



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:06 PM 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 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

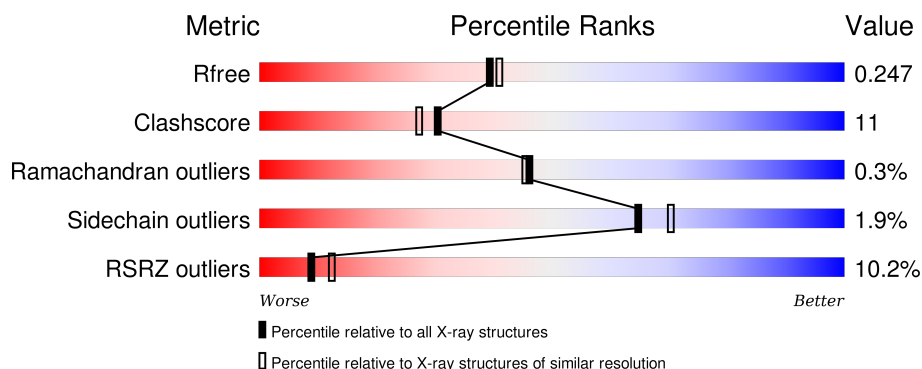
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (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.

Mol	Chain	Length	Quality of chain
1	A	436	<div> <div>7%</div> <div>80%</div> <div>19%</div> </div>
1	B	436	<div> <div>14%</div> <div>82%</div> <div>17%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	XYP	A	452	-	-	-	X
2	XYP	B	952	-	-	X	X
2	XYP	B	956	-	-	-	X
2	XYP	B	957	-	-	-	X
2	XYP	B	958	-	-	-	X
3	XYP	A	456	-	-	-	X
3	XYP	A	457	-	-	-	X
3	XYP	A	471	-	-	-	X
3	XYP	A	472	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7562 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	4	0
			3298	2025	600	656	17			
1	B	436	Total	C	N	O	S	0	4	0
			3297	2024	599	657	17			

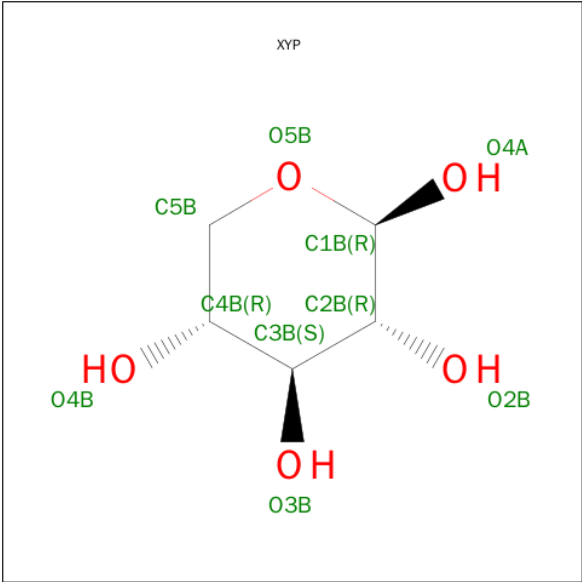
- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

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		

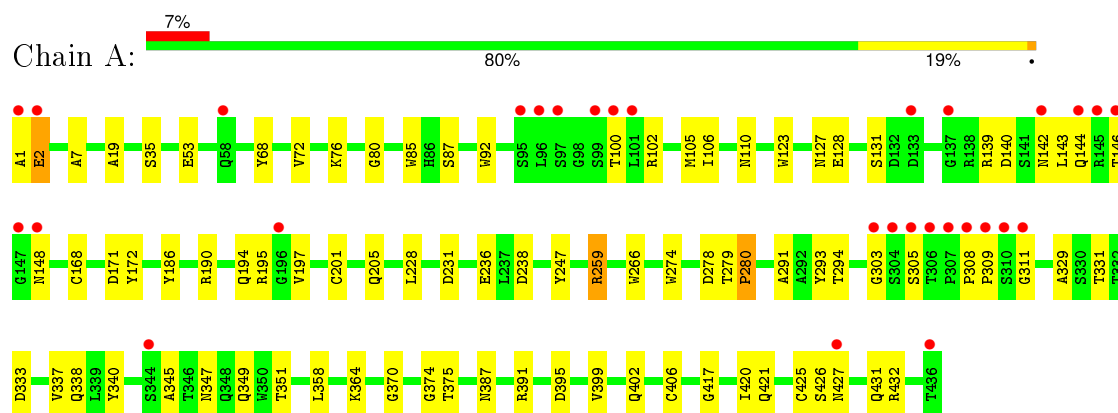
- Molecule 5 is water.

