



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:47 PM GMT

PDB ID : 1V6V  
Title : Crystal Structure Of Xylanase From Streptomyces Olivaceoviridis E-86 Complexed With 3(2)-alpha-L-arabinofuranosyl-xylotriose  
Authors : Fujimoto, Z.; Kaneko, S.; Kuno, A.; Kobayashi, H.; Kusakabe, I.; Mizuno, H.  
Deposited on : 2003-12-04  
Resolution : 2.10 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

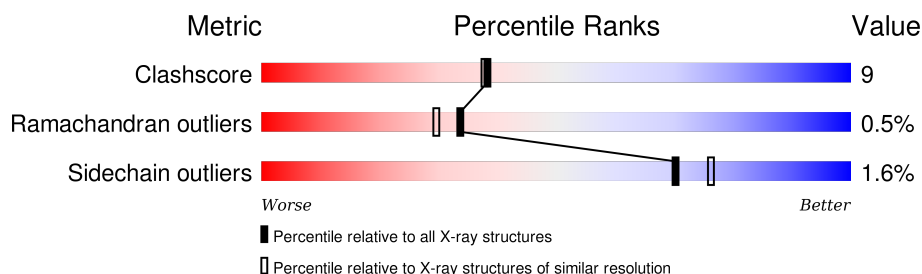
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	436	 85% 14% .
1	B	436	 83% 16% .

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7722 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 ENDO-1,4-BETA-D-XYLANASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	0	0
			3288	2020	596	656	16			
1	B	436	Total	C	N	O	S	0	0	0
			3288	2020	596	656	16			

- Molecule 2 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	4	Total	C	O	0	0
			37	20	17		
2	A	4	Total	C	O	0	0
			37	20	17		
2	B	4	Total	C	O	0	0
			37	20	17		

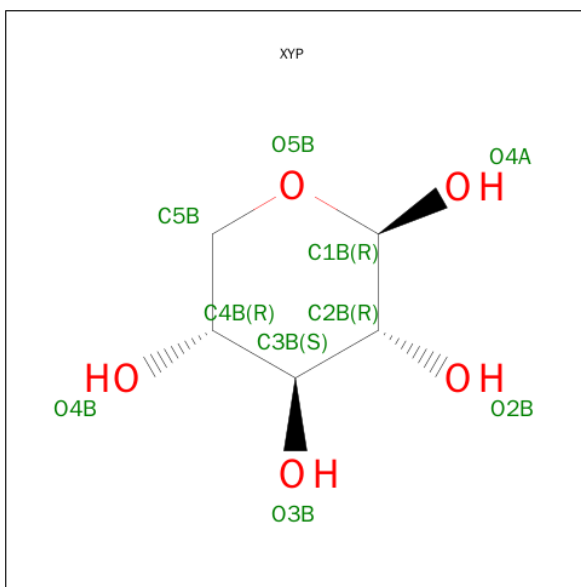
- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	2	Total	C	O	0	0
			19	10	9		
3	B	2	Total	C	O	0	0
			19	10	9		
3	B	2	Total	C	O	0	0
			19	10	9		

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	3	Total	C	O	0	0
			28	15	13		

- Molecule 5 is SUGAR (XYLOPYRANOSE) (three-letter code: XYP) (formula: C<sub>5</sub>H<sub>10</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			10	5	5		

- Molecule 6 is water.

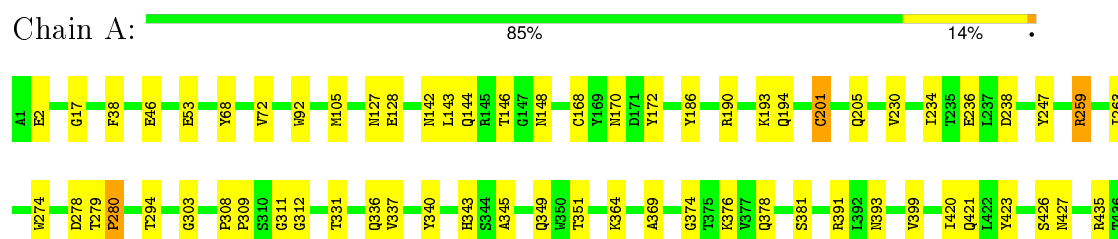
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	420	Total	O	0	0
			420	420		
6	B	520	Total	O	0	0
			520	520		

