



wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 06:10 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 wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

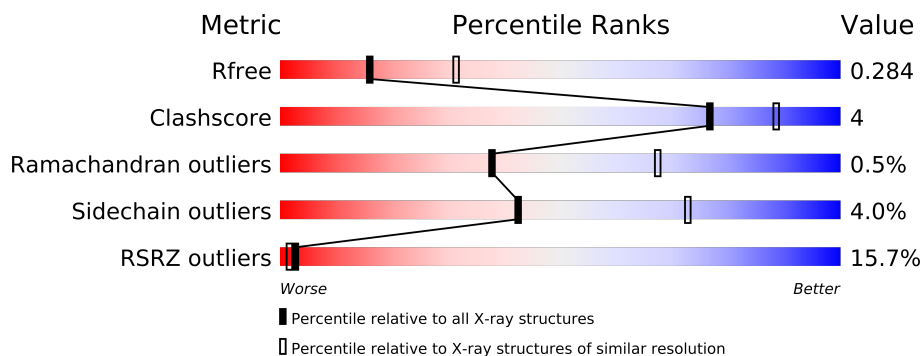
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	401	
1	B	401	
1	C	401	
1	D	401	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12477 atoms, of which 0 are hydrogen and 0 are deuterium.

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

Continued on next page...

Continued from previous page...

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	0	0
			32	17	15		
2	B	3	Total	C	O	0	0
			32	17	15		
2	B	3	Total	C	O	0	0
			31	17	14		
2	C	3	Total	C	O	0	0
			32	17	15		

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

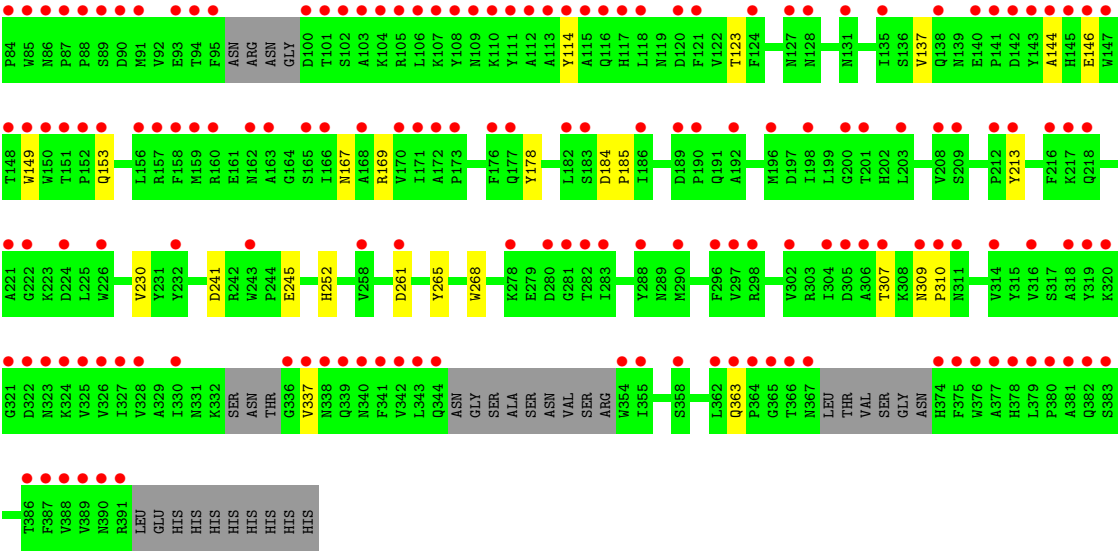
Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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
B	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
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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total 10	O 10	0	0
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, α , β , γ	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) 97.7 (44.67-2.59)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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	2778 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	65.9	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 35.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

The worst 5 of 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

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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	32	0
1	D	2948	0	0	10	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	9019	82	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

The worst 5 of 82 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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: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

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%)	27	53

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	388/401 (97%)	373 (96%)	14 (4%)	1 (0%)	50 77
1	D	357/401 (89%)	316 (88%)	36 (10%)	5 (1%)	16 32
All	All	1524/1604 (95%)	1435 (94%)	80 (5%)	9 (1%)	38 63

5 of 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

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%)	53 82
1	B	334/341 (98%)	321 (96%)	13 (4%)	43 74
1	C	331/341 (97%)	320 (97%)	11 (3%)	50 79
1	D	312/341 (92%)	293 (94%)	19 (6%)	26 50
All	All	1308/1364 (96%)	1255 (96%)	53 (4%)	42 72

