



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:50 AM GMT

PDB ID : 2BFG
Title : crystal structure of beta-xylosidase (fam GH39) in complex with dinitrophenyl-beta-xyloside and covalently bound xyloside
Authors : Czjzek, M.; Bravman, T.; Henrissat, B.; Shoham, Y.
Deposited on : 2004-12-07
Resolution : 2.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at 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.

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

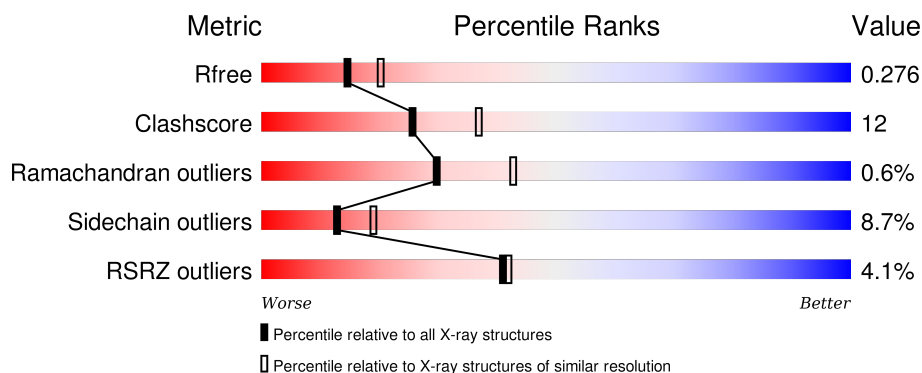
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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 ≥ 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	503	<div> <div>4%</div> <div>71% 25% .</div> </div>
1	B	503	<div> <div>6%</div> <div>68% 27% .</div> </div>
1	C	503	<div> <div>5%</div> <div>68% 28% .</div> </div>
1	D	503	<div> <div>4%</div> <div>70% 26% .</div> </div>
1	E	503	<div> <div>2%</div> <div>71% 26% .</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	503	
1	G	503	
1	H	503	

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	NA	A	1503	-	-	-	X
2	NA	E	1503	-	-	-	X
2	NA	F	1503	-	-	-	X
3	ANX	A	1504	-	-	-	X
3	ANX	D	1504	-	-	-	X
4	XYP	D	1505	X	-	-	-
6	XYS	C	1504	-	-	-	X
6	XYS	E	1504	-	-	-	X
6	XYS	F	1504	-	-	-	X
6	XYS	G	1504	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 34237 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 BETA-XYLOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	501	Total	C	N	O	S	0	0	0
			4087	2641	693	742	11			
1	B	501	Total	C	N	O	S	0	0	0
			4087	2641	693	742	11			
1	C	501	Total	C	N	O	S	0	0	0
			4084	2640	693	740	11			
1	D	501	Total	C	N	O	S	0	0	0
			4087	2641	693	742	11			
1	E	501	Total	C	N	O	S	0	0	0
			4087	2641	693	742	11			
1	F	501	Total	C	N	O	S	0	0	0
			4087	2641	693	742	11			
1	G	501	Total	C	N	O	S	0	0	0
			4087	2641	693	742	11			
1	H	501	Total	C	N	O	S	0	0	0
			4087	2641	693	742	11			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	.	-	LEU	DELETION	UNP Q9ZFM2
A	.	-	GLU	DELETION	UNP Q9ZFM2
A	406	GLU	PHE	CONFLICT	UNP Q9ZFM2
A	445	ARG	PRO	CONFLICT	UNP Q9ZFM2
A	446	GLN	-	INSERTION	UNP Q9ZFM2
A	447	VAL	SER	CONFLICT	UNP Q9ZFM2
B	.	-	LEU	DELETION	UNP Q9ZFM2
B	.	-	GLU	DELETION	UNP Q9ZFM2
B	406	GLU	PHE	CONFLICT	UNP Q9ZFM2
B	445	ARG	PRO	CONFLICT	UNP Q9ZFM2
B	446	GLN	-	INSERTION	UNP Q9ZFM2
B	447	VAL	SER	CONFLICT	UNP Q9ZFM2
C	.	-	LEU	DELETION	UNP Q9ZFM2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	.	-	GLU	DELETION	UNP Q9ZFM2
C	406	GLU	PHE	CONFLICT	UNP Q9ZFM2
C	445	ARG	PRO	CONFLICT	UNP Q9ZFM2
C	446	GLN	-	INSERTION	UNP Q9ZFM2
C	447	VAL	SER	CONFLICT	UNP Q9ZFM2
D	.	-	LEU	DELETION	UNP Q9ZFM2
D	.	-	GLU	DELETION	UNP Q9ZFM2
D	406	GLU	PHE	CONFLICT	UNP Q9ZFM2
D	445	ARG	PRO	CONFLICT	UNP Q9ZFM2
D	446	GLN	-	INSERTION	UNP Q9ZFM2
D	447	VAL	SER	CONFLICT	UNP Q9ZFM2
E	.	-	LEU	DELETION	UNP Q9ZFM2
E	.	-	GLU	DELETION	UNP Q9ZFM2
E	406	GLU	PHE	CONFLICT	UNP Q9ZFM2
E	445	ARG	PRO	CONFLICT	UNP Q9ZFM2
E	446	GLN	-	INSERTION	UNP Q9ZFM2
E	447	VAL	SER	CONFLICT	UNP Q9ZFM2
F	.	-	LEU	DELETION	UNP Q9ZFM2
F	.	-	GLU	DELETION	UNP Q9ZFM2
F	406	GLU	PHE	CONFLICT	UNP Q9ZFM2
F	445	ARG	PRO	CONFLICT	UNP Q9ZFM2
F	446	GLN	-	INSERTION	UNP Q9ZFM2
F	447	VAL	SER	CONFLICT	UNP Q9ZFM2
G	.	-	LEU	DELETION	UNP Q9ZFM2
G	.	-	GLU	DELETION	UNP Q9ZFM2
G	406	GLU	PHE	CONFLICT	UNP Q9ZFM2
G	445	ARG	PRO	CONFLICT	UNP Q9ZFM2
G	446	GLN	-	INSERTION	UNP Q9ZFM2
G	447	VAL	SER	CONFLICT	UNP Q9ZFM2
H	.	-	LEU	DELETION	UNP Q9ZFM2
H	.	-	GLU	DELETION	UNP Q9ZFM2
H	406	GLU	PHE	CONFLICT	UNP Q9ZFM2
H	445	ARG	PRO	CONFLICT	UNP Q9ZFM2
H	446	GLN	-	INSERTION	UNP Q9ZFM2
H	447	VAL	SER	CONFLICT	UNP Q9ZFM2

