wwPDB X-ray Structure Validation Summary Report (i)

Aug 8, 2023 – 12:36 AM EDT

PDB ID	:	1PX4
Title	:	E. COLI (LACZ) BETA-GALACTOSIDASE (G794A) WITH IPTG BOUND
Authors	:	Juers, D.H.; Hakda, S.; Matthews, B.W.; Huber, R.E.
Deposited on	:	2003-07-02
Resolution	:	1.60 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:

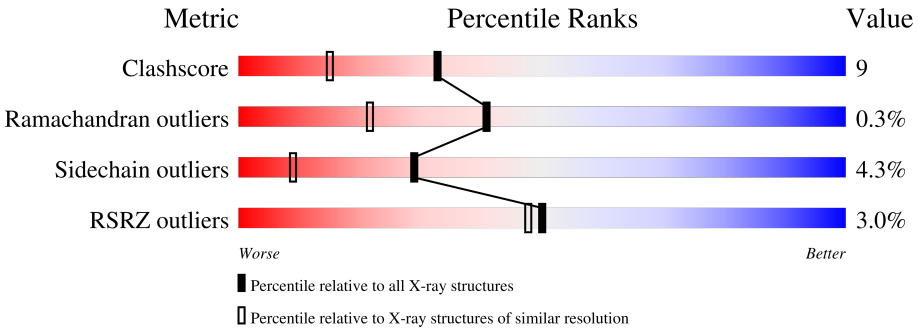
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.60 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))
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	1023	3% 71% 23% 5%
1	B	1023	3% 71% 24%
1	C	1023	2% 68% 25% 5%
1	D	1023	4% 70% 23% 5%

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	MG	A	3105	-	-	-	X
5	DMS	A	8404	-	-	X	-
5	DMS	A	8416	-	-	X	-
5	DMS	B	8506	-	-	X	-
5	DMS	C	8506	-	-	X	-
5	DMS	D	8506	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 36785 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-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1011	Total	C	N	O	S	0	0	0
			8126	5139	1440	1509	38			
1	B	1011	Total	C	N	O	S	0	0	0
			8126	5139	1440	1509	38			
1	C	1011	Total	C	N	O	S	0	0	0
			8126	5139	1440	1509	38			
1	D	1011	Total	C	N	O	S	0	0	0
			8126	5139	1440	1509	38			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP P00722
A	2	SER	-	cloning artifact	UNP P00722
A	3	HIS	-	cloning artifact	UNP P00722
A	4	MET	-	cloning artifact	UNP P00722
A	5	LEU	-	cloning artifact	UNP P00722
A	6	GLU	-	cloning artifact	UNP P00722
A	7	ASP	-	cloning artifact	UNP P00722
A	8	PRO	-	cloning artifact	UNP P00722
A	794	ALA	GLY	engineered mutation	UNP P00722
B	1	GLY	-	cloning artifact	UNP P00722
B	2	SER	-	cloning artifact	UNP P00722
B	3	HIS	-	cloning artifact	UNP P00722
B	4	MET	-	cloning artifact	UNP P00722
B	5	LEU	-	cloning artifact	UNP P00722
B	6	GLU	-	cloning artifact	UNP P00722
B	7	ASP	-	cloning artifact	UNP P00722
B	8	PRO	-	cloning artifact	UNP P00722
B	794	ALA	GLY	engineered mutation	UNP P00722
C	1	GLY	-	cloning artifact	UNP P00722
C	2	SER	-	cloning artifact	UNP P00722
C	3	HIS	-	cloning artifact	UNP P00722

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Chain	Residue	Modelled	Actual	Comment	Reference
C	4	MET	-	cloning artifact	UNP P00722
C	5	LEU	-	cloning artifact	UNP P00722
C	6	GLU	-	cloning artifact	UNP P00722
C	7	ASP	-	cloning artifact	UNP P00722
C	8	PRO	-	cloning artifact	UNP P00722
C	794	ALA	GLY	engineered mutation	UNP P00722
D	1	GLY	-	cloning artifact	UNP P00722
D	2	SER	-	cloning artifact	UNP P00722
D	3	HIS	-	cloning artifact	UNP P00722
D	4	MET	-	cloning artifact	UNP P00722
D	5	LEU	-	cloning artifact	UNP P00722
D	6	GLU	-	cloning artifact	UNP P00722
D	7	ASP	-	cloning artifact	UNP P00722
D	8	PRO	-	cloning artifact	UNP P00722
D	794	ALA	GLY	engineered mutation	UNP P00722

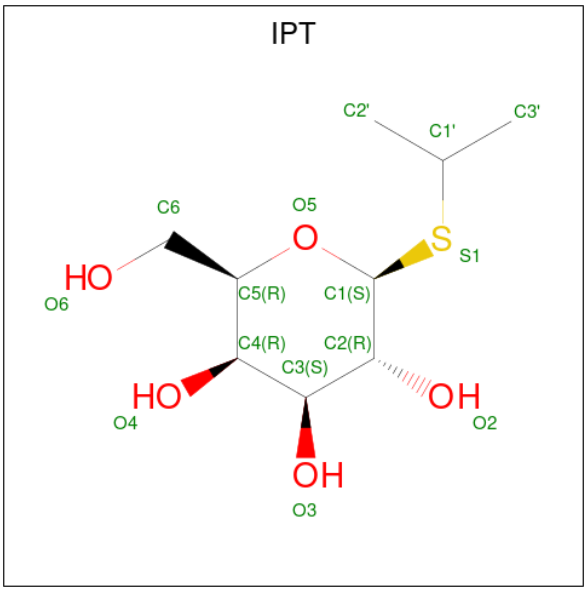
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total Mg 4 4	0	0
2	B	3	Total Mg 3 3	0	0
2	C	5	Total Mg 5 5	0	0
2	D	4	Total Mg 4 4	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

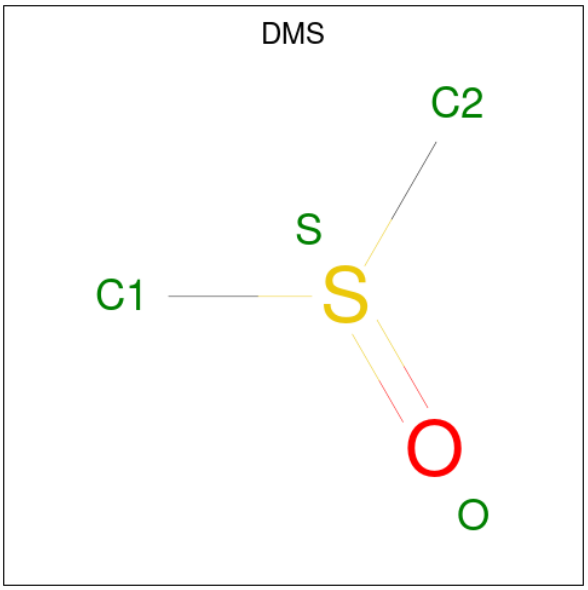
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total Na 4 4	0	0
3	B	4	Total Na 4 4	0	0
3	C	4	Total Na 4 4	0	0
3	D	4	Total Na 4 4	0	0

