wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 03:58 PM GMT

PDB ID	:	4DX5
Title	:	Transport of drugs by the multidrug transporter AcrB involves an access and a deep binding pocket that are separated by a switch-loop
Authors	:	Eicher, T.; Cha, H.; Seeger, M.A.; Brandstaetter, L.; El-Delik, J.; Bohnert, J.A.; Kern, W.V.; Verrey, F.; Gruetter, M.G.; Diederichs, K.; Pos, K.M.
Deposited on	:	2012-02-27
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
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:

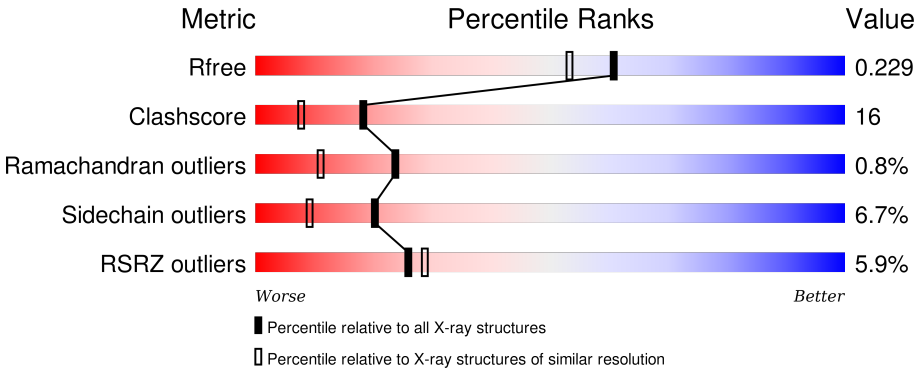
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 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}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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 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	1057	8% 70% 23% 5% •
1	B	1057	5% 78% 17% • •
1	C	1057	4% 79% 16% • •
2	D	169	3% 77% 13% • 8%
2	E	169	14% 63% 23% • • 10%

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
10	C14	B	1109	-	-	-	X
11	LMU	B	1114	-	-	-	X
12	DD9	C	1111	-	-	-	X
14	UND	C	1119	-	-	-	X
3	GOL	A	1101	-	-	-	X
3	GOL	A	1110	-	-	-	X
3	GOL	B	1101	-	-	-	X
3	GOL	B	1102	-	-	-	X
3	GOL	B	1113	-	-	-	X
3	GOL	B	1115	-	-	-	X
3	GOL	B	1116	-	-	X	X
3	GOL	B	1117	-	-	-	X
3	GOL	C	1101	-	-	-	X
3	GOL	C	1114	-	-	-	X
3	GOL	C	1115	-	-	-	X
3	GOL	C	1117	-	-	-	X
3	GOL	D	201	-	-	-	X
3	GOL	D	202	-	-	-	X
4	LMT	A	1102	-	-	-	X
4	LMT	A	1109	-	-	-	X
4	LMT	B	1104	-	-	-	X
4	LMT	B	1110	-	-	-	X
4	LMT	B	1111	-	-	-	X
5	OCT	A	1105	-	-	-	X
5	OCT	C	1106	-	-	-	X
5	OCT	C	1112	-	-	-	X
6	D10	A	1107	-	-	-	X
6	D10	B	1107	-	-	-	X
6	D10	C	1107	-	-	-	X
6	D10	C	1120	-	-	-	X
7	HEX	B	1108	-	-	-	X
7	HEX	B	1112	-	-	-	X
7	HEX	C	1113	-	-	-	X
8	D12	A	1111	-	-	X	-

