wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 08:22 PM GMT

PDB ID	:	1JZ2
Title	:	E. COLI (lacZ) BETA-GALACTOSIDASE-TRAPPED 2-F-GALACTOSYL-ENZYME INTERMEDIATE (ORTHORHOMBIC)
Authors	:	Juers, D.H.; McCarter, J.D.; Mackenzie, L.; Withers, S.G.; Matthews, B.W.
Deposited on	:	2001-09-13
Resolution	:	2.10 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

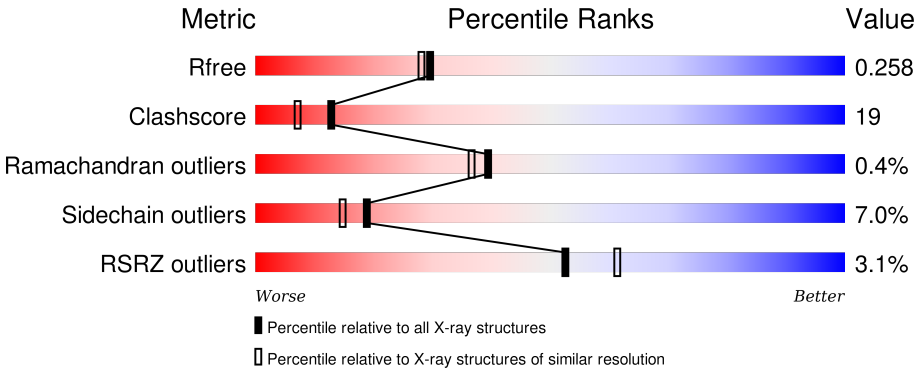
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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 <=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% 53% 36% 9%
1	B	1023	3% 55% 34% 9%
1	C	1023	3% 55% 35% 8%
1	D	1023	3% 57% 34% 7%

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	2FG	A	2001	X	-	-	-
2	2FG	B	2001	X	-	-	-
2	2FG	C	2001	X	-	-	-
2	2FG	D	2001	X	-	-	-
3	MG	B	3002	-	-	-	X
5	DMS	A	8402	-	-	-	X
5	DMS	A	8403	-	-	-	X
5	DMS	A	8406	-	-	X	X
5	DMS	A	8407	-	-	-	X
5	DMS	A	8412	-	-	-	X
5	DMS	A	8414	-	-	X	-
5	DMS	A	8417	-	X	-	X
5	DMS	A	8419	-	-	-	X
5	DMS	A	8423	-	-	-	X
5	DMS	A	8502	-	-	-	X
5	DMS	A	8504	-	-	-	X
5	DMS	B	8405	-	-	-	X
5	DMS	B	8406	-	-	-	X
5	DMS	B	8407	-	-	-	X
5	DMS	B	8411	-	-	-	X
5	DMS	B	8417	-	-	X	-
5	DMS	B	8423	-	-	-	X
5	DMS	B	8425	-	-	-	X
5	DMS	B	8502	-	-	-	X
5	DMS	B	8504	-	-	X	-
5	DMS	B	8506	-	-	X	-
5	DMS	B	8508	-	-	-	X
5	DMS	C	8403	-	-	-	X
5	DMS	C	8404	-	-	-	X
5	DMS	C	8419	-	-	-	X
5	DMS	C	8421	-	-	X	-
5	DMS	D	8406	-	-	-	X
5	DMS	D	8408	-	-	-	X
5	DMS	D	8423	-	-	-	X
6	BTB	B	2002	-	-	X	X
6	BTB	D	2002	-	-	-	X

2 Entry composition

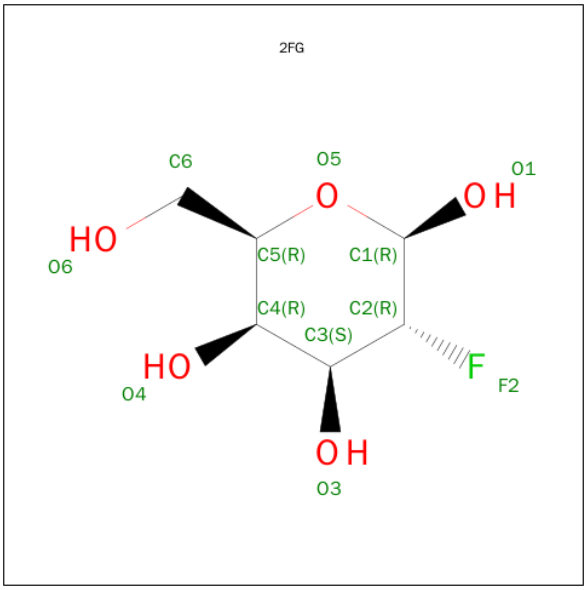
There are 7 unique types of molecules in this entry. The entry contains 35825 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			8125	5138	1440	1509	38			
1	B	1011	Total	C	N	O	S	0	0	0
			8125	5138	1440	1509	38			
1	C	1011	Total	C	N	O	S	0	0	0
			8125	5138	1440	1509	38			
1	D	1011	Total	C	N	O	S	0	0	0
			8125	5138	1440	1509	38			

- Molecule 2 is SUGAR (2-FLUORO-2-DEOXY-BETA-D-GALACTOPYRANOSE) (three-letter code: 2FG) (formula: $C_6H_{11}FO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	F	O	0	0
			11	6	1	4		
2	B	1	Total	C	F	O	0	0
			11	6	1	4		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C F O 11 6 1 4	0	0
2	D	1	Total C F O 11 6 1 4	0	0

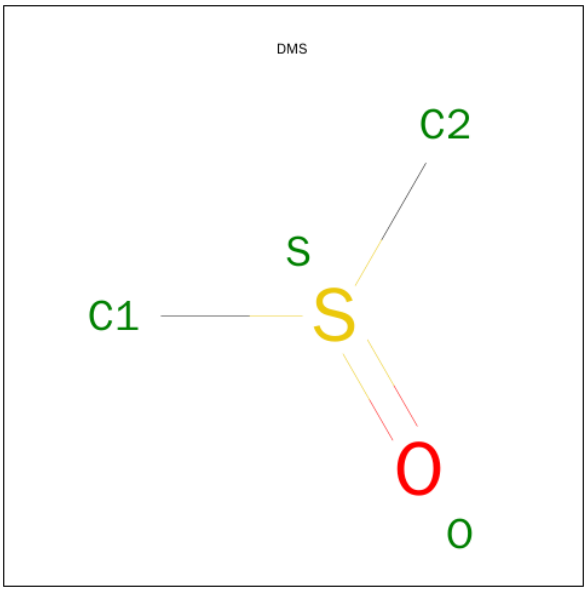
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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

