wwPDB X-ray Structure Validation Summary Report (i)

Aug 16, 2023 – 02:31 AM EDT

PDB ID	:	1YI7
Title	:	Beta-d-xylosidase (selenomethionine) XYND from Clostridium Acetobutylicum
Authors	:	Teplyakov, A.; Fedorov, E.; Gilliland, G.L.; Almo, S.C.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2005-01-11
Resolution	:	1.90 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 (1)) were used in the production of this report:

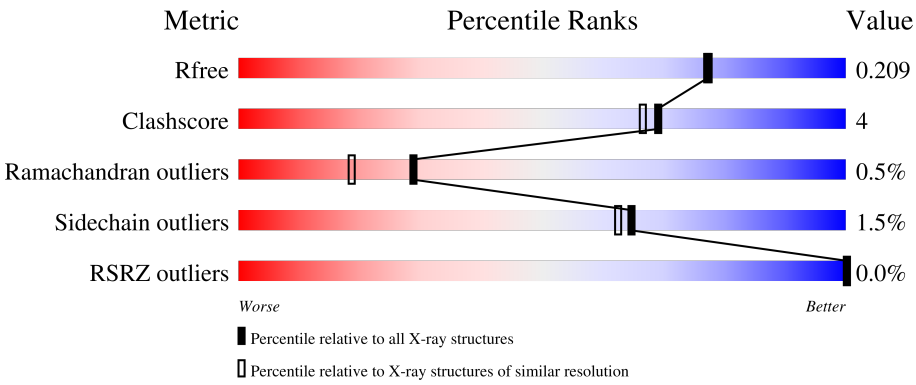
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	542	86% 13% •
1	B	542	86% 12% ••
1	C	542	89% 9% •
1	D	542	88% 9% ••

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 20181 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, family 43 glycosyl hydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	534	4341	2783	723	821	10	4	0	0	0
1	B	534	4345	2785	723	823	10	4	0	1	0
1	C	534	4343	2784	723	821	11	4	0	1	0
1	D	534	4347	2786	723	823	11	4	0	2	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	cloning artifact	UNP Q97DM1
A	2	SER	-	cloning artifact	UNP Q97DM1
A	3	LEU	-	cloning artifact	UNP Q97DM1
A	64	MSE	MET	modified residue	UNP Q97DM1
A	98	MSE	MET	modified residue	UNP Q97DM1
A	144	MSE	MET	modified residue	UNP Q97DM1
A	445	MSE	MET	modified residue	UNP Q97DM1
A	535	GLU	-	expression tag	UNP Q97DM1
A	536	GLY	-	expression tag	UNP Q97DM1
A	537	HIS	-	expression tag	UNP Q97DM1
A	538	HIS	-	expression tag	UNP Q97DM1
A	539	HIS	-	expression tag	UNP Q97DM1
A	540	HIS	-	expression tag	UNP Q97DM1
A	541	HIS	-	expression tag	UNP Q97DM1
A	542	HIS	-	expression tag	UNP Q97DM1
B	1	MSE	-	cloning artifact	UNP Q97DM1
B	2	SER	-	cloning artifact	UNP Q97DM1
B	3	LEU	-	cloning artifact	UNP Q97DM1
B	64	MSE	MET	modified residue	UNP Q97DM1
B	98	MSE	MET	modified residue	UNP Q97DM1
B	144	MSE	MET	modified residue	UNP Q97DM1