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 29010 atoms, of which 587 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 Acriflavine resistance protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1044	Total	C	N	O	S	0	0	0
			7943	5106	1315	1478	44			
1	B	1033	Total	C	N	O	S	0	0	0
			7849	5052	1295	1458	44			
1	C	1033	Total	C	N	O	S	0	0	0
			7849	5052	1295	1458	44			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1050	LEU	-	EXPRESSION TAG	UNP P31224
A	1051	GLU	-	EXPRESSION TAG	UNP P31224
A	1052	HIS	-	EXPRESSION TAG	UNP P31224
A	1053	HIS	-	EXPRESSION TAG	UNP P31224
A	1054	HIS	-	EXPRESSION TAG	UNP P31224
A	1055	HIS	-	EXPRESSION TAG	UNP P31224
A	1056	HIS	-	EXPRESSION TAG	UNP P31224
A	1057	HIS	-	EXPRESSION TAG	UNP P31224
B	1050	LEU	-	EXPRESSION TAG	UNP P31224
B	1051	GLU	-	EXPRESSION TAG	UNP P31224
B	1052	HIS	-	EXPRESSION TAG	UNP P31224
B	1053	HIS	-	EXPRESSION TAG	UNP P31224
B	1054	HIS	-	EXPRESSION TAG	UNP P31224
B	1055	HIS	-	EXPRESSION TAG	UNP P31224
B	1056	HIS	-	EXPRESSION TAG	UNP P31224
B	1057	HIS	-	EXPRESSION TAG	UNP P31224
C	1050	LEU	-	EXPRESSION TAG	UNP P31224
C	1051	GLU	-	EXPRESSION TAG	UNP P31224
C	1052	HIS	-	EXPRESSION TAG	UNP P31224
C	1053	HIS	-	EXPRESSION TAG	UNP P31224
C	1054	HIS	-	EXPRESSION TAG	UNP P31224
C	1055	HIS	-	EXPRESSION TAG	UNP P31224
C	1056	HIS	-	EXPRESSION TAG	UNP P31224

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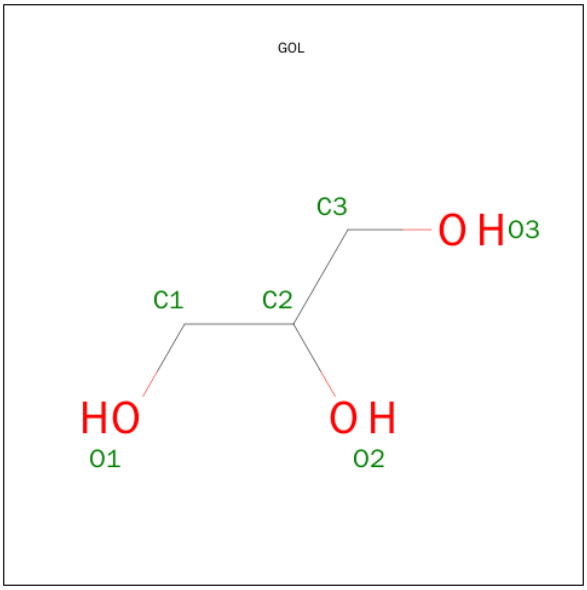
Chain	Residue	Modelled	Actual	Comment	Reference
C	1057	HIS	-	EXPRESSION TAG	UNP P31224

- Molecule 2 is a protein called DARPIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	156	Total	C	N	O	S	0	0	0
			1177	741	206	229	1			
2	E	152	Total	C	N	O	S	0	0	0
			1151	726	202	222	1			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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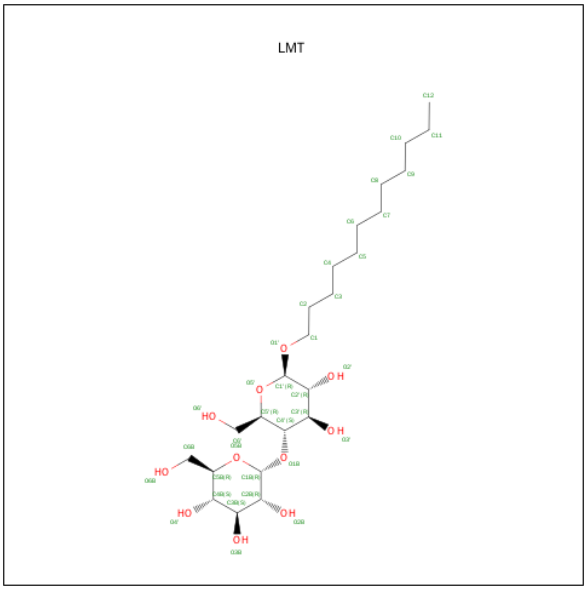
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	D	1	Total C H O 14 3 8 3	0	0