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

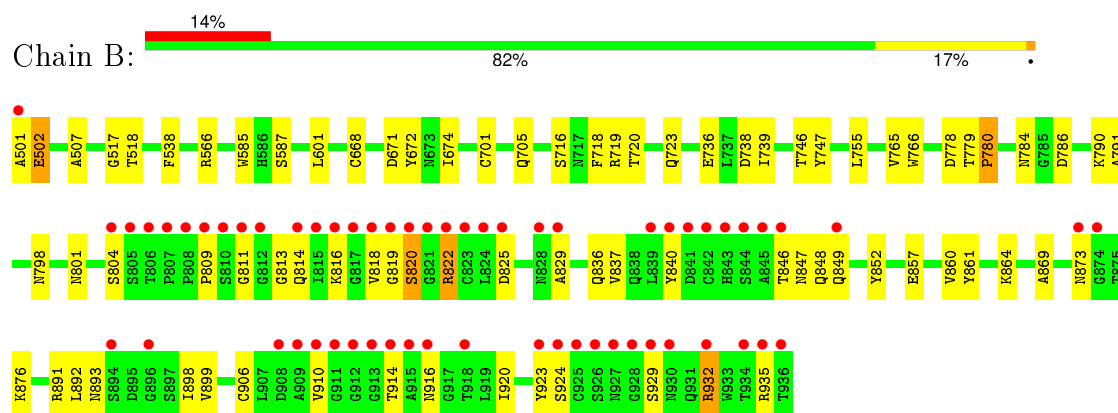
### 3 Residue-property plots [i](#)

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



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



## 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 0.202 , 0.247	Depositor DCC
$R_{free}$ test set	5211 reflections (10.13%)	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> )	0.38 , 62.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	2 of 58491 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.95	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.

<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

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 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	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
All	All	7562	0	6345	144	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 11.

All (144) 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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:190:ARG:NH1	1:A:190:ARG:HB3	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	Interatomic distance (Å)	Clash overlap (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 [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	438/436 (100%)	418 (95%)	20 (5%)	0	100	100
1	B	438/436 (100%)	416 (95%)	19 (4%)	3 (1%)	26	21
All	All	876/872 (100%)	834 (95%)	39 (4%)	3 (0%)	46	45

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	502	GLU
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%)	63	68
1	B	345/341 (101%)	337 (98%)	8 (2%)	58	62
All	All	690/682 (101%)	675 (98%)	15 (2%)	65	64

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

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Mol	Chain	Res	Type
1	A	110	ASN
1	A	173	ASN
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 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 ⓘ

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	9,9,10	0.67	0	12,12,14	0.89	1 (8%)
2	XYP	A	451	2	9,9,10	0.67	0	12,12,14	0.87	1 (8%)
2	XYP	A	452	2	10,10,10	0.50	0	12,14,14	0.69	0
3	XYP	A	456	3	9,9,10	0.85	0	12,12,14	0.83	1 (8%)
3	XYP	A	457	3	10,10,10	0.56	0	12,14,14	0.65	0
3	XYP	A	471	3	9,9,10	0.77	0	12,12,14	0.90	1 (8%)
3	XYP	A	472	3	10,10,10	0.61	0	12,14,14	0.66	0
2	XYP	B	950	2	9,9,10	0.64	0	12,12,14	0.90	1 (8%)
2	XYP	B	951	2	9,9,10	0.65	0	12,12,14	0.86	1 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	XYP	B	952	2	10,10,10	0.50	0	12,14,14	0.70	0
2	XYP	B	956	2	9,9,10	1.02	0	12,12,14	0.82	1 (8%)
2	XYP	B	957	2	9,9,10	0.64	0	12,12,14	1.00	1 (8%)
2	XYP	B	958	2	10,10,10	0.60	0	12,14,14	0.66	0
3	XYP	B	970	3	9,9,10	0.74	0	12,12,14	0.88	1 (8%)
3	XYP	B	971	3	10,10,10	0.62	0	12,14,14	0.64	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.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	957	XYP	C4B-C3B-C2B	-3.10	108.18	111.24
2	B	950	XYP	C4B-C3B-C2B	-2.95	108.32	111.24
3	A	471	XYP	C4B-C3B-C2B	-2.91	108.36	111.24
2	A	450	XYP	C4B-C3B-C2B	-2.90	108.37	111.24
3	B	970	XYP	C4B-C3B-C2B	-2.90	108.37	111.24
2	A	451	XYP	C4B-C3B-C2B	-2.83	108.44	111.24
2	B	951	XYP	C4B-C3B-C2B	-2.78	108.49	111.24
3	A	456	XYP	C4B-C3B-C2B	-2.66	108.61	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	956	XYP	C4B-C3B-C2B	-2.57	108.70	111.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	452	XYP	4	0
3	A	456	XYP	3	0
3	A	472	XYP	1	0
2	B	952	XYP	6	0
2	B	956	XYP	4	0
3	B	970	XYP	1	0
3	B	971	XYP	1	0