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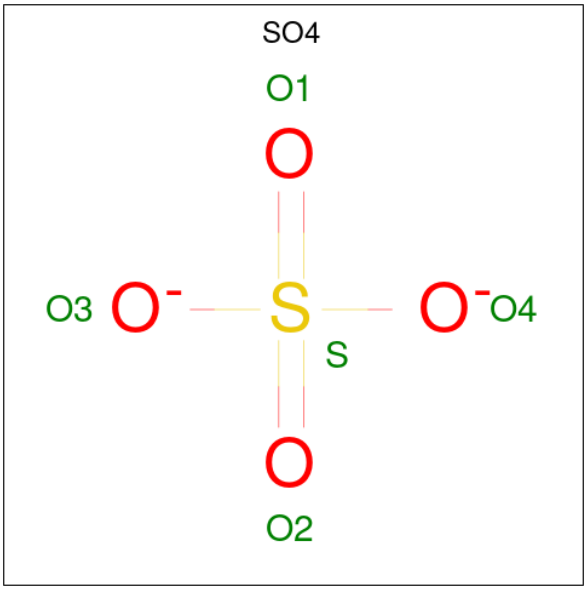
Chain	Residue	Modelled	Actual	Comment	Reference
B	445	MSE	MET	modified residue	UNP Q97DM1
B	535	GLU	-	expression tag	UNP Q97DM1
B	536	GLY	-	expression tag	UNP Q97DM1
B	537	HIS	-	expression tag	UNP Q97DM1
B	538	HIS	-	expression tag	UNP Q97DM1
B	539	HIS	-	expression tag	UNP Q97DM1
B	540	HIS	-	expression tag	UNP Q97DM1
B	541	HIS	-	expression tag	UNP Q97DM1
B	542	HIS	-	expression tag	UNP Q97DM1
C	1	MSE	-	cloning artifact	UNP Q97DM1
C	2	SER	-	cloning artifact	UNP Q97DM1
C	3	LEU	-	cloning artifact	UNP Q97DM1
C	64	MSE	MET	modified residue	UNP Q97DM1
C	98	MSE	MET	modified residue	UNP Q97DM1
C	144	MSE	MET	modified residue	UNP Q97DM1
C	445	MSE	MET	modified residue	UNP Q97DM1
C	535	GLU	-	expression tag	UNP Q97DM1
C	536	GLY	-	expression tag	UNP Q97DM1
C	537	HIS	-	expression tag	UNP Q97DM1
C	538	HIS	-	expression tag	UNP Q97DM1
C	539	HIS	-	expression tag	UNP Q97DM1
C	540	HIS	-	expression tag	UNP Q97DM1
C	541	HIS	-	expression tag	UNP Q97DM1
C	542	HIS	-	expression tag	UNP Q97DM1
D	1	MSE	-	cloning artifact	UNP Q97DM1
D	2	SER	-	cloning artifact	UNP Q97DM1
D	3	LEU	-	cloning artifact	UNP Q97DM1
D	64	MSE	MET	modified residue	UNP Q97DM1
D	98	MSE	MET	modified residue	UNP Q97DM1
D	144	MSE	MET	modified residue	UNP Q97DM1
D	445	MSE	MET	modified residue	UNP Q97DM1
D	535	GLU	-	expression tag	UNP Q97DM1
D	536	GLY	-	expression tag	UNP Q97DM1
D	537	HIS	-	expression tag	UNP Q97DM1
D	538	HIS	-	expression tag	UNP Q97DM1
D	539	HIS	-	expression tag	UNP Q97DM1
D	540	HIS	-	expression tag	UNP Q97DM1
D	541	HIS	-	expression tag	UNP Q97DM1
D	542	HIS	-	expression tag	UNP Q97DM1

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0

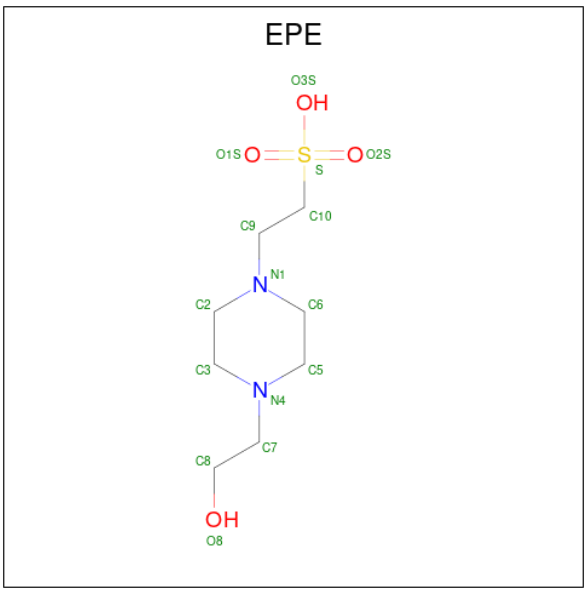
- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