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

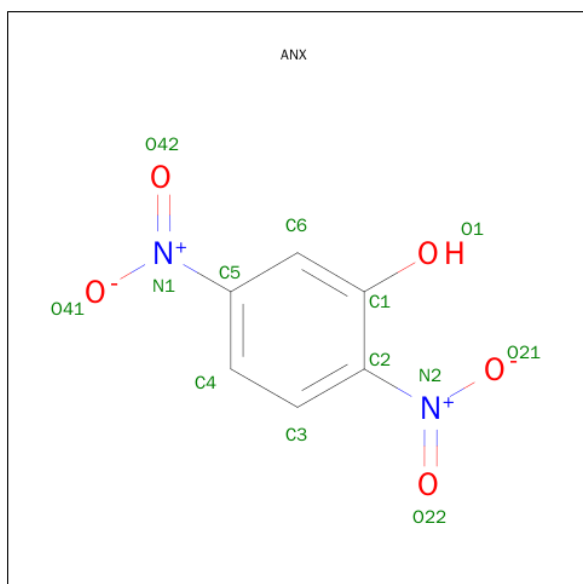
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Na 1 1	0	0
2	D	1	Total Na 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	1	Total	Na	0	0
			1	1		
2	H	1	Total	Na	0	0
			1	1		
2	B	1	Total	Na	0	0
			1	1		
2	C	1	Total	Na	0	0
			1	1		
2	A	1	Total	Na	0	0
			1	1		
2	F	1	Total	Na	0	0
			1	1		

- Molecule 3 is 2,5-DINITROPHENOL (three-letter code: ANX) (formula: C₆H₄N₂O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			13	6	2	5		
3	D	1	Total	C	N	O	0	0
			13	6	2	5		

- 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
			18	10	8		

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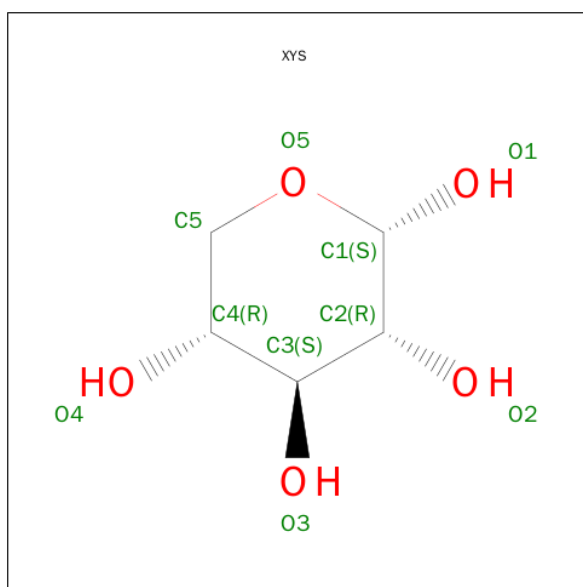
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	2	Total	C	O	0	0
			18	10	8		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is SUGAR (XYLOPYRANOSE) (three-letter code: XYS) (formula: C₅H₁₀O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			9	5	4		
6	C	1	Total	C	O	0	0
			9	5	4		
6	E	1	Total	C	O	0	0
			9	5	4		
6	F	1	Total	C	O	0	0
			9	5	4		
6	G	1	Total	C	O	0	0
			9	5	4		
6	H	1	Total	C	O	0	0
			9	5	4		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	172	Total	O	0	0
			172	172		
7	B	167	Total	O	0	0
			167	167		
7	C	179	Total	O	0	0
			179	179		
7	D	160	Total	O	0	0
			160	160		
7	E	187	Total	O	0	0
			187	187		
7	F	144	Total	O	0	0
			144	144		