## 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	12,14,14	0.65	0
4	XYP	B	961	-	10,10,10	0.67	0	12,14,14	0.64	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.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1461	XYP	3	0
4	B	961	XYP	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	436/436 (100%)	0.51	30 (6%) 20 27	12, 22, 44, 83	0
1	B	436/436 (100%)	0.68	59 (13%) 4 6	12, 20, 65, 77	0
All	All	872/872 (100%)	0.60	89 (10%) 9 12	12, 21, 59, 83	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	306	THR	12.4
1	A	305	SER	9.7
1	B	819	GLY	9.3
1	A	304	SER	8.6
1	B	845	ALA	7.7
1	A	303	GLY	7.3
1	B	923	TYR	7.2
1	B	936	THR	7.2
1	B	810	SER	6.9
1	B	915	ALA	6.9
1	B	805	SER	6.8
1	B	823	CYS	6.4
1	B	844	SER	6.4
1	B	809	PRO	6.2
1	B	926	SER	6.1
1	A	308	PRO	6.1
1	A	311	GLY	5.7
1	B	822	ARG	5.6
1	B	820	SER	5.6
1	B	807	PRO	5.6
1	A	307	PRO	5.6
1	B	839	LEU	5.5
1	B	928	GLY	5.3
1	B	806	THR	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	840	TYR	5.0
1	B	501	ALA	4.9
1	B	911	GLY	4.9
1	A	309	PRO	4.7
1	B	929	SER	4.7
1	B	818	VAL	4.6
1	B	925	CYS	4.6
1	B	927	ASN	4.6
1	A	100	THR	4.6
1	B	829	ALA	4.5
1	B	817	GLY	4.5
1	B	843	HIS	4.3
1	B	932	ARG	4.3
1	B	808	PRO	4.2
1	B	814	GLN	4.2
1	B	811	GLY	4.1
1	B	842	CYS	4.1
1	A	436	THR	4.1
1	B	918	THR	4.0
1	A	310	SER	4.0
1	A	97	SER	3.9
1	B	841	ASP	3.7
1	B	828	ASN	3.6
1	A	133	ASP	3.6
1	B	930	ASN	3.5
1	B	934	THR	3.5
1	A	95	SER	3.4
1	B	874	GLY	3.3
1	B	816	LYS	3.3
1	B	914	THR	3.3
1	B	846	THR	3.3
1	B	894	SER	3.2
1	B	912	GLY	3.1
1	B	935	ARG	3.1
1	A	137	GLY	3.1
1	A	147	GLY	3.0
1	B	824	LEU	3.0
1	A	344	SER	3.0
1	B	873	ASN	3.0
1	B	910	VAL	2.9
1	B	916	ASN	2.8
1	B	909	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	2	GLU	2.7
1	B	913	GLY	2.7
1	A	142	ASN	2.6
1	A	146	THR	2.6
1	B	815	ILE	2.6
1	A	144	GLN	2.5
1	B	924	SER	2.5
1	B	812	GLY	2.4
1	A	148	ASN	2.4
1	A	145	ARG	2.4
1	A	1	ALA	2.4
1	B	849	GLN	2.3
1	A	96	LEU	2.3
1	B	896	GLY	2.3
1	B	825	ASP	2.2
1	A	101	LEU	2.2
1	B	821	GLY	2.2
1	A	99	SER	2.1
1	B	804	SER	2.0
1	A	427	ASN	2.0
1	A	58	GLN	2.0
1	A	196	GLY	2.0
1	B	908	ASP	2.0

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

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

## 6.3 Carbohydrates [i](#)

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
3	XYP	A	456	9/10	0.80	0.23	6.07	48,50,52,52	0
2	XYP	B	957	9/10	0.78	0.20	5.00	33,34,36,37	0
3	XYP	A	472	10/10	0.77	0.26	4.57	34,42,45,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	XYP	A	452	10/10	0.84	0.24	4.01	25,28,35,40	0
2	XYP	B	956	9/10	0.79	0.18	3.92	27,29,32,32	0
3	XYP	A	471	9/10	0.84	0.20	3.47	23,24,28,29	0
2	XYP	B	952	10/10	0.90	0.18	3.25	16,19,25,35	0
3	XYP	A	457	10/10	0.83	0.23	2.87	46,48,49,50	0
2	XYP	B	958	10/10	0.85	0.27	2.83	42,48,52,52	0
3	XYP	B	971	10/10	0.81	0.39	1.15	60,61,61,62	0
2	XYP	A	451	9/10	0.93	0.15	0.04	21,23,26,28	0
2	XYP	B	951	9/10	0.95	0.11	-0.29	16,16,19,24	0
3	XYP	B	970	9/10	0.66	0.34	-	59,60,60,60	0
2	XYP	B	950	9/10	0.81	0.27	-	32,36,41,42	0
2	XYP	A	450	9/10	0.89	0.15	-	33,36,39,40	0

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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( $\text{\AA}^2$ )	Q<0.9
4	XYP	A	1461	10/10	0.95	0.13	0.01	29,30,31,31	0
4	XYP	B	961	10/10	0.78	0.22	-0.74	62,63,63,63	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.