



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:51 PM UTC

PDB ID : 3KL3 / pdb\_00003kl3  
Title : Crystal structure of Ligand bound XynC  
Authors : St John, F.J.; Hurlbert, J.C.; Pozharski, E.  
Deposited on : 2009-11-06  
Resolution : 2.33 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

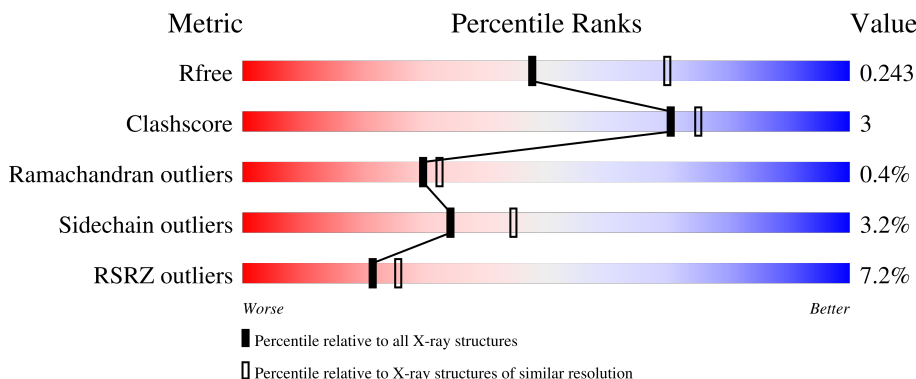
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.33 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))
$R_{free}$	180053	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	401	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>6%</div> <div>..</div> </div> </div>
1	B	401	<div> <div></div> <div>89%</div> <div>8%</div> <div>..</div> </div>
1	C	401	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>8%</div> <div>.</div> </div> </div>
1	D	401	<div> <div>26%</div> <div> <div></div> <div>77%</div> <div>13%</div> <div>.</div> <div>8%</div> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12822 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 Glucuronoxylanase xynC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	0	0
			3095	1959	547	580	9			
1	B	390	Total	C	N	O	S	0	1	0
			3112	1970	551	582	9			
1	C	390	Total	C	N	O	S	0	4	0
			3133	1983	556	585	9			
1	D	368	Total	C	N	O	S	0	0	0
			2940	1869	514	548	9			

There are 44 discrepancies between the modelled and reference sequences:

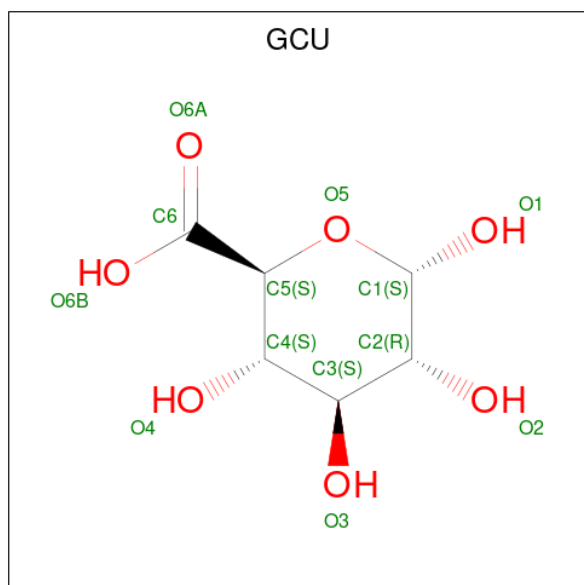
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q45070
A	392	LEU	-	expression tag	UNP Q45070
A	393	GLU	-	expression tag	UNP Q45070
A	394	HIS	-	expression tag	UNP Q45070
A	395	HIS	-	expression tag	UNP Q45070
A	396	HIS	-	expression tag	UNP Q45070
A	397	HIS	-	expression tag	UNP Q45070
A	398	HIS	-	expression tag	UNP Q45070
A	399	HIS	-	expression tag	UNP Q45070
A	400	HIS	-	expression tag	UNP Q45070
A	401	HIS	-	expression tag	UNP Q45070
B	1	MET	-	expression tag	UNP Q45070
B	392	LEU	-	expression tag	UNP Q45070
B	393	GLU	-	expression tag	UNP Q45070
B	394	HIS	-	expression tag	UNP Q45070
B	395	HIS	-	expression tag	UNP Q45070
B	396	HIS	-	expression tag	UNP Q45070
B	397	HIS	-	expression tag	UNP Q45070
B	398	HIS	-	expression tag	UNP Q45070
B	399	HIS	-	expression tag	UNP Q45070
B	400	HIS	-	expression tag	UNP Q45070