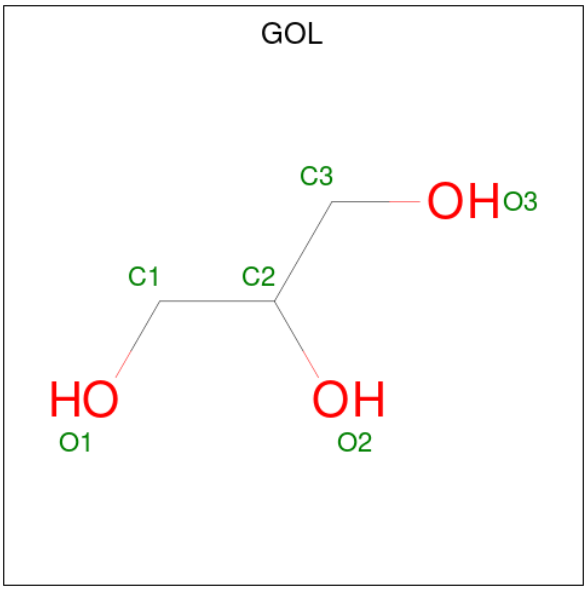
- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID

(three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	15	8	2	4	1	0	0
			Total	C	N	O	S		
4	A	1	15	8	2	4	1	0	0
			Total	C	N	O	S		
4	C	1	15	8	2	4	1	0	0
			Total	C	N	O	S		
4	D	1	15	8	2	4	1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is water.

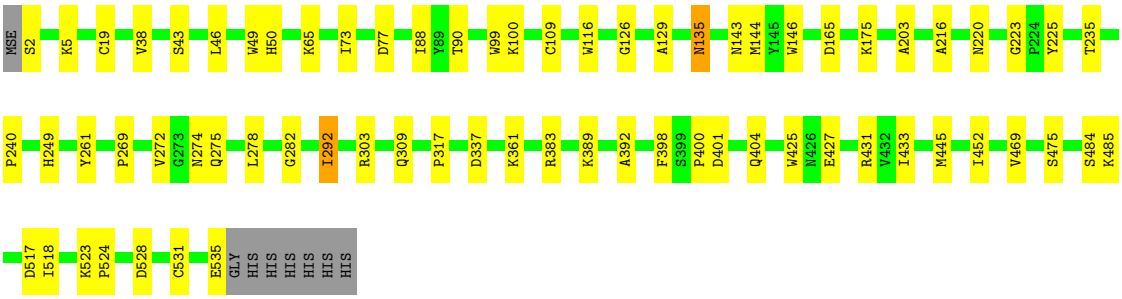
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	683	683	683	0	0
			Total	O		
6	B	614	614	614	0	0
			Total	O		
6	C	656	656	656	0	0
			Total	O		
6	D	633	633	633	0	0

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, family 43 glycosyl hydrolase

Chain A:

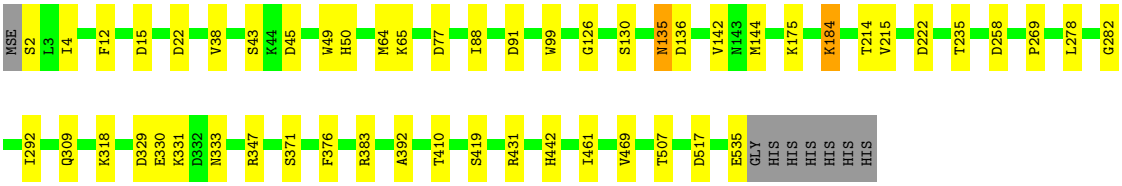


• Molecule 1: Beta-xylosidase, family 43 glycosyl hydrolase

Chain B:

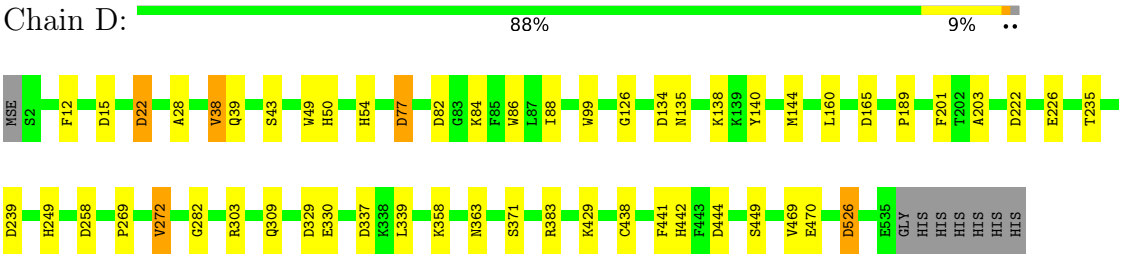
• Molecule 1: Beta-xylosidase, family 43 glycosyl hydrolase

Chain C:



• Molecule 1: Beta-xylosidase, family 43 glycosyl hydrolase

Chain D:


88%
9%
MSE S2 F12 D15 D22 A28 V38 Q39 S43 W49 H50 H54 D77 D82 G83 K84 F85 W86 L87 I88 W99 G126 D134 N135 K138 K139 Y140 M144 L160 D165 P189 F201 T202 A203 D222 E226 T235
D239 H249 D258 P269 V272 G282 R303 Q309 D329 E330 D337 K338 L339 K358 N363 S371 R383 K429 C438 F441 H442 F443 D444 S449 V469 E470 D526 E535 GLY HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	89.13Å 143.73Å 188.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 38.52 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-1.90) 100.0 (38.52-1.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.85 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.142 , 0.202 0.149 , 0.209	Depositor DCC
R_{free} test set	5744 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å^2)	17.6	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 51.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	20181	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: SO4, CA, EPE, GOL

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	0.64	1/4470 (0.0%)	0.80	4/6077 (0.1%)
1	B	0.61	0/4478	0.81	7/6088 (0.1%)
1	C	0.65	0/4476	0.82	9/6085 (0.1%)
1	D	0.64	0/4484	0.83	12/6096 (0.2%)
All	All	0.64	1/17908 (0.0%)	0.82	32/24346 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	19	CYS	CB-SG	-5.69	1.72	1.81

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	528	ASP	CB-CG-OD2	7.31	124.88	118.30
1	B	526	ASP	CB-CG-OD2	7.13	124.72	118.30
1	D	526	ASP	CB-CG-OD2	6.57	124.21	118.30
1	C	15	ASP	CB-CG-OD2	6.40	124.06	118.30
1	D	77	ASP	CB-CG-OD2	6.22	123.90	118.30

There are no chirality outliers.

There are no planarity outliers.

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	4341	0	4127	40	0
1	B	4345	0	4127	32	0
1	C	4343	0	4128	29	0
1	D	4347	0	4128	32	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
3	A	10	0	0	1	0
3	B	10	0	0	0	0
3	C	5	0	0	0	0
3	D	10	0	0	0	0
4	A	30	0	34	0	0
4	C	15	0	17	1	0
4	D	15	0	17	0	0
5	A	30	0	40	0	0
5	B	30	0	40	2	0
5	C	30	0	40	1	0
5	D	30	0	40	0	0
6	A	683	0	0	5	0
6	B	614	0	0	2	0
6	C	656	0	0	5	0
6	D	633	0	0	13	0
All	All	20181	0	16738	126	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 4.

The worst 5 of 126 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:C:331:LYS:HE2	1:C:333:ASN:HD21	1.46	0.79
1:A:475:SER:HB3	1:A:485:LYS:HA	1.63	0.78
1:D:358:LYS:HE3	6:D:3636:HOH:O	1.84	0.77
1:A:65:LYS:HA	6:A:3696:HOH:O	1.87	0.74
1:A:269:PRO:HB3	1:A:282:GLY:HA3	1.71	0.72

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	532/542 (98%)	503 (94%)	27 (5%)	2 (0%)	34	24
1	B	533/542 (98%)	504 (95%)	26 (5%)	3 (1%)	25	15
1	C	533/542 (98%)	503 (94%)	28 (5%)	2 (0%)	34	24
1	D	534/542 (98%)	504 (94%)	27 (5%)	3 (1%)	25	15
All	All	2132/2168 (98%)	2014 (94%)	108 (5%)	10 (0%)	29	18

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	469	VAL
1	B	469	VAL
1	C	469	VAL
1	D	469	VAL
1	B	12	PHE

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	475/477 (100%)	467 (98%)	8 (2%)	60	57
1	B	476/477 (100%)	469 (98%)	7 (2%)	65	62
1	C	476/477 (100%)	469 (98%)	7 (2%)	65	62
1	D	477/477 (100%)	471 (99%)	6 (1%)	69	68
All	All	1904/1908 (100%)	1876 (98%)	28 (2%)	65	62

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	402	THR
1	D	383	ARG
1	C	135	ASN
1	D	222	ASP
1	C	50	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	333	ASN
1	D	135	ASN
1	C	135	ASN
1	B	333	ASN
1	C	333	ASN