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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	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	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	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	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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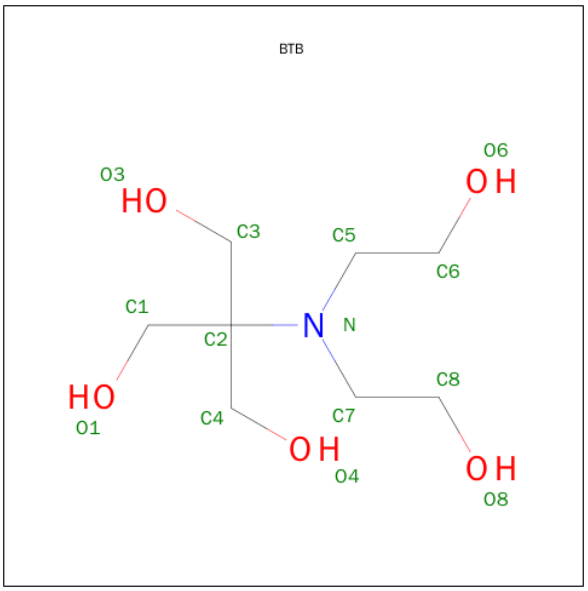
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	O	S	0	0
			4	2	1	1		
5	D	1	Total	C	O	S	0	0
			4	2	1	1		
5	D	1	Total	C	O	S	0	0
			4	2	1	1		
5	D	1	Total	C	O	S	0	0
			4	2	1	1		
5	D	1	Total	C	O	S	0	0
			4	2	1	1		
5	D	1	Total	C	O	S	0	0
			4	2	1	1		
5	D	1	Total	C	O	S	0	0
			4	2	1	1		
5	D	1	Total	C	O	S	0	0
			4	2	1	1		
5	D	1	Total	C	O	S	0	0
			4	2	1	1		
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 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: BTB) (formula: $C_8H_{19}NO_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C N O 14 8 1 5	0	0
6	D	1	Total C N O 14 8 1 5	0	0

- Molecule 7 is water.

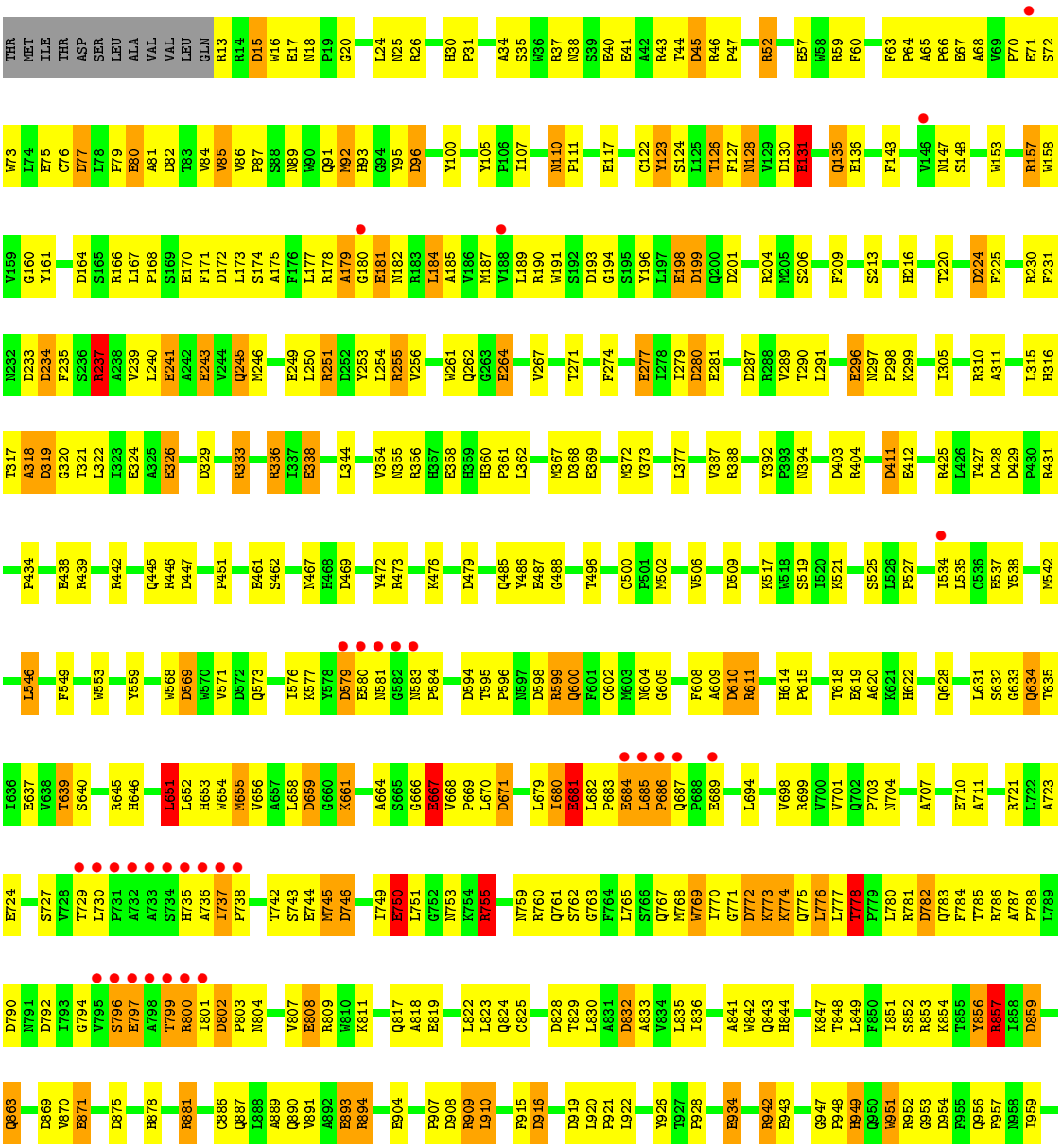
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	753	Total O 753 753	0	0
7	B	734	Total O 734 734	0	0
7	C	716	Total O 716 716	0	0
7	D	754	Total O 754 754	0	0

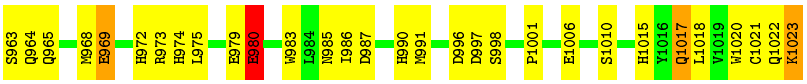
3 Residue-property plots (i)

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 (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