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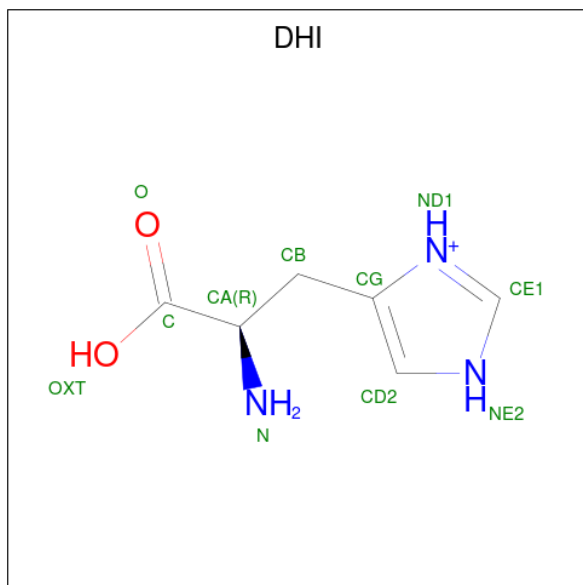
Chain	Residue	Modelled	Actual	Comment	Reference
B	401	HIS	-	expression tag	UNP Q45070
C	1	MET	-	expression tag	UNP Q45070
C	392	LEU	-	expression tag	UNP Q45070
C	393	GLU	-	expression tag	UNP Q45070
C	394	HIS	-	expression tag	UNP Q45070
C	395	HIS	-	expression tag	UNP Q45070
C	396	HIS	-	expression tag	UNP Q45070
C	397	HIS	-	expression tag	UNP Q45070
C	398	HIS	-	expression tag	UNP Q45070
C	399	HIS	-	expression tag	UNP Q45070
C	400	HIS	-	expression tag	UNP Q45070
C	401	HIS	-	expression tag	UNP Q45070
D	1	MET	-	expression tag	UNP Q45070
D	392	LEU	-	expression tag	UNP Q45070
D	393	GLU	-	expression tag	UNP Q45070
D	394	HIS	-	expression tag	UNP Q45070
D	395	HIS	-	expression tag	UNP Q45070
D	396	HIS	-	expression tag	UNP Q45070
D	397	HIS	-	expression tag	UNP Q45070
D	398	HIS	-	expression tag	UNP Q45070
D	399	HIS	-	expression tag	UNP Q45070
D	400	HIS	-	expression tag	UNP Q45070
D	401	HIS	-	expression tag	UNP Q45070

- Molecule 2 is alpha-D-glucopyranuronic acid (CCD ID: GCU) (formula:  $C_6H_{10}O_7$ ).



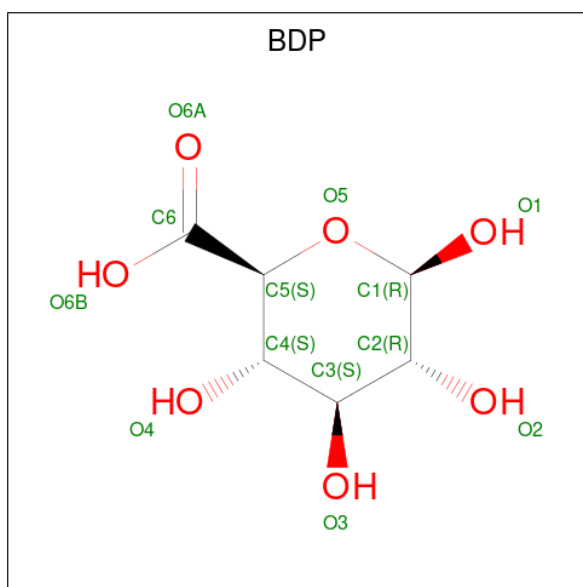
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is D-HISTIDINE (CCD ID: DHI) (formula:  $C_6H_{10}N_3O_2$ ).