- Molecule 4 is 1-methylethyl 1-thio-beta-D-galactopyranoside (three-letter code: IPT) (formula: $C_9H_{18}O_5S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O S 15 9 5 1	0	0
4	B	1	Total C O S 15 9 5 1	0	0
4	C	1	Total C O S 15 9 5 1	0	0
4	D	1	Total C O S 15 9 5 1	0	0

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	D	1	Total	C	O	S	0	0
			4	2	1	1		
5	D	1	Total	C	O	S	0	0
			4	2	1	1		
5	D	1	Total	C	O	S	0	0
			4	2	1	1		
5	D	1	Total	C	O	S	0	0
			4	2	1	1		
5	D	1	Total	C	O	S	0	0
			4	2	1	1		
5	D	1	Total	C	O	S	0	0
			4	2	1	1		
5	D	1	Total	C	O	S	0	0
			4	2	1	1		
5	D	1	Total	C	O	S	0	0
			4	2	1	1		
5	D	1	Total	C	O	S	0	0
			4	2	1	1		
5	D	1	Total	C	O	S	0	0
			4	2	1	1		
5	D	1	Total	C	O	S	0	0
			4	2	1	1		
5	D	1	Total	C	O	S	0	0
			4	2	1	1		
5	D	1	Total	C	O	S	0	0
			4	2	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	O	S	0	0
			4	2	1	1		
5	D	1	Total	C	O	S	0	0
			4	2	1	1		
5	D	1	Total	C	O	S	0	0
			4	2	1	1		
5	D	1	Total	C	O	S	0	0
			4	2	1	1		
5	D	1	Total	C	O	S	0	0
			4	2	1	1		
5	D	1	Total	C	O	S	0	0
			4	2	1	1		
5	D	1	Total	C	O	S	0	0
			4	2	1	1		
5	D	1	Total	C	O	S	0	0
			4	2	1	1		
5	D	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 6 is water.

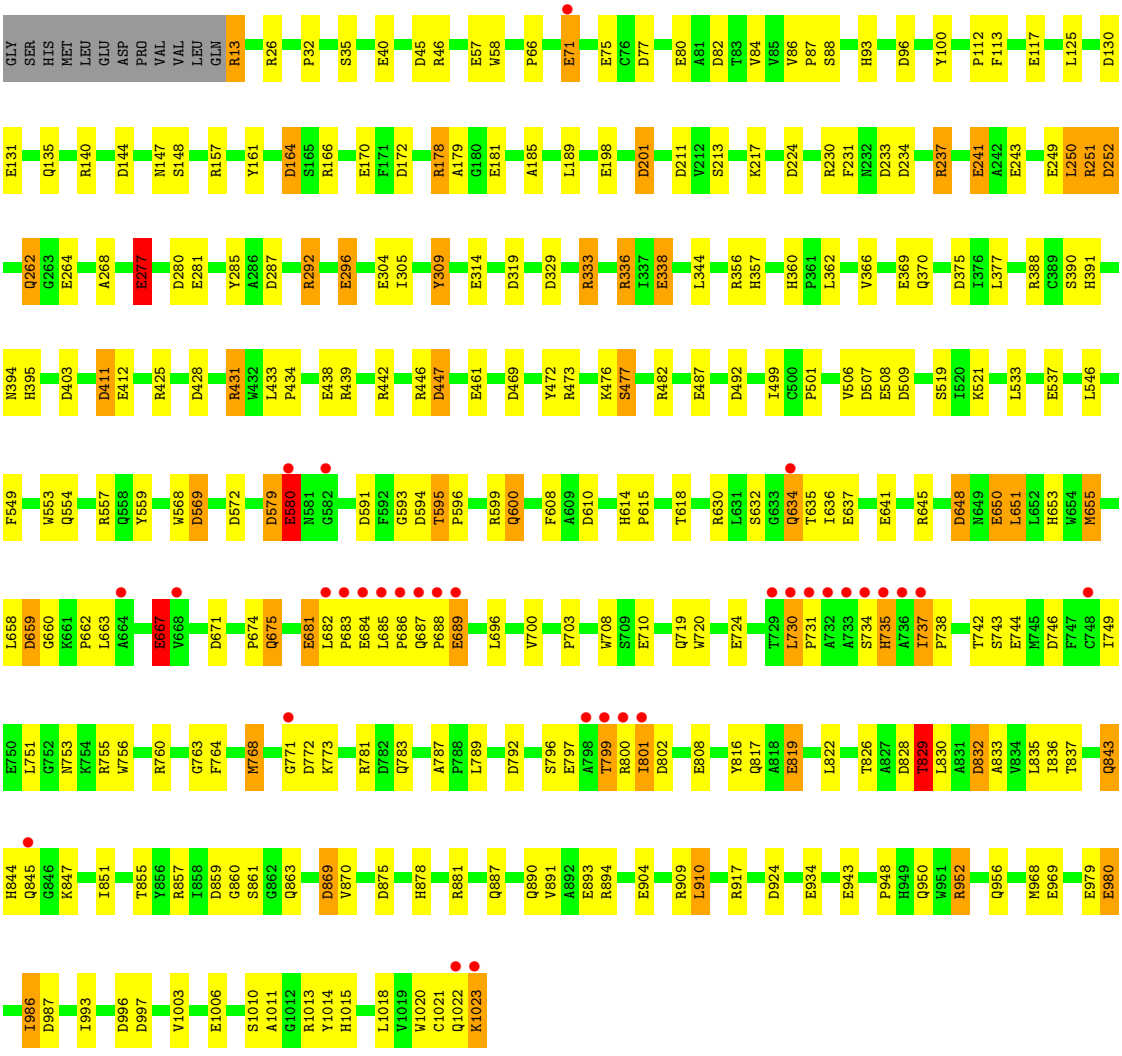
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	950	Total	O	0	0
			950	950		
6	B	971	Total	O	0	0
			971	971		
6	C	943	Total	O	0	0
			943	943		
6	D	949	Total	O	0	0
			949	949		

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.