- Molecule 4 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 35 24 11	0	0
4	A	1	Total C O 35 24 11	0	0
4	A	1	Total C O 35 24 11	0	0

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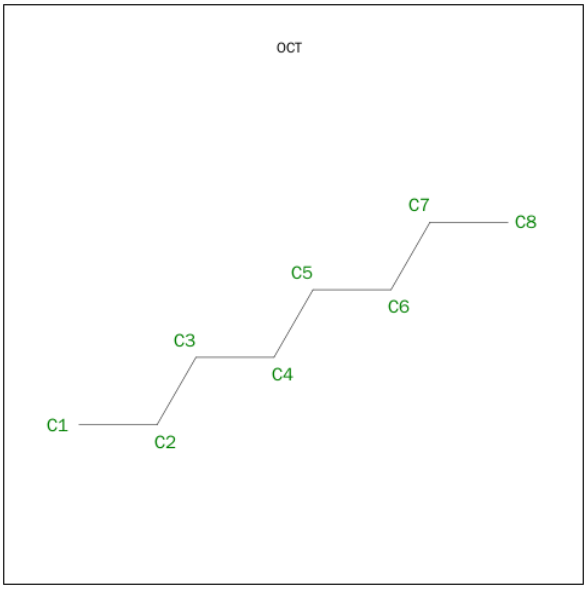
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 35 24 11	0	0
4	B	1	Total C O 35 24 11	0	0
4	B	1	Total C O 35 24 11	0	0
4	B	1	Total C O 35 24 11	0	0
4	C	1	Total C O 35 24 11	0	0

- Molecule 5 is N-OCTANE (three-letter code: OCT) (formula: C_8H_{18}).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C H 26 8 18	0	0
5	A	1	Total C H 26 8 18	0	0
5	C	1	Total C H 26 8 18	0	0
5	C	1	Total C H 26 8 18	0	0
5	C	1	Total C H 26 8 18	0	0
5	C	1	Total C H 26 8 18	0	0

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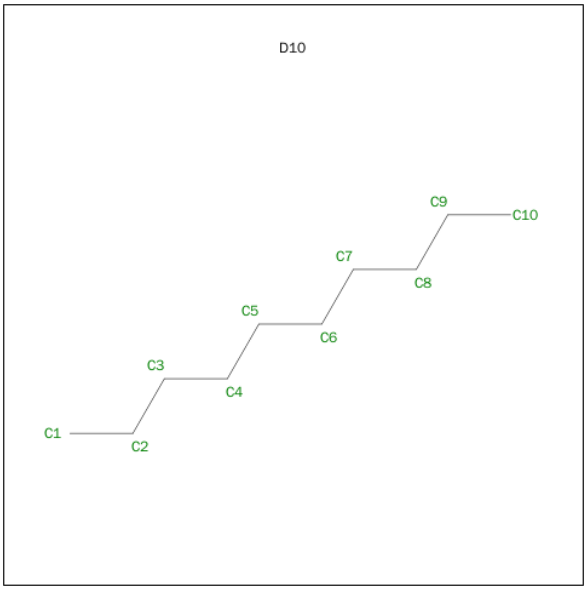
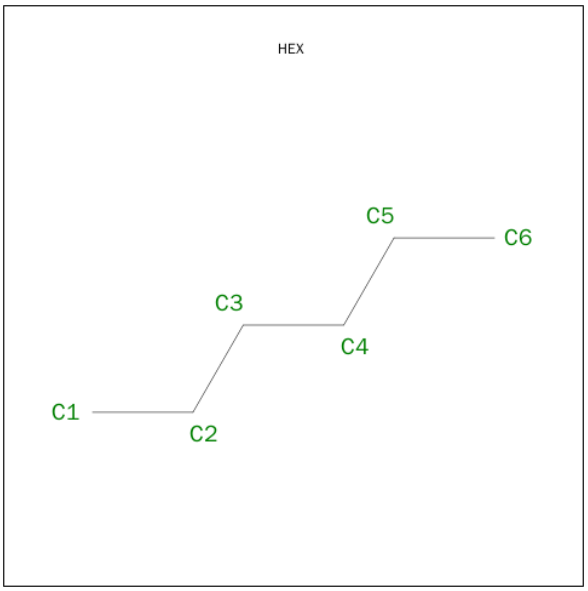
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C H 26 8 18	0	0

- Molecule 6 is DECANE (three-letter code: D10) (formula: $C_{10}H_{22}$).



