



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 02:34 PM 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 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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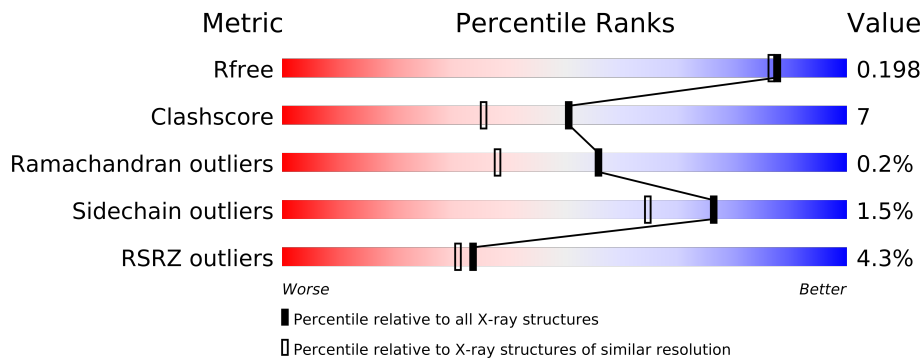
The following versions of software and data (see [references](#)) were used in the production of this report:

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 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))
$R_{free}$	66092	1269 (1.86-1.86)
Clashscore	79885	1470 (1.86-1.86)
Ramachandran outliers	78287	1451 (1.86-1.86)
Sidechain outliers	78261	1451 (1.86-1.86)
RSRZ outliers	66119	1269 (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. 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	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	SO4	A	970	-	X
5	SO4	A	971	-	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 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	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		

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 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		

There are 2 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

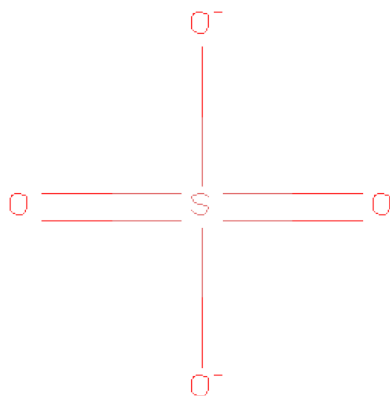
- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

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

There are 4 discrepancies between the modelled and reference sequences:

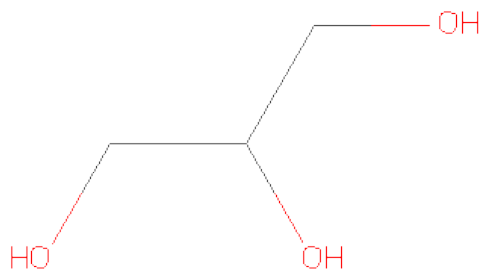
Chain	Residue	Modelled	Actual	Comment	Reference
A	127	SER	ASN	ENGINEERED MUTATION	UNP Q7SI98
A	128	HIS	GLU	ENGINEERED MUTATION	UNP Q7SI98
B	627	SER	ASN	ENGINEERED MUTATION	UNP Q7SI98
B	628	HIS	GLU	ENGINEERED MUTATION	UNP Q7SI98

- Molecule 5 is SULFATE ION (three-letter code: SO<sub>4</sub>) (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:  $C_3H_8O_3$ ).



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		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.70Å 94.09Å 138.37Å 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 1.85Å)	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> )	0.42 , 39.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	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.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, YYS, 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	YYS	C1
2	A	454	YYS	C1
2	A	453	YYS	C1
2	A	452	YYS	C1
2	A	451	YYS	C1
3	A	459	YYS	C1
3	A	458	YYS	C1
3	A	457	YYS	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 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	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

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 7.

All (95) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
1:A:340:TYR:CE1	4:A:957:XYS:H52	2.45	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:XYS: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:XYS:H52	7:A:1272:HOH:O	2.19	0.43
1:A:274:TRP:CH2	2:A:453:XYS: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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:XYS: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%)	38	19
All	All	846/872 (97%)	816 (96%)	28 (3%)	2 (0%)	56	38

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%)	76	65
1	B	334/341 (98%)	329 (98%)	5 (2%)	76	65
All	All	668/682 (98%)	658 (98%)	10 (2%)	76	65

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 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 ⓘ