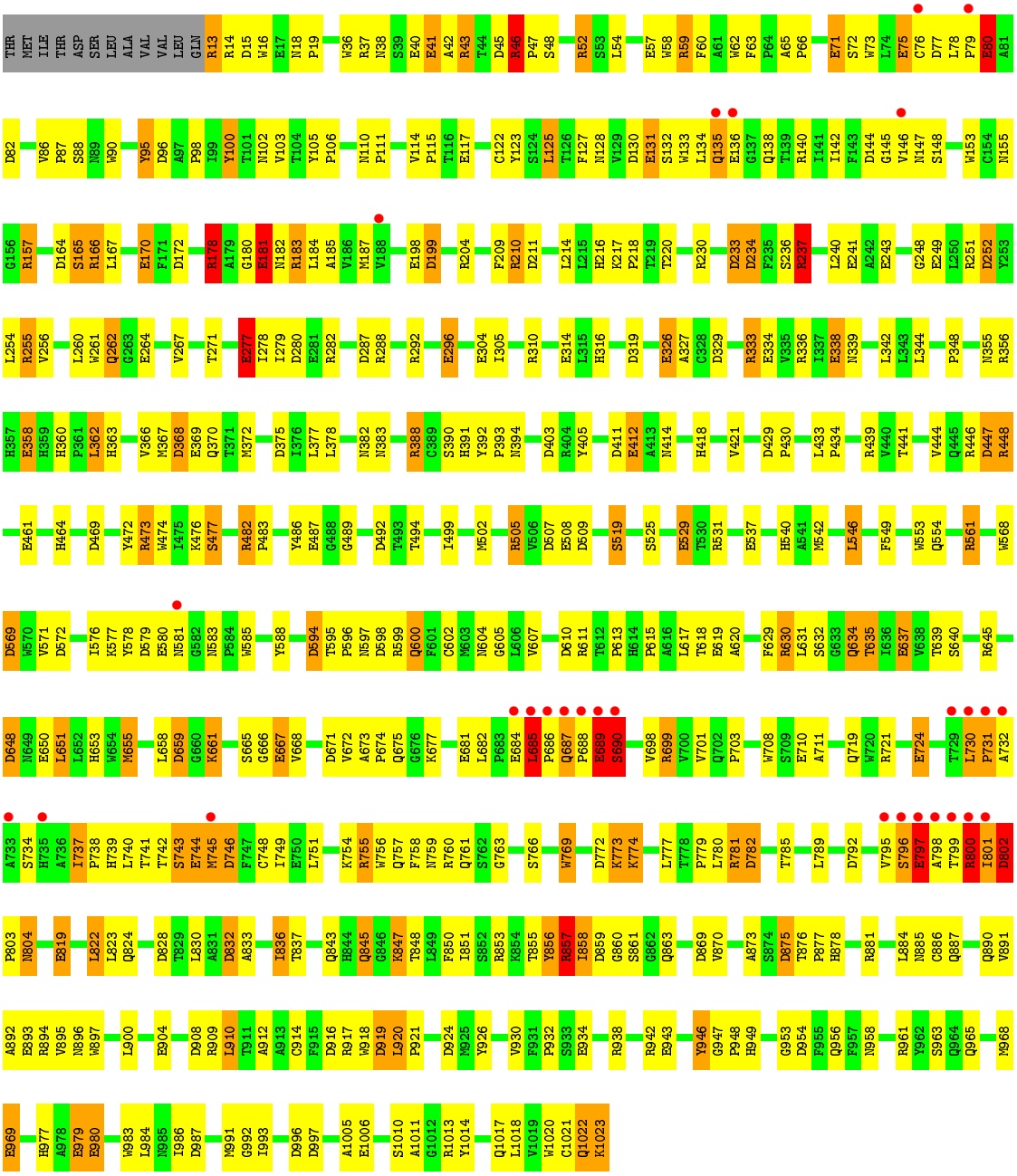
Chain A:





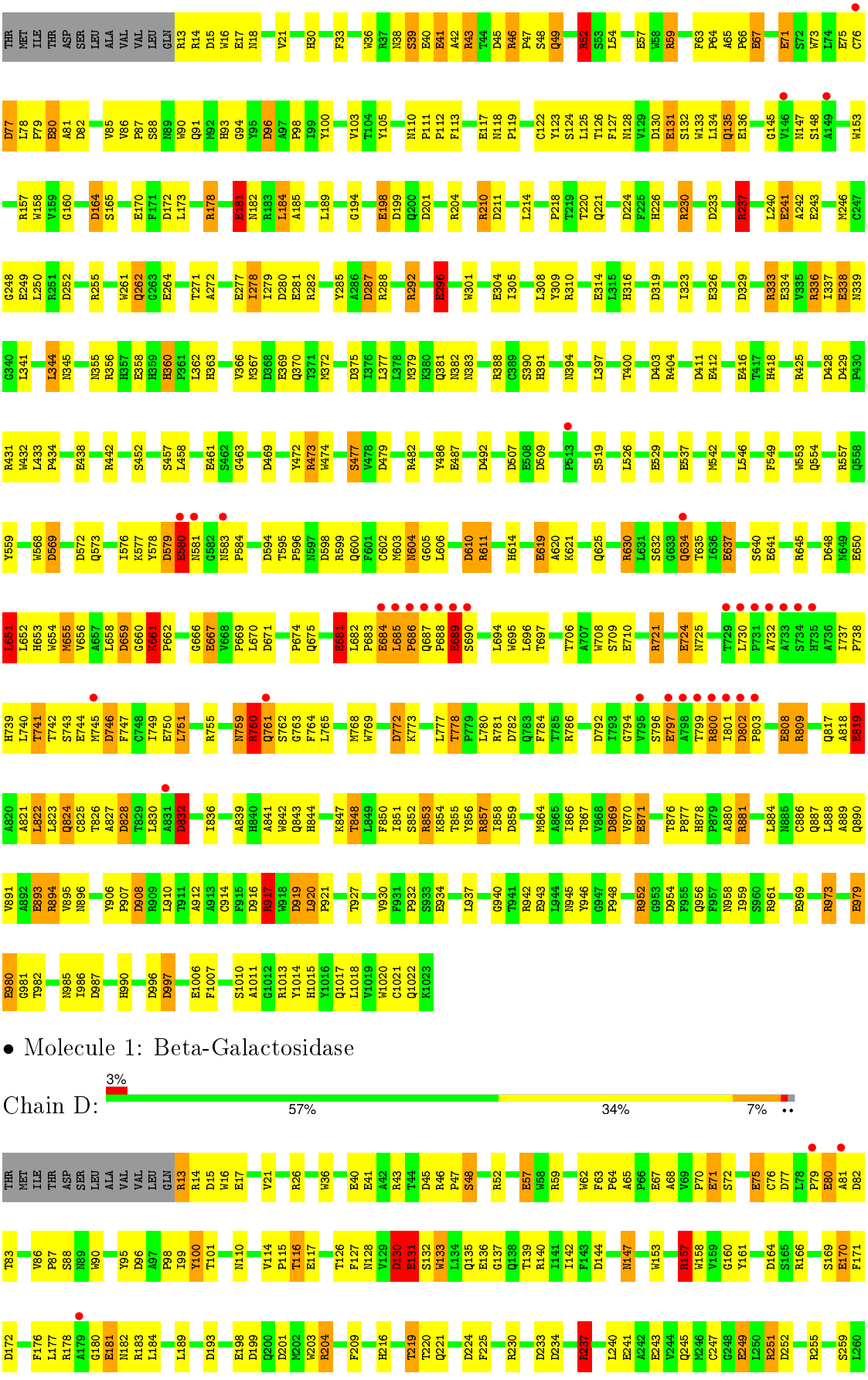
- Molecule 1: Beta-Galactosidase

Chain B:



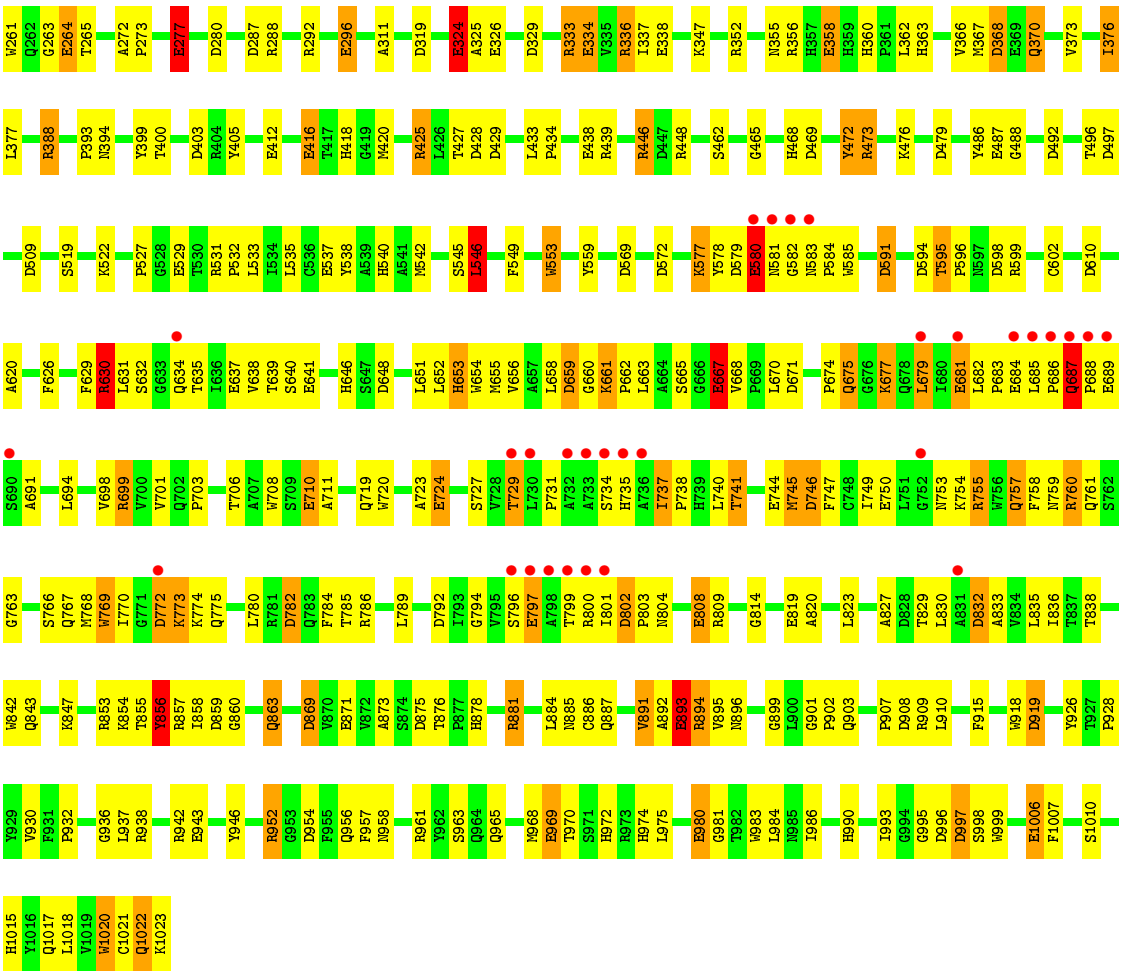
- Molecule 1: Beta-Galactosidase

Chain C:



• Molecule 1: Beta-Galactosidase

Chain D:


W261 Q262 G263 E264 T265 A272 P273 E277 D280 D287 R288 R292 E296 A311 D319 E324 A325 E326 D329 R333 E334 V335 R336 I337 E338 K347 R352 N355 R356 H357 E358 H359 H360 P361 L362 H363 V366 M367 D368 E369 Q370 V373 I376
L377 R388 P393 N394 Y399 T400 D403 R404 Y405 E412 E416 T417 H418 G419 M420 R425 L426 T427 D428 D429 L433 P434 E438 R439 R446 D447 R448 S462 G465 H468 D469 Y472 R473 K476 D479 Y486 E487 G488 D492 T496 D497
D509 S519 K522 P527 G528 E529 T530 R531 P532 L533 I534 L535 C536 E537 Y538 A539 H540 A541 M542 S545 L546 F549 W553 Y559 D569 D572 K577 Y578 D579 E580 N581 G582 N583 P584 W585 D591 D594 T595 P596 N597 D598 R599 C602 D610
A620 F626 F629 R630 L631 S632 G633 Q634 T635 I636 E637 V638 T639 S640 E641 H646 S647 D648 L651 L652 H653 W654 M655 V656 A657 L658 D659 G660 K661 P662 L663 A664 S665 G666 E667 V668 P669 L670 D671 P674 Q675 G676 K677 Q678 L679 I680 E681 L682 P683 E684 L685 P686 Q687 P688 E689
S690 A691 L694 V698 R699 V700 V701 Q702 P703 T706 A707 W708 S709 E710 A711 Q719 W720 A723 E724 S727 V728 T729 L730 P731 A732 A733 S734 H735 A736 I737 P738 H739 L740 T741 E744 M745 D746 F747 C748 I749 E750 L751 G752 N753 K754 R755 W756 Q757 F758 N759 R760 Q761 S762
G763 S766 Q767 M768 W769 I770 G771 D772 K773 K774 Q775 L780 R781 D782 Q783 F784 T785 R786 L789 D792 I793 G794 V795 S796 E797 A798 T799 R800 I801 D802 P803 N804 E808 R809 G814 E819 A820 L823 A827 D828 T829 L830 A831 D832 A833 V834 L835 I836 T837 T838
W842 Q843 K847 R853 K854 T855 Y856 R857 I858 D859 G860 Q863 D869 V870 E871 V872 A873 S874 D875 T876 P877 H878 R881 L884 N885 C886 Q887 V891 A892 E893 R894 V895 N896 G899 L900 G901 P902 Q903 P907 D908 R909 I910 F915 W918 D919 Y926 T927 P928
Y929 V930 F931 P932 G936 L937 R938 R942 E943 Y946 R952 G953 D954 F955 Q956 F957 N958 R961 Y962 S963 Q964 Q965 M968 E969 T970 S971 H972 R973 H974 L975 E980 G981 T982 W983 L984 N985 I986 H990 I993 G994 G995 D996 D997 S998 W999 E1006 F1007 S1010
H1015 Y1016 Q1017 L1018 V1019 W1020 C1021 Q1022 K1023