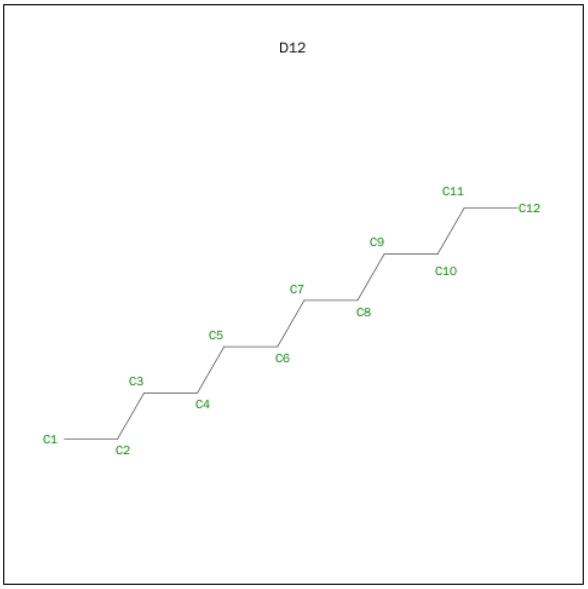
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C H 32 10 22	0	0
6	B	1	Total C H 32 10 22	0	0
6	B	1	Total C H 32 10 22	0	0
6	C	1	Total C H 32 10 22	0	0
6	C	1	Total C H 32 10 22	0	0
6	C	1	Total C H 32 10 22	0	0

- Molecule 7 is HEXANE (three-letter code: HEX) (formula: C_6H_{14}).



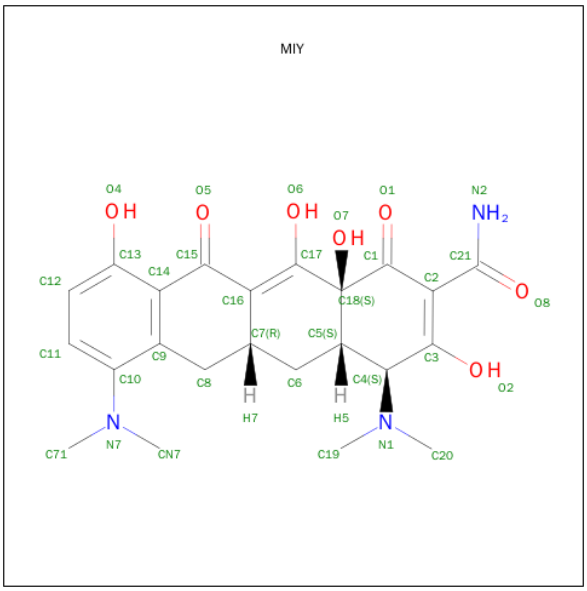
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C H 20 6 14	0	0
7	B	1	Total C H 20 6 14	0	0
7	B	1	Total C H 20 6 14	0	0
7	C	1	Total C H 20 6 14	0	0
7	C	1	Total C H 20 6 14	0	0

- Molecule 8 is DODECANE (three-letter code: D12) (formula: $C_{12}H_{26}$).



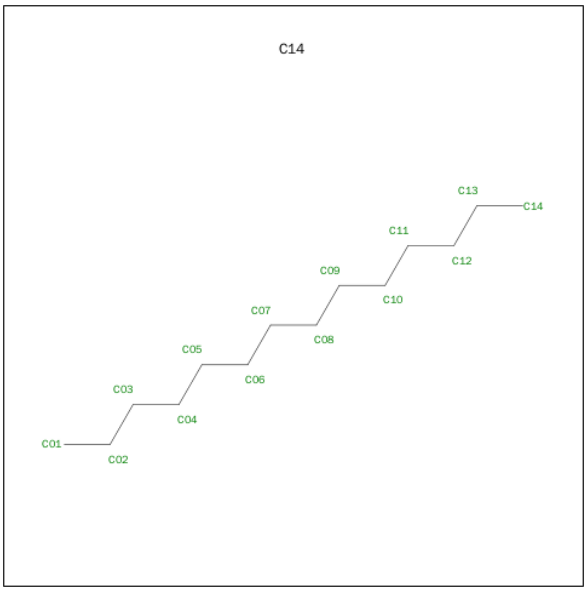
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C H 38 12 26	0	0
8	B	1	Total C H 38 12 26	0	0
8	C	1	Total C H 38 12 26	0	0
8	C	1	Total C H 38 12 26	0	0

