



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 02:53 AM GMT

PDB ID : 1ISX  
Title : Crystal structure of xylanase from *Streptomyces olivaceoviridis* E-86 complexed with xylotriose  
Authors : Fujimoto, Z.; Kuno, A.; Kaneko, S.; Kobayashi, H.; Kusakabe, I.; Mizuno, H.  
Deposited on : 2001-12-27  
Resolution : 2.10 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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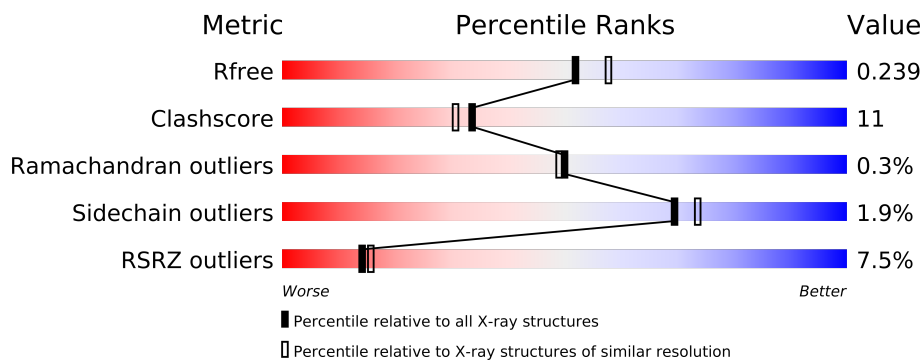
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 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 2.10 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))
$R_{free}$	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (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. 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	436	
1	B	436	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7562 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 endo-1,4-beta-D-xylanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	4	0
			3298	2025	600	656	17			
1	B	436	Total	C	N	O	S	0	4	0
			3297	2024	599	657	17			

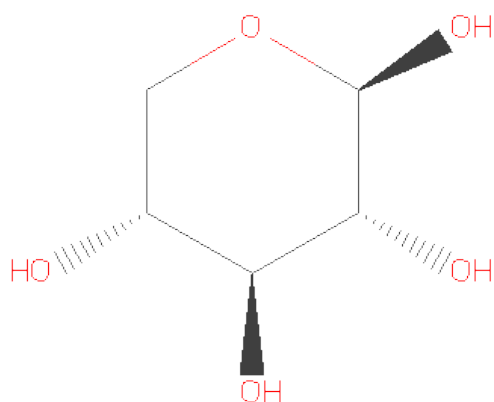
- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

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

- 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	A	2	Total	C	O	0	0
			19	10	9		
3	B	2	Total	C	O	0	0
			19	10	9		

- Molecule 4 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
4	A	1	Total	C	O	0	0
			10	5	5		
4	B	1	Total	C	O	0	0
			10	5	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	398	Total	O	0	0
			398	398		
5	B	408	Total	O	0	0
			408	408		

### 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 ( $\text{RSRZ} > 2$ ). 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.

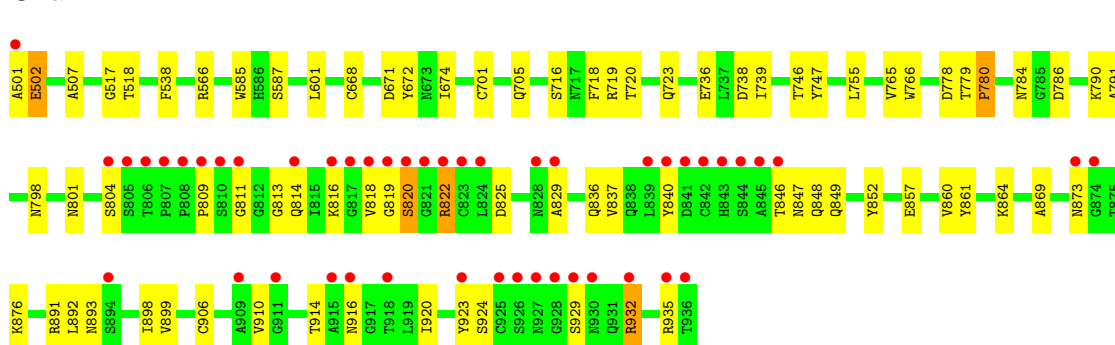
- Molecule 1: endo-1,4-beta-D-xylanase

Chain A:



- Molecule 1: endo-1,4-beta-D-xylanase

Chain B:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.37Å 94.46Å 138.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.82 – 2.10 36.30 – 2.00	Depositor EDS
% Data completeness (in resolution range)	88.2 (29.82-2.10) 86.8 (36.30-2.00)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.55 (at 2.00Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.189 , 0.240 0.194 , 0.239	Depositor DCC
$R_{free}$ test set	5938 reflections (11.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.5	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 48.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	2 of 58491 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7562	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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

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	0.31	0/3389	0.60	0/4599
1	B	0.32	0/3388	0.60	0/4597
All	All	0.31	0/6777	0.60	0/9196

There are no bond length outliers.

There are no bond angle outliers.

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	3298	0	3104	75	0
1	B	3297	0	3098	63	0
2	A	28	0	24	4	0
2	B	56	0	48	6	0
3	A	38	0	34	4	0
3	B	19	0	17	2	0
4	A	10	0	10	3	0
4	B	10	0	10	1	0
5	A	398	0	0	8	0
5	B	408	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7562	0	6345	144	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 11.

All (144) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:736:GLU:OE1	2:B:952:XYP:H1B	1.48	1.12
1:A:236:GLU:OE1	2:A:452:XYP:H1B	1.58	1.01
1:A:139[A]:ARG:HE	1:A:140:ASP:H	1.07	0.99
1:A:1:ALA:HB1	1:A:7:ALA:HB1	1.47	0.97
1:A:139[A]:ARG:HE	1:A:140:ASP:N	1.72	0.87
1:B:822:ARG:HH12	1:B:916:ASN:N	1.84	0.75
1:B:899:VAL:HG22	1:B:906:CYS:SG	2.26	0.74
1:A:139[A]:ARG:NE	1:A:140:ASP:H	1.86	0.71
1:B:813:GLY:H	1:B:849:GLN:NE2	1.89	0.70
1:B:719:ARG:O	1:B:723:GLN:HG3	1.92	0.69
1:B:501:ALA:HB3	1:B:507:ALA:HB1	1.72	0.69
1:A:144:GLN:HE22	1:A:148:ASN:HA	1.57	0.69
1:B:822:ARG:HG2	1:B:822:ARG:HH11	1.60	0.67
1:B:705:GLN:OE1	2:B:952:XYP:O4A	2.14	0.66
1:A:1:ALA:HB3	5:A:1675:HOH:O	1.96	0.64
1:B:840:TYR:CE2	4:B:961:XYP:H1B	2.33	0.64
1:A:85:TRP:CE2	1:A:87:SER:HB2	2.34	0.62
2:B:952:XYP:O4A	2:B:956:XYP:O4B	2.16	0.62
1:B:836:GLN:HB2	1:B:876[A]:LYS:HE3	1.81	0.61
1:B:784[B]:ASN:HB3	5:B:1015:HOH:O	2.01	0.61
1:B:929:SER:HA	1:B:932:ARG:HE	1.66	0.61
1:A:340:TYR:CZ	4:A:1461:XYP:H5B2	2.35	0.60
1:A:432:ARG:HH11	1:A:432:ARG:HG3	1.65	0.60
1:B:671:ASP:HB3	1:B:674:ILE:HD13	1.83	0.60
2:B:952:XYP:C1B	2:B:956:XYP:O4B	2.50	0.59
1:A:395:ASP:O	1:A:432:ARG:HD2	2.03	0.59