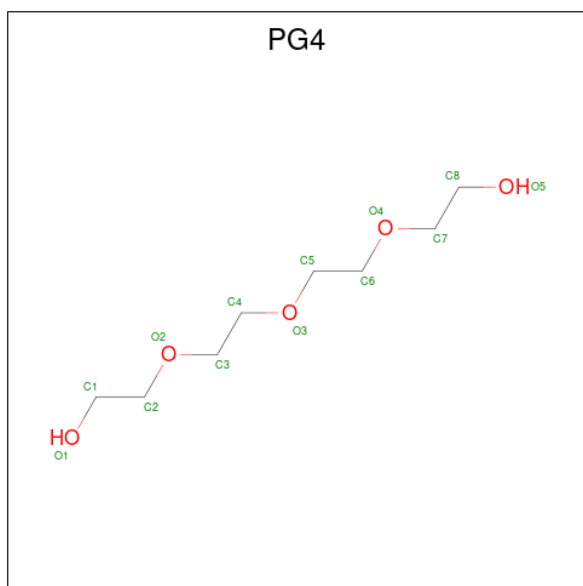
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	6	3	2		
3	B	1	Total	C	N	O	0	0
			11	6	3	2		

- Molecule 4 is beta-D-glucopyranuronic acid (CCD ID: BDP) (formula:  $C_6H_{10}O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 5 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			13	8	5		
5	C	1	Total	C	O	0	0
			10	6	4		

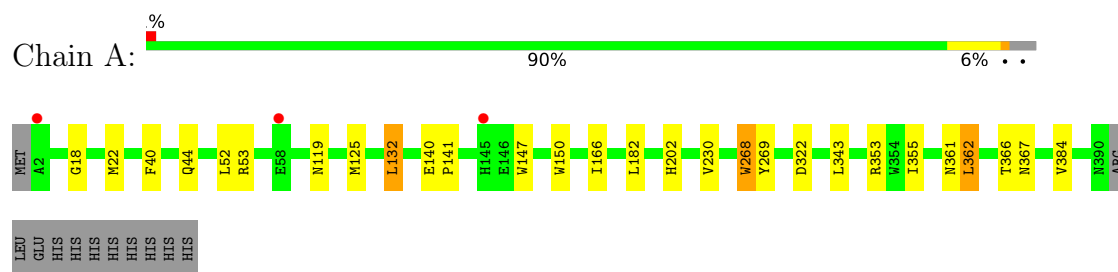
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	112	Total 112	O 112	0	0
6	B	189	Total 189	O 189	0	0
6	C	156	Total 157	O 157	0	1

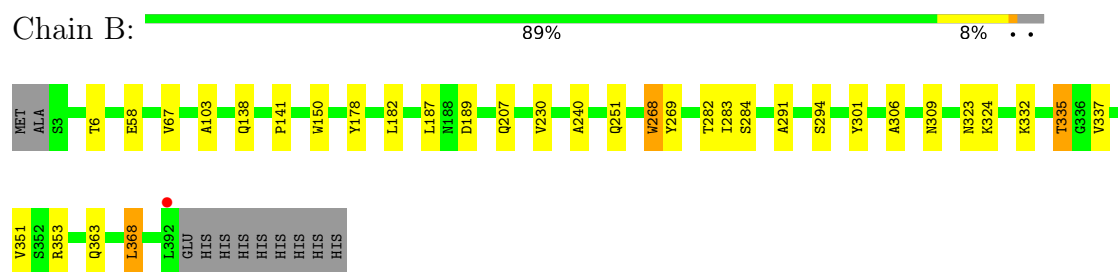
### 3 Residue-property plots [i](#)

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.

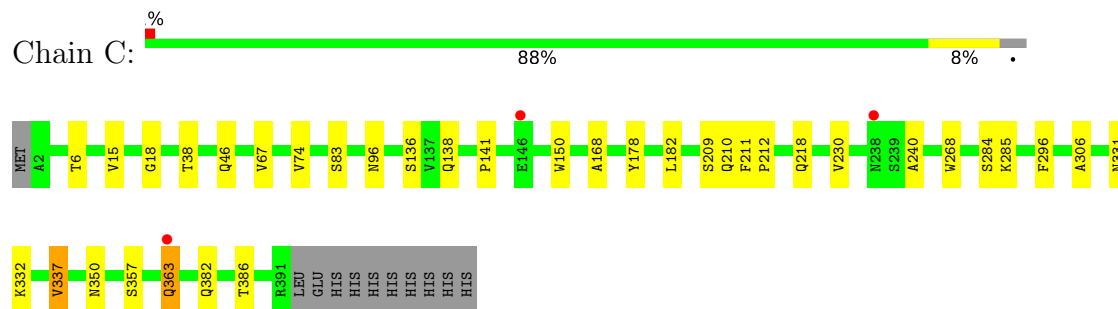
#### • Molecule 1: Glucuronoxylanase xynC



