



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:01 AM GMT

PDB ID : 3KL5  
Title : Structure Analysis of a Xylanase From Glycosyl Hydrolase Family Thirty: Carbohydrate Ligand Complexes Reveal this Family of Enzymes Unique Mechanism of Substrate Specificity and Recognition  
Authors : St John, F.J.; Hurlbert, J.C.; Pozharski, E.  
Deposited on : 2009-11-06  
Resolution : 2.59 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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

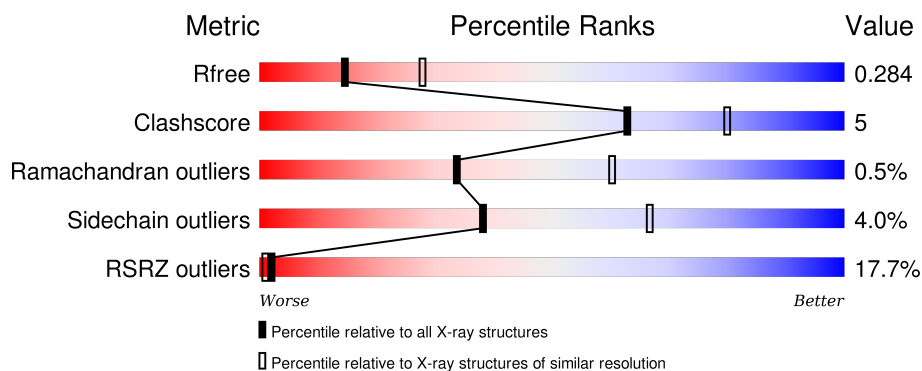
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.59 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))
$R_{free}$	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	401	<div> <div>6%</div> <div>85% 12% .</div> </div>
1	B	401	<div> <div>3%</div> <div>86% 10% ..</div> </div>
1	C	401	<div> <div>2%</div> <div>84% 13% .</div> </div>
1	D	401	<div> <div>56%</div> <div>70% 20% . 8%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	XYP	A	404	-	-	-	X
2	XYP	B	404	-	-	-	X
2	XYP	C	403	-	-	-	X
2	XYP	C	404	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12477 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	1	0
			3109	1966	552	582	9			
1	B	390	Total	C	N	O	S	0	3	0
			3136	1984	557	586	9			
1	C	389	Total	C	N	O	S	0	1	0
			3110	1967	552	582	9			
1	D	367	Total	C	N	O	S	0	0	0
			2948	1878	516	545	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 a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total C O 32 17 15	0	0
2	B	3	Total C O 32 17 15	0	0
2	B	3	Total C O 31 17 14	0	0
2	C	3	Total C O 32 17 15	0	0

- Molecule 3 is water.

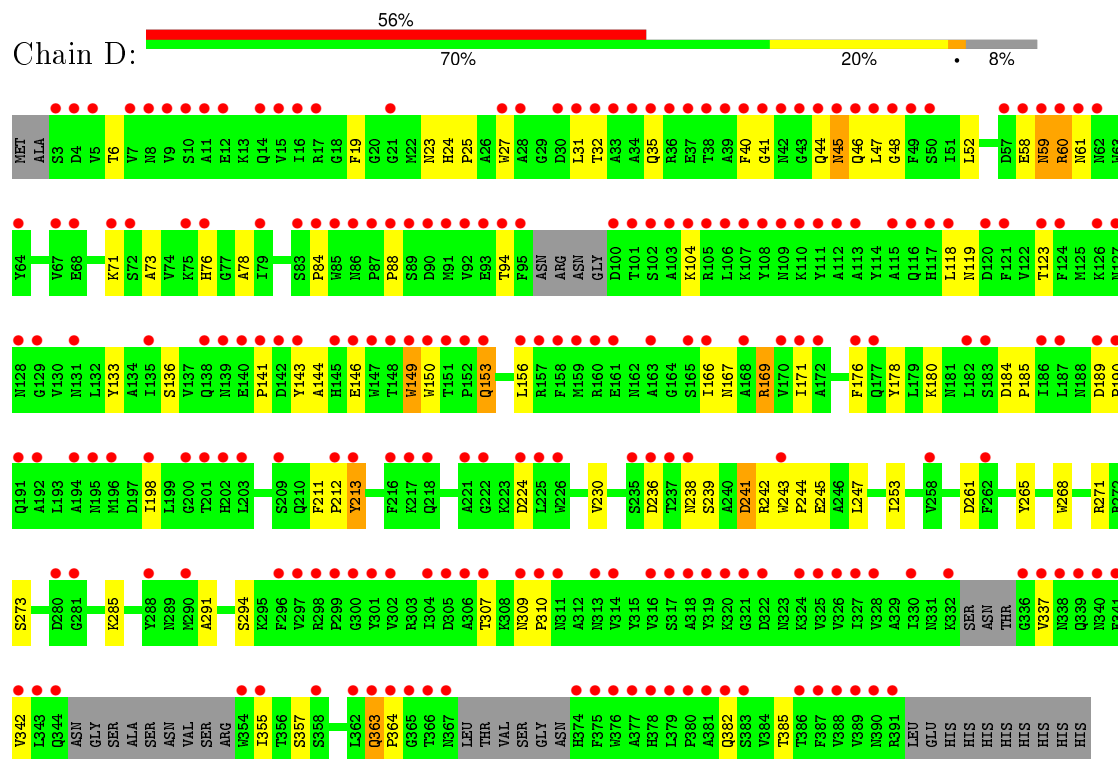
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	10	Total O 10 10	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	17	Total 17	O 17	0	0
3	C	19	Total 19	O 19	0	0
3	D	1	Total 1	O 1	0	0