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	58	GLU
1	C	230	VAL
1	D	261	ASP
1	C	60	ARG
1	C	178	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	345	ASN
1	C	162	ASN
1	C	345	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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	14,14,14	1.45	1 (7%)	20,20,20	1.06	0
2	XYP	A	403	2	9,9,10	1.89	2 (22%)	7,12,14	2.14	2 (28%)
2	XYP	A	404	2	9,9,10	0.81	0	8,12,14	0.98	1 (12%)
2	GCV	B	402	2	14,14,14	0.82	0	20,20,20	1.40	1 (5%)
2	XYP	B	403	2	9,9,10	1.25	1 (11%)	7,12,14	0.84	0
2	XYP	B	404	2	9,9,10	0.98	1 (11%)	8,12,14	1.71	4 (50%)
2	GCV	B	405	2	14,14,14	1.61	2 (14%)	20,20,20	1.51	4 (20%)
2	XYP	B	406	2	9,9,10	2.69	3 (33%)	7,12,14	2.22	1 (14%)
2	XYP	B	407	2	7,8,10	0.87	0	2,10,14	0.39	0
2	GCV	C	402	2	14,14,14	1.55	3 (21%)	20,20,20	2.14	5 (25%)
2	XYP	C	403	2	9,9,10	2.42	2 (22%)	7,12,14	1.30	1 (14%)
2	XYP	C	404	2	9,9,10	1.77	3 (33%)	8,12,14	0.93	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
2	GCV	A	402	2	-	0/6/26/26	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	-	0/6/26/26	0/1/1/1
2	XYP	B	403	2	-	0/0/13/17	0/1/1/1
2	XYP	B	404	2	-	0/0/14/17	0/1/1/1
2	GCV	B	405	2	-	0/6/26/26	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	-	0/6/26/26	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

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	406	XYP	O5B-C1B	6.73	1.50	1.42
2	C	403	XYP	O5B-C1B	5.53	1.48	1.42
2	A	403	XYP	O5B-C1B	4.71	1.47	1.42
2	C	403	XYP	O4A-C1B	3.82	1.49	1.39
2	B	405	GCV	C4-C5	3.69	1.59	1.52

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	402	GCV	O5-C1-C2	6.40	119.77	109.86
2	B	406	XYP	C5B-O5B-C1B	5.39	117.85	111.32
2	B	402	GCV	C3-C4-C5	-4.93	103.05	110.06
2	C	402	GCV	C1-O5-C5	4.45	119.49	112.04
2	A	403	XYP	O4A-C1B-O5B	-4.21	107.24	111.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	389/401 (97%)	0.46	27 (6%) 17 14	42, 58, 72, 80	0
1	B	390/401 (97%)	0.46	9 (2%) 57 54	42, 58, 73, 79	1 (0%)
1	C	389/401 (97%)	0.51	5 (1%) 74 75	42, 58, 72, 79	0
1	D	367/401 (91%)	2.71	202 (55%) 0 0	74, 120, 155, 179	364 (99%)
All	All	1535/1604 (95%)	1.01	243 (15%) 3 2	42, 62, 140, 179	365 (23%)

The worst 5 of 243 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	343	LEU	10.8
1	D	319	TYR	9.4
1	D	108	TYR	8.7
1	D	102	SER	8.6
1	D	103	ALA	8.6

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, 95th 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	XYP	C	404	9/10	0.35	7.84	118,118,118,119	0
2	XYP	C	403	9/10	0.41	5.84	115,116,117,118	0
2	XYP	A	403	9/10	0.26	2.66	92,93,94,95	0
2	XYP	B	404	9/10	0.20	2.24	81,82,83,83	0
2	XYP	A	404	9/10	0.26	2.07	92,94,94,95	0
2	GCV	C	402	14/14	0.25	1.49	112,114,115,116	0
2	GCV	B	402	14/14	0.15	-0.04	73,76,78,79	0
2	GCV	A	402	14/14	0.22	-0.09	91,94,95,95	0
2	XYP	B	406	9/10	0.17	-2.30	88,90,91,91	0
2	XYP	B	403	9/10	0.10	-2.46	77,78,78,80	0
2	GCV	B	405	14/14	0.16	-3.22	86,88,90,90	0
2	XYP	B	407	8/10	0.19	-6.09	91,92,92,93	0

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.