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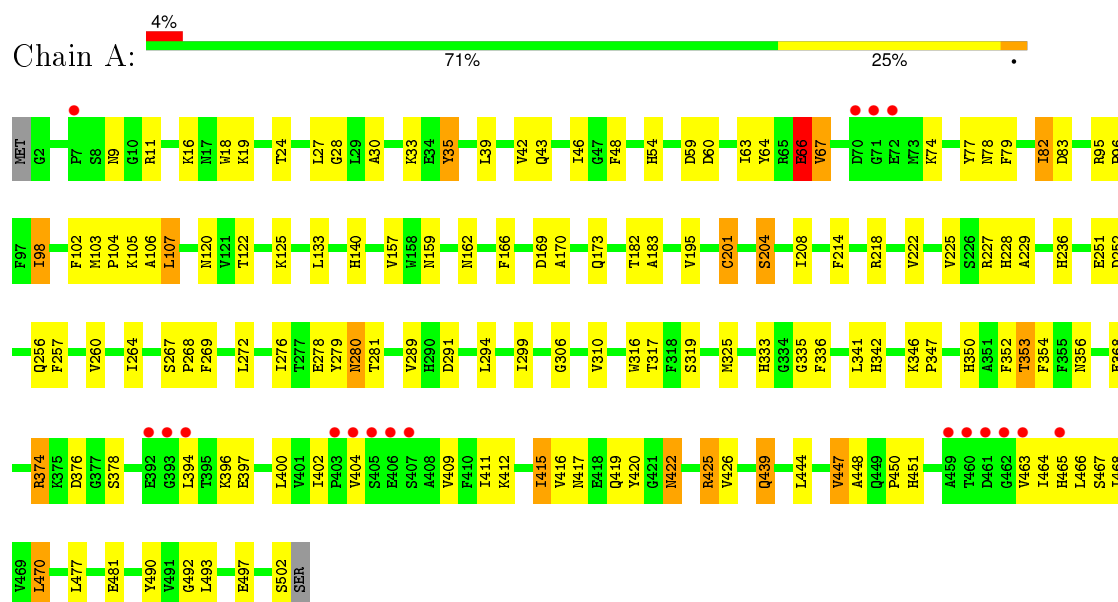
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	178	Total 178	O 178	0	0
7	H	193	Total 193	O 193	0	0

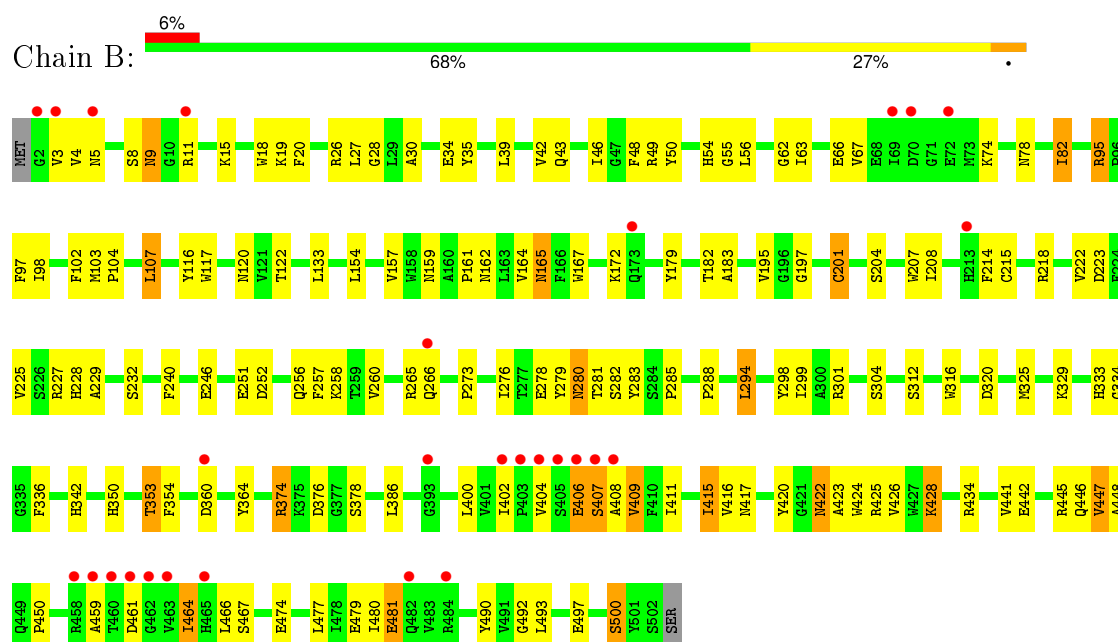
3 Residue-property plots

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.

