



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:25 AM GMT

PDB ID : 2D24  
Title : Crystal structure of ES complex of catalytic-site mutant xylanase from *Streptomyces olivaceoviridis* E-86  
Authors : Suzuki, R.; Kuno, A.; Fujimoto, Z.; Ito, S.; Kawahara, S.I.; Kaneko, S.; Hasegawa, T.; Taira, K.  
Deposited on : 2005-09-02  
Resolution : 1.85 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

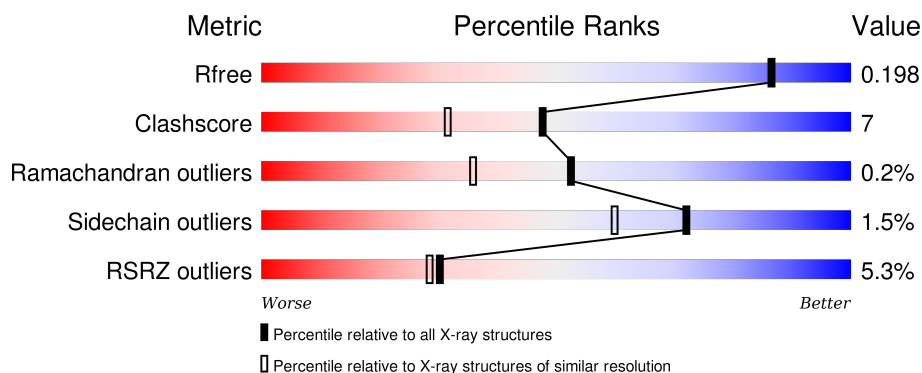
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

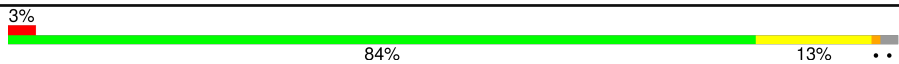
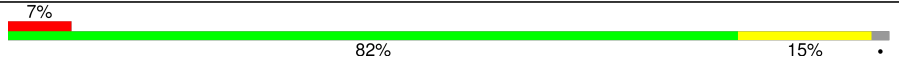
The reported resolution of this entry is 1.85 Å.

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	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

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	 3% 84% 13% ..
1	B	436	 7% 82% 15% .

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	XYS	A	451	X	-	-	-
2	XYS	A	452	X	-	-	-
2	XYS	A	453	X	-	-	-
2	XYS	A	454	X	-	-	-
2	XYS	A	455	X	-	-	-
2	XYS	B	951	X	-	-	-
2	XYS	B	952	X	-	-	-
2	XYS	B	953	X	-	-	X
2	XYS	B	954	X	-	-	-
2	XYS	B	955	X	-	-	X
3	XYS	A	456	X	-	-	-
3	XYS	A	457	X	-	-	X
3	XYS	A	458	X	-	-	-
3	XYS	A	459	X	-	-	X
4	XYS	A	956	X	-	-	X
4	XYS	A	957	X	-	-	X
4	XYS	B	958	X	-	-	-
4	XYS	B	959	X	-	-	-
6	GOL	B	980	-	-	-	X
6	GOL	B	982	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7333 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	427	Total	C	N	O	S	0	0	0
			3233	1988	588	641	16			
1	B	427	Total	C	N	O	S	0	0	0
			3233	1988	588	641	16			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	127	SER	ASN	ENGINEERED MUTATION	UNP Q7SI98
A	128	HIS	GLU	ENGINEERED MUTATION	UNP Q7SI98
B	627	SER	ASN	ENGINEERED MUTATION	UNP Q7SI98
B	628	HIS	GLU	ENGINEERED MUTATION	UNP Q7SI98

- Molecule 2 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	5	Total	C	O	0	0
			46	25	21		
2	B	5	Total	C	O	0	0
			46	25	21		