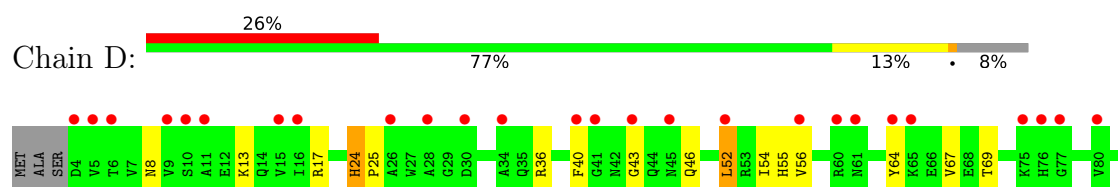
#### • Molecule 1: Glucuronoxylanase xynC



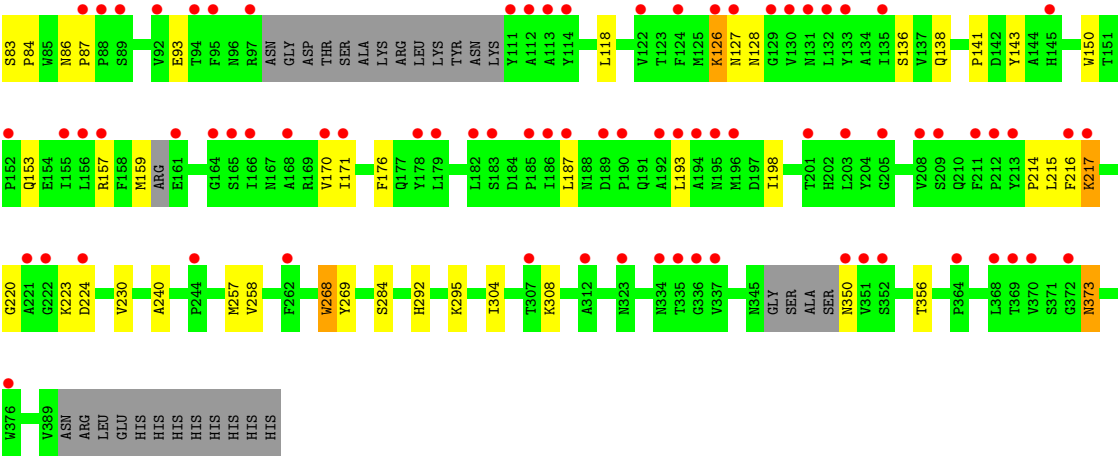
#### • Molecule 1: Glucuronoxylanase xynC



#### • Molecule 1: Glucuronoxylanase xynC







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	137.87Å 192.73Å 65.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.33 50.00 – 2.33	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-2.33) 99.7 (50.00-2.33)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.49 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.195 , 0.248 0.193 , 0.243	Depositor DCC
$R_{free}$ test set	3791 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.2	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 46.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12822	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DHI, PG4, BDP, GCU

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	0.63	0/3182	0.81	1/4335 (0.0%)
1	B	0.69	0/3202	0.85	3/4361 (0.1%)
1	C	0.64	0/3229	0.82	2/4397 (0.0%)
1	D	0.52	0/3023	0.79	2/4119 (0.0%)
All	All	0.62	0/12636	0.82	8/17212 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	189	ASP	CA-C-N	5.79	125.92	119.32
1	B	189	ASP	C-N-CA	5.79	125.92	119.32
1	A	18	GLY	N-CA-C	5.72	118.33	110.56
1	B	67	VAL	N-CA-C	5.58	115.78	110.42
1	D	24	HIS	CA-C-N	5.41	124.59	118.97
1	D	24	HIS	C-N-CA	5.41	124.59	118.97
1	C	18	GLY	N-CA-C	5.12	117.64	110.38
1	C	67	VAL	N-CA-C	5.12	115.33	110.42

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	3095	0	2950	14	0
1	B	3112	0	2974	24	0
1	C	3133	0	2999	18	0
1	D	2940	0	2792	28	0
2	A	13	0	9	0	0
2	B	13	0	9	1	0
3	A	11	0	9	2	0
3	B	11	0	9	0	0
4	B	13	0	9	0	0
5	B	13	0	18	6	0
5	C	10	0	13	1	0
6	A	112	0	0	0	0
6	B	189	0	0	1	0
6	C	157	0	0	0	0
All	All	12822	0	11791	81	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 3.