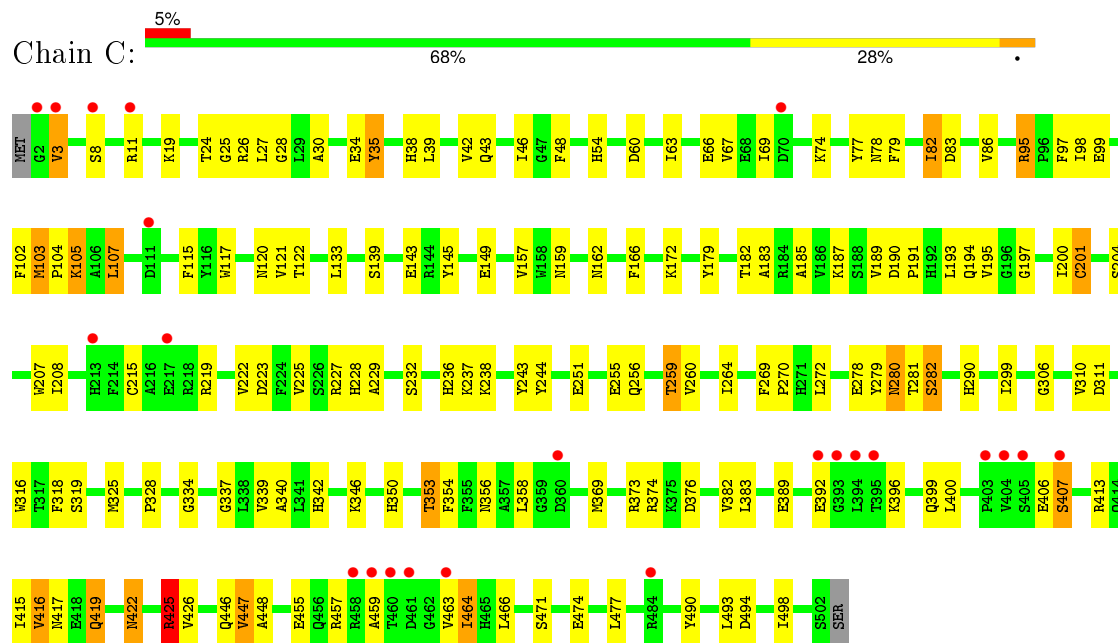
• Molecule 1: BETA-XYLOSIDASE



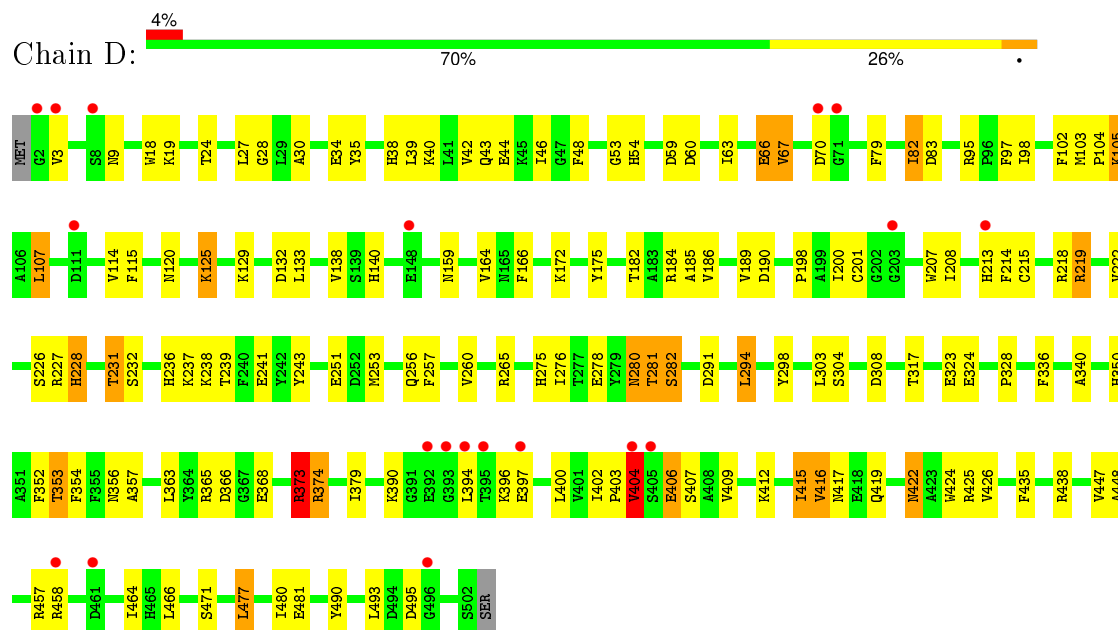
• Molecule 1: BETA-XYLOSIDASE



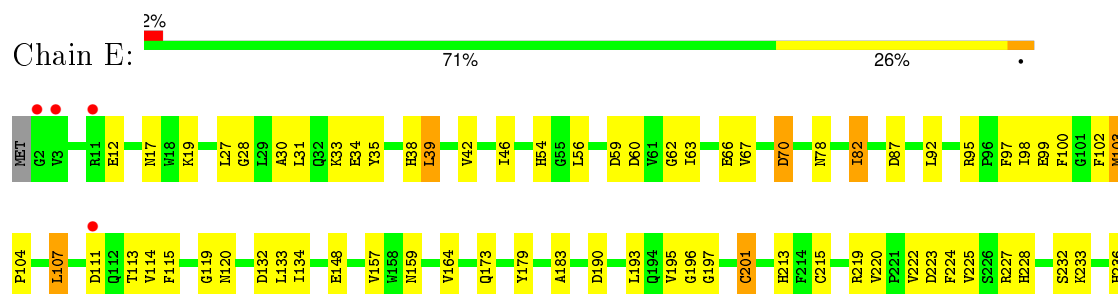
- Molecule 1: BETA-XYLOSIDASE

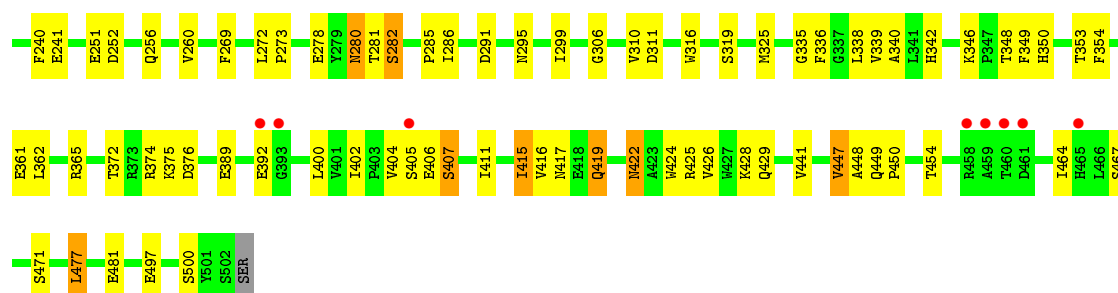


- Molecule 1: BETA-XYLOSIDASE

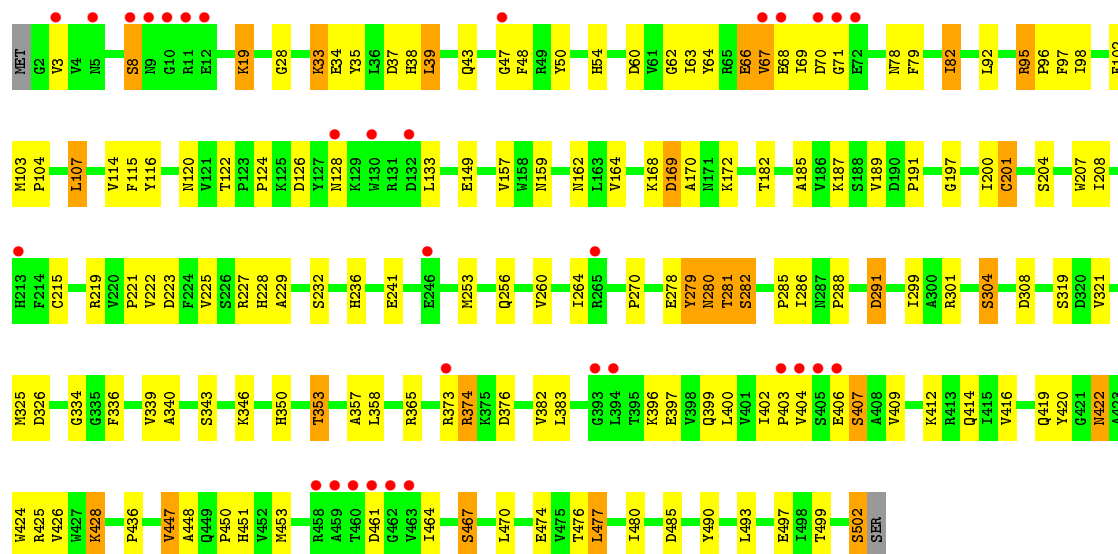


- Molecule 1: BETA-XYLOSIDASE

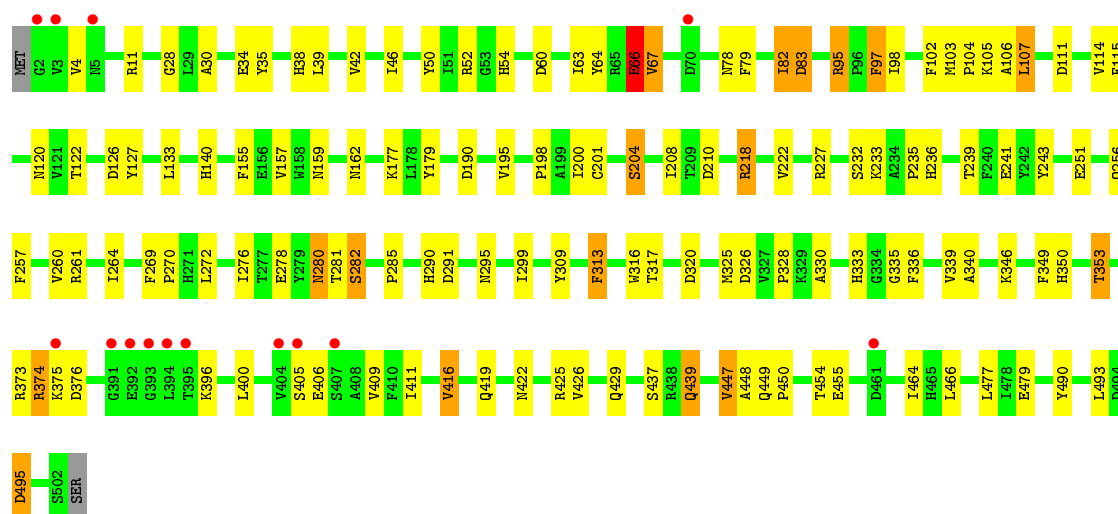




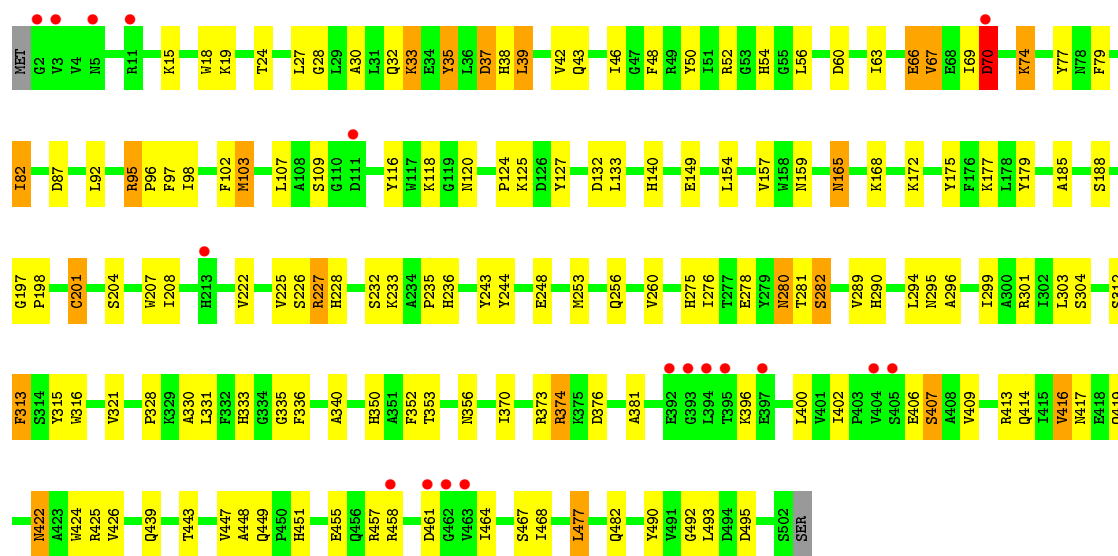
• Molecule 1: BETA-XYLOSIDASE



• Molecule 1: BETA-XYLOSIDASE



• Molecule 1: BETA-XYLOSIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.95Å 162.16Å 308.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.11 – 2.40 39.62 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (40.11-2.40) 99.6 (39.62-2.40)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.194 , 0.270 0.207 , 0.276	Depositor DCC
R_{free} test set	8689 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	18.3	Xtriage
Anisotropy	0.617	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 47.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	3 of 173787 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	34237	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.35 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 7.1498e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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, NA, XYS, ANX, 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	0.75	0/4202	0.86	5/5705 (0.1%)