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

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

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

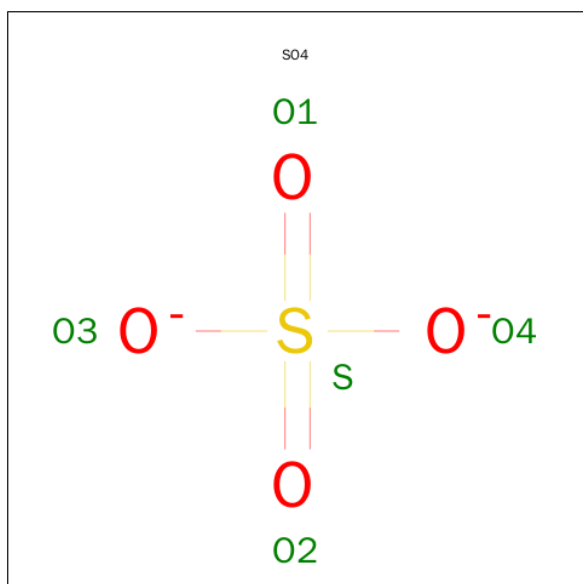
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	2	Total	C	O	0	0
			19	10	9		

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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	318	Total	O	0	0
			318	318		
7	B	354	Total	O	0	0
			354	354		

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.

Chain A:

Chain B:

Segment	Color	Percentage	Labels
1	Red	7%	A501
2	Green	82%	E502, A507, R556, R566, G580, W585, T600, L601, W623, S627, N670, D671, Y672
3	Yellow	15%	W679, Q705, S710, R719, Q723, I734, D738, I739, T746, Y747, I763, S773, W774, R775, S776, T777, D778, T779, P780, I784, G785, D786, T794
4	Grey	4%	N804

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.70 Å 94.09 Å 138.37 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.51 – 1.85 36.51 – 1.85	Depositor EDS
% Data completeness (in resolution range)	(Not available) (36.51-1.85) 99.9 (36.51-1.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	8.21 (at 1.85 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.177 , 0.199 0.177 , 0.198	Depositor DCC
$R_{free}$ test set	4309 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	14.1	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 53.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 84968 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7333	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% 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: GOL, XYS, SO4

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	0/3298	0.61	0/4473
1	B	0.30	0/3298	0.61	0/4473
All	All	0.30	0/6596	0.61	0/8946

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	5	0
2	B	5	0
3	A	4	0
4	A	2	0
4	B	2	0
All	All	18	0

There are no bond length outliers.

There are no bond angle outliers.

All (18) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	455	XYS	C1
2	A	454	XYS	C1
2	A	453	XYS	C1
2	A	452	XYS	C1
2	A	451	XYS	C1
3	A	459	XYS	C1
3	A	458	XYS	C1
3	A	457	XYS	C1

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Mol	Chain	Res	Type	Atom
3	A	456	XYS	C1
4	A	957	XYS	C1
4	A	956	XYS	C1
2	B	955	XYS	C1
2	B	954	XYS	C1
2	B	953	XYS	C1
2	B	952	XYS	C1
2	B	951	XYS	C1
4	B	959	XYS	C1
4	B	958	XYS	C1

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	3233	0	3043	43	0
1	B	3233	0	3040	50	0
2	A	46	0	38	1	0
2	B	46	0	38	1	0
3	A	37	0	31	2	0
4	A	19	0	17	4	0
4	B	19	0	17	1	0
5	A	10	0	0	0	0
6	B	18	0	24	0	0
7	A	318	0	0	3	0
7	B	354	0	0	3	0
All	All	7333	0	6248	95	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 7.