### 3 Residue-property plots

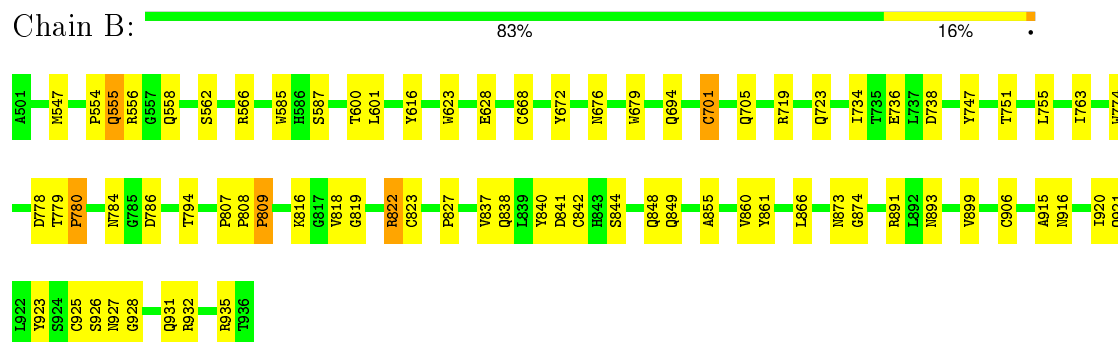
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

#### • Molecule 1: ENDO-1,4-BETA-D-XYLANASE



#### • Molecule 1: ENDO-1,4-BETA-D-XYLANASE



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.56 Å 93.99 Å 139.13 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.97 – 2.10	Depositor
% Data completeness (in resolution range)	98.7 (29.97-2.10)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.06	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.174 , 0.204	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7722	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XYP, AHR

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	0.29	0/3356	0.60	0/4556
1	B	0.31	0/3356	0.60	0/4556
All	All	0.30	0/6712	0.60	0/9112

There are no bond length outliers.

There are no bond angle outliers.

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	3288	0	3093	56	0
1	B	3288	0	3090	63	0
2	A	74	0	62	4	0
2	B	37	0	31	3	0
3	A	19	0	17	4	0
3	B	38	0	34	5	0
4	A	28	0	24	5	0
5	B	10	0	10	3	0
6	A	420	0	0	7	0
6	B	520	0	0	5	0
All	All	7722	0	6361	120	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 9.