1	B	0.75	1/4202 (0.0%)	0.85	7/5705 (0.1%)
1	C	0.73	1/4199 (0.0%)	0.85	4/5701 (0.1%)
1	D	0.70	0/4202	0.86	10/5705 (0.2%)
1	E	0.75	1/4202 (0.0%)	0.88	10/5705 (0.2%)
1	F	0.70	1/4202 (0.0%)	0.84	8/5705 (0.1%)
1	G	0.74	0/4202	0.87	8/5705 (0.1%)
1	H	0.77	1/4202 (0.0%)	0.88	6/5705 (0.1%)
All	All	0.74	5/33613 (0.0%)	0.86	58/45636 (0.1%)

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
1	E	0	1
1	F	0	1
1	G	0	1
4	D	1	0
All	All	1	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	103	MET	SD-CE	-5.55	1.46	1.77
1	H	103	MET	SD-CE	-5.48	1.47	1.77
1	F	447	VAL	CB-CG1	-5.14	1.42	1.52
1	C	425	ARG	CG-CD	5.03	1.64	1.51
1	B	246	GLU	CD-OE1	5.02	1.31	1.25

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	376	ASP	CB-CG-OD2	7.72	125.25	118.30
1	A	376	ASP	CB-CG-OD2	7.55	125.10	118.30
1	D	291	ASP	CB-CG-OD2	7.30	124.87	118.30
1	G	210	ASP	CB-CG-OD2	7.14	124.72	118.30
1	D	83	ASP	CB-CG-OD2	7.02	124.61	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	D	1505	XYP	C1B

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	405	SER	Peptide
1	F	66	GLU	Peptide
1	G	66	GLU	Peptide

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	4087	0	4000	94	0
1	B	4087	0	4000	109	0
1	C	4084	0	3998	99	0
1	D	4087	0	3999	108	0
1	E	4087	0	4000	96	1
1	F	4087	0	4000	114	1
1	G	4087	0	4000	99	0