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	137.72Å 194.01Å 65.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.59 44.67 – 2.59	Depositor EDS
% Data completeness (in resolution range)	97.5 (50.00-2.59) 97.6 (44.67-2.59)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.32 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.241 , 0.290 0.237 , 0.284	Depositor DCC
$R_{free}$ test set	2775 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	65.9	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 43.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 54601 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12477	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: XYP, GCV

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	0.59	0/3196	0.63	4/4353 (0.1%)
1	B	0.58	0/3224	0.70	5/4390 (0.1%)
1	C	0.59	2/3197 (0.1%)	0.70	5/4354 (0.1%)
1	D	0.43	0/3031	0.51	0/4123
All	All	0.55	2/12648 (0.0%)	0.64	14/17220 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	162	ASN	CG-OD1	-5.33	1.12	1.24
1	C	162	ASN	CG-ND2	-5.22	1.19	1.32

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	169	ARG	NE-CZ-NH1	-14.19	113.21	120.30
1	C	60	ARG	NE-CZ-NH2	12.89	126.75	120.30
1	C	60	ARG	NE-CZ-NH1	-12.73	113.93	120.30
1	B	169	ARG	NE-CZ-NH2	12.08	126.34	120.30
1	C	169	ARG	NE-CZ-NH2	-8.86	115.87	120.30
1	A	169	ARG	NE-CZ-NH2	-7.55	116.52	120.30
1	A	60	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	A	60	ARG	NE-CZ-NH2	-7.11	116.74	120.30
1	A	169	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	C	169	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	B	169	ARG	CD-NE-CZ	6.56	132.79	123.60
1	B	60	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	C	60	ARG	CD-NE-CZ	5.96	131.94	123.60
1	B	60	ARG	NE-CZ-NH1	5.95	123.28	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	3109	0	2963	25	0
1	B	3136	0	2993	26	0
1	C	3110	0	2965	34	0
1	D	2948	0	2810	56	0
2	A	32	0	25	2	0
2	B	63	0	48	3	0
2	C	32	0	25	1	0
3	A	10	0	0	2	0
3	B	17	0	0	0	0
3	C	19	0	0	4	0
3	D	1	0	0	0	0
All	All	12477	0	11829	128	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 5.