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	151.50Å 167.70Å 201.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.60 – 2.10 27.59 – 2.10	Depositor EDS
% Data completeness (in resolution range)	92.0 (27.60-2.10) 92.1 (27.59-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.59 (at 2.10Å)	Xtriage
Refinement program	TNT V. 5-E	Depositor
R, R_{free}	0.167 , 0.270 0.165 , 0.258	Depositor DCC
R_{free} test set	3979 reflections (1.47%)	DCC
Wilson B-factor (Å^2)	23.5	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 131.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 273807 reflections (0.000%)	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	35825	wwPDB-VP
Average B, all atoms (Å^2)	33.0	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 44.88 % 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 1.4330e-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, 0.375 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: NA, MG, DMS, 2FG, BTB

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	1.02	52/8367 (0.6%)	1.65	148/11415 (1.3%)
1	B	1.01	50/8367 (0.6%)	1.64	173/11415 (1.5%)
1	C	1.00	49/8367 (0.6%)	1.64	161/11415 (1.4%)
1	D	1.02	45/8367 (0.5%)	1.65	187/11415 (1.6%)
All	All	1.01	196/33468 (0.6%)	1.65	669/45660 (1.5%)

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
1	D	1	0
All	All	2	0

The worst 5 of 196 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	71	GLU	CD-OE2	8.54	1.35	1.25
1	C	198	GLU	CD-OE2	8.05	1.34	1.25
1	C	529	GLU	CD-OE2	7.99	1.34	1.25
1	B	117	GLU	CD-OE2	7.95	1.34	1.25
1	D	667	GLU	CD-OE2	7.55	1.33	1.25

The worst 5 of 669 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	685	LEU	C-N-CD	-18.06	80.87	120.60
1	D	881	ARG	NE-CZ-NH1	16.92	128.76	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	917	ARG	NE-CZ-NH1	-14.85	112.88	120.30
1	A	909	ARG	NE-CZ-NH1	14.21	127.41	120.30
1	D	237	ARG	NE-CZ-NH1	14.04	127.32	120.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	690	SER	CA
1	D	157	ARG	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	8125	0	7716	342	0
1	B	8125	0	7716	320	0
1	C	8125	0	7716	322	0
1	D	8125	0	7716	248	0
2	A	11	0	8	1	0
2	B	11	0	8	0	0
2	C	11	0	8	0	0
2	D	11	0	9	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
4	D	3	0	0	0	0
5	A	76	0	114	26	0
5	B	80	0	120	26	0
5	C	60	0	90	11	0
5	D	60	0	90	4	0
6	B	14	0	19	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	14	0	19	6	0
7	A	753	0	0	22	0
7	B	734	0	0	11	0
7	C	716	0	0	17	0
7	D	754	0	0	18	0
All	All	35825	0	31349	1234	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 19.

The worst 5 of 1234 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:634:GLN:N	1:C:634:GLN:HE21	1.45	1.13
1:B:687:GLN:HG3	1:B:688:PRO:HD2	1.21	1.12
1:C:778:THR:HG23	1:C:887:GLN:HB3	1.33	1.11
1:C:634:GLN:NE2	1:C:634:GLN:H	1.49	1.09
1:A:655:MET:HB3	1:A:699:ARG:HH12	0.95	1.09

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%)	957 (95%)	50 (5%)	2 (0%)	52	53
1	B	1009/1023 (99%)	945 (94%)	58 (6%)	6 (1%)	30	24
1	C	1009/1023 (99%)	948 (94%)	54 (5%)	7 (1%)	26	21
1	D	1009/1023 (99%)	957 (95%)	49 (5%)	3 (0%)	46	45
All	All	4036/4092 (99%)	3807 (94%)	211 (5%)	18 (0%)	39	37

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	690	SER
1	B	732	ALA
1	B	796	SER
1	B	801	ILE
1	B	802	ASP

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%)	802 (93%)	62 (7%)	18	14
1	B	864/875 (99%)	801 (93%)	63 (7%)	17	13
1	C	864/875 (99%)	806 (93%)	58 (7%)	20	16
1	D	864/875 (99%)	806 (93%)	58 (7%)	20	16
All	All	3456/3500 (99%)	3215 (93%)	241 (7%)	19	15