1:B:818:VAL:HG23	1:B:929:SER:HB2	1.85	0.58
2:B:952:XYP:O5B	2:B:956:XYP:O4B	2.21	0.58
1:A:236:GLU:HG2	1:A:266:TRP:CE3	2.38	0.58
1:B:585:TRP:CE2	1:B:587:SER:HB3	2.39	0.58
1:B:736:GLU:HG2	1:B:766:TRP:CE3	2.39	0.57
1:A:105:MET:CE	1:A:143:LEU:HD22	2.35	0.57
1:A:102:ARG:O	1:A:106:ILE:HG13	2.05	0.57
1:A:105:MET:HE3	1:A:143:LEU:HD22	1.87	0.57
1:A:345:ALA:O	1:A:349:GLN:HG2	2.05	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2:GLU:HG2	5:A:1736:HOH:O	2.05	0.56
1:B:502:GLU:HB2	1:B:801:ASN:OD1	2.06	0.56
1:B:720:THR:HG23	5:B:1370:HOH:O	2.05	0.55
1:A:399:VAL:HG22	1:A:406:CYS:SG	2.47	0.55
1:A:231:ASP:OD1	1:A:259:ARG:HG3	2.07	0.55
1:A:53:GLU:HG2	1:A:92:TRP:HZ2	1.71	0.55
1:A:144:GLN:NE2	1:A:148:ASN:HA	2.22	0.55
1:A:190:ARG:O	1:A:194:GLN:HG3	2.07	0.54
1:A:432:ARG:NH1	1:A:432:ARG:HG3	2.23	0.54
1:B:816:LYS:NZ	1:B:816:LYS:HB3	2.23	0.53
1:B:869:ALA:HB3	5:B:1317:HOH:O	2.07	0.53
1:A:294:THR:OG1	1:A:391:ARG:HD2	2.08	0.53
1:A:142:ASN:O	1:A:146:THR:HG23	2.08	0.53
1:B:738:ASP:HB2	1:B:780:PRO:HB2	1.90	0.52
1:B:779:THR:N	1:B:780:PRO:HD3	2.24	0.52
1:A:278:ASP:O	1:A:279:THR:C	2.48	0.52
1:B:873:ASN:ND2	1:B:924:SER:H	2.07	0.52
1:A:128:GLU:HA	1:A:171:ASP:CG	2.31	0.51
1:A:425:CYS:HA	1:A:431:GLN:OE1	2.11	0.51
1:A:238:ASP:HB2	1:A:280:PRO:HB2	1.92	0.50
1:B:778:ASP:O	1:B:779:THR:C	2.49	0.50
1:B:822:ARG:HG2	1:B:822:ARG:NH1	2.26	0.50
1:A:370:GLY:H	1:A:375:THR:HG21	1.75	0.50
1:A:426:SER:O	1:A:427:ASN:HB2	2.11	0.50
1:B:784[B]:ASN:ND2	1:B:790:LYS:HG2	2.27	0.49
1:A:231:ASP:HA	1:A:259:ARG:HG3	1.94	0.49
1:A:426:SER:HB3	3:A:472:XYP:H5B2	1.94	0.49
1:A:68:TYR:CZ	1:A:72[A]:VAL:HG21	2.48	0.48
1:A:303:GLY:HA2	5:A:1837:HOH:O	2.12	0.48
1:B:784[A]:ASN:OD1	1:B:786:ASP:OD1	2.32	0.48
1:B:813:GLY:H	1:B:849:GLN:HE21	1.57	0.48
1:B:739:ILE:HD13	1:B:746:THR:HG22	1.95	0.48
1:B:876[A]:LYS:HG3	5:B:1317:HOH:O	2.12	0.48
1:B:804:SER:HA	5:B:1320:HOH:O	2.13	0.48
1:B:819:GLY:O	1:B:914:THR:HG22	2.14	0.47
1:B:672:TYR:HB3	1:B:705:GLN:OE1	2.14	0.47
1:B:809:PRO:CG	1:B:935:ARG:HB3	2.45	0.47
1:A:205:GLN:OE1	2:A:452:XYP:O4A	2.24	0.47
1:B:798:ASN:HB3	5:B:1298:HOH:O	2.14	0.47
1:B:822:ARG:CZ	1:B:914:THR:O	2.63	0.47
1:A:131:SER:HB2	5:A:1806:HOH:O	2.15	0.46
1:A:340:TYR:CE1	4:A:1461:XYP:H5B2	2.50	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:190:ARG:NH1	1:A:190:ARG:HB3	2.30	0.46
1:B:822:ARG:NH1	1:B:916:ASN:N	2.60	0.46
1:B:860:VAL:O	1:B:861:TYR:HB2	2.16	0.46
1:A:1:ALA:HA	5:A:1795:HOH:O	2.16	0.45
1:B:829:ALA:HA	1:B:847:ASN:CB	2.46	0.45
1:B:892:LEU:CD2	1:B:898:ILE:HG12	2.46	0.45
1:B:819:GLY:CA	1:B:929:SER:HB2	2.47	0.45