All (81) 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:B:103:ALA:HA	2:B:403:GCU:H1	1.42	1.01
1:A:141:PRO:HG2	1:A:182:LEU:HD21	1.71	0.72
1:B:282:THR:HB	5:B:405:PG4:H11	1.71	0.72
1:B:363:GLN:NE2	6:B:481:HOH:O	2.00	0.72
1:B:283:ILE:H	5:B:405:PG4:H32	1.57	0.70
1:C:331:ASN:ND2	1:C:337:VAL:HG12	2.11	0.66
1:C:96:ASN:HD21	5:C:402:PG4:H52	1.59	0.66
1:B:353:ARG:HE	1:B:368:LEU:HD21	1.62	0.65
1:B:335:THR:HG23	1:C:168:ALA:HA	1.81	0.63
1:D:240:ALA:HB1	1:D:284:SER:HB2	1.80	0.62
1:C:363[A]:GLN:HA	1:C:363[A]:GLN:HE21	1.64	0.62
1:D:46:GLN:O	1:D:295:LYS:HE2	2.01	0.61
1:C:240:ALA:HB1	1:C:284:SER:HB2	1.83	0.61
1:D:171:ILE:HG12	1:D:198:ILE:HB	1.82	0.61
1:B:283:ILE:H	5:B:405:PG4:C3	2.12	0.61
1:D:138:GLN:HE21	1:D:150:TRP:HE1	1.49	0.60
1:C:38:THR:HA	1:C:46:GLN:HG2	1.85	0.59
1:C:240:ALA:HB1	1:C:284:SER:CB	2.32	0.59
1:D:258:VAL:HG11	1:D:308:LYS:HG2	1.86	0.58
1:B:141:PRO:HG2	1:B:182:LEU:HD21	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:ASN:O	1:D:304:ILE:HB	2.06	0.56
1:D:138:GLN:HG2	1:D:141:PRO:HB3	1.88	0.55
1:B:282:THR:HB	5:B:405:PG4:C1	2.36	0.55
1:B:324:LYS:HZ2	1:B:324:LYS:HB2	1.70	0.54
1:A:268:TRP:CG	1:A:269:TYR:H	2.26	0.54
1:D:240:ALA:HB1	1:D:284:SER:CB	2.39	0.53
1:A:119:ASN:ND2	1:A:166:ILE:HA	2.24	0.53
1:A:22:MET:SD	1:A:53:ARG:HD3	2.49	0.52
1:A:322:ASP:H	3:A:403:DHI:HB2	1.74	0.52
1:B:207:GLN:HG3	1:C:218[B]:GLN:HA	1.90	0.52
1:B:353:ARG:NE	1:B:368:LEU:HD21	2.24	0.52
1:A:140:GLU:OE2	1:A:202:HIS:HD2	1.93	0.52
1:D:43:GLY:H	1:D:46:GLN:HE21	1.59	0.50
1:D:84:PRO:HG3	1:D:118:LEU:HD21	1.94	0.49
1:D:198:ILE:HG12	1:D:224:ASP:HB2	1.94	0.49
1:D:193:LEU:HD22	1:D:223:LYS:HE3	1.95	0.48
1:A:366:THR:HG22	1:A:367:ASN:O	2.14	0.47
1:B:207:GLN:HG3	1:C:218[A]:GLN:HA	1.94	0.47
1:D:143:TYR:HB2	1:D:176:PHE:CD1	2.50	0.47
1:D:292:HIS:HE1	1:D:356:THR:OG1	1.98	0.47
1:B:351:VAL:HB	1:B:368:LEU:HB2	1.97	0.47
1:A:353:ARG:HD2	1:A:355:ILE:HD11	1.97	0.46
1:B:282:THR:HG22	5:B:405:PG4:H61	1.98	0.46
1:A:40:PHE:HZ	1:A:52:LEU:HD13	1.81	0.46
1:C:83:SER:HA	1:C:136:SER:HB3	1.96	0.46
1:D:214:PRO:O	1:D:217:LYS:HG3	2.16	0.45
1:A:361:ASN:O	1:A:362:LEU:C	2.58	0.45
1:C:138:GLN:HG2	1:C:150:TRP:CD1	2.52	0.45
1:B:240:ALA:HB1	1:B:284:SER:HB2	1.98	0.45
1:C:141:PRO:HG2	1:C:182:LEU:HD21	1.99	0.45
1:C:285:LYS:NZ	1:C:357:SER:O	2.50	0.45
1:A:322:ASP:HB2	3:A:403:DHI:HD2	1.99	0.45
1:D:126:LYS:HD2	1:D:127:ASN:HD22	1.81	0.44
1:A:119:ASN:HD21	1:A:166:ILE:HA	1.82	0.44
1:C:363[A]:GLN:HA	1:C:363[A]:GLN:NE2	2.31	0.44
1:D:86:ASN:HA	1:D:87:PRO:HD2	1.80	0.44
1:B:240:ALA:HB1	1:B:284:SER:CB	2.48	0.43
1:B:309:ASN:HB3	1:C:15:VAL:HG21	2.00	0.43
1:D:159:MET:HE1	1:D:170:VAL:HG12	1.99	0.43
1:C:6:THR:O	1:C:306:ALA:HA	2.18	0.43
1:D:373:ASN:HD22	1:D:373:ASN:H	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:ALA:HA	1:B:294:SER:OG	2.19	0.42
1:D:67:VAL:HG21	1:D:128:ASN:HD22	1.84	0.42
1:D:40:PHE:CZ	1:D:52:LEU:HG	2.55	0.42
1:B:332:LYS:HB3	1:B:332:LYS:HE2	1.93	0.41
1:A:141:PRO:HB2	1:A:150:TRP:HB2	2.02	0.41
1:C:211:PHE:N	1:C:212:PRO:CD	2.83	0.41
1:B:268:TRP:CG	1:B:269:TYR:H	2.38	0.41
1:D:83:SER:HA	1:D:136:SER:HB3	2.01	0.41
5:B:405:PG4:H11	5:B:405:PG4:H31	1.78	0.41
1:B:6:THR:O	1:B:306:ALA:HA	2.21	0.41
1:B:301:TYR:OH	1:B:324:LYS:NZ	2.52	0.41
1:C:296:PHE:CG	1:C:386:THR:HG21	2.56	0.41
1:D:138:GLN:HE21	1:D:150:TRP:NE1	2.14	0.41
1:D:268:TRP:CG	1:D:269:TYR:H	2.39	0.41
1:A:125:MET:HB2	1:A:132:LEU:HD22	2.03	0.40
1:D:24:HIS:HA	1:D:25:PRO:HD3	1.92	0.40
1:D:373:ASN:HD22	1:D:373:ASN:N	2.19	0.40
1:D:216:PHE:O	1:D:220:GLY:N	2.52	0.40
1:B:138:GLN:HG2	1:B:150:TRP:CD1	2.57	0.40
1:D:36:ARG:HD3	1:D:69:THR:HA	2.02	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	387/401 (96%)	370 (96%)	15 (4%)	2 (0%)	24	26
1	B	389/401 (97%)	377 (97%)	11 (3%)	1 (0%)	36	41
1	C	392/401 (98%)	381 (97%)	10 (3%)	1 (0%)	36	41
1	D	360/401 (90%)	338 (94%)	20 (6%)	2 (1%)	21	22
All	All	1528/1604 (95%)	1466 (96%)	56 (4%)	6 (0%)	30	32