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 35 ligands modelled in this entry, 4 are monoatomic - leaving 31 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	SO4	D	3008	-	4,4,4	0.19	0	6,6,6	0.22	0
3	SO4	D	3010	-	4,4,4	0.16	0	6,6,6	0.59	0
3	SO4	B	3009	-	4,4,4	0.14	0	6,6,6	0.20	0
5	GOL	D	3023	-	5,5,5	0.44	0	5,5,5	1.14	0
4	EPE	C	3015	-	15,15,15	0.90	1 (6%)	18,20,20	1.66	3 (16%)
3	SO4	A	3005	-	4,4,4	0.19	0	6,6,6	0.20	0
5	GOL	C	3022	-	5,5,5	0.34	0	5,5,5	0.88	0
5	GOL	B	3021	-	5,5,5	0.36	0	5,5,5	1.40	1 (20%)
5	GOL	D	3031	-	5,5,5	0.23	0	5,5,5	0.57	0
5	GOL	D	3019	-	5,5,5	0.23	0	5,5,5	0.41	0
5	GOL	C	3030	-	5,5,5	0.46	0	5,5,5	0.33	0
5	GOL	D	3027	-	5,5,5	0.39	0	5,5,5	0.41	0
3	SO4	A	3011	-	4,4,4	0.21	0	6,6,6	0.22	0
5	GOL	B	3017	-	5,5,5	0.28	0	5,5,5	0.38	0
5	GOL	D	3035	-	5,5,5	0.43	0	5,5,5	0.30	0
5	GOL	A	3016	-	5,5,5	0.47	0	5,5,5	0.37	0
5	GOL	B	3033	-	5,5,5	0.47	0	5,5,5	0.38	0
4	EPE	A	3013	-	15,15,15	0.82	1 (6%)	18,20,20	1.78	3 (16%)
5	GOL	A	3024	-	5,5,5	0.39	0	5,5,5	0.39	0
4	EPE	D	3014	-	15,15,15	0.77	1 (6%)	18,20,20	1.56	2 (11%)
5	GOL	B	3025	-	5,5,5	0.40	0	5,5,5	0.46	0
5	GOL	B	3029	-	5,5,5	0.39	0	5,5,5	0.86	0
3	SO4	C	3007	-	4,4,4	0.22	0	6,6,6	0.15	0
5	GOL	C	3026	-	5,5,5	0.43	0	5,5,5	0.57	0
5	GOL	A	3032	-	5,5,5	0.55	0	5,5,5	0.41	0
5	GOL	A	3028	-	5,5,5	0.42	0	5,5,5	0.45	0
5	GOL	C	3034	-	5,5,5	0.42	0	5,5,5	0.51	0
5	GOL	A	3020	-	5,5,5	0.49	0	5,5,5	1.28	1 (20%)
4	EPE	A	3012	-	15,15,15	0.82	1 (6%)	18,20,20	1.29	2 (11%)
3	SO4	B	3006	-	4,4,4	0.20	0	6,6,6	0.24	0
5	GOL	C	3018	-	5,5,5	0.46	0	5,5,5	0.54	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	GOL	D	3023	-	-	0/4/4/4	-
4	EPE	C	3015	-	-	1/9/19/19	0/1/1/1
5	GOL	C	3022	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	3021	-	-	0/4/4/4	-
5	GOL	D	3031	-	-	0/4/4/4	-
5	GOL	D	3019	-	-	0/4/4/4	-
5	GOL	C	3030	-	-	1/4/4/4	-
5	GOL	D	3027	-	-	2/4/4/4	-
5	GOL	B	3017	-	-	0/4/4/4	-
5	GOL	D	3035	-	-	1/4/4/4	-
5	GOL	A	3016	-	-	0/4/4/4	-
5	GOL	B	3033	-	-	0/4/4/4	-
4	EPE	A	3013	-	-	0/9/19/19	0/1/1/1
5	GOL	A	3024	-	-	4/4/4/4	-
4	EPE	D	3014	-	-	1/9/19/19	0/1/1/1
5	GOL	B	3025	-	-	4/4/4/4	-
5	GOL	B	3029	-	-	4/4/4/4	-
5	GOL	C	3026	-	-	4/4/4/4	-
5	GOL	A	3032	-	-	0/4/4/4	-
5	GOL	A	3028	-	-	0/4/4/4	-
5	GOL	C	3034	-	-	1/4/4/4	-
5	GOL	A	3020	-	-	0/4/4/4	-
4	EPE	A	3012	-	-	0/9/19/19	0/1/1/1
5	GOL	C	3018	-	-	0/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	3015	EPE	C10-S	2.78	1.81	1.77
4	A	3012	EPE	C10-S	2.71	1.81	1.77
4	A	3013	EPE	C10-S	2.53	1.81	1.77
4	D	3014	EPE	C10-S	2.49	1.81	1.77