1:A:195:ARG:NH2	1:A:197:VAL:HG21	2.31	0.45
1:B:818:VAL:HG23	1:B:819:GLY:N	2.31	0.45
1:A:338:GLN:OE1	1:A:417:GLY:HA2	2.17	0.45
1:A:85:TRP:CZ2	1:A:87:SER:HB2	2.51	0.45
1:B:846:THR:C	1:B:848:GLN:H	2.20	0.45
1:B:736:GLU:HG2	1:B:766:TRP:CZ3	2.52	0.44
1:B:923:TYR:CZ	3:B:971:XYP:H5B2	2.52	0.44
1:B:566:ARG:NH2	5:B:1109:HOH:O	2.46	0.44
1:A:291:ALA:HA	1:A:391:ARG:HG2	2.00	0.44
1:B:910:VAL:HG13	3:B:970:XYP:H4B	2.00	0.44
1:B:822:ARG:N	1:B:822:ARG:HD2	2.33	0.43
1:A:333:ASP:OD1	1:A:364:LYS:HE3	2.18	0.43
1:B:932:ARG:HH11	1:B:932:ARG:HG2	1.84	0.43
1:A:190:ARG:HB3	1:A:190:ARG:HH11	1.82	0.43
1:A:340:TYR:CE2	4:A:1461:XYP:H1B	2.54	0.43
1:A:259:ARG:HB2	5:A:1547:HOH:O	2.17	0.43
1:B:814:GLN:HE21	1:B:848:GLN:HB3	1.83	0.43
1:A:329:ALA:HA	1:A:347:ASN:HB3	2.00	0.43
1:A:231:ASP:HA	1:A:259:ARG:CG	2.49	0.43
1:A:331:THR:O	1:A:364:LYS:HE2	2.19	0.43
2:A:452:XYP:O5B	3:A:456:XYP:O4B	2.37	0.43
1:B:517:GLY:HA2	1:B:538:PHE:HB3	2.00	0.43
1:A:127:ASN:ND2	1:A:128:GLU:HG3	2.34	0.43
1:A:337:VAL:HG23	1:A:420:ILE:HB	2.01	0.42
1:A:387:ASN:HB3	1:A:402:GLN:OE1	2.19	0.42
1:B:860:VAL:O	1:B:864:LYS:HB2	2.19	0.42
1:B:852:TYR:HA	1:B:857:GLU:O	2.18	0.42
1:A:308:PRO:HA	1:A:309:PRO:HD3	1.89	0.42
1:B:820:SER:O	1:B:822:ARG:HD2	2.19	0.42
1:A:279:THR:N	1:A:280:PRO:HD3	2.34	0.42
1:A:311:GLY:HA2	1:A:351:THR:HG23	2.01	0.42
1:A:35:SER:HA	1:A:76:LYS:HE2	2.01	0.42
1:A:80:GLY:HA3	1:A:123:TRP:CE3	2.55	0.42
1:A:374:GLY:HA2	1:A:421:GLN:OE1	2.19	0.42
1:B:825:ASP:OD2	1:B:847:ASN:ND2	2.53	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:452:XYP:O4A	3:A:456:XYP:O4B	2.29	0.42
1:A:53:GLU:HG2	1:A:92:TRP:CZ2	2.55	0.41
1:B:791:ALA:HA	1:B:891:ARG:HG2	2.02	0.41
1:A:106:ILE:HG22	1:A:110:ASN:ND2	2.35	0.41
1:A:186:TYR:CE1	1:A:228:LEU:HD11	2.56	0.41
1:A:305:SER:HB2	5:A:1845:HOH:O	2.20	0.41
1:B:893:ASN:ND2	1:B:899:VAL:HG23	2.36	0.41
1:B:518:THR:HA	1:B:765:VAL:O	2.21	0.41
1:A:236:GLU:HG2	1:A:266:TRP:CZ3	2.55	0.41
1:A:172:TYR:CD1	3:A:456:XYP:H5B2	2.55	0.41
1:A:19:ALA:HB2	1:A:266:TRP:CE3	2.56	0.41
1:A:100:THR:HG22	5:A:1766:HOH:O	2.20	0.41
1:A:358:LEU:HD23	1:A:358:LEU:HA	1.97	0.41
2:B:952:XYP:C1B	2:B:956:XYP:HO4B	2.23	0.40
1:B:813:GLY:N	1:B:849:GLN:NE2	2.64	0.40
1:A:293:TYR:CD1	1:A:293:TYR:C	2.95	0.40
1:B:716:SER:C	1:B:718:PHE:H	2.25	0.40
1:B:837:VAL:HG23	1:B:920:ILE:HB	2.04	0.40
1:B:873:ASN:HD21	1:B:924:SER:H	1.69	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	438/436 (100%)	418 (95%)	20 (5%)	0	100	100
1	B	438/436 (100%)	416 (95%)	19 (4%)	3 (1%)	30	23
All	All	876/872 (100%)	834 (95%)	39 (4%)	3 (0%)	50	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	502	GLU