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	268	TRP
1	D	268	TRP
1	C	268	TRP
1	D	64	TYR
1	A	147	TRP
1	A	268	TRP

### 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	329/341 (96%)	323 (98%)	6 (2%)	51	64
1	B	332/341 (97%)	323 (97%)	9 (3%)	39	51
1	C	334/341 (98%)	323 (97%)	11 (3%)	33	43
1	D	313/341 (92%)	296 (95%)	17 (5%)	20	24
All	All	1308/1364 (96%)	1265 (97%)	43 (3%)	34	43

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	132	LEU
1	A	230	VAL
1	A	343	LEU
1	A	362	LEU
1	A	384	VAL
1	B	58	GLU
1	B	178	TYR
1	B	187	LEU
1	B	230	VAL
1	B	251	GLN
1	B	323	ASN
1	B	335	THR
1	B	337	VAL

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Mol	Chain	Res	Type
1	B	368	LEU
1	C	74	VAL
1	C	178	TYR
1	C	209	SER
1	C	210	GLN
1	C	230	VAL
1	C	332	LYS
1	C	337	VAL
1	C	350	ASN
1	C	363[A]	GLN
1	C	363[B]	GLN
1	C	382	GLN
1	D	13	LYS
1	D	17	ARG
1	D	52	LEU
1	D	54	ILE
1	D	55	HIS
1	D	56	VAL
1	D	93	GLU
1	D	126	LYS
1	D	153	GLN
1	D	157	ARG
1	D	187	LEU
1	D	215	LEU
1	D	217	LYS
1	D	230	VAL
1	D	257	MET
1	D	350	ASN
1	D	373	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	128	ASN
1	A	153	GLN
1	A	309	ASN
1	A	339	GLN
1	B	86	ASN
1	B	131	ASN
1	B	251	GLN
1	B	255	ASN