5 of 241 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	804	ASN
1	C	165	SER
1	D	735	HIS
1	B	845	GLN
1	B	956	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	49	GLN
1	C	675	GLN
1	D	817	GLN
1	C	135	GLN
1	C	583	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 95 ligands modelled in this entry, 20 are monoatomic - leaving 75 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	$\#\|Z\| > 2$
2	2FG	A	2001	1,4	11,11,12	0.87	0	11,15,17	2.35	2 (18%)
5	DMS	A	8401	-	3,3,3	1.31	0	3,3,3	0.34	0
5	DMS	A	8402	-	3,3,3	2.24	2 (66%)	3,3,3	0.52	0
5	DMS	A	8403	-	3,3,3	0.75	0	3,3,3	0.38	0
5	DMS	A	8404	-	3,3,3	0.73	0	3,3,3	0.35	0
5	DMS	A	8405	-	3,3,3	1.09	0	3,3,3	0.22	0
5	DMS	A	8406	-	3,3,3	0.86	0	3,3,3	0.45	0
5	DMS	A	8407	-	3,3,3	1.20	0	3,3,3	0.80	0
5	DMS	A	8408	-	3,3,3	0.50	0	3,3,3	0.30	0
5	DMS	A	8409	-	3,3,3	1.71	2 (66%)	3,3,3	0.34	0
5	DMS	A	8410	-	3,3,3	0.68	0	3,3,3	0.09	0
5	DMS	A	8411	-	3,3,3	0.42	0	3,3,3	0.86	0
5	DMS	A	8412	-	3,3,3	0.43	0	3,3,3	0.34	0
5	DMS	A	8414	-	3,3,3	1.03	0	3,3,3	0.31	0
5	DMS	A	8417	-	3,3,3	2.07	2 (66%)	3,3,3	1.18	1 (33%)
5	DMS	A	8419	-	3,3,3	0.77	0	3,3,3	0.19	0
5	DMS	A	8423	-	3,3,3	1.10	0	3,3,3	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	DMS	A	8501	-	3,3,3	0.31	0	3,3,3	0.26	0
5	DMS	A	8502	-	3,3,3	0.99	0	3,3,3	0.11	0
5	DMS	A	8504	-	3,3,3	1.00	0	3,3,3	0.10	0
2	2FG	B	2001	1,4	11,11,12	1.23	1 (9%)	11,15,17	2.11	3 (27%)
6	BTB	B	2002	-	12,13,13	1.31	2 (16%)	8,16,16	0.96	1 (12%)
5	DMS	B	8401	-	3,3,3	1.86	1 (33%)	3,3,3	0.28	0
5	DMS	B	8402	-	3,3,3	0.76	0	3,3,3	0.40	0
5	DMS	B	8403	-	3,3,3	1.24	0	3,3,3	0.43	0
5	DMS	B	8404	-	3,3,3	0.53	0	3,3,3	0.41	0
5	DMS	B	8405	-	3,3,3	0.96	0	3,3,3	0.12	0
5	DMS	B	8406	-	3,3,3	0.81	0	3,3,3	0.26	0
5	DMS	B	8407	-	3,3,3	1.19	0	3,3,3	1.07	0
5	DMS	B	8408	-	3,3,3	0.72	0	3,3,3	0.63	0
5	DMS	B	8409	-	3,3,3	1.42	0	3,3,3	0.11	0
5	DMS	B	8411	-	3,3,3	1.02	0	3,3,3	0.39	0
5	DMS	B	8412	-	3,3,3	1.05	0	3,3,3	0.09	0
5	DMS	B	8414	-	3,3,3	1.65	1 (33%)	3,3,3	0.61	0
5	DMS	B	8417	-	3,3,3	0.58	0	3,3,3	0.13	0
5	DMS	B	8421	-	3,3,3	0.78	0	3,3,3	0.24	0
5	DMS	B	8423	-	3,3,3	0.99	0	3,3,3	0.09	0
5	DMS	B	8425	-	3,3,3	1.13	0	3,3,3	0.21	0
5	DMS	B	8502	-	3,3,3	1.40	1 (33%)	3,3,3	0.81	0
5	DMS	B	8504	-	3,3,3	0.68	0	3,3,3	0.34	0
5	DMS	B	8506	-	3,3,3	1.17	0	3,3,3	0.56	0
5	DMS	B	8508	-	3,3,3	1.83	1 (33%)	3,3,3	0.76	0
2	2FG	C	2001	1,4	11,11,12	1.17	1 (9%)	11,15,17	1.96	3 (27%)
5	DMS	C	8401	-	3,3,3	1.33	1 (33%)	3,3,3	1.07	0
5	DMS	C	8402	-	3,3,3	0.84	0	3,3,3	0.31	0
5	DMS	C	8403	-	3,3,3	0.95	0	3,3,3	0.91	0
5	DMS	C	8404	-	3,3,3	1.27	0	3,3,3	0.40	0
5	DMS	C	8405	-	3,3,3	0.85	0	3,3,3	0.14	0
5	DMS	C	8408	-	3,3,3	1.01	0	3,3,3	0.58	0
5	DMS	C	8409	-	3,3,3	1.31	0	3,3,3	0.22	0
5	DMS	C	8411	-	3,3,3	1.06	0	3,3,3	0.42	0
5	DMS	C	8412	-	3,3,3	0.86	0	3,3,3	0.14	0
5	DMS	C	8414	-	3,3,3	0.36	0	3,3,3	0.15	0
5	DMS	C	8417	-	3,3,3	0.61	0	3,3,3	0.26	0
5	DMS	C	8419	-	3,3,3	0.81	0	3,3,3	0.15	0
5	DMS	C	8421	-	3,3,3	1.29	1 (33%)	3,3,3	0.69	0
5	DMS	C	8423	-	3,3,3	1.25	0	3,3,3	0.21	0
5	DMS	C	8504	-	3,3,3	0.58	0	3,3,3	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	2FG	D	2001	1,4	11,11,12	1.37	2 (18%)	11,15,17	2.28	3 (27%)
6	BTB	D	2002	-	12,13,13	1.23	2 (16%)	8,16,16	0.71	0
5	DMS	D	8401	-	3,3,3	1.12	0	3,3,3	0.59	0
5	DMS	D	8402	-	3,3,3	1.84	2 (66%)	3,3,3	0.11	0
5	DMS	D	8403	-	3,3,3	1.63	1 (33%)	3,3,3	0.62	0
5	DMS	D	8405	-	3,3,3	1.18	0	3,3,3	0.09	0
5	DMS	D	8406	-	3,3,3	0.63	0	3,3,3	0.59	0
5	DMS	D	8408	-	3,3,3	0.47	0	3,3,3	0.63	0
5	DMS	D	8409	-	3,3,3	1.50	1 (33%)	3,3,3	0.13	0
5	DMS	D	8411	-	3,3,3	0.86	0	3,3,3	0.21	0
5	DMS	D	8412	-	3,3,3	1.63	1 (33%)	3,3,3	0.29	0
5	DMS	D	8414	-	3,3,3	0.32	0	3,3,3	0.40	0
5	DMS	D	8416	-	3,3,3	0.64	0	3,3,3	0.63	0
5	DMS	D	8421	-	3,3,3	0.68	0	3,3,3	0.11	0
5	DMS	D	8423	-	3,3,3	0.96	0	3,3,3	0.20	0
5	DMS	D	8427	-	3,3,3	1.16	0	3,3,3	0.78	0
5	DMS	D	8501	-	3,3,3	0.28	0	3,3,3	0.32	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2FG	A	2001	1,4	1/1/4/5	0/2/19/22	0/1/1/1
5	DMS	A	8401	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8402	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8403	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8404	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8405	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8406	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8407	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8408	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8409	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8410	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8411	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8412	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8414	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8417	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8419	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8423	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DMS	A	8501	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8502	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8504	-	-	0/0/0/0	0/0/0/0
2	2FG	B	2001	1,4	1/1/4/5	0/2/19/22	0/1/1/1
6	BTB	B	2002	-	-	0/21/21/21	0/0/0/0
5	DMS	B	8401	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8402	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8403	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8404	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8405	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8406	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8407	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8408	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8409	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8411	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8412	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8414	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8417	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8421	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8423	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8425	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8502	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8504	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8506	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8508	-	-	0/0/0/0	0/0/0/0
2	2FG	C	2001	1,4	1/1/4/5	0/2/19/22	0/1/1/1
5	DMS	C	8401	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8402	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8403	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8404	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8405	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8408	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8409	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8411	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8412	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8414	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8417	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8419	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8421	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8423	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8504	-	-	0/0/0/0	0/0/0/0
2	2FG	D	2001	1,4	1/1/4/5	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BTB	D	2002	-	-	0/21/21/21	0/0/0/0
5	DMS	D	8401	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8402	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8403	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8405	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8406	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8408	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8409	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8411	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8412	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8414	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8416	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8421	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8423	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8427	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8501	-	-	0/0/0/0	0/0/0/0