All (120) 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:774:TRP:HH2	3:B:956:XYP:H4B	1.43	0.83
2:A:470:AHR:O2'	2:A:470:AHR:H5'1	1.78	0.83
1:A:274:TRP:HH2	3:A:456:XYP:H4B	1.46	0.81
1:B:927:ASN:HA	1:B:932:ARG:CZ	2.13	0.78
1:A:144:GLN:HE22	1:A:148:ASN:HA	1.55	0.71
1:B:736:GLU:OE1	2:B:952:XYP:H1B	1.92	0.70
1:A:193:LYS:HD2	1:A:230:VAL:HG13	1.77	0.67
1:A:236:GLU:OE1	2:A:452:XYP:H1B	1.95	0.66
1:B:840:TYR:CE2	5:B:961:XYP:H1B	2.30	0.66
1:A:105:MET:CE	1:A:143:LEU:HD22	2.27	0.65
1:A:343:HIS:CE1	4:A:462:XYP:H5B2	2.31	0.65
1:A:238:ASP:HB2	1:A:280:PRO:HB2	1.80	0.63
1:B:547:MET:HE1	1:B:623:TRP:CH2	2.34	0.63
1:A:331:THR:O	1:A:364:LYS:HE2	2.00	0.62
1:A:337:VAL:HG23	1:A:420:ILE:HB	1.82	0.61
1:A:193:LYS:HD2	1:A:230:VAL:CG1	2.33	0.58
1:B:816:LYS:HZ3	1:B:816:LYS:HB3	1.69	0.58
1:A:426:SER:O	1:A:427:ASN:HB2	2.04	0.57
1:A:46:GLU:HG2	6:A:701:HOH:O	2.02	0.57
1:B:841:ASP:H	1:B:916:ASN:HD21	1.52	0.57
1:A:172:TYR:HB3	1:A:205:GLN:NE2	2.20	0.57
1:B:842:CYS:HA	1:B:848:GLN:OE1	2.05	0.57
1:B:841:ASP:H	1:B:916:ASN:ND2	2.02	0.57
1:A:144:GLN:NE2	1:A:148:ASN:HA	2.19	0.56
1:B:547:MET:HE3	1:B:616:TYR:CE2	2.41	0.56
1:A:193:LYS:HE2	1:A:193:LYS:HA	1.87	0.56
1:A:105:MET:HE2	1:A:143:LEU:HD22	1.86	0.56
1:B:784:ASN:OD1	1:B:786:ASP:OD2	2.24	0.56
1:B:899:VAL:HG22	1:B:906:CYS:SG	2.47	0.55
1:B:672:TYR:CD2	3:B:956:XYP:H5B2	2.41	0.55
1:B:676:ASN:HB3	1:B:679:TRP:CD2	2.41	0.55
1:B:874:GLY:HA2	1:B:921:GLN:OE1	2.06	0.55
1:A:274:TRP:CH2	3:A:456:XYP:H4B	2.36	0.54
1:A:336:GLN:CD	1:A:376:LYS:HG3	2.27	0.54
1:A:343:HIS:ND1	4:A:462:XYP:H5B2	2.23	0.53
1:A:142:ASN:O	1:A:146:THR:HG23	2.08	0.53
1:A:172:TYR:CD2	3:A:456:XYP:H5B2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:TYR:CZ	4:A:461:XYP:H5B2	2.44	0.53
1:A:309:PRO:HD2	1:A:435:ARG:NH2	2.25	0.52
1:B:778:ASP:O	1:B:779:THR:C	2.48	0.52