All (128) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:HIS:HD2	3:C:411:HOH:O	1.57	0.87
1:B:244[B]:PRO:O	1:B:245[B]:GLU:HB2	1.76	0.82
1:B:244[B]:PRO:O	1:B:245[B]:GLU:CB	2.30	0.76
1:D:144:ALA:HB3	1:D:149:TRP:HD1	1.53	0.74
1:B:315:TYR:OH	1:C:222:GLY:HA2	1.86	0.74
1:B:229:GLU:OE2	2:B:404:XYP:H1B	1.91	0.71
1:C:238:ASN:OD1	1:D:27:TRP:HA	1.92	0.69
1:B:353[A]:ARG:HD2	1:B:355:ILE:HD11	1.75	0.68
1:D:141:PRO:HB3	1:D:150:TRP:HB2	1.76	0.68
1:C:145:HIS:ND1	1:C:149:TRP:HZ2	1.93	0.67
1:D:144:ALA:HB3	1:D:149:TRP:CD1	2.30	0.67
1:B:353[A]:ARG:HH21	1:B:368:LEU:HD21	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:HIS:CG	1:D:27:TRP:HB2	2.31	0.65
1:D:24:HIS:CE1	1:D:27:TRP:CD1	2.85	0.65
1:D:156:LEU:HD13	1:D:185:PRO:O	1.97	0.65
1:D:59:ASN:HB2	1:D:88:PRO:HB3	1.79	0.65
1:A:141:PRO:HG2	1:A:182:LEU:HD21	1.80	0.61
1:D:23:ASN:HB3	1:D:52:LEU:HD11	1.83	0.60
1:A:42:ASN:ND2	1:B:98:ASN:OD1	2.34	0.60
1:D:243:TRP:CE2	1:D:247:LEU:HD11	2.38	0.59
1:A:324:LYS:HE3	1:B:100:ASP:HB2	1.84	0.58
1:D:239:SER:HB3	1:D:242:ARG:HH11	1.69	0.58
1:C:145:HIS:ND1	1:C:149:TRP:CZ2	2.72	0.58
1:C:25:PRO:HB3	1:C:30:ASP:HB2	1.87	0.57
1:B:25:PRO:HB3	1:B:30:ASP:HB2	1.87	0.57
1:A:25:PRO:HB3	1:A:30:ASP:HB2	1.87	0.56
1:A:353:ARG:HD2	1:A:355:ILE:HD11	1.86	0.56
1:B:141:PRO:HG2	1:B:182:LEU:HD21	1.87	0.56
1:D:198:ILE:HG12	1:D:224:ASP:HB2	1.86	0.56
1:C:141:PRO:HG2	1:C:182:LEU:HD21	1.86	0.56
1:D:241:ASP:HA	1:D:285:LYS:HB2	1.86	0.56
2:A:402:GCV:O2	2:A:404:XYP:H5B1	2.06	0.56
1:D:143:TYR:HB2	1:D:176:PHE:CD2	2.41	0.56
1:D:144:ALA:C	1:D:146:GLU:H	2.09	0.55
1:C:218:GLN:HG3	3:C:417:HOH:O	2.07	0.54
1:D:355:ILE:HG12	1:D:385:THR:HG23	1.90	0.53
1:C:6:THR:O	1:C:306:ALA:HA	2.10	0.52
1:C:254:HIS:CD2	3:C:411:HOH:O	2.43	0.52
1:D:44:GLN:O	1:D:45:ASN:CB	2.58	0.52
1:C:238:ASN:OD1	1:D:27:TRP:CG	2.64	0.51
1:D:244:PRO:HB3	1:D:382:GLN:CG	2.41	0.51
1:B:353[A]:ARG:O	1:B:353[A]:ARG:HG3	2.09	0.51
1:C:310:PRO:O	1:C:311:ASN:ND2	2.41	0.51
1:D:236:ASP:HB2	1:D:239:SER:HB3	1.92	0.50
1:A:285:LYS:NZ	1:A:357:SER:O	2.42	0.50
1:D:180:LYS:HD2	1:D:213:TYR:CE1	2.47	0.50
1:B:315:TYR:CZ	1:C:222:GLY:HA2	2.46	0.50
1:A:138:GLN:HG2	1:A:150:TRP:CD1	2.47	0.50
1:D:40:PHE:HZ	1:D:52:LEU:HD13	1.77	0.50
1:C:5:VAL:HG22	1:C:310:PRO:HG3	1.94	0.49
1:D:94:THR:HG22	1:D:104:LYS:HG2	1.94	0.49
1:D:31:LEU:HA	1:D:271:ARG:HH22	1.77	0.49
1:D:244:PRO:HB3	1:D:382:GLN:HG3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:THR:HB	1:C:168:ALA:HA	1.94	0.49
1:A:167[B]:ASN:CG	1:A:167[B]:ASN:O	2.51	0.49
1:B:138:GLN:HG2	1:B:150:TRP:CD1	2.47	0.49
1:B:140:GLU:OE2	2:B:404:XYP:O4A	2.31	0.49
1:D:291:ALA:HA	1:D:294:SER:HB3	1.94	0.49
1:D:238:ASN:H	1:D:273:SER:HB2	1.78	0.49
1:D:153:GLN:H	1:D:153:GLN:HE21	1.60	0.48
1:A:165:SER:HA	1:C:309:ASN:O	2.12	0.48
1:D:32:THR:OG1	1:D:35:GLN:HB2	2.14	0.48
1:D:84:PRO:HG3	1:D:118:LEU:HD21	1.96	0.48
1:A:243:TRP:CH2	1:A:247:LEU:HD13	2.49	0.47
1:D:184:ASP:N	1:D:185:PRO:CD	2.77	0.47