All (95) 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:935:ARG:HA	1:B:936:THR:HB	1.45	0.96
1:B:836:GLN:HB2	1:B:876:LYS:HE3	1.59	0.84
1:A:1:ALA:HB1	7:A:1194:HOH:O	1.85	0.77
1:B:926:SER:O	1:B:927:ASN:HB2	1.87	0.73
1:A:340:TYR:CZ	4:A:957:XYS:H52	2.24	0.71
1:B:816:LYS:HG2	1:B:823:CYS:SG	2.34	0.68
1:A:2:GLU:HB2	1:A:301:ASN:OD1	1.94	0.67
1:A:54:PRO:HB2	1:A:55:GLN:NE2	2.10	0.66
3:A:457:XYS:H4	3:A:456:XYS:O2	1.95	0.65
1:B:816:LYS:HE2	1:B:936:THR:HG21	1.80	0.64
1:A:336:GLN:HB2	1:A:376:LYS:HE3	1.79	0.64
1:B:501:ALA:N	1:B:507:ALA:HB1	2.12	0.63
1:B:935:ARG:CA	1:B:936:THR:HB	2.25	0.62
1:A:340:TYR:CE2	4:A:957:XYS:H1	2.34	0.62
1:A:54:PRO:HB2	1:A:55:GLN:HE22	1.64	0.61
1:A:234:ILE:HD12	1:A:263:ILE:HG12	1.82	0.61
1:A:176:ASN:HB3	1:A:179:TRP:CD2	2.35	0.61
1:A:238:ASP:HB2	1:A:280:PRO:HB2	1.82	0.61
1:B:502:GLU:HG3	1:B:801:ASN:OD1	2.01	0.60
1:A:1:ALA:HB3	1:A:7:ALA:HB1	1.83	0.60
1:A:97:SER:O	1:A:100:THR:HG22	2.04	0.58
1:B:855:ALA:O	1:B:889:LYS:HD2	2.04	0.57
1:B:822:ARG:HE	1:B:915:ALA:HA	1.70	0.57
1:A:294:THR:OG1	1:A:391:ARG:HD2	2.05	0.56
1:A:190:ARG:O	1:A:194:GLN:HG3	2.06	0.56
1:B:501:ALA:HB3	7:B:1062:HOH:O	2.05	0.55
1:B:831:THR:O	1:B:831:THR:HG22	2.05	0.55
1:A:337:VAL:HG23	1:A:420:ILE:HB	1.88	0.55
1:B:679:TRP:HE3	7:B:1064:HOH:O	1.89	0.54
1:B:738:ASP:HB2	1:B:780:PRO:HB2	1.89	0.54
1:B:903:SER:HB2	1:B:905:LEU:HD13	1.89	0.53
1:A:376:LYS:HE2	1:A:378:GLN:OE1	2.08	0.53
1:B:822:ARG:HG2	1:B:822:ARG:HH11	1.73	0.53
4:A:957:XYS:H51	4:A:956:XYS:O2	2.08	0.53
1:B:779:THR:N	1:B:780:PRO:HD3	2.24	0.52
1:A:426:SER:O	1:A:427:ASN:HB2	2.10	0.52
1:B:778:ASP:O	1:B:779:THR:C	2.48	0.52
1:A:279:THR:N	1:A:280:PRO:HD3	2.25	0.52
1:B:719:ARG:O	1:B:723:GLN:HG3	2.10	0.51
1:A:278:ASP:O	1:A:279:THR:C	2.48	0.51
1:A:55:GLN:HB2	1:A:58:GLN:HB2	1.91	0.51
1:A:128:HIS:HE1	1:A:205:GLN:OE1	1.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:TYR:CE1	4:A:957:XY5:H52	2.45	0.50
1:B:910:VAL:HA	1:B:921:GLN:NE2	2.27	0.50
1:B:773:SER:OG	1:B:776:SER:HA	2.12	0.49
1:B:837:VAL:HG23	1:B:920:ILE:HB	1.95	0.48
1:B:774:TRP:CH2	2:B:953:XY5:H4	2.49	0.48
1:A:236:GLU:HG2	1:A:266:TRP:CE3	2.49	0.48
1:B:627:SER:HA	1:B:670:ASN:O	2.13	0.47
1:A:127:SER:HA	1:A:170:ASN:O	2.14	0.47
1:B:935:ARG:HH11	1:B:935:ARG:HG2	1.79	0.47
1:A:128:HIS:CE1	1:A:205:GLN:OE1	2.67	0.47