1:B:738:ASP:HB2	1:B:780:PRO:HB2	1.92	0.51
1:B:779:THR:N	1:B:780:PRO:HD3	2.26	0.51
1:A:303:GLY:HA2	6:A:786:HOH:O	2.11	0.51
1:A:190:ARG:HD2	6:A:756:HOH:O	2.08	0.51
1:A:168:CYS:HA	1:A:201:CYS:O	2.09	0.51
1:B:816:LYS:NZ	1:B:816:LYS:HB3	2.26	0.50
1:A:279:THR:N	1:A:280:PRO:HD3	2.26	0.50
1:B:672:TYR:CG	3:B:956:XYP:H5B2	2.46	0.50
1:A:311:GLY:HA2	1:A:351:THR:HG23	1.94	0.50
1:B:893:ASN:HD21	1:B:899:VAL:CG2	2.24	0.50
1:A:343:HIS:CG	4:A:462:XYP:H5B2	2.47	0.49
1:B:585:TRP:CE2	1:B:587:SER:HB3	2.47	0.49
1:B:837:VAL:HG23	1:B:920:ILE:HB	1.94	0.49
1:A:278:ASP:O	1:A:279:THR:C	2.50	0.49
1:B:893:ASN:ND2	1:B:899:VAL:HG23	2.28	0.49
1:B:925:CYS:HB3	6:B:1322:HOH:O	2.13	0.49
1:B:628:GLU:OE2	2:B:952:XYP:O4A	2.31	0.49
1:B:827:PRO:HG3	1:B:838:GLN:HG2	1.95	0.48
1:B:923:TYR:CZ	3:B:971:XYP:H5B2	2.48	0.48
1:B:822:ARG:HH12	1:B:915:ALA:HA	1.79	0.48
1:A:68:TYR:CZ	1:A:72:VAL:HG21	2.49	0.47
1:B:555:GLN:NE2	1:B:558:GLN:NE2	2.62	0.47
1:A:336:GLN:HB2	1:A:376:LYS:HD3	1.95	0.47
1:B:855:ALA:HA	6:B:1248:HOH:O	2.14	0.47
1:B:926:SER:O	1:B:927:ASN:HB2	2.15	0.47
1:A:186:TYR:HE2	1:A:190:ARG:HH21	1.60	0.47
1:B:823:CYS:HB3	6:B:1106:HOH:O	2.15	0.47
1:A:172:TYR:CG	3:A:456:XYP:H5B2	2.50	0.46
1:B:927:ASN:HA	1:B:932:ARG:NH1	2.30	0.46
1:A:345:ALA:O	1:A:349:GLN:HG2	2.15	0.46
1:A:381:SER:HB2	6:A:875:HOH:O	2.14	0.46
1:B:925:CYS:HA	1:B:931:GLN:OE1	2.14	0.46
1:A:234:ILE:HD12	1:A:263:ILE:HG12	1.97	0.46
1:A:369:ALA:HB2	1:A:378:GLN:NE2	2.31	0.46
1:A:128:GLU:OE2	2:A:452:XYP:O4A	2.33	0.46
1:B:719:ARG:O	1:B:723:GLN:HG3	2.16	0.46
1:A:127:ASN:HD22	1:A:170:ASN:HB3	1.82	0.45
1:B:562:SER:O	1:B:566:ARG:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:ARG:HH11	1:A:259:ARG:HG3	1.82	0.45
1:B:840:TYR:CZ	5:B:961:XYP:H5B2	2.51	0.45
1:A:53:GLU:HG2	1:A:92:TRP:HZ2	1.80	0.45
1:B:705:GLN:OE1	2:B:952:XYP:O4A	2.34	0.44
1:A:435:ARG:HD2	6:A:653:HOH:O	2.18	0.44
