wwPDB X-ray Structure Validation Summary Report (i)

Dec 3, 2023 – 06:54 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

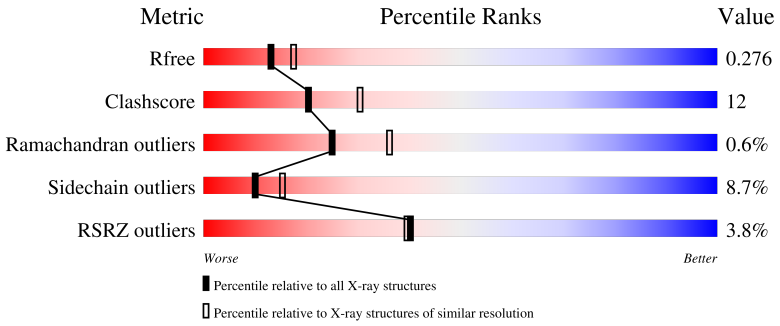
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	4% 72% 25% ·
1	B	503	5% 68% 27% ·
1	C	503	4% 68% 28% ·
1	D	503	3% 70% 25% ·
1	E	503	2% 71% 26% ·

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Mol	Chain	Length	Quality of chain
1	F	503	6% 69% 26% 5%
1	G	503	3% 73% 23%
1	H	503	3% 69% 26%

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
3	ANX	A	1504	-	-	-	X

2 Entry composition (i)

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	A	1	Total Na 1 1	0	0
2	B	1	Total Na 1 1	0	0

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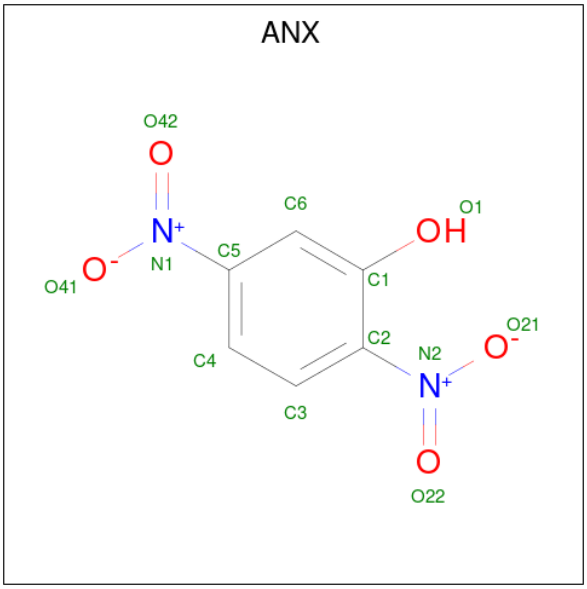
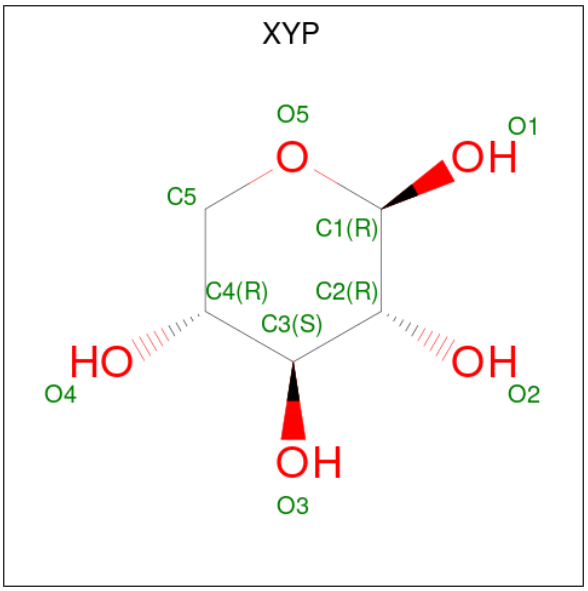
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total Na 1 1	0	0
2	D	1	Total Na 1 1	0	0
2	E	1	Total Na 1 1	0	0
2	F	1	Total Na 1 1	0	0
2	G	1	Total Na 1 1	0	0
2	H	1	Total Na 1 1	0	0

- Molecule 3 is 2,5-DINITROPHENOL (three-letter code: ANX) (formula: $C_6H_4N_2O_5$).