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Mol	Chain	Res	Type
1	B	811	GLY
1	B	820	SER

### 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	345/341 (101%)	338 (98%)	7 (2%)	68	72
1	B	345/341 (101%)	337 (98%)	8 (2%)	63	66
All	All	690/682 (101%)	675 (98%)	15 (2%)	69	68

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	201[A]	CYS
1	A	201[B]	CYS
1	A	247	TYR
1	A	259	ARG
1	A	274	TRP
1	A	280	PRO
1	B	601	LEU
1	B	701[A]	CYS
1	B	701[B]	CYS
1	B	747	TYR
1	B	755	LEU
1	B	780	PRO
1	B	822	ARG
1	B	932	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	110	ASN
1	A	173	ASN

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Mol	Chain	Res	Type
1	A	284	ASN
1	A	314	GLN
1	B	814	GLN
1	B	848	GLN
1	B	849	GLN
1	B	921	GLN

### 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 ⓘ

15 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	XYP	A	450	2	8,9,10	0.53	0	8,12,14	0.75	0
2	XYP	A	451	2	8,9,10	0.58	0	8,12,14	0.71	0
2	XYP	A	452	2	10,10,10	0.50	0	14,14,14	0.65	0
3	XYP	A	456	3	8,9,10	0.74	0	8,12,14	0.73	0
3	XYP	A	457	3	10,10,10	0.56	0	14,14,14	0.61	0
3	XYP	A	471	3	8,9,10	0.59	0	8,12,14	0.75	0
3	XYP	A	472	3	10,10,10	0.61	0	14,14,14	0.61	0
2	XYP	B	950	2	8,9,10	0.51	0	8,12,14	0.76	0
2	XYP	B	951	2	8,9,10	0.52	0	8,12,14	0.71	0
2	XYP	B	952	2	10,10,10	0.50	0	14,14,14	0.66	0
2	XYP	B	956	2	8,9,10	0.89	0	8,12,14	0.77	0
2	XYP	B	957	2	8,9,10	0.53	0	8,12,14	0.76	0
2	XYP	B	958	2	10,10,10	0.60	0	14,14,14	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	XYP	B	970	3	8,9,10	0.60	0	8,12,14	0.74	0
3	XYP	B	971	3	10,10,10	0.62	0	14,14,14	0.59	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	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
3	XYP	A	471	3	-	0/0/14/17	0/1/1/1
3	XYP	A	472	3	-	0/0/17/17	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
2	XYP	B	956	2	-	0/0/14/17	0/1/1/1
2	XYP	B	957	2	-	0/0/14/17	0/1/1/1
2	XYP	B	958	2	-	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.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	XYP	A	1461	-	10,10,10	0.61	0	14,14,14	0.60	0
4	XYP	B	961	-	10,10,10	0.67	0	14,14,14	0.60	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
4	XYP	A	1461	-	-	0/0/17/17	0/1/1/1
4	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.