1:B:751:THR:O	1:B:755:LEU:HD23	2.18	0.44
1:B:935:ARG:HH11	1:B:935:ARG:HG3	1.82	0.44
1:B:554:PRO:HB2	1:B:555:GLN:NE2	2.31	0.44
1:B:566:ARG:NE	6:B:1400:HOH:O	2.45	0.44
1:B:932:ARG:HD2	1:B:932:ARG:N	2.32	0.43
1:B:849:GLN:HA	1:B:849:GLN:NE2	2.33	0.43
1:B:818:VAL:HG23	1:B:819:GLY:N	2.33	0.43
1:A:340:TYR:CE1	4:A:461:XYP:H5B2	2.54	0.43
1:B:807:PRO:HA	1:B:808:PRO:HD3	1.90	0.43
1:B:860:VAL:O	1:B:861:TYR:HB2	2.19	0.43
1:B:694:GLN:NE2	6:B:1399:HOH:O	2.51	0.43
1:A:46:GLU:CG	6:A:701:HOH:O	2.65	0.42
1:B:928:GLY:O	1:B:932:ARG:HD3	2.19	0.42
1:A:311:GLY:HA2	6:A:550:HOH:O	2.19	0.42
1:B:556:ARG:HH12	1:B:600:THR:CG2	2.33	0.42
1:B:873:ASN:OD1	1:B:923:TYR:HA	2.20	0.42
1:A:393:ASN:HD21	1:A:399:VAL:HG21	1.85	0.42
1:B:822:ARG:HG2	1:B:822:ARG:HH11	1.84	0.42
1:A:294:THR:OG1	1:A:391:ARG:HD2	2.20	0.42
1:A:190:ARG:O	1:A:194:GLN:HG3	2.20	0.41
1:B:668:CYS:HA	1:B:701:CYS:O	2.20	0.41
1:B:774:TRP:CH2	3:B:956:XYP:H4B	2.36	0.41
1:B:841:ASP:CG	1:B:916:ASN:HD21	2.23	0.41
1:A:374:GLY:HA2	1:A:421:GLN:OE1	2.20	0.41
1:A:17:GLY:HA2	1:A:38:PHE:HB3	2.00	0.41
1:B:734:ILE:HD12	1:B:763:ILE:HG12	2.02	0.41
1:B:840:TYR:CE1	5:B:961:XYP:H5B2	2.55	0.41
1:A:127:ASN:ND2	1:A:170:ASN:HB3	2.36	0.41
1:B:849:GLN:HA	1:B:849:GLN:HE21	1.85	0.41
1:B:866:LEU:HD12	1:B:866:LEU:HA	1.95	0.41
1:A:205:GLN:NE2	2:A:452:XYP:O4A	2.54	0.41
1:B:893:ASN:HD21	1:B:899:VAL:HG21	1.86	0.41
1:A:308:PRO:HA	1:A:309:PRO:HD3	1.94	0.41
1:A:53:GLU:HG2	1:A:92:TRP:CZ2	2.55	0.41
1:B:794:THR:OG1	1:B:891:ARG:HD2	2.20	0.41
1:B:808:PRO:HA	1:B:809:PRO:HD3	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:MET:HE3	1:A:143:LEU:HD22	2.00	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	434/436 (100%)	419 (96%)	13 (3%)	2 (0%)	34	30
1	B	434/436 (100%)	417 (96%)	15 (4%)	2 (0%)	34	30
All	All	868/872 (100%)	836 (96%)	28 (3%)	4 (0%)	34	30