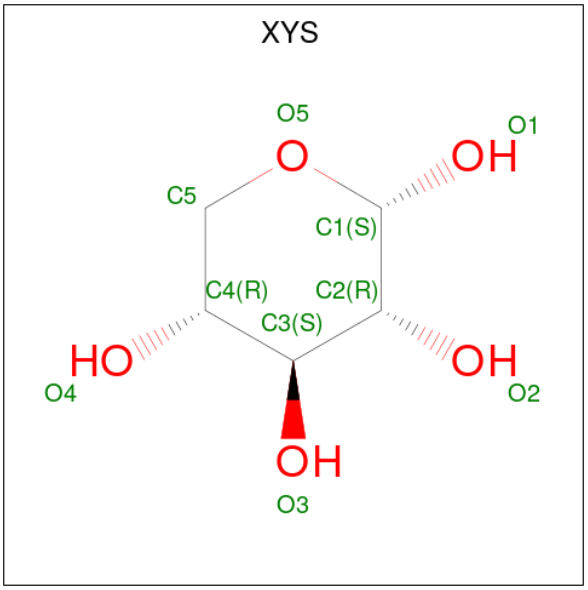
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 13 6 2 5	0	0
3	D	1	Total C N O 13 6 2 5	0	0

- Molecule 4 is beta-D-xylopyranose (three-letter code: XYP) (formula: $C_5H_{10}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 9 5 4	0	0
4	D	1	Total C O 9 5 4	0	0

- Molecule 5 is alpha-D-xylopyranose (three-letter code: XYS) (formula: $C_5H_{10}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 9 5 4	0	0
5	B	1	Total C O 9 5 4	0	0

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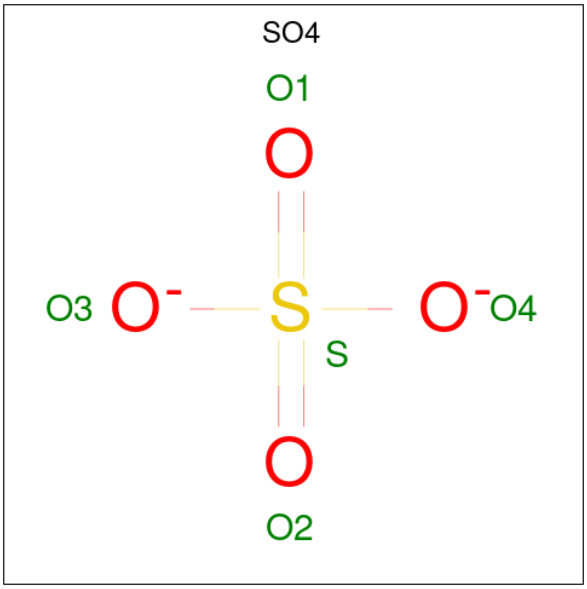
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 9 5 4	0	0
5	D	1	Total C O 9 5 4	0	0
5	E	1	Total C O 9 5 4	0	0
5	F	1	Total C O 9 5 4	0	0
5	G	1	Total C O 9 5 4	0	0
5	H	1	Total C O 9 5 4	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	1	Total O S 5 4 1	0	0
6	G	1	Total O S 5 4 1	0	0
6	H	1	Total O S 5 4 1	0	0

- Molecule 7 is water.

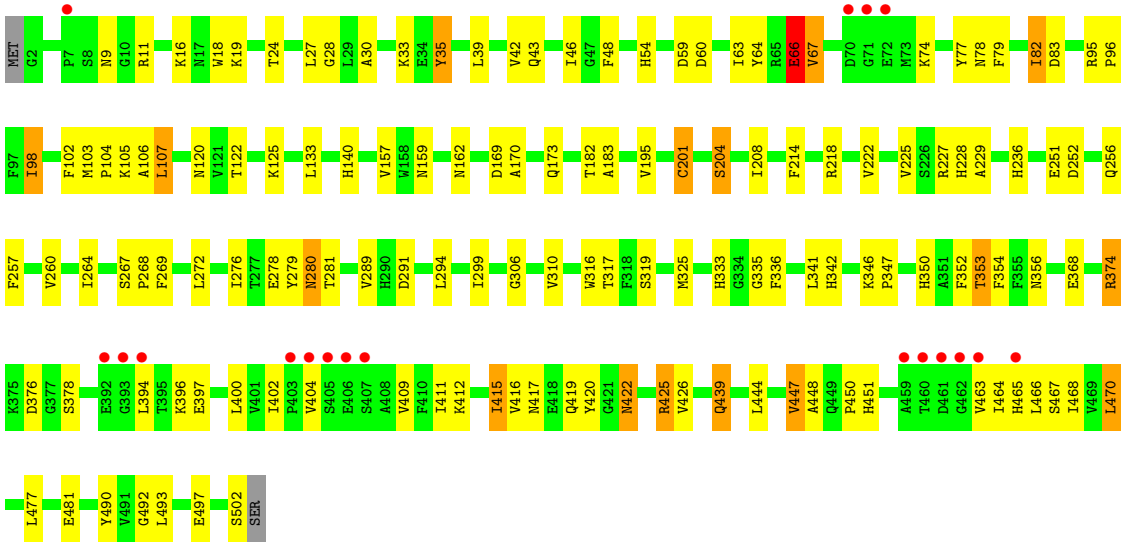
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	172	Total O 172 172	0	0
7	B	167	Total O 167 167	0	0
7	C	179	Total O 179 179	0	0
7	D	160	Total O 160 160	0	0
7	E	187	Total O 187 187	0	0
7	F	144	Total O 144 144	0	0
7	G	178	Total O 178 178	0	0
7	H	193	Total O 193 193	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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 (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.

