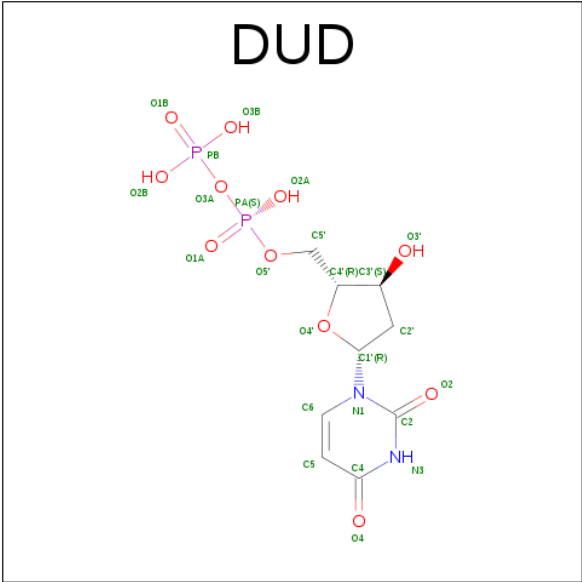
Chain	Residue	Modelled	Actual	Comment	Reference
A	12	SER	-	EXPRESSION TAG	UNP Q9RN61
B	-9	MET	-	EXPRESSION TAG	UNP Q9RN61
B	-8	HIS	-	EXPRESSION TAG	UNP Q9RN61
B	-7	HIS	-	EXPRESSION TAG	UNP Q9RN61
B	-6	HIS	-	EXPRESSION TAG	UNP Q9RN61
B	-5	HIS	-	EXPRESSION TAG	UNP Q9RN61
B	-4	HIS	-	EXPRESSION TAG	UNP Q9RN61
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		

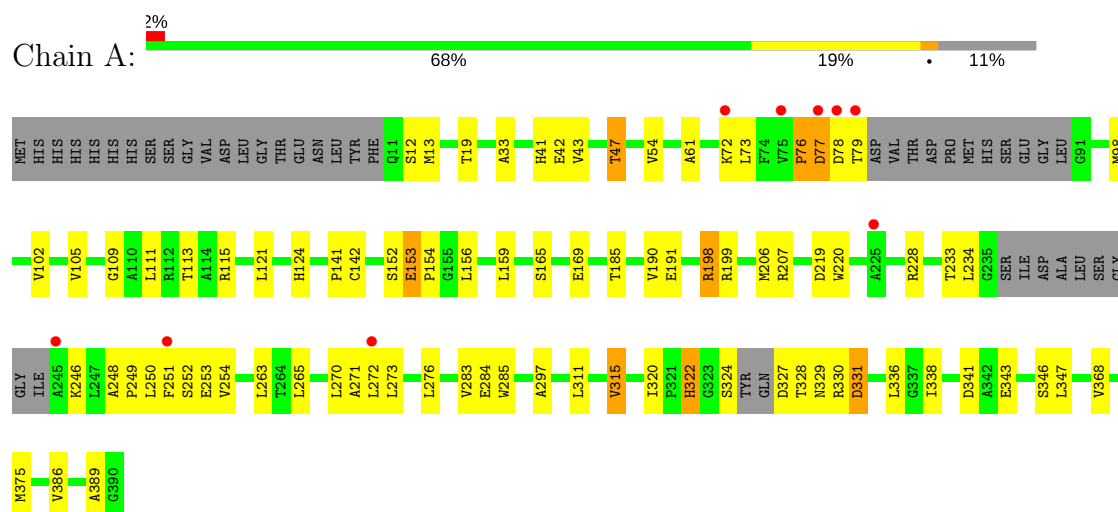
- Molecule 3 is water.