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	312	GLY
1	B	844	SER
1	A	2	GLU
1	B	809	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	341/341 (100%)	336 (98%)	5 (2%)	72	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	341/341 (100%)	335 (98%)	6 (2%)	66	72
All	All	682/682 (100%)	671 (98%)	11 (2%)	70	76

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	201	CYS
1	A	247	TYR
1	A	259	ARG
1	A	280	PRO
1	A	423	TYR
1	B	555	GLN
1	B	601	LEU
1	B	701	CYS
1	B	747	TYR
1	B	780	PRO
1	B	822	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	ASN
1	A	127	ASN
1	A	170	ASN
1	A	173	ASN
1	A	205	GLN
1	A	349	GLN
1	B	511	GLN
1	B	555	GLN
1	B	673	ASN
1	B	694	GLN
1	B	814	GLN
1	B	849	GLN
1	B	893	ASN

### 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 ⓘ

21 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	AHR	A	449	2	9,9,10	0.70	0	12,12,14	1.37	1 (8%)
2	XYP	A	450	2	9,9,10	0.63	0	12,12,14	0.96	1 (8%)
2	XYP	A	451	2	9,9,10	0.62	0	12,12,14	1.16	1 (8%)
2	XYP	A	452	2	10,10,10	0.44	0	12,14,14	0.75	0
3	XYP	A	456	3	9,9,10	0.61	0	12,12,14	0.95	1 (8%)
3	XYP	A	457	3	10,10,10	0.51	0	12,14,14	0.71	0
4	XYP	A	461	4	9,9,10	0.63	0	12,12,14	0.95	1 (8%)
4	XYP	A	462	4	9,9,10	0.63	0	12,12,14	0.89	1 (8%)
4	XYP	A	463	4	10,10,10	0.56	0	12,14,14	0.68	0
2	AHR	A	470	2	9,9,10	0.68	0	12,12,14	1.42	1 (8%)
2	XYP	A	471	2	9,9,10	0.61	0	12,12,14	1.02	1 (8%)
2	XYP	A	472	2	9,9,10	0.65	0	12,12,14	1.02	1 (8%)
2	XYP	A	473	2	10,10,10	0.50	0	12,14,14	0.67	0
2	AHR	B	949	2	9,9,10	0.77	0	12,12,14	1.37	1 (8%)
2	XYP	B	950	2	9,9,10	0.61	0	12,12,14	0.99	1 (8%)
2	XYP	B	951	2	9,9,10	0.62	0	12,12,14	1.11	1 (8%)
2	XYP	B	952	2	10,10,10	0.43	0	12,14,14	0.73	0
3	XYP	B	956	3	9,9,10	0.65	0	12,12,14	0.96	1 (8%)
3	XYP	B	957	3	10,10,10	0.53	0	12,14,14	0.68	0
3	XYP	B	970	3	9,9,10	0.64	0	12,12,14	0.97	1 (8%)
3	XYP	B	971	3	10,10,10	0.52	0	12,14,14	0.71	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	AHR	A	449	2	-	0/2/15/18	0/1/1/1
2	XYP	A	450	2	-	0/0/14/17	0/1/1/1
2	XYP	A	451	2	-	0/0/14/17	0/1/1/1
2	XYP	A	452	2	-	0/0/17/17	0/1/1/1
3	XYP	A	456	3	-	0/0/14/17	0/1/1/1
3	XYP	A	457	3	-	0/0/17/17	0/1/1/1
4	XYP	A	461	4	-	0/0/14/17	0/1/1/1
4	XYP	A	462	4	-	0/0/14/17	0/1/1/1
4	XYP	A	463	4	-	0/0/17/17	0/1/1/1
2	AHR	A	470	2	-	0/2/15/18	0/1/1/1
2	XYP	A	471	2	-	0/0/14/17	0/1/1/1
2	XYP	A	472	2	-	0/0/14/17	0/1/1/1
2	XYP	A	473	2	-	0/0/17/17	0/1/1/1
2	AHR	B	949	2	-	0/2/15/18	0/1/1/1
2	XYP	B	950	2	-	0/0/14/17	0/1/1/1
2	XYP	B	951	2	-	0/0/14/17	0/1/1/1
2	XYP	B	952	2	-	0/0/17/17	0/1/1/1
3	XYP	B	956	3	-	0/0/14/17	0/1/1/1
3	XYP	B	957	3	-	0/0/17/17	0/1/1/1
3	XYP	B	970	3	-	0/0/14/17	0/1/1/1
3	XYP	B	971	3	-	0/0/17/17	0/1/1/1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	470	AHR	C1'-C2'-C3'	-3.93	95.32	101.64
2	A	449	AHR	C1'-O4'-C4'	-3.69	98.79	108.08
2	B	949	AHR	C1'-O4'-C4'	-3.64	98.94	108.08
2	B	951	XYP	C4B-C3B-C2B	-3.37	107.91	111.24
2	A	451	XYP	C4B-C3B-C2B	-3.33	107.94	111.24
2	B	950	XYP	C4B-C3B-C2B	-3.10	108.17	111.24
3	B	970	XYP	C4B-C3B-C2B	-3.08	108.19	111.24
3	B	956	XYP	C4B-C3B-C2B	-3.04	108.23	111.24
2	A	471	XYP	C4B-C3B-C2B	-3.03	108.24	111.24
2	A	450	XYP	C4B-C3B-C2B	-3.02	108.26	111.24
3	A	456	XYP	C4B-C3B-C2B	-3.00	108.28	111.24
4	A	461	XYP	C4B-C3B-C2B	-2.88	108.39	111.24
2	A	472	XYP	C4B-C3B-C2B	-2.61	108.66	111.24
4	A	462	XYP	C4B-C3B-C2B	-2.52	108.74	111.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	452	XYP	3	0
3	A	456	XYP	4	0
4	A	461	XYP	2	0
4	A	462	XYP	3	0
2	A	470	AHR	1	0
2	B	952	XYP	3	0
3	B	956	XYP	4	0
3	B	971	XYP	1	0

## 5.6 Ligand geometry ⓘ

1 ligand is 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$
5	XYP	B	961	-	10,10,10	0.53	0	12,14,14	0.70	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
5	XYP	B	961	-	-	0/0/17/17	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	961	XYP	3	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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.