1:B:734:ILE:HD12	1:B:763:ILE:HG12	1.97	0.47
1:A:141:SER:O	1:A:145:ARG:HG3	2.15	0.47
1:B:814:GLN:OE1	1:B:842:CYS:HB3	2.15	0.46
1:B:818:VAL:O	1:B:929:SER:HB2	2.15	0.46
1:B:502:GLU:O	1:B:502:GLU:HG2	2.15	0.46
1:B:874:GLY:HA2	1:B:921:GLN:OE1	2.16	0.46
1:B:556:ARG:HH12	1:B:600:THR:HG22	1.81	0.46
1:A:168:CYS:HA	1:A:201:CYS:O	2.16	0.46
1:B:784:ASN:OD1	1:B:786:ASP:OD1	2.34	0.45
1:A:403:SER:HB2	1:A:405:LEU:HD13	1.97	0.45
1:A:128:HIS:HD2	7:A:1106:HOH:O	1.99	0.45
1:B:822:ARG:NH1	1:B:841:ASP:OD1	2.50	0.45
1:B:739:ILE:HD13	1:B:746:THR:HG22	1.99	0.44
1:A:142:ASN:O	1:A:146:THR:HG23	2.17	0.44
1:B:869:ALA:HB2	1:B:878:GLN:HE22	1.83	0.44
1:B:899:VAL:HG22	1:B:906:CYS:SG	2.58	0.43
1:A:435:ARG:HG3	1:A:435:ARG:HH11	1.82	0.43
1:A:378:GLN:NE2	1:B:710:SER:HB2	2.33	0.43
1:A:358:LEU:HD23	1:A:358:LEU:HA	1.91	0.43
1:A:27:ASP:HB3	1:A:30:TYR:HB3	2.00	0.43
1:A:68:TYR:OH	1:A:119:LYS:HB3	2.17	0.43
1:A:172:TYR:HB3	1:A:205:GLN:NE2	2.33	0.43
1:B:566:ARG:NH2	7:B:1033:HOH:O	2.43	0.43
1:A:374:GLY:HA2	1:A:421:GLN:OE1	2.19	0.43
3:A:458:XY5:H52	7:A:1272:HOH:O	2.19	0.43
1:A:274:TRP:CH2	2:A:453:XY5:H4	2.54	0.43
1:B:794:THR:OG1	1:B:891:ARG:HD2	2.19	0.43
1:B:672:TYR:HB3	1:B:705:GLN:NE2	2.34	0.43
1:B:556:ARG:HH12	1:B:600:THR:CG2	2.32	0.42
1:B:580:GLY:HA3	1:B:623:TRP:CE3	2.55	0.42
1:B:816:LYS:CE	1:B:936:THR:HG21	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:GLY:HA3	1:A:123:TRP:CE3	2.55	0.42
1:A:425:CYS:HA	1:A:431:GLN:OE1	2.20	0.42
1:B:840:TYR:CD1	1:B:916:ASN:HB3	2.55	0.41
1:B:840:TYR:HA	1:B:916:ASN:OD1	2.20	0.41
1:B:926:SER:O	1:B:927:ASN:CB	2.64	0.41
1:B:822:ARG:NH1	1:B:822:ARG:HG2	2.36	0.41
1:B:923:TYR:CZ	4:B:959:XY5:H52	2.55	0.41
1:B:828:ASN:N	1:B:828:ASN:ND2	2.69	0.41
1:A:236:GLU:HG2	1:A:266:TRP:CZ3	2.56	0.40
1:A:329:ALA:HA	1:A:347:ASN:HB3	2.03	0.40
1:A:435:ARG:N	1:A:435:ARG:HD3	2.37	0.40
1:B:828:ASN:N	1:B:828:ASN:HD22	2.19	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	423/436 (97%)	410 (97%)	13 (3%)	0	100	100
1	B	423/436 (97%)	406 (96%)	15 (4%)	2 (0%)	34	17
All	All	846/872 (97%)	816 (96%)	28 (3%)	2 (0%)	52	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	927	ASN
1	B	844	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	334/341 (98%)	329 (98%)	5 (2%)	72	60
1	B	334/341 (98%)	329 (98%)	5 (2%)	72	60
All	All	668/682 (98%)	658 (98%)	10 (2%)	72	60