1:A:161:GLU:O	1:C:312:ALA:HA	2.14	0.47
1:B:22:MET:HG3	1:B:23:ASN:N	2.28	0.47
1:A:3:SER:N	1:A:311:ASN:HD21	2.13	0.47
1:A:229:GLU:OE2	2:A:404:XYP:H1B	2.15	0.47
1:C:119:ASN:ND2	1:C:166:ILE:HA	2.30	0.47
1:D:60:ARG:N	1:D:60:ARG:HD2	2.30	0.47
1:B:207:GLN:HG2	1:C:218:GLN:HA	1.96	0.46
1:C:138:GLN:HG2	1:C:150:TRP:CD1	2.51	0.46
1:C:238:ASN:CG	1:D:27:TRP:CD1	2.88	0.46
1:C:119:ASN:ND2	1:C:165:SER:O	2.43	0.46
1:B:24:HIS:CE1	1:B:26:ALA:HB3	2.50	0.46
1:A:35:GLN:HA	3:A:405:HOH:O	2.15	0.46
1:B:54:ILE:O	1:B:82:ALA:HA	2.16	0.46
1:D:119:ASN:HD21	1:D:166:ILE:HA	1.81	0.46
1:C:231:TYR:OH	2:C:404:XYP:H5B2	2.16	0.46
1:D:239:SER:CB	1:D:242:ARG:HH11	2.29	0.46
1:C:42:ASN:OD1	1:C:295:LYS:HG2	2.16	0.46
1:B:32:THR:O	1:B:36:ARG:HG3	2.16	0.46
1:B:6:THR:O	1:B:306:ALA:HA	2.15	0.46
1:C:5:VAL:CG2	1:C:310:PRO:HG3	2.46	0.45
1:D:19:PHE:CD1	1:D:265:TYR:HB3	2.52	0.45
1:D:243:TRP:CZ2	1:D:357:SER:HA	2.52	0.45
1:D:144:ALA:C	1:D:146:GLU:N	2.70	0.45
1:C:238:ASN:OD1	1:D:27:TRP:CD1	2.70	0.45
1:B:251:GLN:OE1	1:C:222:GLY:HA3	2.17	0.44
1:D:253:ILE:HG12	1:D:265:TYR:CE2	2.53	0.44
1:A:165:SER:HB3	3:A:409:HOH:O	2.17	0.44
1:D:363:GLN:HA	1:D:364:PRO:HD3	1.88	0.44
1:C:24:HIS:CE1	1:C:26:ALA:HB3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:TYR:O	1:D:169:ARG:HD3	2.17	0.44
1:D:41:GLY:O	1:D:48:GLY:N	2.51	0.44
1:C:27:TRP:CD1	1:D:238:ASN:HB2	2.53	0.44
1:D:31:LEU:HA	1:D:271:ARG:NH2	2.33	0.43
1:A:24:HIS:CE1	1:A:26:ALA:HB3	2.53	0.43
2:B:402:GCV:O2	2:B:404:XYP:H5B1	2.18	0.43
1:A:22:MET:HG3	1:A:23:ASN:N	2.33	0.43
1:A:6:THR:O	1:A:306:ALA:HA	2.18	0.43
1:C:53:ARG:HD2	1:C:81:PHE:CZ	2.53	0.43
1:D:141:PRO:CB	1:D:150:TRP:HB2	2.47	0.43
1:A:268:TRP:O	1:A:269:TYR:C	2.57	0.43
1:A:20:GLY:HA2	1:A:49:PHE:CG	2.54	0.43
1:A:5:VAL:HG22	1:A:310:PRO:HG3	2.01	0.43
1:D:24:HIS:HA	1:D:25:PRO:HD3	1.86	0.43
1:D:47:LEU:HD23	1:D:291:ALA:HB2	1.99	0.43
1:A:232:TYR:CG	1:A:233:PRO:HA	2.54	0.42
1:C:22:MET:HG3	1:C:23:ASN:N	2.33	0.42
1:D:61:ASN:H	1:D:61:ASN:HD22	1.67	0.42
1:C:143:TYR:HB2	1:C:176:PHE:CD2	2.55	0.42
1:B:313:ASN:OD1	1:C:197:ASP:HB3	2.19	0.41
1:D:243:TRP:CZ2	1:D:247:LEU:HD11	2.54	0.41
1:D:189:ASP:HA	1:D:190:PRO:HD3	1.81	0.41
1:B:335:THR:HG21	3:C:422:HOH:O	2.20	0.41
1:A:363:GLN:HA	1:A:364:PRO:HD3	1.97	0.41
1:D:211:PHE:N	1:D:212:PRO:HD2	2.34	0.41
1:B:240:ALA:HB1	1:B:284:SER:HB2	2.02	0.41
1:B:319:TYR:CD2	1:B:319:TYR:N	2.89	0.41
1:A:319:TYR:N	1:A:319:TYR:CD2	2.88	0.41
1:D:73:ALA:O	1:D:78:ALA:HB3	2.21	0.41
1:D:136:SER:HA	1:D:171:ILE:HB	2.03	0.41
1:A:240:ALA:HB1	1:A:284:SER:HB2	2.04	0.40
1:C:363:GLN:HA	1:C:364:PRO:HD3	1.98	0.40
1:D:6:THR:HA	1:D:342:VAL:HG22	2.03	0.40
1:D:84:PRO:HD2	1:D:136:SER:HB3	2.04	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	388/401 (97%)	373 (96%)	15 (4%)	0	100	100
1	B	391/401 (98%)	373 (95%)	15 (4%)	3 (1%)	24	46
1	C	388/401 (97%)	373 (96%)	14 (4%)	1 (0%)	46	72
1	D	357/401 (89%)	316 (88%)	36 (10%)	5 (1%)	14	28
All	All	1524/1604 (95%)	1435 (94%)	80 (5%)	9 (1%)	34	56