- Molecule 9 is (4S,4AS,5AR,12AS)-4,7-BIS(DIMETHYLAMINO)-3,10,12,12A-TETRAHYDROXY-1,11-DIOXO-1,4,4A,5,5A,6,11,12A-OCTAHYDROTETRACENE-2-CARBOXAMIDE (three-letter code: MIY) (formula: $C_{23}H_{27}N_3O_7$).



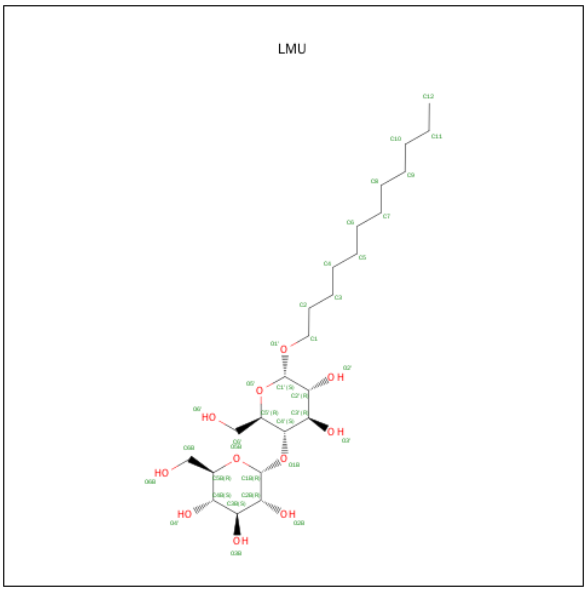
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C H N O 60 23 27 3 7	0	0

- Molecule 10 is TETRADECANE (three-letter code: C14) (formula: $C_{14}H_{30}$).



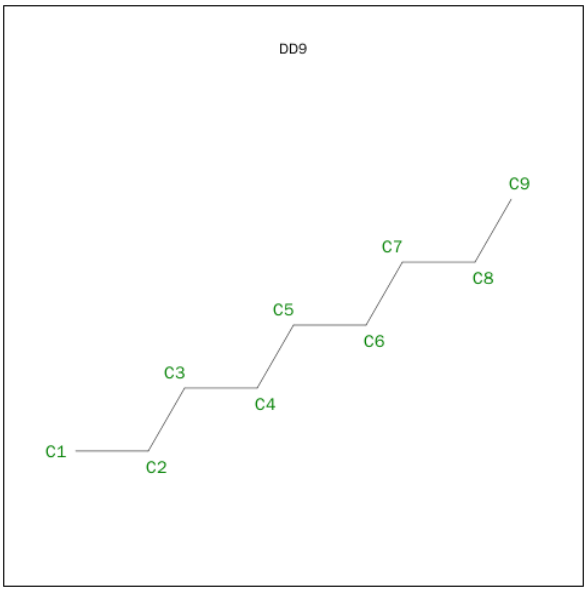
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	H	0	0
			44	14	30		

- Molecule 11 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula: $C_{24}H_{46}O_{11}$).