## 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, 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	436/436 (100%)	0.16	19 (4%) 33 37	12, 22, 44, 83	0
1	B	436/436 (100%)	0.28	47 (10%) 6 7	12, 20, 65, 77	0
All	All	872/872 (100%)	0.22	66 (7%) 14 15	12, 21, 59, 83	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	306	THR	10.5
1	A	304	SER	8.3
1	A	305	SER	8.0
1	B	819	GLY	6.0
1	B	845	ALA	5.9
1	A	303	GLY	5.9
1	B	915	ALA	5.9
1	B	936	THR	5.7
1	B	805	SER	5.7
1	B	840	TYR	5.3
1	A	308	PRO	5.2
1	B	844	SER	5.1
1	B	926	SER	5.1
1	A	309	PRO	5.0
1	B	822	ARG	5.0
1	B	818	VAL	4.7
1	A	311	GLY	4.7
1	A	307	PRO	4.6
1	B	923	TYR	4.6
1	B	839	LEU	4.5
1	B	810	SER	4.5
1	B	928	GLY	4.4
1	B	843	HIS	4.3
1	B	807	PRO	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	823	CYS	4.2
1	B	829	ALA	4.0
1	A	436	THR	4.0
1	B	929	SER	4.0
1	B	932	ARG	3.9
1	B	501	ALA	3.9
1	B	820	SER	3.8
1	B	806	THR	3.6
1	B	809	PRO	3.6
1	B	927	ASN	3.6
1	B	925	CYS	3.4
1	B	911	GLY	3.3
1	A	310	SER	3.3
1	B	814	GLN	3.1
1	B	894	SER	3.0
1	B	930	ASN	2.9
1	B	817	GLY	2.9
1	B	842	CYS	2.9
1	A	97	SER	2.9
1	B	816	LYS	2.8
1	B	808	PRO	2.8
1	A	100	THR	2.7
1	B	846	THR	2.7
1	B	918	THR	2.7
1	B	828	ASN	2.7
1	A	133	ASP	2.6
1	B	916	ASN	2.6
1	A	2	GLU	2.6
1	B	873	ASN	2.5
1	B	811	GLY	2.4
1	B	874	GLY	2.4
1	A	1	ALA	2.4
1	B	804	SER	2.4
1	A	147	GLY	2.4
1	B	821	GLY	2.3
1	B	909	ALA	2.2
1	B	935	ARG	2.2
1	B	841	ASP	2.2
1	A	344	SER	2.1
1	A	139[A]	ARG	2.1
1	A	137	GLY	2.0
1	B	824	LEU	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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	XYP	B	950	9/10	0.24	47.00	32,36,41,42	0
3	XYP	A	456	9/10	0.22	7.34	48,50,52,52	0
3	XYP	A	472	10/10	0.22	5.05	34,42,45,48	0
2	XYP	B	957	9/10	0.19	4.39	33,34,36,37	0
2	XYP	A	452	10/10	0.22	4.13	25,28,35,40	0
2	XYP	B	956	9/10	0.17	3.75	27,29,32,32	0
3	XYP	A	457	10/10	0.22	3.19	46,48,49,50	0
3	XYP	A	471	9/10	0.16	2.71	23,24,28,29	0
2	XYP	A	450	9/10	0.14	2.64	33,36,39,40	0
2	XYP	B	958	10/10	0.25	2.62	42,48,52,52	0
2	XYP	B	952	10/10	0.15	2.35	16,19,25,35	0
3	XYP	B	971	10/10	0.34	1.49	60,61,61,62	0
3	XYP	B	970	9/10	0.28	0.46	59,60,60,60	0
2	XYP	A	451	9/10	0.12	-0.14	21,23,26,28	0
2	XYP	B	951	9/10	0.09	-0.35	16,16,19,24	0

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	XYP	A	1461	10/10	0.13	0.43	29,30,31,31	0
4	XYP	B	961	10/10	0.23	-0.33	62,63,63,63	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.