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		

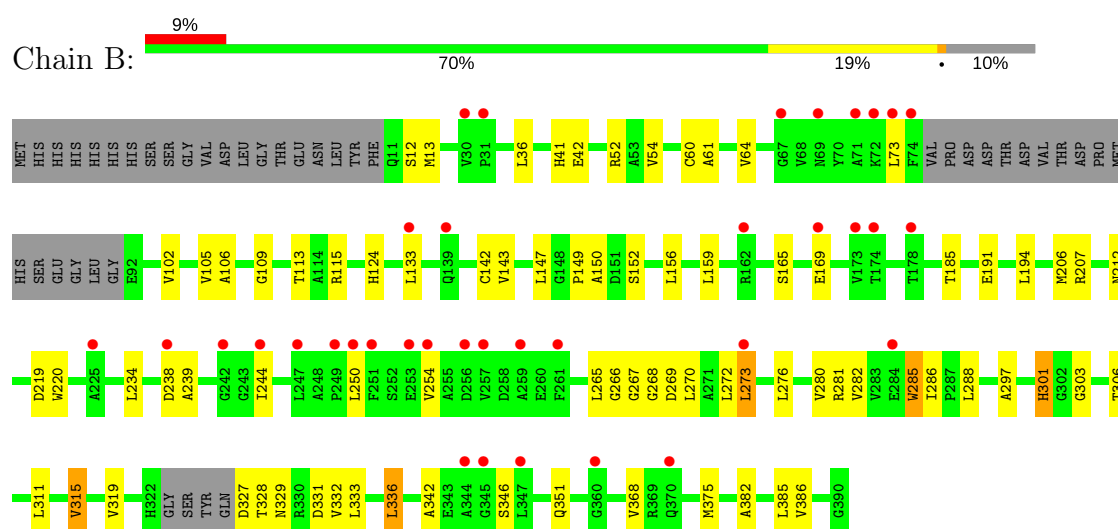
### 3 Residue-property plots

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

#### • Molecule 1: GLYCOSYL TRANSFERASE

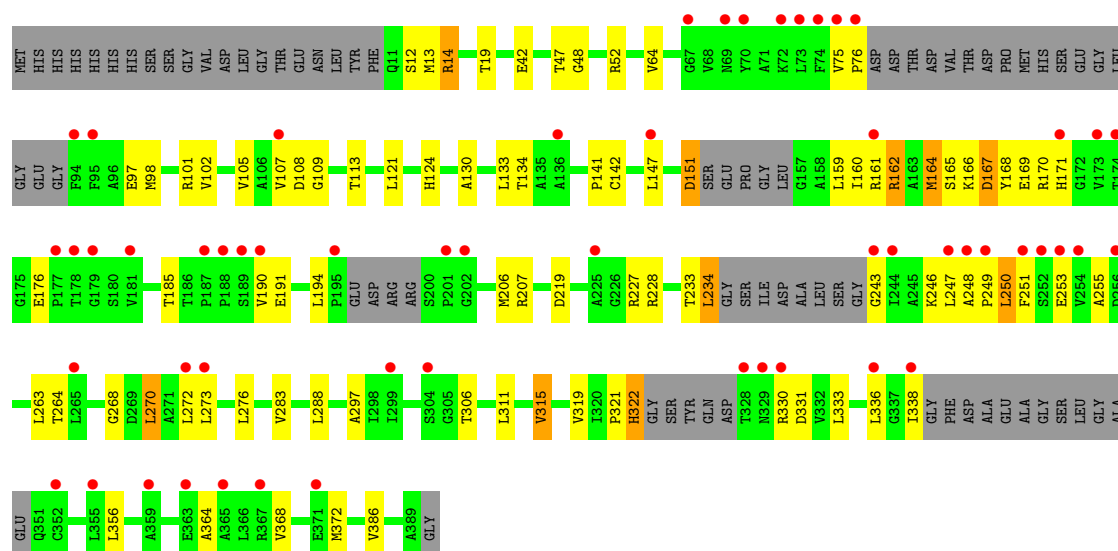


#### • Molecule 1: GLYCOSYL TRANSFERASE

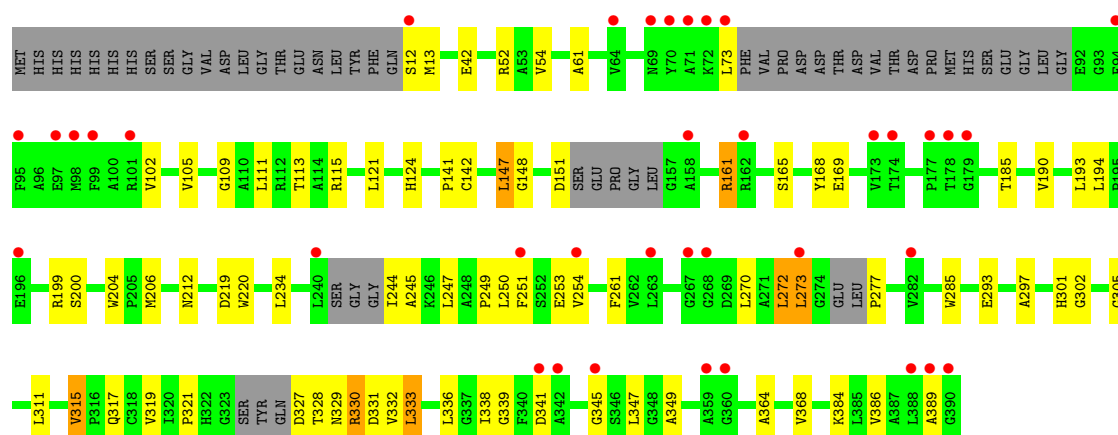


#### • Molecule 1: GLYCOSYL TRANSFERASE





### • Molecule 1: GLYCOSYL TRANSFERASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	70.2	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 69.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: 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(°)	Ideal(°)
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 [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	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

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	349/400 (87%)	330 (95%)	17 (5%)	2 (1%)	28	56
1	B	354/400 (88%)	339 (96%)	14 (4%)	1 (0%)	44	73
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%)	51	79

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

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%)	22	48
1	B	269/303 (89%)	256 (95%)	13 (5%)	30	59
1	C	248/303 (82%)	229 (92%)	19 (8%)	15	34
1	D	258/303 (85%)	246 (95%)	12 (5%)	30	60
All	All	1042/1212 (86%)	982 (94%)	60 (6%)	24	50

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 ⓘ