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Mol	Chain	Res	Type
1	B	311	ASN
1	B	339	GLN
1	C	23	ASN
1	C	210	GLN
1	C	334	ASN
1	C	338	ASN
1	C	344	GLN
1	D	24	HIS
1	D	46	GLN
1	D	127	ASN
1	D	138	GLN
1	D	167	ASN
1	D	181	ASN
1	D	195	ASN
1	D	238	ASN
1	D	251	GLN
1	D	255	ASN
1	D	292	HIS
1	D	339	GLN
1	D	363	GLN
1	D	373	ASN
1	D	382	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

7 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
3	DHI	A	403	-	10,11,11	1.23	2 (20%)	10,14,14	1.35	1 (10%)
2	GCU	A	402	-	13,13,13	0.71	0	18,19,19	2.05	2 (11%)
3	DHI	B	404	-	10,11,11	1.21	1 (10%)	10,14,14	1.26	1 (10%)
5	PG4	B	405	-	12,12,12	0.49	0	11,11,11	0.37	0
4	BDP	B	402	-	13,13,13	0.68	0	18,19,19	1.12	0
2	GCU	B	403	-	13,13,13	0.85	0	18,19,19	2.00	3 (16%)
5	PG4	C	402	-	9,9,12	0.46	0	8,8,11	0.37	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
3	DHI	A	403	-	-	5/8/8/8	0/1/1/1
2	GCU	A	402	-	-	0/4/24/24	0/1/1/1
3	DHI	B	404	-	-	6/8/8/8	0/1/1/1
5	PG4	B	405	-	-	7/10/10/10	-
4	BDP	B	402	-	-	0/4/24/24	0/1/1/1
2	GCU	B	403	-	-	0/4/24/24	0/1/1/1
5	PG4	C	402	-	-	3/7/7/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	403	DHI	OXT-C	-2.25	1.23	1.30
3	B	404	DHI	OXT-C	-2.15	1.23	1.30
3	A	403	DHI	CG-ND1	-2.01	1.33	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	402	GCU	C1-O5-C5	6.97	122.47	112.22
2	B	403	GCU	C1-O5-C5	6.01	121.07	112.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	403	GCU	O5-C1-C2	4.28	117.83	110.30
2	A	402	GCU	O5-C1-C2	3.10	115.75	110.30
3	A	403	DHI	OXT-C-O	-2.87	117.58	124.08
3	B	404	DHI	OXT-C-O	-2.74	117.87	124.08
2	B	403	GCU	O5-C5-C4	2.54	114.50	109.48

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	403	DHI	O-C-CA-N
3	A	403	DHI	N-CA-CB-CG
5	B	405	PG4	O1-C1-C2-O2
5	B	405	PG4	C1-C2-O2-C3
5	B	405	PG4	O2-C3-C4-O3
3	A	403	DHI	OXT-C-CA-N
5	C	402	PG4	O3-C5-C6-O4
5	B	405	PG4	O4-C7-C8-O5
3	B	404	DHI	CA-CB-CG-CD2
3	B	404	DHI	CA-CB-CG-ND1
3	B	404	DHI	O-C-CA-N
5	C	402	PG4	O2-C3-C4-O3
5	B	405	PG4	C8-C7-O4-C6
5	C	402	PG4	C6-C5-O3-C4
5	B	405	PG4	C3-C4-O3-C5
3	B	404	DHI	N-CA-CB-CG
3	B	404	DHI	C-CA-CB-CG
3	A	403	DHI	O-C-CA-CB
3	B	404	DHI	OXT-C-CA-N
3	A	403	DHI	OXT-C-CA-CB
5	B	405	PG4	O3-C5-C6-O4

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	403	DHI	2	0
5	B	405	PG4	6	0
2	B	403	GCU	1	0
5	C	402	PG4	1	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	389/401 (97%)	-0.02	3 (0%) 82 85	20, 36, 54, 72	0
1	B	390/401 (97%)	-0.33	1 (0%) 90 91	12, 27, 42, 50	1 (0%)
1	C	390/401 (97%)	-0.11	3 (0%) 82 85	14, 31, 49, 57	4 (1%)
1	D	368/401 (91%)	1.54	104 (28%) 1 1	31, 60, 86, 115	366 (99%)
All	All	1537/1604 (95%)	0.25	111 (7%) 21 25	12, 36, 74, 115	371 (24%)