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	TRP
1	A	128	HIS
1	A	247	TYR
1	A	280	PRO
1	A	435	ARG
1	B	585	TRP
1	B	601	LEU
1	B	747	TYR
1	B	780	PRO
1	B	927	ASN

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

Mol	Chain	Res	Type
1	A	55	GLN
1	A	60	ASN
1	A	128	HIS
1	A	205	GLN
1	A	343	HIS
1	A	349	GLN
1	B	511	GLN
1	B	628	HIS
1	B	705	GLN
1	B	828	ASN
1	B	849	GLN
1	B	927	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 ⓘ

18 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	XYS	A	451	2	9,9,10	0.69	0	12,12,14	0.84	1 (8%)
2	XYS	A	452	2	9,9,10	1.86	2 (22%)	12,12,14	1.97	3 (25%)
2	XYS	A	453	2	9,9,10	0.98	0	12,12,14	1.13	1 (8%)
2	XYS	A	454	2	9,9,10	0.79	0	12,12,14	1.03	1 (8%)
2	XYS	A	455	2	10,10,10	0.56	0	12,14,14	0.67	0
3	XYS	A	456	3	9,9,10	0.66	0	12,12,14	0.94	1 (8%)
3	XYS	A	457	3	9,9,10	0.72	0	12,12,14	0.84	1 (8%)
3	XYS	A	458	3	9,9,10	0.64	0	12,12,14	0.90	1 (8%)
3	XYS	A	459	3	10,10,10	0.59	0	12,14,14	0.68	0
4	XYS	A	956	4	9,9,10	0.70	0	12,12,14	0.94	1 (8%)
4	XYS	A	957	4	10,10,10	0.56	0	12,14,14	0.68	0
2	XYS	B	951	2	9,9,10	0.62	0	12,12,14	0.87	1 (8%)
2	XYS	B	952	2	9,9,10	1.89	3 (33%)	12,12,14	2.01	3 (25%)
2	XYS	B	953	2	9,9,10	1.00	1 (11%)	12,12,14	1.14	2 (16%)
2	XYS	B	954	2	9,9,10	0.84	0	12,12,14	1.15	1 (8%)
2	XYS	B	955	2	10,10,10	0.50	0	12,14,14	0.73	1 (8%)
4	XYS	B	958	4	9,9,10	0.64	0	12,12,14	0.94	1 (8%)
4	XYS	B	959	4	10,10,10	0.52	0	12,14,14	0.67	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	XYS	A	451	2	1/1/3/4	0/0/14/17	0/1/1/1
2	XYS	A	452	2	1/1/3/4	0/0/14/17	1/1/1/1
2	XYS	A	453	2	1/1/3/4	0/0/14/17	0/1/1/1
2	XYS	A	454	2	1/1/3/4	0/0/14/17	0/1/1/1
2	XYS	A	455	2	1/1/4/4	0/0/17/17	0/1/1/1
3	XYS	A	456	3	1/1/3/4	0/0/14/17	0/1/1/1
3	XYS	A	457	3	1/1/3/4	0/0/14/17	0/1/1/1
3	XYS	A	458	3	1/1/3/4	0/0/14/17	0/1/1/1
3	XYS	A	459	3	1/1/4/4	0/0/17/17	0/1/1/1
4	XYS	A	956	4	1/1/3/4	0/0/14/17	0/1/1/1
4	XYS	A	957	4	1/1/4/4	0/0/17/17	0/1/1/1
2	XYS	B	951	2	1/1/3/4	0/0/14/17	0/1/1/1
2	XYS	B	952	2	1/1/3/4	0/0/14/17	1/1/1/1
2	XYS	B	953	2	1/1/3/4	0/0/14/17	0/1/1/1
2	XYS	B	954	2	1/1/3/4	0/0/14/17	0/1/1/1
2	XYS	B	955	2	1/1/4/4	0/0/17/17	0/1/1/1
4	XYS	B	958	4	1/1/3/4	0/0/14/17	0/1/1/1
4	XYS	B	959	4	1/1/4/4	0/0/17/17	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	953	XYS	O5-C5	2.01	1.46	1.42
2	B	952	XYS	C5-C4	2.04	1.57	1.52
2	A	452	XYS	O5-C5	2.49	1.47	1.42
2	B	952	XYS	O5-C5	2.49	1.47	1.42
2	B	952	XYS	C2-C3	3.59	1.57	1.52
2	A	452	XYS	C2-C3	3.61	1.57	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	952	XYS	C4-C3-C2	-4.45	106.84	111.24
2	A	452	XYS	C4-C3-C2	-4.35	106.94	111.24
2	A	452	XYS	C5-C4-C3	-3.90	104.93	109.54
2	B	952	XYS	C5-C4-C3	-3.81	105.03	109.54
4	B	958	XYS	C4-C3-C2	-3.04	108.24	111.24
3	A	456	XYS	C4-C3-C2	-2.93	108.34	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	956	XYS	C4-C3-C2	-2.88	108.39	111.24
2	B	954	XYS	C4-C3-C2	-2.86	108.41	111.24
3	A	458	XYS	C4-C3-C2	-2.85	108.42	111.24
2	A	453	XYS	C4-C3-C2	-2.81	108.46	111.24
2	B	951	XYS	C4-C3-C2	-2.68	108.59	111.24
2	A	451	XYS	C4-C3-C2	-2.55	108.72	111.24
2	B	953	XYS	C4-C3-C2	-2.40	108.87	111.24
2	A	454	XYS	C4-C3-C2	-2.29	108.98	111.24
3	A	457	XYS	C4-C3-C2	-2.26	109.00	111.24
2	B	955	XYS	C4-C3-C2	-2.03	107.60	111.04
2	B	953	XYS	O4-C4-C5	2.11	113.43	109.21
2	A	452	XYS	C1-C2-C3	2.18	112.12	109.54
2	B	952	XYS	C1-C2-C3	2.41	112.39	109.54