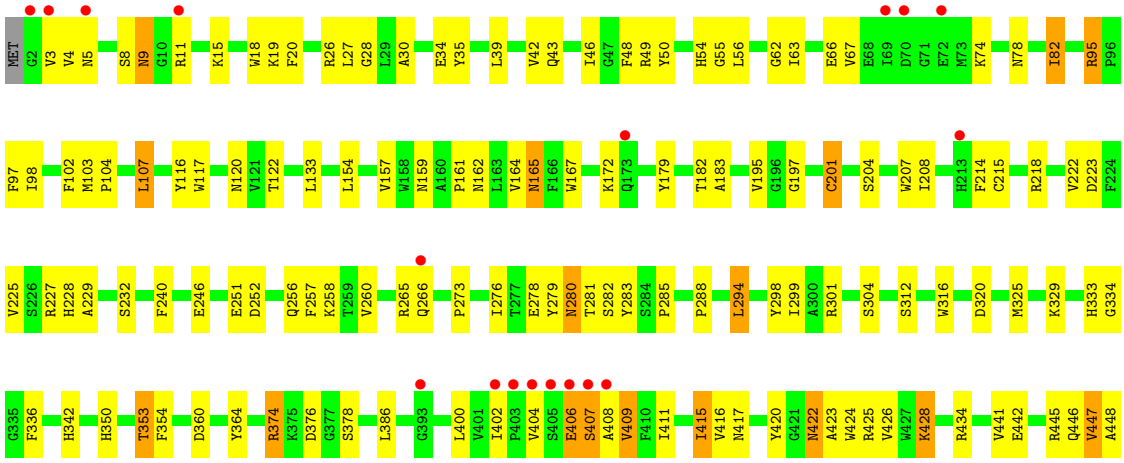
• Molecule 1: BETA-XYLOSIDASE

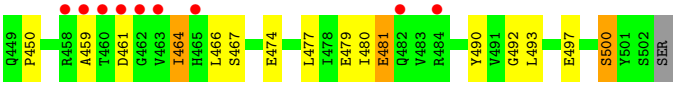
Chain A:



• Molecule 1: BETA-XYLOSIDASE

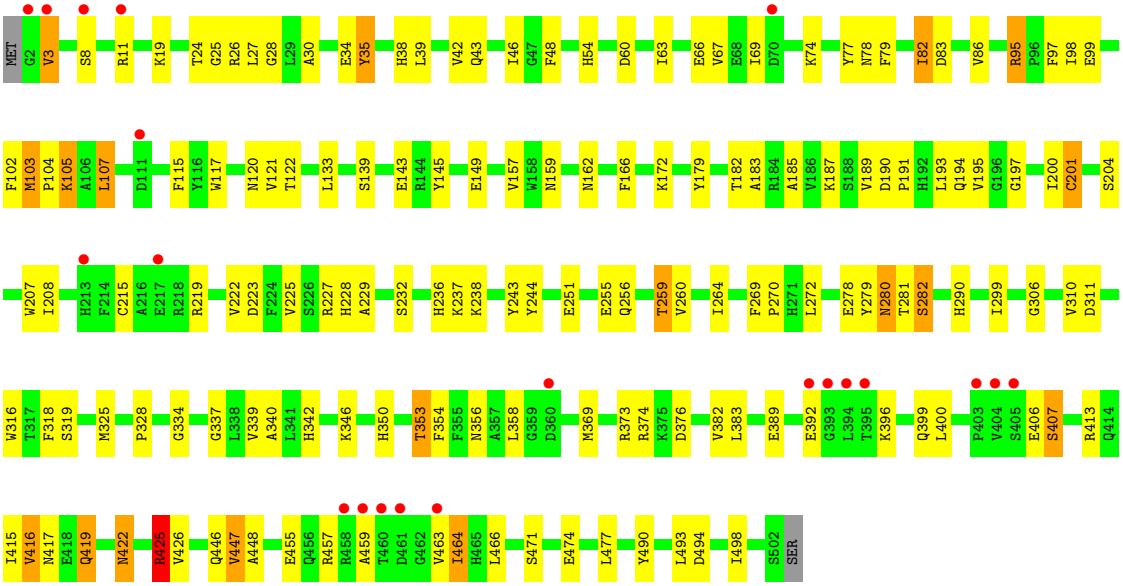
Chain B:





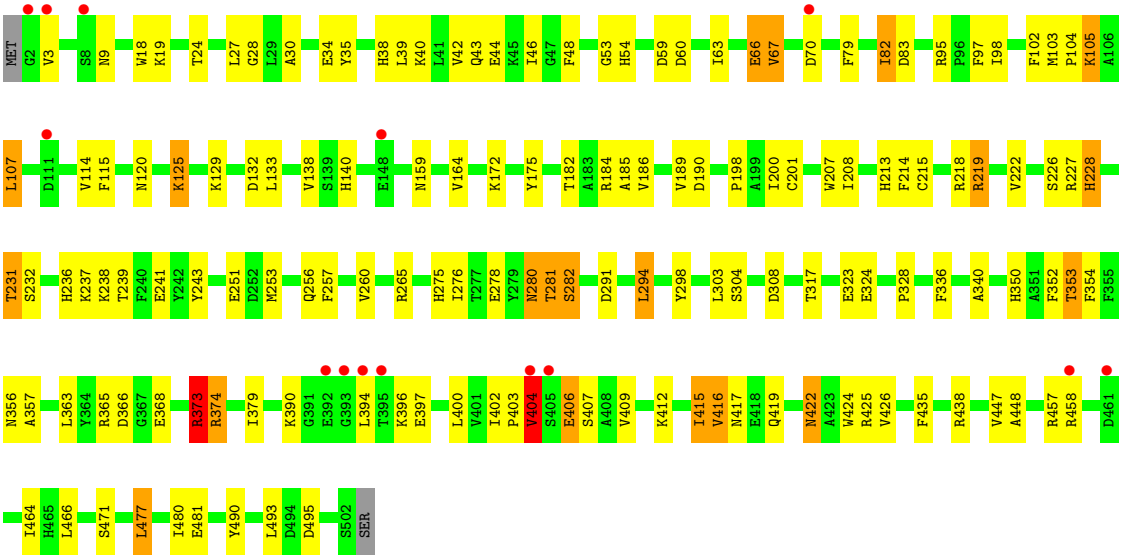
• Molecule 1: BETA-XYLOSIDASE

Chain C:



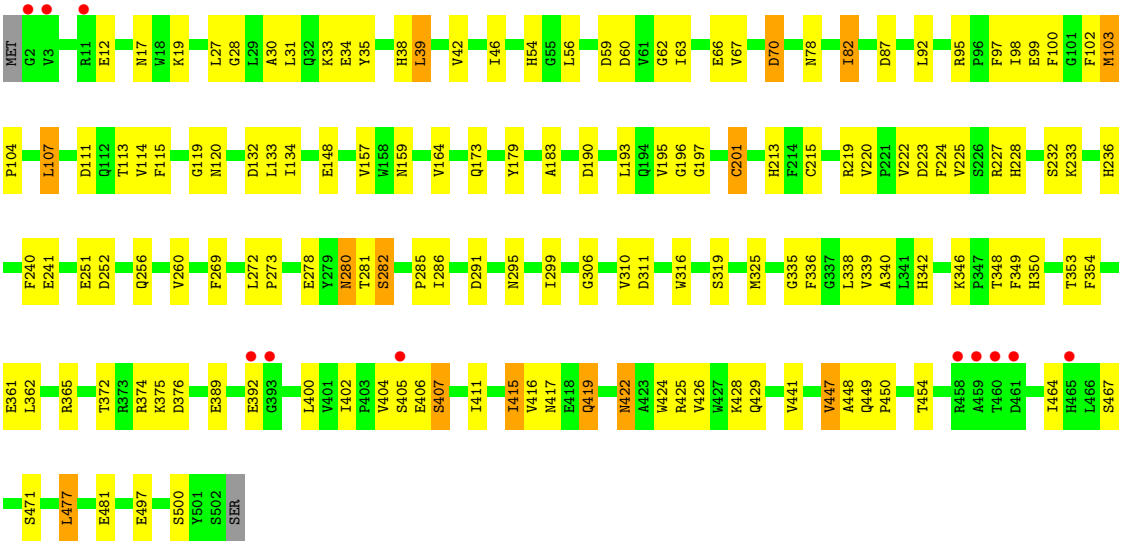
• Molecule 1: BETA-XYLOSIDASE

Chain D:



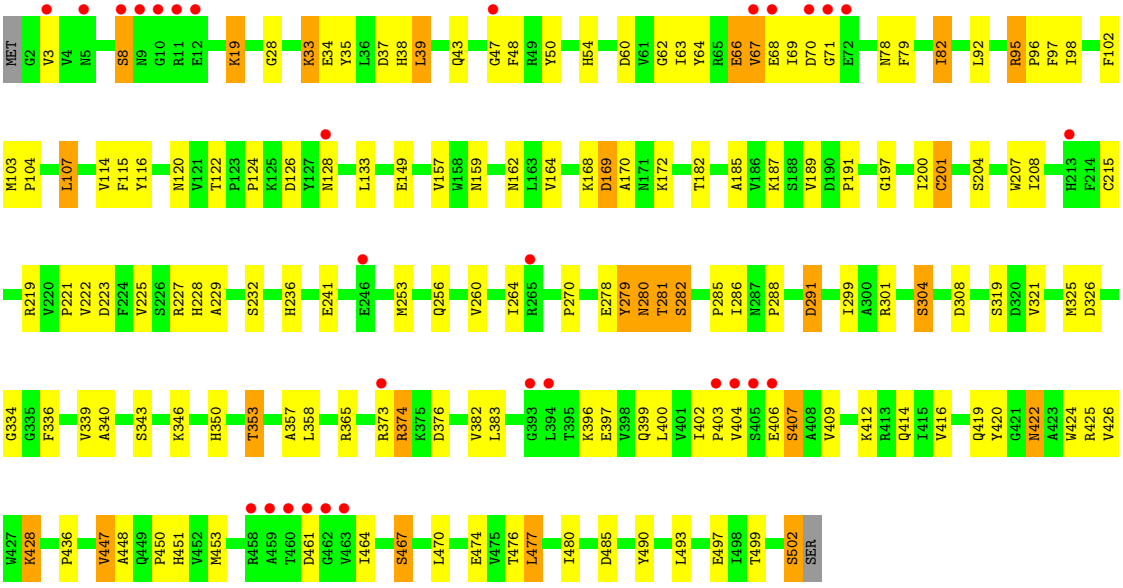
• Molecule 1: BETA-XYLOSIDASE

Chain E:



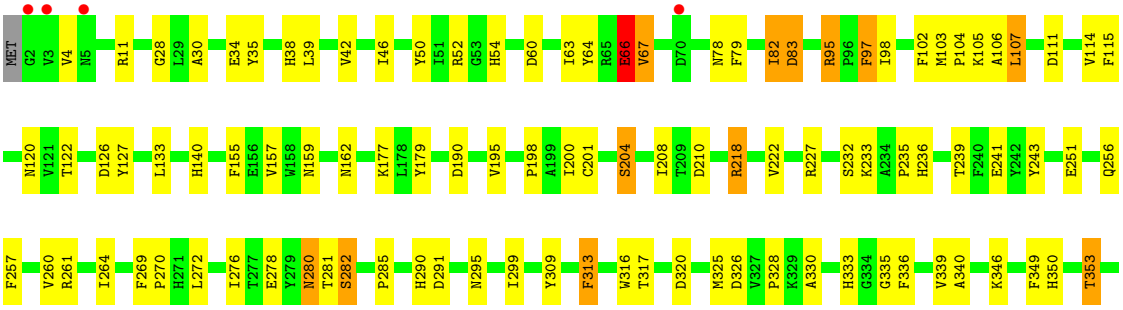
• Molecule 1: BETA-XYLOSIDASE

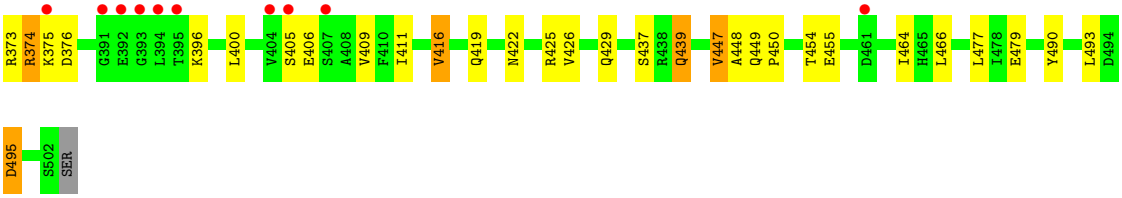
Chain F:



• Molecule 1: BETA-XYLOSIDASE

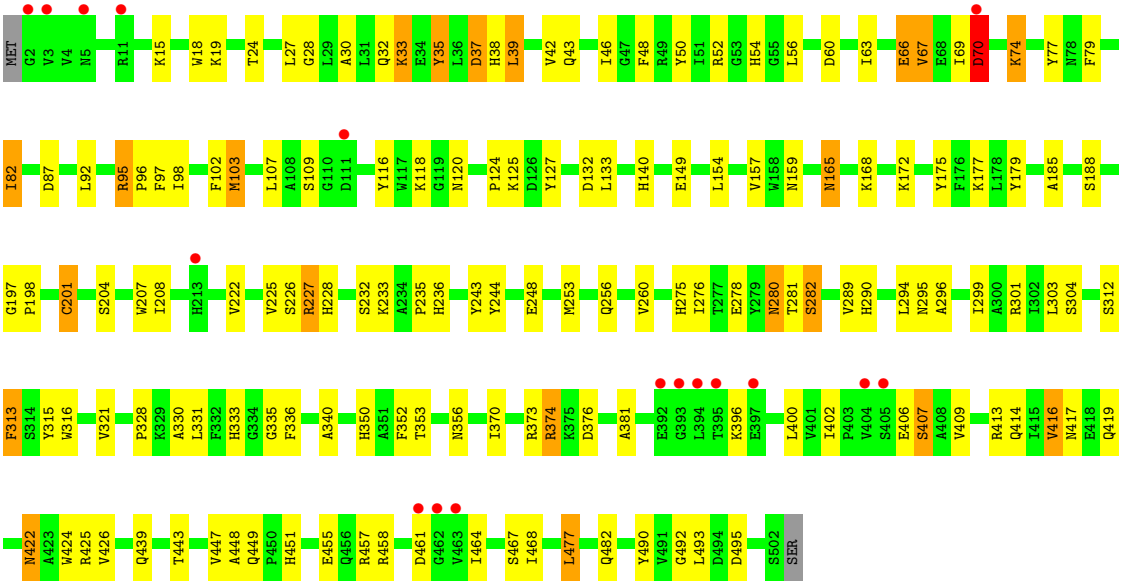
Chain G:





- Molecule 1: BETA-XYLOSIDASE

Chain H:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	18.3	Xtriage
Anisotropy	0.617	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 47.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	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 $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ANX, XYP, SO4, XYS, NA

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
All	All	0	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(^{o})	Ideal(^{o})
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

There are no chirality outliers.

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 (i)

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	93	0
1	B	4087	0	4000	109	0
1	C	4084	0	3998	99	0
1	D	4087	0	3999	107	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
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	9	0	0	1	0
4	D	9	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	9	0	3	1	0
5	B	9	0	8	1	0
5	C	9	0	8	1	0
5	D	9	0	2	1	0
5	E	9	0	8	0	0
5	F	9	0	8	0	0
5	G	9	0	8	1	0
5	H	9	0	8	2	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
6	C	5	0	0	0	0
6	D	5	0	0	0	0
6	E	5	0	0	0	0
6	F	5	0	0	0	0
6	G	5	0	0	1	0
6	H	5	0	0	1	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	32056	807	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 807 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%)	34	48
1	B	499/503 (99%)	469 (94%)	28 (6%)	2 (0%)	34	48
1	C	499/503 (99%)	475 (95%)	22 (4%)	2 (0%)	34	48
1	D	499/503 (99%)	466 (93%)	29 (6%)	4 (1%)	19	29
1	E	499/503 (99%)	470 (94%)	27 (5%)	2 (0%)	34	48
1	F	499/503 (99%)	468 (94%)	28 (6%)	3 (1%)	25	36
1	G	499/503 (99%)	469 (94%)	27 (5%)	3 (1%)	25	36
1	H	499/503 (99%)	469 (94%)	25 (5%)	5 (1%)	15	23
All	All	3992/4024 (99%)	3751 (94%)	218 (6%)	23 (1%)	25	36