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	268	TRP
1	B	245[A]	GLU
1	B	245[B]	GLU
1	B	4	ASP
1	D	58	GLU
1	D	59	ASN
1	D	310	PRO
1	C	268	TRP
1	D	45	ASN

### 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	331/341 (97%)	321 (97%)	10 (3%)	48	76
1	B	334/341 (98%)	321 (96%)	13 (4%)	39	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	331/341 (97%)	320 (97%)	11 (3%)	45	73
1	D	312/341 (92%)	293 (94%)	19 (6%)	23	46
All	All	1308/1364 (96%)	1255 (96%)	53 (4%)	38	66

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	GLU
1	A	60	ARG
1	A	178	TYR
1	A	209	SER
1	A	213	TYR
1	A	230	VAL
1	A	324	LYS
1	A	335	THR
1	A	337	VAL
1	A	369	THR
1	B	58	GLU
1	B	60	ARG
1	B	178	TYR
1	B	209	SER
1	B	230	VAL
1	B	251	GLN
1	B	324	LYS
1	B	335	THR
1	B	337	VAL
1	B	353[A]	ARG
1	B	353[B]	ARG
1	B	369	THR
1	B	392	LEU
1	C	58	GLU
1	C	60	ARG
1	C	89	SER
1	C	178	TYR
1	C	209	SER
1	C	213	TYR
1	C	230	VAL
1	C	324	LYS
1	C	335	THR
1	C	337	VAL
1	C	369	THR

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Mol	Chain	Res	Type
1	D	46	GLN
1	D	60	ARG
1	D	71	LYS
1	D	76	HIS
1	D	123	THR
1	D	149	TRP
1	D	153	GLN
1	D	167	ASN
1	D	169	ARG
1	D	178	TYR
1	D	213	TYR
1	D	230	VAL
1	D	241	ASP
1	D	245	GLU
1	D	261	ASP
1	D	307	THR
1	D	309	ASN
1	D	337	VAL
1	D	363	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	345	ASN
1	C	162	ASN
1	C	345	ASN
1	D	24	HIS
1	D	61	ASN
1	D	76	HIS
1	D	145	HIS
1	D	153	GLN
1	D	309	ASN
1	D	313	ASN
1	D	339	GLN
1	D	363	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

12 carbohydrates 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	GCV	A	402	2	11,14,14	1.63	1 (9%)	14,20,20	1.14	1 (7%)
2	XYP	A	403	2	9,9,10	1.84	4 (44%)	10,12,14	1.40	2 (20%)
2	XYP	A	404	2	9,9,10	1.16	1 (11%)	11,12,14	0.89	1 (9%)
2	GCV	B	402	2	11,14,14	0.81	0	14,20,20	0.88	0
2	XYP	B	403	2	9,9,10	1.05	0	10,12,14	1.32	2 (20%)
2	XYP	B	404	2	9,9,10	1.32	2 (22%)	11,12,14	1.58	5 (45%)
2	GCV	B	405	2	11,14,14	1.76	2 (18%)	14,20,20	1.30	2 (14%)
2	XYP	B	406	2	9,9,10	2.44	4 (44%)	10,12,14	1.22	2 (20%)
2	XYP	B	407	2	8,8,10	1.25	0	9,10,14	2.08	2 (22%)
2	GCV	C	402	2	11,14,14	1.76	3 (27%)	14,20,20	2.49	4 (28%)
2	XYP	C	403	2	9,9,10	2.46	4 (44%)	10,12,14	2.08	2 (20%)
2	XYP	C	404	2	9,9,10	1.81	2 (22%)	11,12,14	1.75	1 (9%)