1	H	4087	0	4000	114	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	13	0	3	1	0
3	D	13	0	3	0	0
4	A	18	0	6	3	0
4	D	18	0	6	5	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0
5	E	5	0	0	0	0
5	F	5	0	0	0	0
5	G	5	0	0	1	0
5	H	5	0	0	1	0
6	B	9	0	8	1	0
6	C	9	0	8	1	0
6	E	9	0	8	0	0
6	F	9	0	8	0	0
6	G	9	0	8	1	0
6	H	9	0	8	2	0
7	A	172	0	0	7	0
7	B	167	0	0	13	0
7	C	179	0	0	6	0
7	D	160	0	0	8	0
7	E	187	0	0	13	0
7	F	144	0	0	14	0
7	G	178	0	0	11	0
7	H	193	0	0	18	0
All	All	34237	0	32063	809	1

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 12.

The worst 5 of 809 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:350:HIS:CE1	7:B:2120:HOH:O	1.89	1.20
1:A:201:CYS:SG	3:A:1504:ANX:O21	1.99	1.20
1:E:103:MET:SD	7:E:2061:HOH:O	2.10	1.10
1:F:426:VAL:HG21	1:F:447:VAL:HG11	1.34	1.07
1:B:280:ASN:HD22	1:B:281:THR:H	1.06	1.02

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:392:GLU:O	1:F:399:GLN:NE2[1_655]	2.19	0.01

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	499/503 (99%)	465 (93%)	32 (6%)	2 (0%)	39	56
1	B	499/503 (99%)	469 (94%)	28 (6%)	2 (0%)	39	56
1	C	499/503 (99%)	475 (95%)	22 (4%)	2 (0%)	39	56
1	D	499/503 (99%)	466 (93%)	29 (6%)	4 (1%)	24	35
1	E	499/503 (99%)	470 (94%)	27 (5%)	2 (0%)	39	56
1	F	499/503 (99%)	468 (94%)	28 (6%)	3 (1%)	30	43
1	G	499/503 (99%)	469 (94%)	27 (5%)	3 (1%)	30	43
1	H	499/503 (99%)	469 (94%)	25 (5%)	5 (1%)	19	28
All	All	3992/4024 (99%)	3751 (94%)	218 (6%)	23 (1%)	30	43