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	179	LEU	4.7
1	D	221	ALA	4.2
1	D	192	ALA	4.1
1	D	64	TYR	4.1
1	D	11	ALA	4.0
1	D	15	VAL	3.8
1	D	185	PRO	3.8
1	D	26	ALA	3.7
1	D	212	PRO	3.6
1	D	89	SER	3.6
1	D	43	GLY	3.6
1	D	60	ARG	3.6
1	D	95	PHE	3.5
1	D	178	TYR	3.5
1	D	213	TYR	3.5
1	D	88	PRO	3.5
1	D	112	ALA	3.5
1	D	156	LEU	3.3
1	D	127	ASN	3.3
1	D	368	LEU	3.3
1	D	94	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	113	ALA	3.2
1	D	190	PRO	3.2
1	D	186	ILE	3.2
1	D	211	PHE	3.1
1	D	369	THR	3.1
1	D	92	VAL	3.1
1	C	363[A]	GLN	3.0
1	B	392	LEU	2.9
1	D	165	SER	2.9
1	D	126	LYS	2.8
1	D	164	GLY	2.8
1	D	351	VAL	2.8
1	D	370	VAL	2.8
1	D	40	PHE	2.8
1	D	9	VAL	2.8
1	D	157	ARG	2.8
1	D	133	TYR	2.8
1	D	124	PHE	2.7
1	D	170	VAL	2.7
1	D	352	SER	2.7
1	D	182	LEU	2.7
1	D	131	ASN	2.7
1	D	222	GLY	2.7
1	D	183	SER	2.6
1	D	132	LEU	2.6
1	D	80	VAL	2.6
1	D	122	VAL	2.6
1	D	10	SER	2.6
1	D	376	TRP	2.6
1	D	189	ASP	2.6
1	D	205	GLY	2.6
1	D	130	VAL	2.6
1	D	168	ALA	2.5
1	D	196	MET	2.5
1	D	244	PRO	2.5
1	D	209	SER	2.5
1	D	312	ALA	2.5
1	D	145	HIS	2.5
1	D	97	ARG	2.5
1	D	41	GLY	2.5
1	D	187	LEU	2.4
1	D	34	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	194	ALA	2.4
1	D	350	ASN	2.4
1	A	145	HIS	2.4
1	D	87	PRO	2.4
1	D	208	VAL	2.3
1	D	337	VAL	2.3
1	D	129	GLY	2.3
1	C	238	ASN	2.3
1	D	30	ASP	2.3
1	D	61	ASN	2.3
1	D	372	GLY	2.3
1	D	76	HIS	2.3
1	D	16	ILE	2.3
1	D	155	ILE	2.3
1	D	323	ASN	2.2
1	D	334	ASN	2.2
1	D	152	PRO	2.2
1	D	335	THR	2.2
1	D	262	PHE	2.2
1	D	364	PRO	2.2
1	D	77	GLY	2.2
1	D	6	THR	2.2
1	D	166	ILE	2.2
1	A	58	GLU	2.2
1	D	201	THR	2.2
1	D	307	THR	2.2
1	D	52	LEU	2.2
1	D	4	ASP	2.2
1	D	171	ILE	2.1
1	D	45	ASN	2.1
1	D	161	GLU	2.1
1	D	216	PHE	2.1
1	D	336	GLY	2.1
1	D	114	TYR	2.1
1	D	65	LYS	2.1
1	D	193	LEU	2.1
1	D	203	LEU	2.1
1	A	2	ALA	2.1
1	D	217	LYS	2.1
1	C	146	GLU	2.1
1	D	111	TYR	2.1
1	D	224	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	135	ILE	2.1
1	D	5	VAL	2.1
1	D	56	VAL	2.1
1	D	28	ALA	2.0
1	D	195	ASN	2.0
1	D	75	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides 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<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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	DHI	A	403	11/11	0.73	0.21	88,89,89,89	0
3	DHI	B	404	11/11	0.79	0.19	75,76,77,77	0
2	GCU	B	403	13/13	0.81	0.12	50,54,54,55	0
4	BDP	B	402	13/13	0.84	0.12	58,61,63,64	0
5	PG4	B	405	13/13	0.92	0.08	34,37,46,47	0
2	GCU	A	402	13/13	0.93	0.07	44,47,48,48	0
5	PG4	C	402	10/13	0.95	0.08	36,37,40,41	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.