All (18) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	951	XYS	C1
3	A	459	XYS	C1
3	A	456	XYS	C1
2	A	455	XYS	C1
2	A	452	XYS	C1
4	B	959	XYS	C1
3	A	458	XYS	C1
2	A	451	XYS	C1
2	B	954	XYS	C1
2	A	454	XYS	C1
4	A	956	XYS	C1
2	B	953	XYS	C1
3	A	457	XYS	C1
4	B	958	XYS	C1
2	A	453	XYS	C1
2	B	952	XYS	C1
2	B	955	XYS	C1
4	A	957	XYS	C1

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	952	XYS	C1-C2-C3-C4-C5-O5
2	A	452	XYS	C1-C2-C3-C4-C5-O5

8 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	453	XYS	1	0
3	A	456	XYS	1	0
3	A	457	XYS	1	0
3	A	458	XYS	1	0
4	A	956	XYS	1	0
4	A	957	XYS	4	0
2	B	953	XYS	1	0
4	B	959	XYS	1	0

## 5.6 Ligand geometry [i](#)

5 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	$\# Z  > 2$
5	SO4	A	970	-	4,4,4	0.22	0	6,6,6	0.08	0
5	SO4	A	971	-	4,4,4	0.22	0	6,6,6	0.10	0
6	GOL	B	980	-	5,5,5	0.16	0	5,5,5	0.30	0
6	GOL	B	981	-	5,5,5	0.14	0	5,5,5	0.30	0
6	GOL	B	982	-	5,5,5	0.17	0	5,5,5	0.30	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	SO4	A	970	-	-	0/0/0/0	0/0/0/0
5	SO4	A	971	-	-	0/0/0/0	0/0/0/0
6	GOL	B	980	-	-	0/4/4/4	0/0/0/0
6	GOL	B	981	-	-	0/4/4/4	0/0/0/0
6	GOL	B	982	-	-	0/4/4/4	0/0/0/0

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.