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	404	VAL
1	E	67	VAL
1	E	407	SER
1	F	67	VAL
1	G	67	VAL

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	439/441 (100%)	397 (90%)	42 (10%)	10	15
1	B	439/441 (100%)	395 (90%)	44 (10%)	9	14
1	C	438/441 (99%)	398 (91%)	40 (9%)	12	17
1	D	439/441 (100%)	396 (90%)	43 (10%)	10	14
1	E	439/441 (100%)	401 (91%)	38 (9%)	13	19
1	F	439/441 (100%)	403 (92%)	36 (8%)	14	21
1	G	439/441 (100%)	409 (93%)	30 (7%)	20	31
1	H	439/441 (100%)	407 (93%)	32 (7%)	17	27
All	All	3511/3528 (100%)	3206 (91%)	305 (9%)	13	19

5 of 305 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	125	LYS
1	E	19	LYS
1	H	95	ARG
1	D	228	HIS
1	D	394	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 104 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	266	GLN
1	E	256	GLN
1	H	266	GLN
1	D	280	ASN
1	D	385	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 ⓘ

4 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$
4	XYP	A	1505	3,4	9,9,10	2.58	2 (22%)	12,12,14	1.53	2 (16%)
4	XYS	A	1507	1,4	9,9,10	1.90	3 (33%)	12,12,14	1.80	3 (25%)
4	XYP	D	1505	3,4	9,9,10	2.65	2 (22%)	12,12,14	1.78	2 (16%)
4	XYS	D	1507	1,4	9,9,10	1.92	3 (33%)	12,12,14	2.11	5 (41%)

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	1505	3,4	-	0/0/14/17	0/1/1/1
4	XYS	A	1507	1,4	-	0/0/14/17	0/1/1/1
4	XYP	D	1505	3,4	1/1/3/4	0/0/14/17	1/1/1/1
4	XYS	D	1507	1,4	-	0/0/14/17	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1505	XYP	O2B-C2B	-7.19	1.27	1.43
4	A	1505	XYP	O2B-C2B	-6.85	1.28	1.43
4	D	1507	XYS	C4-C3	2.04	1.55	1.52
4	A	1507	XYS	O5-C5	2.64	1.48	1.42
4	A	1507	XYS	C4-C3	2.65	1.56	1.52

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1507	XYS	C4-C3-C2	-3.91	107.38	111.24
4	D	1507	XYS	C4-C3-C2	-3.89	107.39	111.24
4	D	1507	XYS	C1-C2-C3	-3.47	105.44	109.54
4	D	1505	XYP	C4B-C3B-C2B	-3.36	107.92	111.24
4	A	1507	XYS	C1-C2-C3	-3.02	105.97	109.54

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	D	1505	XYP	C1B

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1505	XYP	C1B-C2B-C3B-C4B-C5B-O5B

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1505	XYP	2	0
4	A	1507	XYS	1	0
4	D	1505	XYP	4	0
4	D	1507	XYS	1	0

5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 for Mogul analysis.

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$
3	ANX	A	1504	4	8,13,13	4.26	2 (25%)	10,18,18	2.17	4 (40%)
5	SO4	A	1506	-	4,4,4	0.24	0	6,6,6	0.33	0
6	XYS	B	1504	1	9,9,10	2.13	3 (33%)	12,12,14	2.09	3 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	B	1505	-	4,4,4	0.36	0	6,6,6	0.33	0
6	XYS	C	1504	1	9,9,10	2.24	4 (44%)	12,12,14	2.68	4 (33%)
5	SO4	C	1505	-	4,4,4	0.35	0	6,6,6	0.25	0
3	ANX	D	1504	1,4	8,13,13	4.04	2 (25%)	10,18,18	2.90	4 (40%)
5	SO4	D	1506	-	4,4,4	0.29	0	6,6,6	0.19	0
6	XYS	E	1504	1	9,9,10	2.23	4 (44%)	12,12,14	2.85	5 (41%)
5	SO4	E	1505	-	4,4,4	0.21	0	6,6,6	0.69	0
6	XYS	F	1504	1	9,9,10	2.29	4 (44%)	12,12,14	2.72	3 (25%)
5	SO4	F	1505	-	4,4,4	0.39	0	6,6,6	0.37	0
6	XYS	G	1504	1	9,9,10	2.03	3 (33%)	12,12,14	2.74	5 (41%)
5	SO4	G	1505	-	4,4,4	0.47	0	6,6,6	0.74	0
6	XYS	H	1504	1	9,9,10	2.27	4 (44%)	12,12,14	2.51	6 (50%)
5	SO4	H	1505	-	4,4,4	0.45	0	6,6,6	0.26	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
3	ANX	A	1504	4	-	2/7/8/8	0/1/1/1
5	SO4	A	1506	-	-	0/0/0/0	0/0/0/0
6	XYS	B	1504	1	-	0/0/14/17	0/1/1/1
5	SO4	B	1505	-	-	0/0/0/0	0/0/0/0
6	XYS	C	1504	1	-	0/0/14/17	0/1/1/1
5	SO4	C	1505	-	-	0/0/0/0	0/0/0/0
3	ANX	D	1504	1,4	-	0/7/8/8	0/1/1/1
5	SO4	D	1506	-	-	0/0/0/0	0/0/0/0
6	XYS	E	1504	1	-	0/0/14/17	0/1/1/1
5	SO4	E	1505	-	-	0/0/0/0	0/0/0/0
6	XYS	F	1504	1	-	0/0/14/17	0/1/1/1
5	SO4	F	1505	-	-	0/0/0/0	0/0/0/0
6	XYS	G	1504	1	-	0/0/14/17	0/1/1/1
5	SO4	G	1505	-	-	0/0/0/0	0/0/0/0
6	XYS	H	1504	1	-	0/0/14/17	0/1/1/1
5	SO4	H	1505	-	-	0/0/0/0	0/0/0/0