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	GCV	A	402	2	-	0/2/26/26	0/1/1/1
2	XYP	A	403	2	-	0/0/13/17	0/1/1/1
2	XYP	A	404	2	-	0/0/14/17	0/1/1/1
2	GCV	B	402	2	-	0/2/26/26	0/1/1/1
2	XYP	B	403	2	-	0/0/13/17	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	XYP	B	404	2	-	0/0/14/17	0/1/1/1
2	GCV	B	405	2	-	0/2/26/26	0/1/1/1
2	XYP	B	406	2	-	0/0/13/17	0/1/1/1
2	XYP	B	407	2	-	0/0/11/17	0/1/1/1
2	GCV	C	402	2	-	0/2/26/26	0/1/1/1
2	XYP	C	403	2	-	0/0/13/17	0/1/1/1
2	XYP	C	404	2	-	0/0/14/17	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	403	XYP	C4B-C3B	2.06	1.55	1.52
2	A	403	XYP	O5B-C5B	2.07	1.47	1.43
2	C	402	GCV	O1-C1	2.10	1.46	1.39
2	B	404	XYP	O5B-C1B	2.23	1.46	1.43
2	B	406	XYP	O5B-C5B	2.38	1.47	1.43
2	A	403	XYP	C4B-C3B	2.42	1.55	1.52
2	A	404	XYP	C4B-C3B	2.44	1.55	1.52
2	A	403	XYP	C2B-C3B	2.63	1.57	1.52
2	A	403	XYP	O5B-C1B	2.75	1.47	1.41
2	C	404	XYP	O5B-C1B	2.81	1.47	1.43
2	B	404	XYP	C4B-C3B	2.90	1.56	1.52
2	B	405	GCV	O5-C5	2.98	1.48	1.43
2	C	402	GCV	O5-C5	3.14	1.48	1.43
2	B	406	XYP	C2B-C1B	3.19	1.58	1.51
2	C	403	XYP	O5B-C1B	3.21	1.48	1.41
2	C	403	XYP	C2B-C1B	3.23	1.58	1.51
2	C	402	GCV	O5-C1	3.33	1.49	1.43
2	A	402	GCV	O5-C5	3.43	1.48	1.43
2	B	405	GCV	C4-C5	3.53	1.59	1.52
2	C	404	XYP	C4B-C3B	3.57	1.57	1.52
2	B	406	XYP	O5B-C1B	3.88	1.50	1.41
2	B	406	XYP	O4A-C1B	4.03	1.48	1.39
2	C	403	XYP	O4A-C1B	4.66	1.49	1.39

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	403	XYP	C1B-C2B-C3B	-5.96	101.02	111.23
2	B	407	XYP	C5B-C4B-C3B	-5.03	103.50	110.33
2	B	405	GCV	O4-C4-C3	-3.19	102.87	110.21
2	B	403	XYP	O4A-C1B-C2B	-2.99	94.81	111.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	404	XYP	C1B-C2B-C3B	-2.77	106.31	110.43
2	A	403	XYP	O4A-C1B-C2B	-2.62	96.91	111.73
2	A	404	XYP	C5B-C4B-C3B	-2.38	107.10	110.33
2	B	404	XYP	O4A-C1B-C2B	-2.15	103.45	109.21
2	B	404	XYP	C4B-C3B-C2B	-2.15	109.02	111.39
2	C	403	XYP	O5B-C5B-C4B	2.03	114.15	110.86
2	A	402	GCV	O4-C4-C3	2.04	114.91	110.21
2	B	404	XYP	O2B-C2B-C3B	2.06	113.72	110.00
2	B	404	XYP	O4A-C1B-O5B	2.06	115.77	109.90
2	B	406	XYP	C1B-C2B-C3B	2.19	114.98	111.23
2	A	403	XYP	C1B-C2B-C3B	2.36	115.28	111.23
2	B	405	GCV	O5-C5-C4	2.47	114.55	109.44
2	B	403	XYP	C1B-C2B-C3B	2.48	115.48	111.23
2	B	406	XYP	C5B-O5B-C1B	2.59	117.85	113.36
2	C	402	GCV	C1-C2-C3	2.67	114.41	110.43
2	C	402	GCV	O5-C5-C4	2.99	115.63	109.44
2	B	407	XYP	C5B-O5B-C1B	3.31	115.09	109.95
2	C	402	GCV	C1-O5-C5	4.94	119.49	112.22
2	C	404	XYP	O5B-C5B-C4B	4.96	118.54	110.76
2	C	402	GCV	O5-C1-C2	6.25	119.77	109.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	402	GCV	1	0
2	A	404	XYP	2	0
2	B	402	GCV	1	0
2	B	404	XYP	3	0
2	C	404	XYP	1	0

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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%)	0.48	26 (6%)	21 15	42, 58, 72, 80	0
1	B	390/401 (97%)	0.49	11 (2%)	56 49	42, 58, 73, 79	1 (0%)
1	C	389/401 (97%)	0.57	10 (2%)	59 53	42, 58, 72, 79	0
1	D	367/401 (91%)	2.89	224 (61%)	0 0	74, 120, 155, 179	364 (99%)
All	All	1535/1604 (95%)	1.08	271 (17%)	2 1	42, 62, 140, 179	365 (23%)

All (271) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	102	SER	10.5
1	D	343	LEU	10.1
1	D	103	ALA	9.7
1	D	100	ASP	9.4
1	D	319	TYR	8.2
1	D	337	VAL	8.1
1	D	11	ALA	8.1
1	D	306	ALA	7.9
1	D	387	PHE	7.8
1	D	302	VAL	7.7
1	D	38	THR	7.7
1	D	101	THR	7.6
1	D	183	SER	7.5
1	D	95	PHE	7.3
1	D	17	ARG	7.2
1	D	389	VAL	7.1
1	D	307	THR	7.1
1	D	8	ASN	7.1
1	D	355	ILE	6.9
1	D	108	TYR	6.9
1	D	192	ALA	6.8