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	8,9,10	0.56	0	8,12,14	0.73	0
2	XYS	A	452	2	8,9,10	1.46	1 (12%)	8,12,14	1.71	2 (25%)
2	XYS	A	453	2	8,9,10	0.88	0	8,12,14	1.14	0
2	XYS	A	454	2	8,9,10	0.73	0	8,12,14	0.96	0
2	XYS	A	455	2	10,10,10	0.56	0	14,14,14	0.63	0
3	XYS	A	456	3	8,9,10	0.55	0	8,12,14	0.78	0
3	XYS	A	457	3	8,9,10	0.64	0	8,12,14	0.67	0
3	XYS	A	458	3	8,9,10	0.53	0	8,12,14	0.73	0
3	XYS	A	459	3	10,10,10	0.59	0	14,14,14	0.65	0
4	XYS	A	956	4	8,9,10	0.53	0	8,12,14	0.76	0
4	XYS	A	957	4	10,10,10	0.56	0	14,14,14	0.64	0
2	XYS	B	951	2	8,9,10	0.53	0	8,12,14	0.75	0
2	XYS	B	952	2	8,9,10	1.47	1 (12%)	8,12,14	1.70	2 (25%)
2	XYS	B	953	2	8,9,10	0.91	0	8,12,14	1.21	1 (12%)
2	XYS	B	954	2	8,9,10	0.78	0	8,12,14	1.01	0
2	XYS	B	955	2	10,10,10	0.50	0	14,14,14	0.67	0
4	XYS	B	958	4	8,9,10	0.54	0	8,12,14	0.76	0
4	XYS	B	959	4	10,10,10	0.52	0	14,14,14	0.62	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	452	XYS	C3-C2	2.07	1.57	1.52
2	B	952	XYS	C3-C2	2.06	1.57	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	452	XYS	C5-C4-C3	-3.80	104.93	109.71
2	B	952	XYS	C5-C4-C3	-3.71	105.03	109.71
2	B	952	XYS	C4-C3-C2	-2.55	106.84	110.53
2	A	452	XYS	C4-C3-C2	-2.48	106.94	110.53
2	B	953	XYS	O4-C4-C5	2.07	113.43	109.14

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

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

## 5.6 Ligand geometry

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	0.26	0	6,6,6	0.07	0
5	SO4	A	971	-	4,4,4	0.26	0	6,6,6	0.08	0
6	GOL	B	980	-	5,5,5	0.16	0	5,5,5	0.29	0
6	GOL	B	981	-	5,5,5	0.15	0	5,5,5	0.28	0
6	GOL	B	982	-	5,5,5	0.18	0	5,5,5	0.27	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.

## 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%)	-0.02	10 (2%) 57 56	8, 14, 27, 46	0
1	B	427/436 (97%)	0.06	25 (5%) 22 20	6, 12, 38, 54	0
All	All	854/872 (97%)	0.02	35 (4%) 34 33	6, 13, 32, 54	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	936	THR	7.2
1	A	303	GLY	6.3
1	B	818	VAL	5.7
1	A	436	THR	5.5
1	B	501	ALA	5.4
1	A	1	ALA	4.9
1	B	927	ASN	4.5
1	B	844	SER	4.2
1	B	845	ALA	3.8
1	B	822	ARG	3.6
1	B	935	ARG	3.5
1	B	911	GLY	3.4
1	B	846	THR	3.4
1	A	26	GLY	3.3
1	B	923	TYR	3.1
1	B	934	THR	3.1
1	B	926	SER	3.0
1	A	435	ARG	3.0
1	B	840	TYR	2.9
1	B	820	SER	2.8
1	B	816	LYS	2.7
1	A	344	SER	2.7
1	B	803	GLY	2.6
1	B	843	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	140	ASP	2.5
1	B	915	ALA	2.5
1	B	817	GLY	2.5
1	A	145	ARG	2.4
1	A	427	ASN	2.4
1	B	932	ARG	2.2
1	B	842	CYS	2.1
1	B	849	GLN	2.1
1	A	137	GLY	2.0
1	B	814	GLN	2.0
1	B	910	VAL	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
4	XYS	A	956	9/10	0.58	15.88	40,42,44,45	0
3	XYS	A	457	9/10	0.25	8.13	31,34,39,45	0
2	XYS	A	455	10/10	0.36	7.68	29,40,43,44	0
3	XYS	A	456	9/10	0.61	6.39	50,54,55,55	0
2	XYS	B	955	10/10	0.35	3.48	22,36,41,43	0
4	XYS	A	957	10/10	0.21	3.27	21,28,31,33	0
2	XYS	B	953	9/10	0.14	3.23	13,13,15,16	0
3	XYS	A	459	10/10	0.18	2.76	26,29,31,35	0
2	XYS	A	453	9/10	0.14	1.94	16,19,20,21	0
3	XYS	A	458	9/10	0.12	1.60	17,21,23,26	0
2	XYS	A	452	9/10	0.13	1.33	12,13,16,16	0
2	XYS	A	454	9/10	0.13	0.93	18,20,22,24	0
2	XYS	B	951	9/10	0.09	0.90	8,9,10,12	0
4	XYS	B	959	10/10	0.23	0.80	42,44,46,47	0
2	XYS	B	952	9/10	0.10	0.29	7,11,13,13	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	XYS	B	958	9/10	0.24	0.27	48,49,50,50	0
2	XYS	B	954	9/10	0.10	0.24	12,13,16,18	0
2	XYS	A	451	9/10	0.10	-0.17	12,13,14,14	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( $\text{\AA}^2$ )	Q<0.9
5	SO4	A	970	5/5	0.35	34.60	77,77,78,78	0
5	SO4	A	971	5/5	0.24	8.15	56,56,56,56	0
6	GOL	B	982	6/6	0.22	7.32	41,43,43,43	0
6	GOL	B	980	6/6	0.19	7.06	34,35,35,35	0
6	GOL	B	981	6/6	0.15	-0.66	42,43,43,44	0

## 6.5 Other polymers

There are no such residues in this entry.