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	1504	XYS	C2-C3	2.07	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	1504	XYS	O5-C5	2.20	1.47	1.42
6	B	1504	XYS	C5-C4	2.21	1.57	1.52
6	F	1504	XYS	C4-C3	2.25	1.55	1.52
6	E	1504	XYS	O5-C5	2.33	1.47	1.42

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	1504	XYS	C1-C2-C3	-5.82	102.66	109.54
6	E	1504	XYS	C1-C2-C3	-5.71	102.79	109.54
6	G	1504	XYS	O5-C1-C2	-5.58	99.88	110.31
6	C	1504	XYS	C1-C2-C3	-5.49	103.04	109.54
6	F	1504	XYS	C1-C2-C3	-5.46	103.08	109.54

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1504	ANX	C6-C5-N1-O42
3	A	1504	ANX	C4-C5-N1-O42

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1504	ANX	1	0
6	B	1504	XYS	1	0
6	C	1504	XYS	1	0
6	G	1504	XYS	1	0
5	G	1505	SO4	1	0
6	H	1504	XYS	2	0
5	H	1505	SO4	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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 ²)	Q<0.9
1	A	501/503 (99%)	0.19	18 (3%) 46 47	17, 24, 43, 51	0
1	B	501/503 (99%)	0.27	28 (5%) 28 28	16, 24, 44, 52	0
1	C	501/503 (99%)	0.16	23 (4%) 36 37	16, 24, 43, 52	0
1	D	501/503 (99%)	0.25	19 (3%) 44 45	16, 24, 43, 51	0
1	E	501/503 (99%)	0.14	12 (2%) 62 61	15, 24, 41, 51	0
1	F	501/503 (99%)	0.35	32 (6%) 23 23	16, 24, 44, 52	0
1	G	501/503 (99%)	0.16	14 (2%) 56 55	16, 23, 42, 51	0
1	H	501/503 (99%)	0.14	18 (3%) 46 47	15, 23, 43, 51	0
All	All	4008/4024 (99%)	0.21	164 (4%) 41 42	15, 24, 43, 52	0

The worst 5 of 164 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	405	SER	9.0
1	D	405	SER	8.3
1	H	2	GLY	8.2
1	G	2	GLY	8.0
1	G	405	SER	6.0

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, 95th 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 ²)	Q<0.9
4	XYS	A	1507	9/10	0.91	0.21	1.87	37,37,37,38	9
4	XYP	A	1505	9/10	0.91	0.20	1.38	37,37,38,38	9
4	XYS	D	1507	9/10	0.92	0.23	1.30	39,39,40,40	9
4	XYP	D	1505	9/10	0.90	0.20	0.73	39,39,40,41	9

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, 95th 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 ²)	Q<0.9
3	ANX	A	1504	13/13	0.57	0.47	15.43	43,50,53,54	13
3	ANX	D	1504	13/13	0.77	0.38	5.89	41,44,46,46	13
6	XYS	F	1504	9/10	0.79	0.25	4.99	40,42,42,42	0
2	NA	A	1503	1/1	0.99	0.36	4.84	19,19,19,19	0
6	XYS	C	1504	9/10	0.76	0.26	3.26	35,38,40,41	0
6	XYS	G	1504	9/10	0.86	0.24	2.80	35,36,36,38	0
2	NA	E	1503	1/1	0.99	0.23	2.24	6,6,6,6	0
2	NA	F	1503	1/1	0.98	0.21	2.20	9,9,9,9	0
6	XYS	E	1504	9/10	0.77	0.25	2.14	36,37,38,39	0
5	SO4	H	1505	5/5	0.96	0.31	1.99	64,64,65,66	0
6	XYS	H	1504	9/10	0.84	0.20	1.94	29,29,32,33	0
6	XYS	B	1504	9/10	0.83	0.23	1.74	39,39,41,42	0
2	NA	D	1503	1/1	0.99	0.19	1.61	10,10,10,10	0
5	SO4	G	1505	5/5	0.96	0.31	1.18	55,55,55,56	0
2	NA	G	1503	1/1	0.99	0.22	0.88	9,9,9,9	0
5	SO4	A	1506	5/5	0.96	0.26	0.76	55,56,57,57	0
5	SO4	E	1505	5/5	0.96	0.24	0.69	56,58,58,59	0
5	SO4	F	1505	5/5	0.94	0.28	0.54	56,56,57,58	0
2	NA	C	1503	1/1	0.99	0.20	0.49	7,7,7,7	0
2	NA	B	1503	1/1	0.99	0.21	0.11	5,5,5,5	0
5	SO4	C	1505	5/5	0.96	0.21	-0.00	60,60,62,62	0
2	NA	H	1503	1/1	0.99	0.17	-0.04	4,4,4,4	0
5	SO4	B	1505	5/5	0.97	0.22	-0.07	58,59,60,61	0
5	SO4	D	1506	5/5	0.98	0.17	-0.45	58,59,59,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.