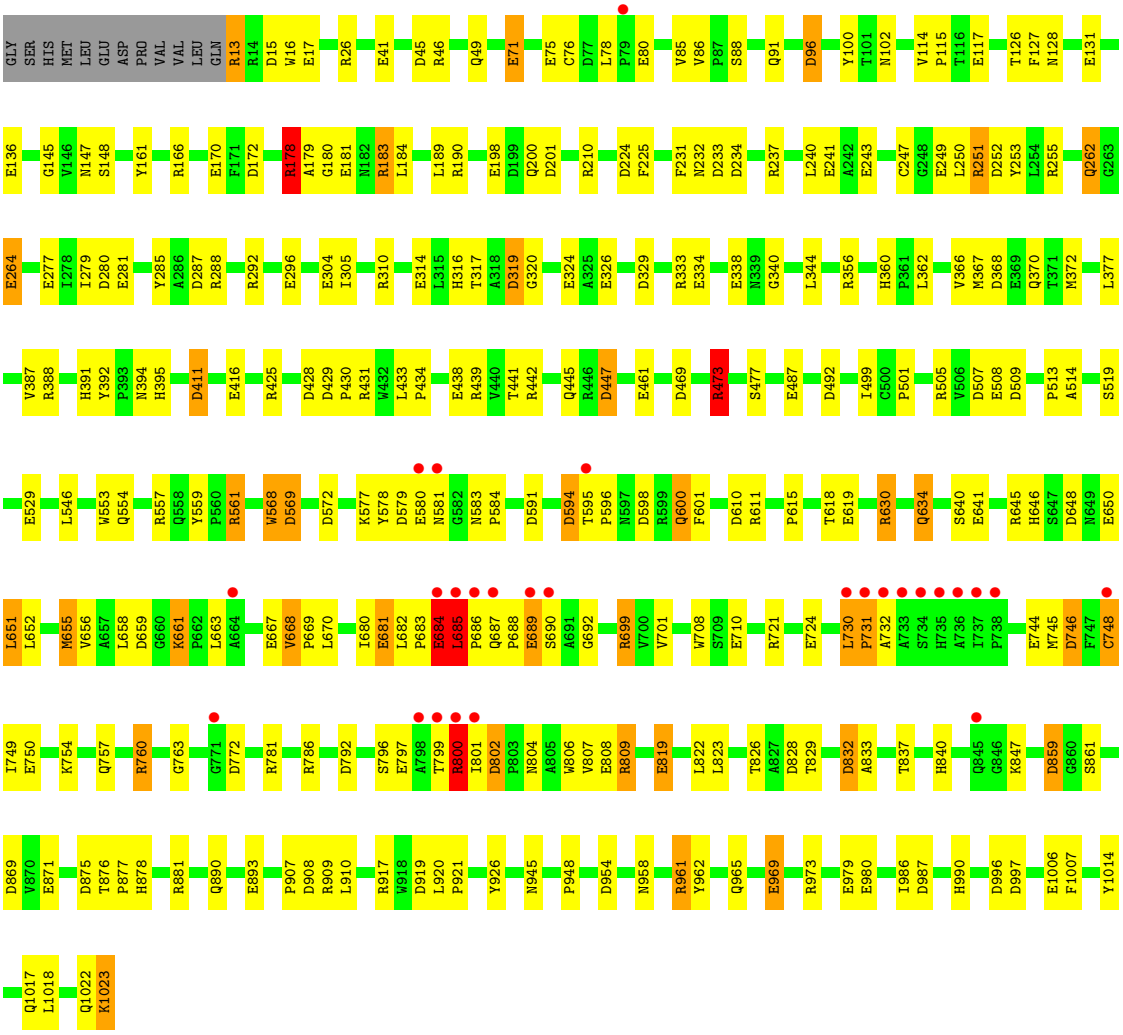
• Molecule 1: beta-galactosidase

Chain A:



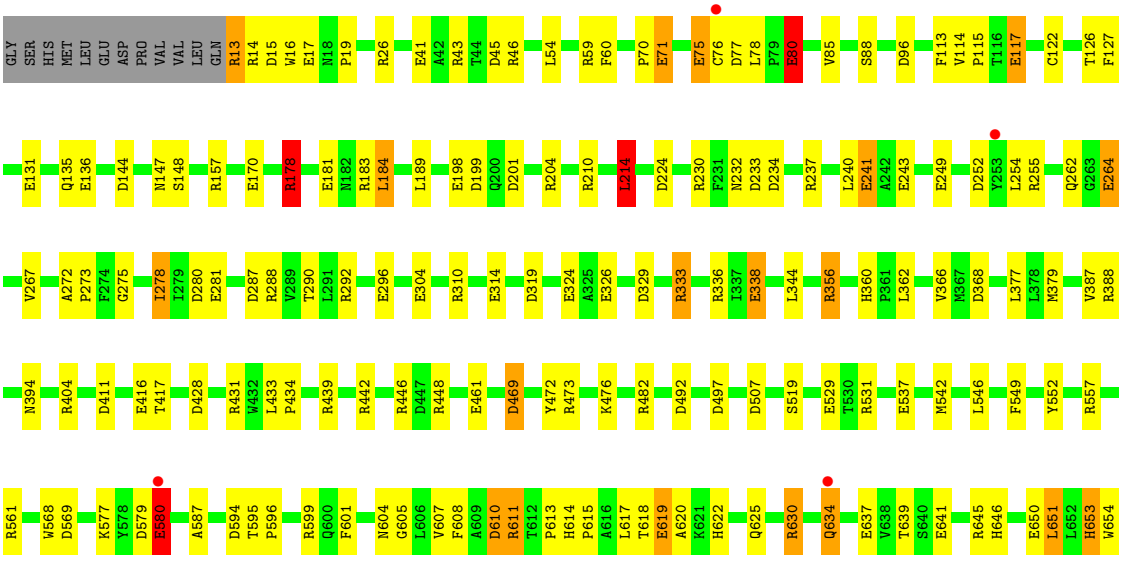
• Molecule 1: beta-galactosidase

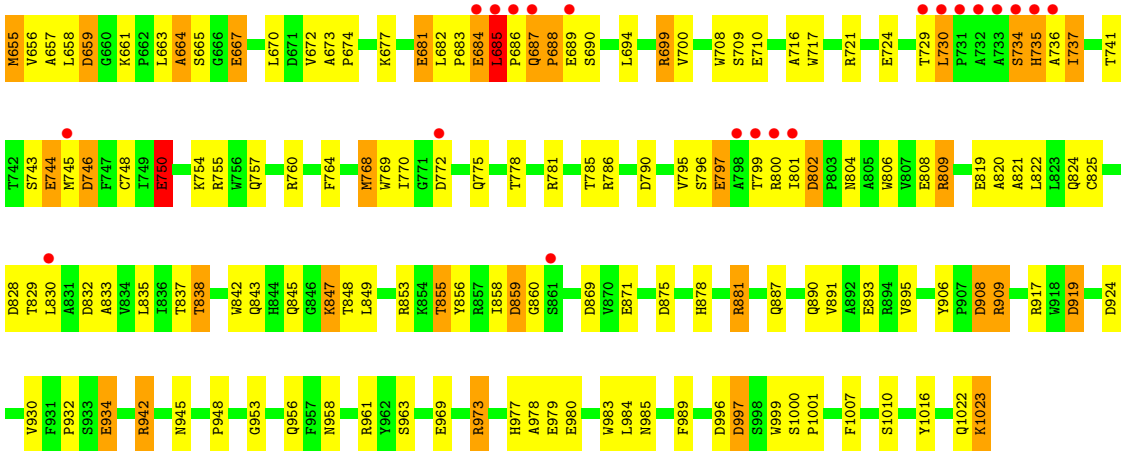
Chain B:

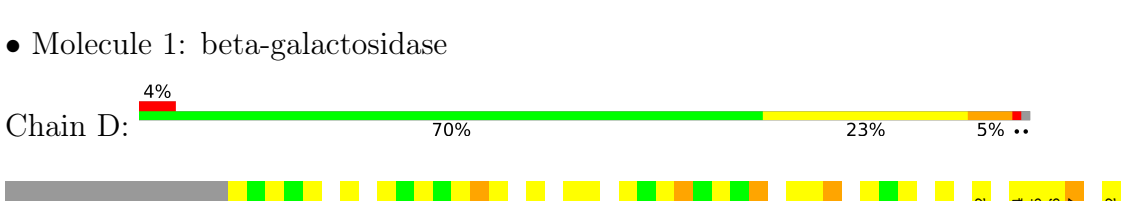


• Molecule 1: beta-galactosidase

Chain C:

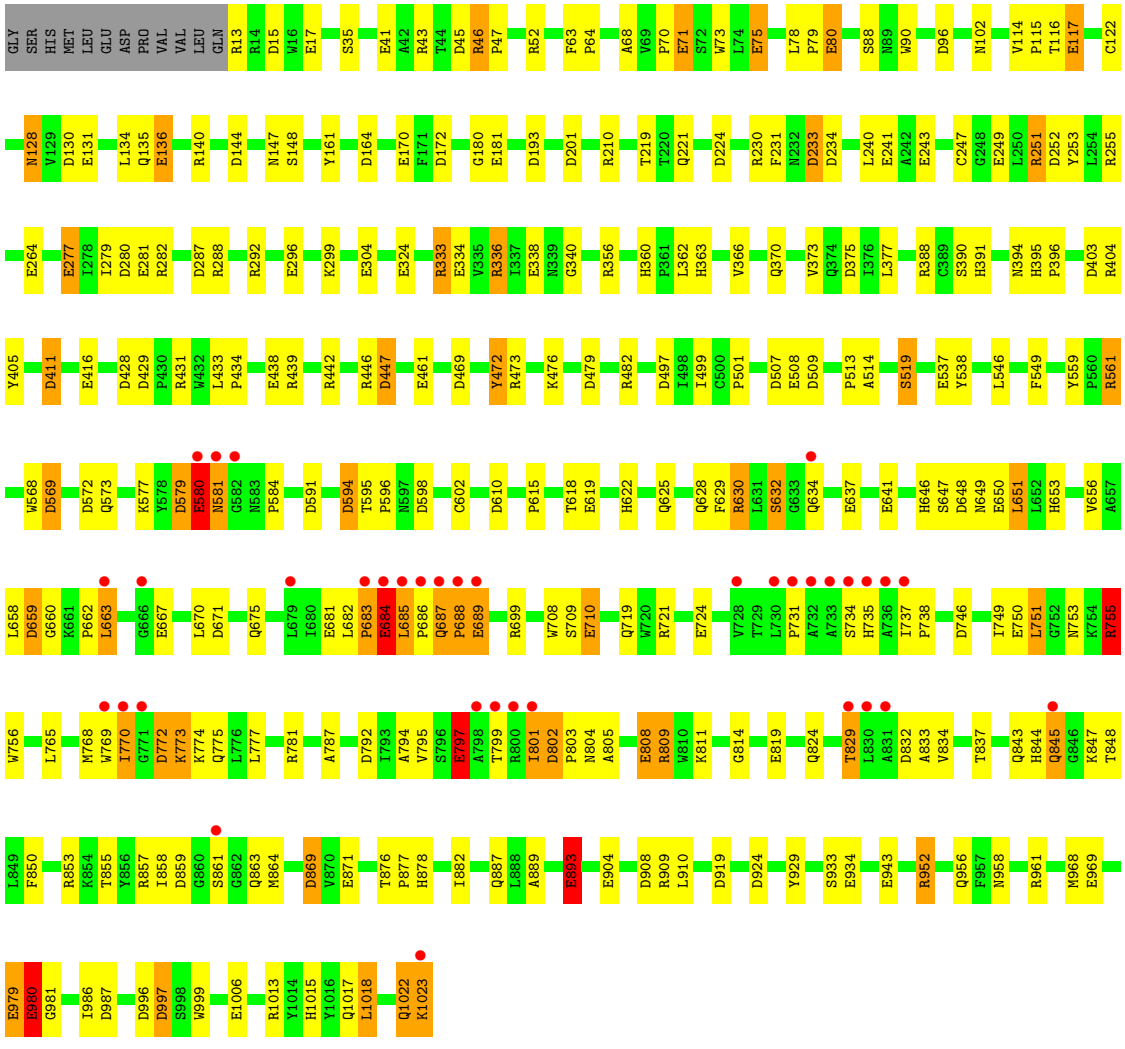






• Molecule 1: beta-galactosidase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	149.49Å 168.29Å 200.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.50 – 1.60 31.50 – 1.60	Depositor EDS
% Data completeness (in resolution range)	94.8 (31.50-1.60) 90.8 (31.50-1.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.19 (at 1.60Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.187 , 0.239 0.200 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	13.8	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 82.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	36785	wwPDB-VP
Average B, all atoms (Å^2)	22.0	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 36.39 % 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 5.0375e-04. 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: IPT, DMS, NA, MG

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	1.09	48/8368 (0.6%)	1.61	153/11417 (1.3%)
1	B	1.11	49/8368 (0.6%)	1.63	154/11417 (1.3%)
1	C	1.10	46/8368 (0.5%)	1.61	155/11417 (1.4%)
1	D	1.12	48/8368 (0.6%)	1.64	170/11417 (1.5%)
All	All	1.10	191/33472 (0.6%)	1.62	632/45668 (1.4%)