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Mol	Chain	Res	Type	RSRZ
1	A	345	ASN	6.7
1	D	112	ALA	6.6
1	D	304	ILE	6.6
1	D	363	GLN	6.6
1	D	280	ASP	6.3
1	D	354	TRP	6.2
1	D	33	ALA	6.2
1	D	149	TRP	6.0
1	D	388	VAL	6.0
1	D	366	THR	5.9
1	D	341	PHE	5.7
1	D	91	MET	5.7
1	D	27	TRP	5.6
1	D	325	VAL	5.6
1	D	106	LEU	5.6
1	D	7	VAL	5.5
1	D	68	GLU	5.5
1	D	9	VAL	5.5
1	D	61	ASN	5.5
1	D	157	ARG	5.4
1	D	143	TYR	5.4
1	D	148	THR	5.3
1	D	67	VAL	5.2
1	D	37	GLU	5.2
1	D	318	ALA	5.2
1	D	190	PRO	5.2
1	D	146	GLU	5.1
1	D	140	GLU	5.1
1	D	339	GLN	5.1
1	D	43	GLY	5.0
1	D	311	ASN	5.0
1	D	342	VAL	5.0
1	D	109	ASN	5.0
1	D	281	GLY	4.9
1	D	5	VAL	4.9
1	D	386	THR	4.8
1	D	10	SER	4.8
1	D	336	GLY	4.8
1	D	322	ASP	4.8
1	D	182	LEU	4.7
1	D	310	PRO	4.7
1	D	4	ASP	4.7