There are no RNA molecules in this entry.

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

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	A	384	1	10,10,11	0.50	0	8,11,13	1.14	1 (12%)
1	MLY	B	384	1	10,10,11	0.56	0	8,11,13	1.09	1 (12%)
1	MLY	C	384	1	10,10,11	0.49	0	8,11,13	1.00	0
1	MLY	D	384	1	10,10,11	0.52	0	8,11,13	1.04	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	A	384	1	-	0/7/9/11	0/0/0/0
1	MLY	B	384	1	-	0/7/9/11	0/0/0/0
1	MLY	C	384	1	-	0/7/9/11	0/0/0/0
1	MLY	D	384	1	-	0/7/9/11	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	384	MLY	CB-CA-C	-2.56	107.44	111.65
1	B	384	MLY	CB-CA-C	-2.30	107.87	111.65

There are no chirality outliers.

There are no torsion outliers.

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 carbohydrates in this entry.

## 5.6 Ligand geometry

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	DUD	B	401	-	20,25,25	0.75	1 (5%)	23,38,38	2.12	2 (8%)
2	DUD	D	401	-	20,25,25	0.80	1 (5%)	23,38,38	1.95	2 (8%)

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	B	401	-	-	0/12/28/28	0/2/2/2
2	DUD	D	401	-	-	0/12/28/28	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 (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	DUD	O4'-C1'-N1	2.91	112.69	107.78
2	B	401	DUD	O4'-C1'-N1	3.26	113.28	107.78
2	D	401	DUD	C4-N3-C2	8.01	121.01	114.13
2	B	401	DUD	C4-N3-C2	8.34	121.30	114.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	DUD	5	0
2	D	401	DUD	2	0