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	B	1	0

The worst 5 of 191 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	537	GLU	CD-OE2	9.16	1.35	1.25
1	C	304	GLU	CD-OE2	8.84	1.35	1.25
1	C	281	GLU	CD-OE2	8.69	1.35	1.25
1	D	281	GLU	CD-OE2	8.64	1.35	1.25
1	D	893	GLU	CD-OE2	8.64	1.35	1.25

The worst 5 of 632 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	809	ARG	NE-CZ-NH1	21.02	130.81	120.30
1	B	809	ARG	NE-CZ-NH2	-17.60	111.50	120.30
1	D	473	ARG	NE-CZ-NH1	14.07	127.33	120.30
1	C	699	ARG	NE-CZ-NH1	13.78	127.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	356	ARG	NE-CZ-NH1	13.66	127.13	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	685	LEU	CA

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	8126	0	7718	148	0
1	B	8126	0	7718	121	0
1	C	8126	0	7718	161	0
1	D	8126	0	7718	131	0
2	A	4	0	0	0	0
2	B	3	0	0	0	0
2	C	5	0	0	0	0
2	D	4	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
4	A	15	0	17	1	0
4	B	15	0	17	0	0
4	C	15	0	17	0	0
4	D	15	0	17	1	0
5	A	96	0	144	16	0
5	B	88	0	132	10	0
5	C	100	0	150	7	0
5	D	92	0	138	13	0
6	A	950	0	0	12	0
6	B	971	0	0	12	0
6	C	943	0	0	14	0
6	D	949	0	0	17	0
All	All	36785	0	31504	562	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 9.

The worst 5 of 562 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:687:GLN:HG3	1:C:688:PRO:HD2	1.36	1.06
1:D:651:LEU:HD11	1:D:653:HIS:CE1	2.01	0.95
1:A:600:GLN:H	1:A:600:GLN:HE21	1.18	0.89
1:D:773:LYS:HG2	1:D:775:GLN:HE22	1.39	0.88
1:B:634:GLN:HG3	1:B:682:LEU:HB2	1.58	0.85

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	1009/1023 (99%)	971 (96%)	37 (4%)	1 (0%)	51 29
1	B	1009/1023 (99%)	967 (96%)	35 (4%)	7 (1%)	22 7
1	C	1009/1023 (99%)	962 (95%)	46 (5%)	1 (0%)	51 29
1	D	1009/1023 (99%)	969 (96%)	36 (4%)	4 (0%)	34 15
All	All	4036/4092 (99%)	3869 (96%)	154 (4%)	13 (0%)	41 21

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	688	PRO
1	B	690	SER
1	B	731	PRO
1	C	1022	GLN
1	D	580	GLU

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	864/875 (99%)	831 (96%)	33 (4%)	33	10
1	B	864/875 (99%)	827 (96%)	37 (4%)	29	9
1	C	864/875 (99%)	820 (95%)	44 (5%)	24	6
1	D	864/875 (99%)	828 (96%)	36 (4%)	30	9
All	All	3456/3500 (99%)	3306 (96%)	150 (4%)	29	9