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 (i)

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%)	8 12
1	B	439/441 (100%)	395 (90%)	44 (10%)	7 11
1	C	438/441 (99%)	398 (91%)	40 (9%)	9 14
1	D	439/441 (100%)	396 (90%)	43 (10%)	8 11
1	E	439/441 (100%)	401 (91%)	38 (9%)	10 15
1	F	439/441 (100%)	403 (92%)	36 (8%)	11 17
1	G	439/441 (100%)	409 (93%)	30 (7%)	16 25
1	H	439/441 (100%)	407 (93%)	32 (7%)	14 22
All	All	3511/3528 (100%)	3206 (91%)	305 (9%)	10 15

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

Mol	Chain	Res	Type
1	F	374	ARG
1	H	222	VAL
1	F	453	MET
1	G	313	PHE
1	H	457	ARG

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

Mol	Chain	Res	Type
1	E	236	HIS
1	F	399	GLN
1	H	356	ASN
1	E	280	ASN
1	F	43	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 28 ligands modelled in this entry, 8 are monoatomic - leaving 20 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	$\#\|Z\|>2$
6	SO4	E	1505	-	4,4,4	0.10	0	6,6,6	0.49	0
6	SO4	H	1505	-	4,4,4	0.19	0	6,6,6	0.30	0
4	XYP	D	1505	3	9,9,10	2.76	2 (22%)	10,12,14	1.86	2 (20%)
4	XYP	A	1505	3	9,9,10	2.67	2 (22%)	10,12,14	1.63	1 (10%)
3	ANX	D	1504	4,1	11,13,13	4.15	3 (27%)	13,18,18	2.32	4 (30%)
5	XYS	B	1504	1	9,9,10	2.16	4 (44%)	10,12,14	1.66	2 (20%)
5	XYS	A	1507	1	9,9,10	1.89	3 (33%)	10,12,14	1.64	2 (20%)
3	ANX	A	1504	4	11,13,13	4.38	4 (36%)	13,18,18	1.90	4 (30%)
6	SO4	G	1505	-	4,4,4	0.24	0	6,6,6	0.78	0
5	XYS	F	1504	1	9,9,10	2.31	4 (44%)	10,12,14	2.33	2 (20%)
5	XYS	C	1504	1	9,9,10	2.22	4 (44%)	10,12,14	2.15	2 (20%)
6	SO4	D	1506	-	4,4,4	0.25	0	6,6,6	0.30	0
6	SO4	F	1505	-	4,4,4	0.23	0	6,6,6	0.43	0
5	XYS	H	1504	1	9,9,10	2.25	3 (33%)	10,12,14	2.21	5 (50%)
5	XYS	G	1504	1	9,9,10	2.03	4 (44%)	10,12,14	2.35	4 (40%)
5	XYS	E	1504	1	9,9,10	2.20	4 (44%)	10,12,14	2.43	3 (30%)
6	SO4	A	1506	-	4,4,4	0.16	0	6,6,6	0.40	0
6	SO4	B	1505	-	4,4,4	0.21	0	6,6,6	0.26	0
6	SO4	C	1505	-	4,4,4	0.24	0	6,6,6	0.19	0
5	XYS	D	1507	1	9,9,10	1.92	2 (22%)	10,12,14	1.96	4 (40%)

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	XYS	D	1507	1	-	-	0/1/1/1
5	XYS	B	1504	1	-	-	0/1/1/1
5	XYS	C	1504	1	-	-	0/1/1/1
5	XYS	F	1504	1	-	-	0/1/1/1
5	XYS	G	1504	1	-	-	0/1/1/1
5	XYS	E	1504	1	-	-	0/1/1/1
5	XYS	H	1504	1	-	-	0/1/1/1
4	XYP	A	1505	3	-	-	0/1/1/1
3	ANX	D	1504	4,1	-	2/4/8/8	0/1/1/1
4	XYP	D	1505	3	-	-	1/1/1/1
5	XYS	A	1507	1	-	-	0/1/1/1
3	ANX	A	1504	4	-	2/4/8/8	0/1/1/1

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1504	ANX	O42-N1	13.02	1.44	1.22
3	D	1504	ANX	O42-N1	12.51	1.44	1.22
4	D	1505	XYP	O2-C2	-7.62	1.27	1.43
4	A	1505	XYP	O2-C2	-7.27	1.28	1.43
5	H	1504	XYS	O5-C1	4.77	1.52	1.42