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2001	2FG	O5-C1	-2.80	1.39	1.43
6	D	2002	BTB	C1-C2	-2.61	1.49	1.53
6	B	2002	BTB	C1-C2	-2.50	1.50	1.53
5	A	8409	DMS	O-S	2.00	1.63	1.50
6	D	2002	BTB	C3-C2	2.03	1.55	1.53

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2001	2FG	O5-C1-C2	-6.79	101.51	111.78
2	D	2001	2FG	O5-C1-C2	-6.15	102.48	111.78
2	B	2001	2FG	O5-C1-C2	-4.88	104.40	111.78
2	C	2001	2FG	O5-C1-C2	-4.16	105.49	111.78
2	C	2001	2FG	C6-C5-C4	-2.77	106.19	113.02

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	2001	2FG	C1
2	A	2001	2FG	C1
2	B	2001	2FG	C1
2	C	2001	2FG	C1

There are no torsion outliers.

There are no ring outliers.

29 monomers are involved in 81 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	2FG	1	0
5	A	8402	DMS	3	0
5	A	8404	DMS	1	0
5	A	8406	DMS	5	0
5	A	8407	DMS	2	0
5	A	8410	DMS	1	0
5	A	8412	DMS	3	0
5	A	8414	DMS	4	0
5	A	8419	DMS	3	0
5	A	8501	DMS	2	0
5	A	8504	DMS	2	0
6	B	2002	BTB	7	0
5	B	8409	DMS	2	0
5	B	8411	DMS	2	0
5	B	8412	DMS	2	0
5	B	8417	DMS	4	0
5	B	8425	DMS	2	0
5	B	8502	DMS	1	0
5	B	8504	DMS	8	0
5	B	8506	DMS	5	0
5	C	8404	DMS	1	0
5	C	8412	DMS	2	0
5	C	8417	DMS	1	0
5	C	8419	DMS	2	0
5	C	8421	DMS	5	0
6	D	2002	BTB	6	0
5	D	8403	DMS	1	0
5	D	8411	DMS	1	0
5	D	8427	DMS	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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%)	-0.30	32 (3%)	51	60	14, 27, 61, 100	0
1	B	1011/1023 (98%)	-0.24	28 (2%)	56	64	15, 28, 64, 100	0
1	C	1011/1023 (98%)	-0.24	33 (3%)	50	59	14, 28, 62, 100	0
1	D	1011/1023 (98%)	-0.33	33 (3%)	50	59	12, 27, 62, 99	0
All	All	4044/4092 (98%)	-0.28	126 (3%)	52	61	12, 28, 63, 100	0

The worst 5 of 126 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	798	ALA	9.8
1	A	732	ALA	8.1
1	C	732	ALA	7.8
1	C	799	THR	7.7
1	A	735	HIS	7.7