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	3015	EPE	C5-N4-C3	4.70	119.40	108.83
4	D	3014	EPE	C5-N4-C3	4.63	119.25	108.83
4	A	3013	EPE	C5-N4-C3	4.02	117.88	108.83
4	A	3013	EPE	O1S-S-C10	3.42	111.03	106.92
4	A	3012	EPE	C5-N4-C3	3.17	115.96	108.83

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	3024	GOL	C1-C2-C3-O3
5	B	3025	GOL	O1-C1-C2-C3
5	B	3025	GOL	C1-C2-C3-O3
5	B	3029	GOL	C1-C2-C3-O3
5	C	3026	GOL	O1-C1-C2-C3

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	3015	EPE	1	0
5	C	3030	GOL	1	0
3	A	3011	SO4	1	0
5	B	3033	GOL	1	0
5	B	3029	GOL	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	530/542 (97%)	-0.41	0 100 100	13, 20, 40, 67	0
1	B	530/542 (97%)	-0.34	1 (0%) 95 95	16, 22, 40, 75	0
1	C	530/542 (97%)	-0.44	0 100 100	14, 21, 41, 91	0
1	D	530/542 (97%)	-0.51	0 100 100	14, 20, 39, 77	0
All	All	2120/2168 (97%)	-0.42	1 (0%) 100 100	13, 21, 40, 91	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	265	LEU	2.0

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

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

6.3 Carbohydrates (i)

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, 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	B-factors(Å^2)	Q<0.9
5	GOL	C	3026	6/6	0.87	0.19	30,37,41,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	B	3025	6/6	0.91	0.18	33,50,59,78	0
5	GOL	A	3024	6/6	0.91	0.17	31,42,49,51	0
5	GOL	D	3027	6/6	0.93	0.15	37,45,47,49	0
5	GOL	C	3034	6/6	0.94	0.14	21,28,46,56	0
3	SO4	A	3011	5/5	0.95	0.28	64,65,75,78	0
4	EPE	A	3012	15/15	0.95	0.10	18,27,50,56	0
3	SO4	A	3005	5/5	0.95	0.18	37,54,59,63	0
5	GOL	D	3023	6/6	0.95	0.18	16,23,26,30	0
5	GOL	A	3032	6/6	0.95	0.14	20,25,33,42	0
5	GOL	D	3031	6/6	0.95	0.08	27,34,40,44	0
3	SO4	C	3007	5/5	0.96	0.19	38,44,58,125	0
3	SO4	B	3009	5/5	0.96	0.19	30,40,53,67	0
5	GOL	B	3017	6/6	0.96	0.08	20,24,25,27	0
4	EPE	C	3015	15/15	0.96	0.08	17,25,42,46	0
5	GOL	B	3033	6/6	0.96	0.14	20,32,43,44	0
3	SO4	D	3008	5/5	0.97	0.17	44,47,50,75	0
4	EPE	D	3014	15/15	0.97	0.06	18,24,45,49	0
5	GOL	C	3018	6/6	0.97	0.08	17,20,23,25	0
5	GOL	C	3022	6/6	0.97	0.21	19,24,25,43	0
5	GOL	A	3020	6/6	0.97	0.23	11,17,25,28	0
5	GOL	C	3030	6/6	0.97	0.15	27,37,39,39	0
3	SO4	D	3010	5/5	0.97	0.09	31,37,52,54	0
3	SO4	B	3006	5/5	0.97	0.16	40,46,56,68	0
4	EPE	A	3013	15/15	0.97	0.08	17,24,38,52	0
5	GOL	B	3021	6/6	0.97	0.21	15,19,25,28	0
5	GOL	D	3019	6/6	0.98	0.07	14,16,22,22	0
5	GOL	A	3016	6/6	0.98	0.07	16,19,22,22	0
5	GOL	A	3028	6/6	0.98	0.07	24,39,43,44	0
5	GOL	B	3029	6/6	0.98	0.08	28,32,35,38	0
5	GOL	D	3035	6/6	0.98	0.13	20,28,38,56	0
2	CA	C	3003	1/1	0.99	0.15	38,38,38,38	0
2	CA	D	3004	1/1	0.99	0.08	41,41,41,41	0
2	CA	B	3002	1/1	0.99	0.19	42,42,42,42	0
2	CA	A	3001	1/1	1.00	0.17	43,43,43,43	0

6.5 Other polymers (i)

There are no such residues in this entry.