No monomer is involved in short contacts.

## 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	427/436 (97%)	0.06	14 (3%) 50 47	8, 14, 27, 46	0
1	B	427/436 (97%)	0.15	31 (7%) 18 17	6, 12, 38, 54	0
All	All	854/872 (97%)	0.10	45 (5%) 30 28	6, 13, 32, 54	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	936	THR	7.4
1	A	303	GLY	7.3
1	B	818	VAL	7.2
1	B	501	ALA	6.0
1	A	1	ALA	5.6
1	B	844	SER	5.3
1	A	436	THR	5.2
1	B	927	ASN	4.7
1	B	846	THR	4.0
1	B	822	ARG	4.0
1	B	845	ALA	3.7
1	B	911	GLY	3.7
1	B	935	ARG	3.6
1	B	934	THR	3.4
1	B	820	SER	3.4
1	B	926	SER	3.4
1	A	435	ARG	3.3
1	B	923	TYR	3.3
1	A	26	GLY	3.2
1	A	427	ASN	3.1
1	B	840	TYR	3.0
1	B	915	ALA	2.9
1	B	843	HIS	2.9
1	B	816	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	140	ASP	2.7
1	A	145	ARG	2.7
1	B	932	ARG	2.7
1	B	842	CYS	2.7
1	B	817	GLY	2.7
1	A	344	SER	2.6
1	B	849	GLN	2.6
1	B	928	GLY	2.5
1	A	137	GLY	2.5
1	B	803	GLY	2.5
1	B	823	CYS	2.4
1	B	839	LEU	2.4
1	B	910	VAL	2.3
1	B	814	GLN	2.2
1	A	394	SER	2.2
1	B	828	ASN	2.2
1	A	58	GLN	2.1
1	A	97	SER	2.1
1	B	924	SER	2.0
1	A	55	GLN	2.0
1	B	841	ASP	2.0

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

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

## 6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	XYS	A	956	9/10	0.52	0.53	12.84	40,42,44,45	0
3	XYS	A	457	9/10	0.65	0.24	8.52	31,34,39,45	0
2	XYS	B	955	10/10	0.71	0.35	3.59	22,36,41,43	0
4	XYS	A	957	10/10	0.85	0.18	3.01	21,28,31,33	0
2	XYS	B	953	9/10	0.92	0.14	2.97	13,13,15,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	XYS	A	459	10/10	0.83	0.16	2.03	26,29,31,35	0
2	XYS	A	453	9/10	0.90	0.14	1.79	16,19,20,21	0
2	XYS	A	452	9/10	0.94	0.14	1.40	12,13,16,16	0
2	XYS	A	454	9/10	0.93	0.14	1.03	18,20,22,24	0
3	XYS	A	458	9/10	0.95	0.10	0.67	17,21,23,26	0
2	XYS	B	951	9/10	0.97	0.09	0.64	8,9,10,12	0
2	XYS	B	952	9/10	0.95	0.10	0.58	7,11,13,13	0
4	XYS	B	959	10/10	0.75	0.22	0.50	42,44,46,47	0
2	XYS	B	954	9/10	0.96	0.10	0.25	12,13,16,18	0
2	XYS	A	451	9/10	0.96	0.11	-0.29	12,13,14,14	0
3	XYS	A	456	9/10	0.52	0.60	-	50,54,55,55	0
4	XYS	B	958	9/10	0.78	0.26	-	48,49,50,50	0
2	XYS	A	455	10/10	0.73	0.38	-	29,40,43,44	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
6	GOL	B	982	6/6	0.68	0.22	7.48	41,43,43,43	0
6	GOL	B	980	6/6	0.69	0.19	6.83	34,35,35,35	0
6	GOL	B	981	6/6	0.61	0.16	-0.55	42,43,43,44	0
5	SO4	A	970	5/5	0.73	0.34	-	77,77,78,78	0
5	SO4	A	971	5/5	0.90	0.23	-	56,56,56,56	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.