5 of 150 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	90	TRP
1	D	910	LEU
1	D	394	ASN
1	D	734	SER
1	B	600	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	878	HIS
1	D	761	GLN
1	D	102	ASN
1	D	363	HIS
1	D	824	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 130 ligands modelled in this entry, 32 are monoatomic - leaving 98 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	$\#\|Z\| > 2$
5	DMS	C	8504	-	3,3,3	0.66	0	3,3,3	0.74	0
5	DMS	C	8407	-	3,3,3	0.87	0	3,3,3	0.12	0
4	IPT	B	2001	3	14,15,15	0.61	0	18,21,21	1.86	4 (22%)
5	DMS	C	8409	-	3,3,3	2.14	1 (33%)	3,3,3	0.26	0
5	DMS	D	8503	-	3,3,3	0.95	0	3,3,3	0.38	0
5	DMS	D	8410	-	3,3,3	1.12	0	3,3,3	0.53	0
5	DMS	D	8421	-	3,3,3	0.63	0	3,3,3	0.94	0
5	DMS	A	8414	-	3,3,3	0.95	0	3,3,3	0.17	0
5	DMS	C	8602	-	3,3,3	0.89	0	3,3,3	0.55	0
5	DMS	A	8503	-	3,3,3	1.70	1 (33%)	3,3,3	0.42	0
5	DMS	C	8411	-	3,3,3	0.48	0	3,3,3	0.27	0
5	DMS	C	8413	-	3,3,3	1.11	0	3,3,3	0.62	0
5	DMS	C	8417	-	3,3,3	0.40	0	3,3,3	0.77	0
5	DMS	A	8421	-	3,3,3	1.13	0	3,3,3	0.13	0
5	DMS	C	8503	-	3,3,3	0.33	0	3,3,3	0.79	0
5	DMS	D	8413	-	3,3,3	1.25	1 (33%)	3,3,3	0.42	0
5	DMS	B	8502	-	3,3,3	1.30	0	3,3,3	0.98	0
5	DMS	A	8502	-	3,3,3	1.88	1 (33%)	3,3,3	1.07	0
5	DMS	D	8406	-	3,3,3	0.95	0	3,3,3	0.50	0
5	DMS	D	8416	-	3,3,3	0.96	0	3,3,3	0.21	0
5	DMS	B	8601	-	3,3,3	1.43	0	3,3,3	0.90	0
5	DMS	C	8420	-	3,3,3	0.67	0	3,3,3	0.20	0
5	DMS	A	8405	-	3,3,3	1.39	1 (33%)	3,3,3	0.36	0
5	DMS	C	8501	-	3,3,3	1.68	1 (33%)	3,3,3	0.66	0
5	DMS	B	8410	-	3,3,3	1.06	0	3,3,3	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	DMS	A	8416	-	3,3,3	3.05	1 (33%)	3,3,3	0.46	0
5	DMS	A	8407	-	3,3,3	1.30	0	3,3,3	0.33	0
5	DMS	A	8412	-	3,3,3	1.12	0	3,3,3	0.39	0
5	DMS	D	8403	-	3,3,3	1.42	0	3,3,3	0.84	0
5	DMS	C	8412	-	3,3,3	1.17	0	3,3,3	0.10	0
5	DMS	D	8417	-	3,3,3	0.44	0	3,3,3	1.19	1 (33%)
5	DMS	A	8413	-	3,3,3	1.97	2 (66%)	3,3,3	0.40	0
5	DMS	D	8409	-	3,3,3	1.87	1 (33%)	3,3,3	0.73	0
5	DMS	C	8425	3	3,3,3	1.09	0	3,3,3	0.52	0
5	DMS	B	8416	-	3,3,3	0.61	0	3,3,3	0.34	0
5	DMS	C	8423	-	3,3,3	0.48	0	3,3,3	0.37	0
5	DMS	B	8423	-	3,3,3	0.35	0	3,3,3	0.16	0
5	DMS	A	8406	-	3,3,3	1.36	0	3,3,3	0.44	0
5	DMS	D	8408	-	3,3,3	1.15	0	3,3,3	0.34	0
5	DMS	B	8413	-	3,3,3	0.96	0	3,3,3	0.29	0
5	DMS	B	8425	3	3,3,3	1.24	0	3,3,3	0.41	0
5	DMS	D	8703	-	3,3,3	0.97	0	3,3,3	0.39	0
5	DMS	C	8410	-	3,3,3	0.52	0	3,3,3	0.32	0
5	DMS	A	8420	-	3,3,3	0.68	0	3,3,3	0.27	0
5	DMS	A	8410	-	3,3,3	0.75	0	3,3,3	0.66	0
5	DMS	A	8417	-	3,3,3	0.71	0	3,3,3	0.66	0
5	DMS	B	8405	-	3,3,3	2.03	2 (66%)	3,3,3	0.48	0
4	IPT	C	2001	3	14,15,15	0.61	0	18,21,21	1.35	3 (16%)
5	DMS	D	8401	-	3,3,3	1.76	0	3,3,3	0.36	0
5	DMS	C	8404	-	3,3,3	1.40	0	3,3,3	1.63	1 (33%)
5	DMS	C	8408	-	3,3,3	0.43	0	3,3,3	1.41	1 (33%)
5	DMS	B	8411	-	3,3,3	1.32	0	3,3,3	0.51	0
5	DMS	D	8701	-	3,3,3	2.25	2 (66%)	3,3,3	0.81	0
5	DMS	B	8417	-	3,3,3	0.44	0	3,3,3	0.63	0
5	DMS	A	8401	-	3,3,3	0.88	0	3,3,3	0.55	0
5	DMS	B	8402	-	3,3,3	1.70	1 (33%)	3,3,3	0.52	0
5	DMS	A	8402	-	3,3,3	1.53	0	3,3,3	0.34	0
5	DMS	A	8411	-	3,3,3	0.45	0	3,3,3	0.39	0
5	DMS	D	8412	-	3,3,3	1.38	0	3,3,3	0.73	0
5	DMS	D	8705	-	3,3,3	2.09	1 (33%)	3,3,3	0.85	0
5	DMS	A	8501	-	3,3,3	1.30	0	3,3,3	0.43	0
5	DMS	A	8425	3	3,3,3	1.20	0	3,3,3	0.58	0
5	DMS	D	8506	-	3,3,3	0.58	0	3,3,3	0.35	0
5	DMS	C	8415	-	3,3,3	1.86	1 (33%)	3,3,3	0.41	0
5	DMS	D	8414	-	3,3,3	0.20	0	3,3,3	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	DMS	B	8401	-	3,3,3	0.62	0	3,3,3	0.39	0
5	DMS	C	8402	-	3,3,3	1.88	1 (33%)	3,3,3	0.39	0
5	DMS	A	8602	-	3,3,3	0.88	0	3,3,3	0.19	0
5	DMS	C	8405	-	3,3,3	1.61	1 (33%)	3,3,3	0.90	0
5	DMS	D	8404	-	3,3,3	0.65	0	3,3,3	0.71	0
5	DMS	B	8421	-	3,3,3	1.14	0	3,3,3	0.62	0
5	DMS	A	8403	-	3,3,3	1.60	0	3,3,3	0.62	0
5	DMS	A	8409	-	3,3,3	2.07	1 (33%)	3,3,3	0.23	0
5	DMS	B	8504	-	3,3,3	1.02	0	3,3,3	0.04	0
4	IPT	D	2001	3	14,15,15	0.84	0	18,21,21	2.13	8 (44%)
4	IPT	A	2001	3	14,15,15	0.61	0	18,21,21	1.72	4 (22%)
5	DMS	C	8414	-	3,3,3	1.06	0	3,3,3	0.66	0
5	DMS	B	8508	-	3,3,3	1.83	1 (33%)	3,3,3	0.53	0
5	DMS	A	8408	-	3,3,3	0.90	0	3,3,3	0.51	0
5	DMS	B	8409	-	3,3,3	2.50	1 (33%)	3,3,3	0.48	0
5	DMS	C	8506	-	3,3,3	1.46	1 (33%)	3,3,3	0.67	0
5	DMS	D	8405	-	3,3,3	1.14	0	3,3,3	0.96	0
5	DMS	C	8401	-	3,3,3	1.57	0	3,3,3	0.73	0
5	DMS	B	8506	-	3,3,3	0.99	0	3,3,3	1.20	1 (33%)
5	DMS	B	8408	-	3,3,3	1.48	1 (33%)	3,3,3	0.29	0
5	DMS	D	8501	-	3,3,3	0.92	0	3,3,3	0.60	0
5	DMS	D	8508	-	3,3,3	1.89	2 (66%)	3,3,3	0.38	0
5	DMS	C	8403	-	3,3,3	0.71	0	3,3,3	0.76	0
5	DMS	D	8411	-	3,3,3	0.99	0	3,3,3	0.25	0
5	DMS	B	8414	-	3,3,3	0.60	0	3,3,3	0.58	0
5	DMS	B	8403	-	3,3,3	0.69	0	3,3,3	0.55	0
5	DMS	A	8504	-	3,3,3	0.98	0	3,3,3	0.87	0
5	DMS	D	8402	-	3,3,3	1.81	1 (33%)	3,3,3	0.26	0
5	DMS	B	8404	-	3,3,3	0.90	0	3,3,3	0.40	0
5	DMS	A	8404	-	3,3,3	1.29	0	3,3,3	0.41	0
5	DMS	B	8412	-	3,3,3	1.06	0	3,3,3	0.24	0
5	DMS	C	8421	-	3,3,3	0.44	0	3,3,3	0.97	0
5	DMS	C	8601	-	3,3,3	1.28	1 (33%)	3,3,3	0.61	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
4	IPT	A	2001	3	-	1/6/26/26	0/1/1/1
4	IPT	C	2001	3	-	1/6/26/26	0/1/1/1
4	IPT	D	2001	3	-	1/6/26/26	0/1/1/1
4	IPT	B	2001	3	-	1/6/26/26	0/1/1/1