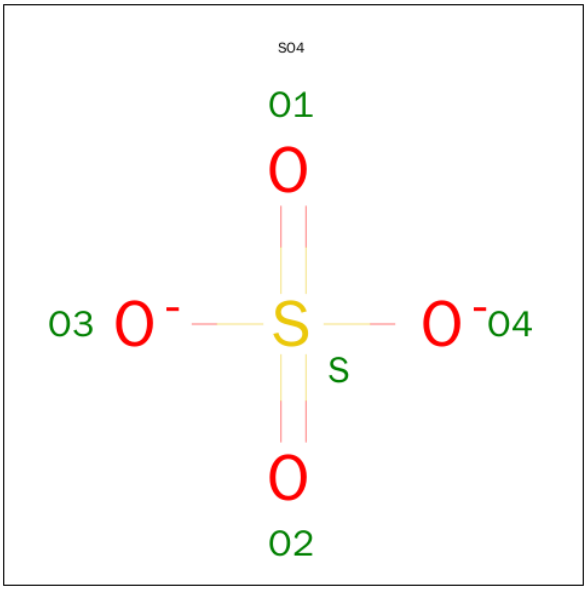
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	H	O	0	0
			81	24	46	11		

- Molecule 12 is NONANE (three-letter code: DD9) (formula: C_9H_{20}).



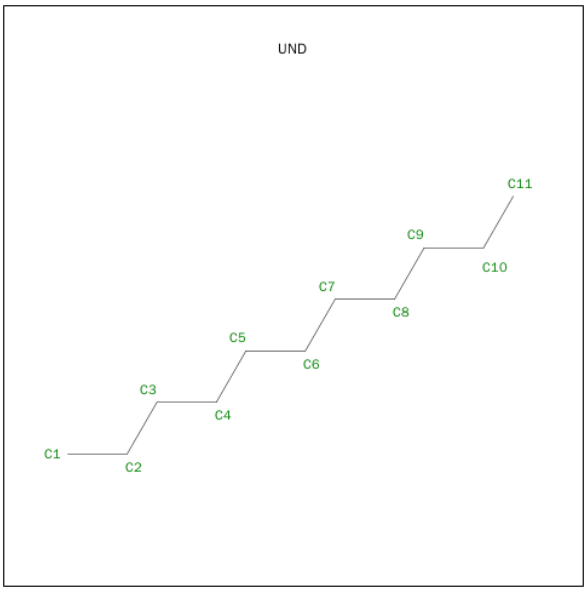
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	C	1	Total C H 29 9 20	0	0

- Molecule 13 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 14 is UNDECANE (three-letter code: UND) (formula: $C_{11}H_{24}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	C	1	Total C H 35 11 24	0	0

- Molecule 15 is water.

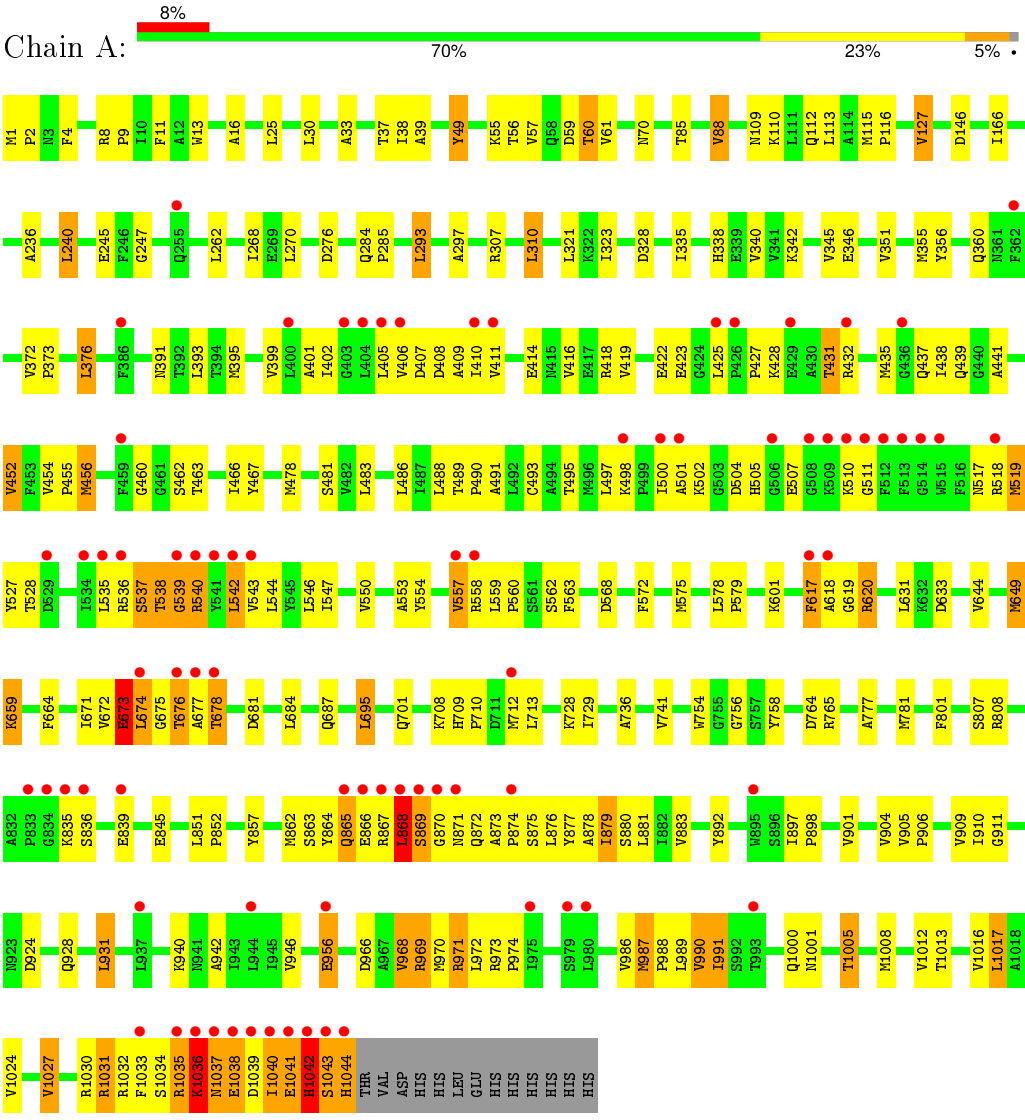
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	540	Total O 540 540	0	0
15	B	531	Total O 531 531	0	0
15	D	87	Total O 87 87	0	0
15	E	42	Total O 42 42	0	0
15	C	583	Total O 583 583	0	0