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{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	LLDF	B-factors(Å^2)	Q<0.9
5	DMS	B	8508	4/4	0.69	0.24	9.59	41,70,84,100	0
5	DMS	D	8423	4/4	0.90	0.16	9.46	40,91,100,100	0
5	DMS	D	8408	4/4	0.98	0.19	5.68	28,52,55,88	0
5	DMS	A	8419	4/4	0.93	0.23	5.67	54,61,62,77	0
5	DMS	B	8407	4/4	0.76	0.21	5.18	26,40,100,100	0
5	DMS	A	8412	4/4	0.95	0.22	5.06	31,40,69,100	0
5	DMS	C	8419	4/4	0.89	0.30	4.97	43,81,100,100	0
5	DMS	B	8423	4/4	0.95	0.20	4.34	59,81,83,100	0
5	DMS	A	8406	4/4	0.95	0.16	4.12	41,54,65,100	0
5	DMS	A	8402	4/4	0.96	0.13	4.11	24,49,63,100	0
5	DMS	A	8423	4/4	0.90	0.15	3.91	65,80,99,100	0
5	DMS	A	8502	4/4	0.94	0.17	3.65	35,83,93,100	0
5	DMS	A	8407	4/4	0.79	0.19	3.48	41,44,100,100	0
5	DMS	C	8404	4/4	0.88	0.13	3.39	22,47,56,100	0
5	DMS	B	8502	4/4	0.90	0.16	3.35	38,65,97,100	0
5	DMS	C	8403	4/4	0.99	0.14	3.19	33,35,40,41	0
3	MG	B	3002	1/1	0.96	0.11	2.98	27,27,27,27	0
6	BTB	B	2002	14/14	0.93	0.15	2.96	12,53,100,100	0
5	DMS	B	8425	4/4	0.80	0.23	2.94	65,81,100,100	0
5	DMS	B	8405	4/4	0.97	0.13	2.64	29,48,83,100	0
5	DMS	D	8406	4/4	0.95	0.13	2.60	29,61,81,100	0
5	DMS	A	8504	4/4	0.97	0.15	2.56	55,69,100,100	0
5	DMS	B	8411	4/4	0.98	0.15	2.55	35,40,41,50	0
5	DMS	B	8406	4/4	0.94	0.18	2.51	67,84,100,100	0
5	DMS	A	8403	4/4	0.98	0.14	2.23	21,37,52,98	0
6	BTB	D	2002	14/14	0.92	0.16	2.08	23,49,100,100	0
5	DMS	A	8417	4/4	0.80	0.20	2.03	44,45,60,100	0
5	DMS	C	8423	4/4	0.74	0.14	1.87	38,49,66,90	0
4	NA	C	3103	1/1	0.96	0.19	1.80	48,48,48,48	0
5	DMS	A	8404	4/4	0.87	0.15	1.46	24,30,52,100	0
5	DMS	D	8402	4/4	0.97	0.12	1.44	24,44,46,100	0
5	DMS	B	8417	4/4	0.94	0.20	1.25	37,100,100,100	0
5	DMS	A	8401	4/4	0.99	0.11	1.20	23,24,26,27	0
3	MG	D	3002	1/1	1.00	0.11	1.15	26,26,26,26	0
5	DMS	D	8405	4/4	0.97	0.09	1.09	25,38,56,79	0
5	DMS	D	8401	4/4	0.99	0.11	1.00	21,23,30,34	0
5	DMS	A	8408	4/4	0.98	0.11	0.79	40,50,100,100	0
5	DMS	B	8402	4/4	0.96	0.10	0.68	35,39,52,74	0
5	DMS	C	8412	4/4	0.97	0.15	0.60	29,31,58,80	0
5	DMS	B	8412	4/4	0.97	0.13	0.49	34,50,86,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	DMS	C	8401	4/4	0.99	0.10	0.48	18,25,29,36	0
4	NA	D	3102	1/1	0.93	0.12	0.42	30,30,30,30	0
5	DMS	B	8401	4/4	0.99	0.10	0.39	21,26,29,38	0
5	DMS	B	8408	4/4	0.97	0.10	0.37	30,62,100,100	0
5	DMS	B	8404	4/4	0.95	0.10	0.36	23,45,47,96	0
5	DMS	C	8408	4/4	0.96	0.10	0.36	21,53,78,100	0
5	DMS	A	8501	4/4	0.89	0.14	0.26	46,49,91,100	0
2	2FG	D	2001	11/12	0.98	0.11	0.25	18,23,24,26	0
2	2FG	A	2001	11/12	0.98	0.10	0.22	14,22,28,29	0
5	DMS	C	8411	4/4	0.96	0.12	0.22	42,47,52,56	0
5	DMS	A	8405	4/4	0.96	0.10	0.21	35,37,65,100	0
5	DMS	D	8412	4/4	0.98	0.13	0.20	26,44,50,100	0
5	DMS	D	8501	4/4	0.95	0.12	0.19	32,52,88,100	0
5	DMS	C	8417	4/4	0.95	0.15	0.16	43,51,92,100	0
4	NA	C	3102	1/1	0.98	0.10	0.07	23,23,23,23	0
2	2FG	B	2001	11/12	0.98	0.10	-0.00	17,24,29,29	0
5	DMS	B	8504	4/4	0.95	0.14	-0.10	43,79,90,100	0
5	DMS	D	8403	4/4	0.99	0.08	-0.12	30,33,36,37	0
2	2FG	C	2001	11/12	0.98	0.10	-0.19	19,23,26,26	0
5	DMS	C	8405	4/4	0.97	0.08	-0.27	39,42,52,97	0
5	DMS	C	8402	4/4	0.98	0.09	-0.33	19,27,40,49	0
5	DMS	A	8411	4/4	0.98	0.09	-0.37	40,42,43,51	0
5	DMS	B	8403	4/4	0.99	0.10	-0.68	21,32,32,53	0
4	NA	A	3102	1/1	0.98	0.09	-0.70	31,31,31,31	0
4	NA	B	3103	1/1	0.96	0.08	-1.07	40,40,40,40	0
4	NA	A	3103	1/1	0.97	0.08	-1.26	42,42,42,42	0
4	NA	B	3102	1/1	0.98	0.04	-1.57	20,20,20,20	0
4	NA	D	3103	1/1	0.97	0.07	-1.66	39,39,39,39	0
4	NA	C	3101	1/1	0.98	0.08	-1.73	19,19,19,19	0
3	MG	C	3002	1/1	0.95	0.04	-1.88	26,26,26,26	0
3	MG	B	3001	1/1	0.99	0.06	-1.99	21,21,21,21	0
4	NA	B	3101	1/1	1.00	0.08	-2.30	19,19,19,19	0
4	NA	D	3101	1/1	1.00	0.07	-2.44	21,21,21,21	0
3	MG	A	3002	1/1	0.98	0.04	-2.47	27,27,27,27	0
3	MG	A	3001	1/1	0.96	0.05	-2.67	26,26,26,26	0
3	MG	C	3001	1/1	0.99	0.04	-3.29	23,23,23,23	0
3	MG	D	3001	1/1	0.99	0.03	-3.76	19,19,19,19	0
4	NA	A	3101	1/1	0.99	0.04	-4.58	21,21,21,21	0
5	DMS	B	8409	4/4	0.88	0.20	-	34,48,100,100	0
5	DMS	D	8409	4/4	0.92	0.13	-	38,41,72,100	0
5	DMS	B	8421	4/4	0.94	0.16	-	39,46,73,100	0
5	DMS	B	8414	4/4	0.94	0.07	-	34,37,53,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	DMS	D	8411	4/4	0.98	0.11	-	44,53,66,100	0
5	DMS	A	8409	4/4	0.93	0.09	-	33,36,40,75	0
5	DMS	C	8409	4/4	0.93	0.12	-	46,57,75,75	0
5	DMS	D	8421	4/4	0.92	0.16	-	47,80,81,100	0
5	DMS	C	8414	4/4	0.96	0.12	-	31,48,89,100	0
5	DMS	C	8421	4/4	0.88	0.18	-	44,48,73,100	0
5	DMS	A	8410	4/4	0.92	0.30	-	44,82,100,100	0
5	DMS	C	8504	4/4	0.97	0.08	-	42,65,81,81	0
5	DMS	D	8414	4/4	0.97	0.17	-	30,60,62,81	0
5	DMS	D	8416	4/4	0.94	0.20	-	47,57,62,100	0
5	DMS	D	8427	4/4	0.73	0.34	-	63,100,100,100	0
5	DMS	A	8414	4/4	0.94	0.18	-	26,74,75,100	0
5	DMS	B	8506	4/4	0.92	0.11	-	20,33,57,90	0

6.5 Other polymers

There are no such residues in this entry.