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	8416	DMS	C1-S	-4.99	1.38	1.75
5	B	8409	DMS	O-S	3.97	1.77	1.50
5	C	8409	DMS	O-S	3.52	1.74	1.50
5	A	8409	DMS	O-S	3.43	1.73	1.50
5	D	8705	DMS	O-S	3.34	1.72	1.50

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	2001	IPT	C6-C5-C4	5.04	124.82	113.00
4	D	2001	IPT	C2-C1-S1	-4.57	104.26	111.30
4	A	2001	IPT	O5-C5-C6	-4.29	95.77	106.44
4	D	2001	IPT	O5-C5-C6	-4.27	95.81	106.44
4	B	2001	IPT	C2-C1-S1	-3.73	105.56	111.30

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2001	IPT	O5-C5-C6-O6
4	C	2001	IPT	O5-C5-C6-O6
4	D	2001	IPT	O5-C5-C6-O6
4	B	2001	IPT	O5-C5-C6-O6

There are no ring outliers.

24 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	8414	DMS	1	0
5	A	8421	DMS	1	0
5	D	8413	DMS	1	0
5	D	8406	DMS	1	0
5	A	8416	DMS	6	0
5	C	8412	DMS	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	8417	DMS	1	0
5	A	8413	DMS	1	0
5	B	8413	DMS	1	0
5	B	8425	DMS	1	0
5	A	8417	DMS	1	0
5	B	8417	DMS	1	0
5	D	8412	DMS	2	0
5	D	8705	DMS	2	0
5	A	8425	DMS	1	0
5	D	8506	DMS	6	0
5	C	8415	DMS	1	0
5	A	8602	DMS	1	0
4	D	2001	IPT	1	0
4	A	2001	IPT	1	0
5	C	8506	DMS	5	0
5	B	8506	DMS	6	0
5	A	8404	DMS	4	0
5	B	8412	DMS	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	1011/1023 (98%)	0.12	32 (3%)	47	44	9, 17, 46, 98	0
1	B	1011/1023 (98%)	0.03	27 (2%)	54	52	8, 17, 43, 100	0
1	C	1011/1023 (98%)	-0.02	25 (2%)	57	55	10, 17, 48, 98	0
1	D	1011/1023 (98%)	0.05	36 (3%)	42	40	9, 17, 49, 98	0
All	All	4044/4092 (98%)	0.05	120 (2%)	50	48	8, 17, 47, 100	0

The worst 5 of 120 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	686	PRO	11.9
1	A	735	HIS	8.8
1	C	732	ALA	8.6
1	B	733	ALA	8.3
1	B	732	ALA	7.8