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Mol	Chain	Res	Type	RSRZ
1	D	135	ILE	4.7
1	D	375	PHE	4.7
1	A	104	LYS	4.7
1	D	376	TRP	4.7
1	D	94	THR	4.6
1	D	3	SER	4.6
1	D	105	ARG	4.6
1	D	83	SER	4.6
1	D	116	GLN	4.5
1	D	113	ALA	4.5
1	D	222	GLY	4.4
1	D	358	SER	4.4
1	D	32	THR	4.4
1	A	391	ARG	4.4
1	D	156	LEU	4.4
1	D	107	LYS	4.3
1	D	305	ASP	4.3
1	D	62	ASN	4.2
1	D	320	LYS	4.2
1	D	64	TYR	4.2
1	D	42	ASN	4.2
1	D	89	SER	4.2
1	A	95	PHE	4.2
1	D	203	LEU	4.2
1	D	298	ARG	4.1
1	D	364	PRO	4.1
1	D	59	ASN	4.1
1	D	141	PRO	4.1
1	D	124	PHE	4.1
1	D	380	PRO	4.1
1	D	128	ASN	4.1
1	D	115	ALA	4.1
1	D	221	ALA	4.1
1	D	104	LYS	4.0
1	D	47	LEU	4.0
1	D	142	ASP	4.0
1	D	159	MET	4.0
1	D	76	HIS	3.9
1	A	103	ALA	3.9
1	D	209	SER	3.9
1	D	391	ARG	3.9
1	D	362	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	145	HIS	3.9
1	D	120	ASP	3.9
1	D	36	ARG	3.9
1	D	147	TRP	3.8
1	D	297	VAL	3.8
1	D	338	ASN	3.8
1	D	326	VAL	3.7
1	D	153	GLN	3.7
1	D	131	ASN	3.7
1	D	212	PRO	3.7
1	D	30	ASP	3.6
1	D	145	HIS	3.6
1	D	85	TRP	3.6
1	D	163	ALA	3.6
1	A	101	THR	3.6
1	D	88	PRO	3.6
1	A	96	ASN	3.5
1	D	152	PRO	3.5
1	D	288	TYR	3.5
1	D	16	ILE	3.5
1	D	198	ILE	3.5
1	D	46	GLN	3.5
1	D	172	ALA	3.5
1	D	365	GLY	3.5
1	D	35	GLN	3.5
1	D	344	GLN	3.5
1	D	110	LYS	3.5
1	D	151	THR	3.5
1	D	177	GLN	3.5
1	A	143	TYR	3.4
1	A	274	TYR	3.4
1	D	390	ASN	3.4
1	D	84	PRO	3.4
1	D	290	MET	3.4
1	D	200	GLY	3.4
1	D	117	HIS	3.4
1	D	12	GLU	3.4
1	D	317	SER	3.4
1	D	150	TRP	3.4
1	D	44	GLN	3.3
1	D	330	ILE	3.3
1	D	28	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	176	PHE	3.3
1	D	15	VAL	3.3
1	D	171	ILE	3.2
1	D	60	ARG	3.2
1	D	296	PHE	3.2
1	A	344	GLN	3.2
1	D	138	GLN	3.2
1	B	193	LEU	3.2
1	D	41	GLY	3.2
1	D	186	ILE	3.2
1	A	99	GLY	3.2
1	D	31	LEU	3.1
1	A	144	ALA	3.1
1	D	111	TYR	3.1
1	D	196	MET	3.1
1	D	79	ILE	3.1
1	A	98	ASN	3.1
1	D	45	ASN	3.1
1	C	348	ALA	3.1
1	D	121	PHE	3.1
1	D	168	ALA	3.1
1	D	170	VAL	3.1
1	D	258	VAL	3.1
1	D	321	GLY	3.1
1	D	316	VAL	3.0
1	D	87	PRO	3.0
1	D	189	ASP	3.0
1	D	118	LEU	3.0
1	D	213	TYR	3.0
1	D	243	TRP	2.9
1	D	374	HIS	2.9
1	D	314	VAL	2.9
1	D	327	ILE	2.9
1	D	86	ASN	2.9
1	D	40	PHE	2.8
1	D	324	LYS	2.8
1	D	218	GLN	2.8
1	D	217	LYS	2.8
1	A	237	THR	2.8
1	D	166	ILE	2.8
1	D	216	PHE	2.7
1	D	332	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	201	THR	2.7
1	D	194	ALA	2.7
1	D	382	GLN	2.7
1	D	367	ASN	2.7
1	A	273	SER	2.7
1	D	160	ARG	2.7
1	A	373	ASN	2.7
1	D	93	GLU	2.7
1	D	49	PHE	2.7
1	D	328	VAL	2.7
1	A	149	TRP	2.7
1	A	348	ALA	2.7
1	A	102	SER	2.7
1	D	237	THR	2.6
1	D	224	ASP	2.6
1	D	34	ALA	2.6
1	B	218	GLN	2.6
1	A	106	LEU	2.5
1	A	157	ARG	2.5
1	C	373	ASN	2.5
1	D	57	ASP	2.5
1	B	3	SER	2.5
1	D	299	PRO	2.5
1	D	90	ASP	2.5
1	D	301	TYR	2.5
1	D	139	ASN	2.5
1	D	381	ALA	2.5
1	C	226	TRP	2.5
1	D	71	LYS	2.5
1	D	129	GLY	2.5
1	D	191	GLN	2.5
1	B	312	ALA	2.4
1	C	15	VAL	2.4
1	D	127	ASN	2.4
1	D	72	SER	2.4
1	D	187	LEU	2.4
1	D	377	ALA	2.3
1	D	313	ASN	2.3
1	D	48	GLY	2.3
1	C	124	PHE	2.3
1	D	50	SER	2.3
1	D	309	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	127	ASN	2.3
1	A	100	ASP	2.3
1	D	126	LYS	2.3
1	D	226	TRP	2.3
1	D	158	PHE	2.2
1	D	378	HIS	2.2
1	D	225	LEU	2.2
1	C	265	TYR	2.2
1	B	362	LEU	2.2
1	D	58	GLU	2.2
1	D	21	GLY	2.2
1	D	75	LYS	2.2
1	D	14	GLN	2.2
1	D	383	SER	2.2
1	D	236	ASP	2.2
1	D	300	GLY	2.1
1	C	345	ASN	2.1
1	C	22	MET	2.1
1	B	355	ILE	2.1
1	D	379	LEU	2.1
1	B	335	THR	2.1
1	C	99	GLY	2.1
1	A	358	SER	2.1
1	B	388	VAL	2.1
1	D	92	VAL	2.1
1	D	39	ALA	2.1
1	A	231	TYR	2.1
1	D	165	SER	2.1
1	D	340	ASN	2.1
1	B	356	THR	2.1
1	B	386	THR	2.1
1	D	235	SER	2.1
1	D	238	ASN	2.0
1	B	222	GLY	2.0
1	D	202	HIS	2.0
1	C	228	THR	2.0
1	D	123	THR	2.0
1	D	262	PHE	2.0
1	D	161	GLU	2.0
1	D	195	ASN	2.0

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

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

## 6.3 Carbohydrates ⓘ

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(Å <sup>2</sup> )	Q<0.9
2	XYP	C	404	9/10	0.44	0.38	9.60	118,118,118,119	0
2	XYP	C	403	9/10	0.46	0.43	5.44	115,116,117,118	0
2	XYP	A	404	9/10	0.89	0.31	2.82	92,94,94,95	0
2	XYP	B	404	9/10	0.82	0.21	2.01	81,82,83,83	0
2	GCV	C	402	14/14	0.82	0.28	1.40	112,114,115,116	0
2	GCV	A	402	14/14	0.88	0.28	0.87	91,94,95,95	0
2	GCV	B	402	14/14	0.94	0.16	0.06	73,76,78,79	0
2	GCV	B	405	14/14	0.86	0.17	-1.83	86,88,90,90	0
2	XYP	B	403	9/10	0.92	0.12	-2.08	77,78,78,80	0
2	XYP	A	403	9/10	0.80	0.29	-	92,93,94,95	0
2	XYP	B	407	8/10	0.91	0.19	-	91,92,92,93	0
2	XYP	B	406	9/10	0.78	0.17	-	88,90,91,91	0

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.