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	1504	XYS	C1-C2-C3	-5.70	102.66	109.67
5	E	1504	XYS	C1-C2-C3	-5.60	102.79	109.67
5	C	1504	XYS	C1-C2-C3	-5.39	103.04	109.67
5	F	1504	XYS	C1-C2-C3	-5.36	103.08	109.67
3	D	1504	ANX	C5-C6-C1	5.35	123.34	118.75

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1505	XYP	C1-C2-C3-C4-C5-O5

11 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	1505	SO4	1	0
4	D	1505	XYP	3	0
4	A	1505	XYP	1	0
5	B	1504	XYS	1	0
5	A	1507	XYS	1	0
3	A	1504	ANX	1	0
6	G	1505	SO4	1	0
5	C	1504	XYS	1	0
5	H	1504	XYS	2	0
5	G	1504	XYS	1	0
5	D	1507	XYS	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^{th} 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%)	0.13	18 (3%)	42	42	17, 24, 43, 51	0
1	B	501/503 (99%)	0.21	27 (5%)	25	24	16, 24, 44, 52	0
1	C	501/503 (99%)	0.10	21 (4%)	36	35	16, 24, 43, 52	0
1	D	501/503 (99%)	0.19	14 (2%)	53	51	16, 24, 43, 51	0
1	E	501/503 (99%)	0.08	11 (2%)	62	60	15, 24, 41, 51	0
1	F	501/503 (99%)	0.28	30 (5%)	21	20	16, 24, 44, 52	0
1	G	501/503 (99%)	0.10	14 (2%)	53	51	16, 23, 42, 51	0
1	H	501/503 (99%)	0.08	17 (3%)	45	44	15, 23, 43, 51	0
All	All	4008/4024 (99%)	0.15	152 (3%)	40	39	15, 24, 43, 52	0

The worst 5 of 152 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	405	SER	8.8
1	D	405	SER	8.1
1	H	2	GLY	7.9
1	G	2	GLY	7.7
1	G	405	SER	5.8

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

There are no monosaccharides in this entry.

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. The B-factors column lists the minimum, median, 95^{th} 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	B-factors(Å^2)	Q<0.9
3	ANX	A	1504	13/13	0.57	0.47	43,50,53,54	13
5	XYS	C	1504	9/10	0.76	0.26	35,38,40,41	0
3	ANX	D	1504	13/13	0.77	0.38	41,44,46,46	13
5	XYS	E	1504	9/10	0.77	0.25	36,37,38,39	0
5	XYS	F	1504	9/10	0.79	0.25	40,42,42,42	0
5	XYS	B	1504	9/10	0.84	0.23	39,39,41,42	0
5	XYS	H	1504	9/10	0.84	0.20	29,29,32,33	0
5	XYS	G	1504	9/10	0.86	0.24	35,36,36,38	0
4	XYP	D	1505	9/10	0.90	0.20	39,39,40,41	9
4	XYP	A	1505	9/10	0.91	0.20	37,37,38,38	9
5	XYS	A	1507	9/10	0.91	0.21	37,37,37,38	9
5	XYS	D	1507	9/10	0.92	0.23	39,39,40,40	9
6	SO4	F	1505	5/5	0.94	0.28	56,56,57,58	0
6	SO4	C	1505	5/5	0.96	0.22	60,60,62,62	0
6	SO4	E	1505	5/5	0.96	0.24	56,58,58,59	0
6	SO4	A	1506	5/5	0.96	0.26	55,56,57,57	0
6	SO4	G	1505	5/5	0.96	0.31	55,55,55,56	0
6	SO4	H	1505	5/5	0.96	0.31	64,64,65,66	0
6	SO4	B	1505	5/5	0.97	0.22	58,59,60,61	0
2	NA	F	1503	1/1	0.98	0.21	9,9,9,9	0
6	SO4	D	1506	5/5	0.98	0.17	58,59,59,60	0
2	NA	H	1503	1/1	0.99	0.17	4,4,4,4	0
2	NA	B	1503	1/1	0.99	0.21	5,5,5,5	0
2	NA	C	1503	1/1	0.99	0.20	7,7,7,7	0
2	NA	D	1503	1/1	0.99	0.19	10,10,10,10	0
2	NA	E	1503	1/1	0.99	0.23	6,6,6,6	0
2	NA	A	1503	1/1	0.99	0.35	19,19,19,19	0
2	NA	G	1503	1/1	0.99	0.22	9,9,9,9	0

6.5 Other polymers (i)

There are no such residues in this entry.