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	357/400 (89%)	0.21	9 (2%) 58 58	26, 49, 95, 131	0
1	B	358/400 (89%)	0.62	36 (10%) 8 6	32, 73, 116, 123	0
1	C	327/400 (81%)	1.04	56 (17%) 2 1	58, 98, 136, 152	0
1	D	347/400 (86%)	0.88	37 (10%) 7 5	57, 98, 130, 157	0
All	All	1389/1600 (86%)	0.68	138 (9%) 8 6	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	5.5
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	73	LEU	4.8
1	D	72	LYS	4.8
1	C	329	ASN	4.7
1	C	243	GLY	4.7
1	D	273	LEU	4.6
1	B	74	PHE	4.6
1	C	336	LEU	4.6
1	C	178	THR	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	4.2
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	B	250	LEU	3.8
1	C	201	PRO	3.7
1	A	75	VAL	3.7
1	C	225	ALA	3.7
1	B	257	VAL	3.7
1	D	254	VAL	3.7
1	B	225	ALA	3.6
1	C	136	ALA	3.6
1	A	225	ALA	3.6
1	A	72	LYS	3.5
1	D	359	ALA	3.5
1	C	179	GLY	3.5
1	D	251	PHE	3.4
1	C	190	VAL	3.4
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	265	LEU	3.2
1	C	72	LYS	3.2
1	C	273	LEU	3.1
1	D	196	GLU	3.1
1	C	355	LEU	3.1
1	B	251	PHE	3.1
1	C	248	ALA	3.1
1	B	174	THR	3.1
1	A	78	ASP	3.0
1	D	268	GLY	3.0
1	C	359	ALA	3.0
1	C	171	HIS	3.0
1	A	251	PHE	3.0
1	C	69	ASN	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	D	64	VAL	2.9
1	C	272	LEU	2.8
1	D	97	GLU	2.8
1	D	99	PHE	2.8
1	C	195	PRO	2.8
1	D	98	MET	2.8
1	C	75	VAL	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	B	249	PRO	2.7
1	D	12	SER	2.6
1	C	371	GLU	2.6
1	B	173	VAL	2.6
1	B	244	ILE	2.6
1	B	253	GLU	2.6
1	B	69	ASN	2.5
1	B	256	ASP	2.5
1	B	284	GLU	2.5
1	B	345	GLY	2.5
1	D	388	LEU	2.5
1	B	139	GLN	2.4
1	C	188	PRO	2.4
1	D	342	ALA	2.4
1	B	273	LEU	2.4
1	B	254	VAL	2.4
1	D	177	PRO	2.4
1	C	189	SER	2.4
1	A	272	LEU	2.4
1	B	247	LEU	2.4
1	B	67	GLY	2.4
1	C	181	VAL	2.4
1	D	95	PHE	2.4
1	B	261	PHE	2.3
1	C	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	C	161	ARG	2.3
1	C	67	GLY	2.2
1	C	202	GLY	2.2
1	B	344	ALA	2.2
1	D	341	ASP	2.2
1	B	31	PRO	2.2
1	B	71	ALA	2.2
1	D	360	GLY	2.2
1	B	370	GLN	2.2
1	B	242	GLY	2.2
1	C	177	PRO	2.2
1	D	158	ALA	2.2
1	B	238	ASP	2.2
1	B	169	GLU	2.1
1	C	107	VAL	2.1
1	B	178	THR	2.1
1	D	174	THR	2.1
1	D	282	VAL	2.1
1	B	73	LEU	2.1
1	B	133	LEU	2.1
1	D	71	ALA	2.1
1	C	70	TYR	2.1
1	C	252	SER	2.1
1	C	299	ILE	2.1
1	B	360	GLY	2.1
1	C	187	PRO	2.1
1	B	162	ARG	2.1
1	D	345	GLY	2.1
1	D	69	ASN	2.1
1	D	101	ARG	2.1
1	C	365	ALA	2.0
1	D	179	GLY	2.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	MLY	C	384	11/12	0.95	0.20	-	75,82,85,90	0
1	MLY	D	384	11/12	0.94	0.29	-	70,78,83,84	0
1	MLY	A	384	11/12	0.97	0.18	-	34,36,39,46	0
1	MLY	B	384	11/12	0.94	0.23	-	48,52,63,65	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	DUD	B	401	24/24	0.91	0.17	-0.66	65,77,90,92	0
2	DUD	D	401	24/24	0.94	0.15	-1.60	75,85,98,103	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.