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

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
2	MG	A	3105	1/1	0.58	0.90	97,97,97,97	1
2	MG	D	3105	1/1	0.77	0.17	38,38,38,38	1
5	DMS	B	8413	4/4	0.77	0.19	33,40,53,58	0
2	MG	B	3105	1/1	0.78	0.18	28,28,28,28	1
5	DMS	C	8504	4/4	0.79	0.17	39,52,72,76	0
5	DMS	C	8407	4/4	0.82	0.23	51,100,100,100	0
5	DMS	A	8407	4/4	0.82	0.19	29,50,51,89	0
2	MG	C	3006	1/1	0.83	0.17	53,53,53,53	0
5	DMS	A	8425	4/4	0.84	0.22	37,55,76,100	0
3	NA	B	3104	1/1	0.84	0.13	32,32,32,32	0
3	NA	D	3104	1/1	0.84	0.17	44,44,44,44	0
2	MG	C	3004	1/1	0.84	0.11	53,53,53,53	0
5	DMS	C	8413	4/4	0.85	0.18	49,59,61,97	0
5	DMS	B	8508	4/4	0.85	0.15	36,41,54,56	0
3	NA	A	3103	1/1	0.86	0.14	32,32,32,32	0
5	DMS	B	8425	4/4	0.86	0.13	23,37,39,46	0
5	DMS	C	8503	4/4	0.87	0.15	25,32,50,52	0
5	DMS	D	8416	4/4	0.87	0.22	32,43,61,100	0
5	DMS	A	8417	4/4	0.88	0.15	26,29,59,100	0
3	NA	A	3104	1/1	0.88	0.12	30,30,30,30	0
5	DMS	A	8406	4/4	0.89	0.18	15,52,66,83	0
5	DMS	D	8404	4/4	0.89	0.13	26,27,54,57	0
5	DMS	A	8503	4/4	0.89	0.15	36,51,55,100	0
5	DMS	D	8501	4/4	0.89	0.12	22,29,41,50	0
5	DMS	D	8705	4/4	0.89	0.13	30,42,42,44	0
5	DMS	B	8421	4/4	0.90	0.14	26,42,54,55	0
5	DMS	C	8417	4/4	0.90	0.17	30,31,51,69	0
5	DMS	D	8703	4/4	0.90	0.16	37,48,53,98	0
5	DMS	C	8423	4/4	0.90	0.14	32,34,67,76	0
5	DMS	B	8417	4/4	0.91	0.17	24,30,61,69	0
5	DMS	B	8410	4/4	0.91	0.20	28,33,34,70	0
5	DMS	A	8404	4/4	0.91	0.12	17,30,39,41	0
5	DMS	C	8415	4/4	0.91	0.14	25,36,60,100	0
5	DMS	C	8602	4/4	0.91	0.14	21,61,62,71	0
5	DMS	A	8416	4/4	0.92	0.18	13,32,46,66	0
5	DMS	C	8506	4/4	0.92	0.17	42,45,48,100	0
3	NA	D	3103	1/1	0.92	0.11	30,30,30,30	0
5	DMS	A	8421	4/4	0.92	0.21	45,52,72,81	0
5	DMS	D	8413	4/4	0.92	0.16	46,49,51,100	0
5	DMS	B	8414	4/4	0.92	0.13	29,54,62,88	0
5	DMS	A	8409	4/4	0.92	0.13	27,29,29,54	0
5	DMS	A	8501	4/4	0.92	0.13	20,25,31,36	0
5	DMS	A	8502	4/4	0.92	0.16	29,29,52,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	DMS	A	8413	4/4	0.93	0.18	34,36,42,47	0
5	DMS	C	8420	4/4	0.93	0.13	38,50,61,100	0
3	NA	B	3103	1/1	0.93	0.10	25,25,25,25	0
5	DMS	C	8501	4/4	0.93	0.11	22,25,38,53	0
5	DMS	D	8417	4/4	0.93	0.14	23,27,70,75	0
5	DMS	D	8421	4/4	0.93	0.17	40,48,96,100	0
5	DMS	B	8416	4/4	0.93	0.17	37,43,47,100	0
5	DMS	D	8503	4/4	0.93	0.14	28,58,59,61	0
5	DMS	D	8508	4/4	0.93	0.15	37,42,52,100	0
5	DMS	B	8409	4/4	0.93	0.12	22,26,44,51	0
3	NA	C	3104	1/1	0.93	0.14	29,29,29,29	0
5	DMS	B	8423	4/4	0.94	0.11	46,55,57,100	0
5	DMS	C	8404	4/4	0.94	0.09	20,22,32,35	0
5	DMS	D	8409	4/4	0.94	0.12	27,29,31,37	0
5	DMS	A	8504	4/4	0.94	0.12	25,38,42,100	0
5	DMS	C	8601	4/4	0.95	0.15	34,44,46,100	0
3	NA	C	3103	1/1	0.95	0.10	25,25,25,25	0
5	DMS	A	8414	4/4	0.95	0.11	24,47,55,91	0
5	DMS	C	8414	4/4	0.95	0.09	20,35,36,43	0
2	MG	D	3005	1/1	0.95	0.07	25,25,25,25	0
2	MG	A	3005	1/1	0.95	0.07	30,30,30,30	0
5	DMS	B	8405	4/4	0.95	0.09	23,30,31,32	0
5	DMS	A	8420	4/4	0.95	0.14	47,53,82,100	0
5	DMS	C	8425	4/4	0.95	0.16	34,41,43,45	0
5	DMS	B	8502	4/4	0.95	0.12	26,29,36,42	0
5	DMS	B	8506	4/4	0.95	0.16	44,100,100,100	0
5	DMS	A	8408	4/4	0.95	0.10	17,35,41,100	0
2	MG	C	3105	1/1	0.95	0.08	28,28,28,28	1
5	DMS	C	8405	4/4	0.96	0.08	21,26,27,28	0
5	DMS	B	8402	4/4	0.96	0.10	14,15,20,21	0
5	DMS	C	8409	4/4	0.96	0.10	26,38,39,40	0
5	DMS	C	8410	4/4	0.96	0.13	24,36,40,80	0
5	DMS	D	8408	4/4	0.96	0.10	19,29,31,38	0
5	DMS	B	8404	4/4	0.96	0.08	23,25,35,55	0
5	DMS	D	8411	4/4	0.96	0.12	29,30,34,100	0
3	NA	D	3101	1/1	0.96	0.08	17,17,17,17	0
5	DMS	B	8408	4/4	0.96	0.12	27,28,35,59	0
4	IPT	D	2001	15/15	0.96	0.09	13,17,22,22	0
5	DMS	A	8411	4/4	0.96	0.14	26,27,30,100	0
5	DMS	B	8504	4/4	0.96	0.10	26,38,43,54	0
5	DMS	B	8411	4/4	0.96	0.10	28,32,38,43	0
5	DMS	D	8506	4/4	0.96	0.11	42,52,59,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	DMS	A	8412	4/4	0.96	0.19	31,36,40,100	0
5	DMS	B	8601	4/4	0.96	0.11	34,36,44,49	0
5	DMS	A	8403	4/4	0.96	0.11	22,26,29,32	0
3	NA	A	3102	1/1	0.97	0.06	12,12,12,12	0
2	MG	D	3002	1/1	0.97	0.07	14,14,14,14	0
5	DMS	D	8402	4/4	0.97	0.10	17,20,21,22	0
5	DMS	C	8411	4/4	0.97	0.13	24,28,32,100	0
5	DMS	D	8405	4/4	0.97	0.11	25,26,30,35	0
5	DMS	D	8406	4/4	0.97	0.09	22,25,25,30	0
5	DMS	C	8412	4/4	0.97	0.16	34,37,75,100	0
2	MG	A	3001	1/1	0.97	0.07	15,15,15,15	0
5	DMS	D	8410	4/4	0.97	0.10	23,33,34,37	0
3	NA	B	3101	1/1	0.97	0.10	15,15,15,15	0
2	MG	B	3002	1/1	0.97	0.06	15,15,15,15	0
5	DMS	D	8414	4/4	0.97	0.12	26,42,83,100	0
4	IPT	A	2001	15/15	0.97	0.09	11,16,24,28	0
5	DMS	A	8410	4/4	0.97	0.13	33,37,47,61	0
5	DMS	C	8421	4/4	0.97	0.09	35,46,47,62	0
4	IPT	B	2001	15/15	0.97	0.08	14,16,23,27	0
5	DMS	C	8402	4/4	0.97	0.10	18,18,26,30	0
4	IPT	C	2001	15/15	0.97	0.07	14,17,28,28	0
3	NA	A	3101	1/1	0.97	0.08	16,16,16,16	0
5	DMS	D	8701	4/4	0.97	0.11	16,18,20,41	0
5	DMS	A	8602	4/4	0.97	0.14	31,53,100,100	0
5	DMS	C	8408	4/4	0.97	0.06	26,28,30,33	0
5	DMS	A	8402	4/4	0.98	0.09	15,18,21,25	0
5	DMS	D	8401	4/4	0.98	0.08	13,14,18,19	0
2	MG	D	3001	1/1	0.98	0.06	13,13,13,13	0
5	DMS	D	8403	4/4	0.98	0.07	20,26,28,36	0
2	MG	B	3001	1/1	0.98	0.06	12,12,12,12	0
5	DMS	C	8401	4/4	0.98	0.08	16,20,20,27	0
5	DMS	B	8403	4/4	0.98	0.06	22,25,28,30	0
5	DMS	C	8403	4/4	0.98	0.07	21,22,26,29	0
5	DMS	B	8412	4/4	0.98	0.08	25,29,33,35	0
3	NA	C	3101	1/1	0.98	0.07	15,15,15,15	0
2	MG	A	3002	1/1	0.98	0.06	16,16,16,16	0
5	DMS	D	8412	4/4	0.98	0.09	20,20,30,92	0
2	MG	C	3001	1/1	0.99	0.05	14,14,14,14	0
2	MG	C	3002	1/1	0.99	0.06	14,14,14,14	0
5	DMS	B	8401	4/4	0.99	0.09	18,19,20,20	0
3	NA	B	3102	1/1	0.99	0.05	12,12,12,12	0
5	DMS	A	8405	4/4	0.99	0.10	24,25,25,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NA	D	3102	1/1	0.99	0.05	12,12,12,12	0
3	NA	C	3102	1/1	0.99	0.06	14,14,14,14	0
5	DMS	A	8401	4/4	0.99	0.10	13,14,15,16	0

6.5 Other polymers (i)

There are no such residues in this entry.