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.

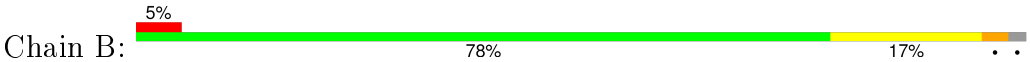
- Molecule 1: Acriflavine resistance protein B

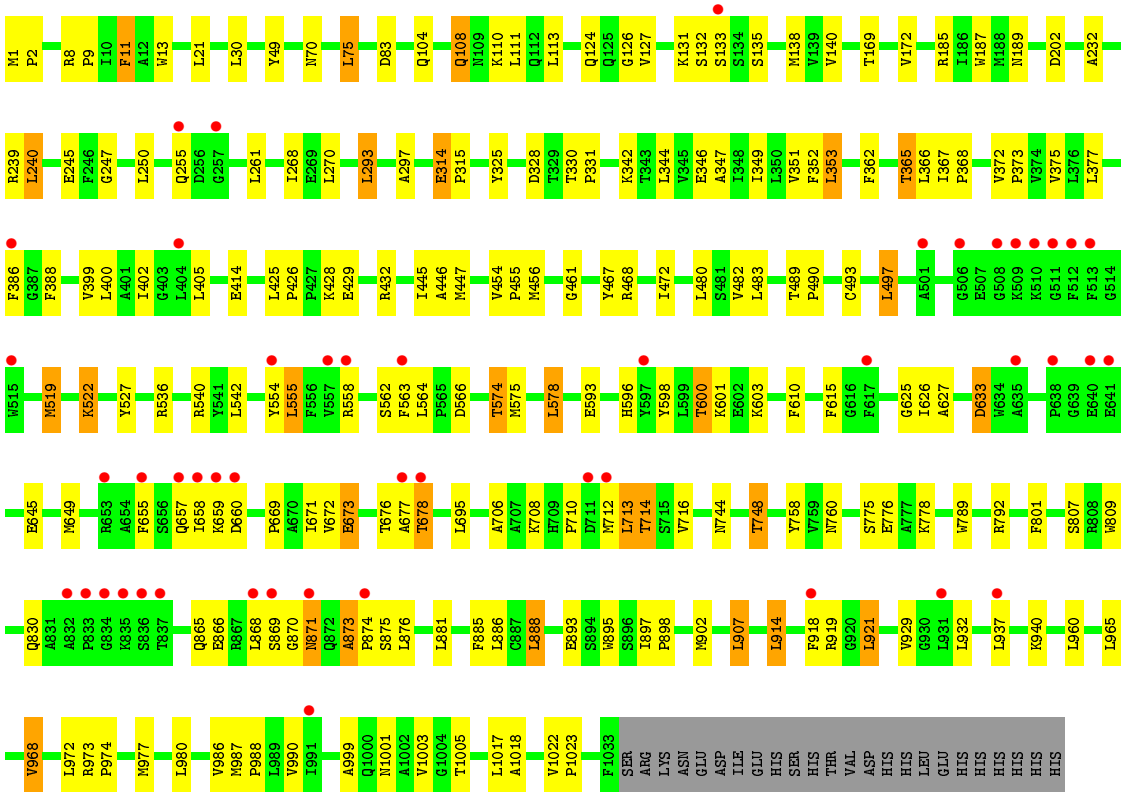
Chain A:



- Molecule 1: Acriflavine resistance protein B

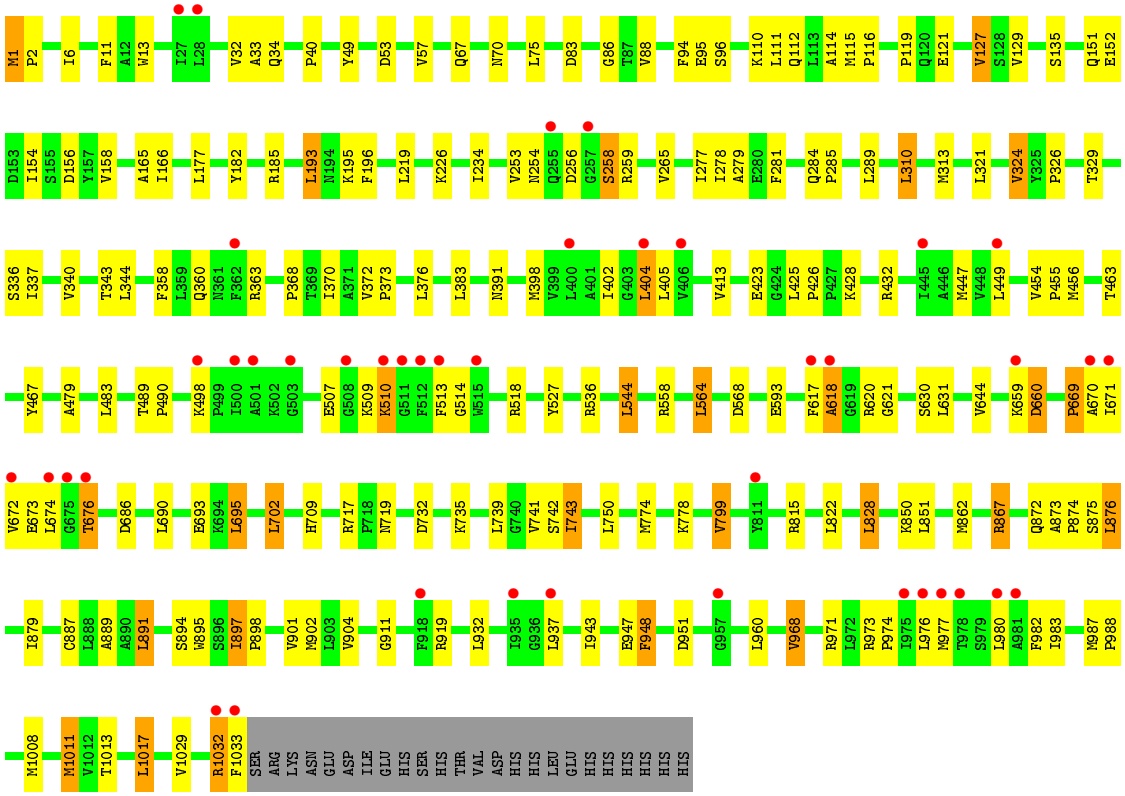
Chain B:





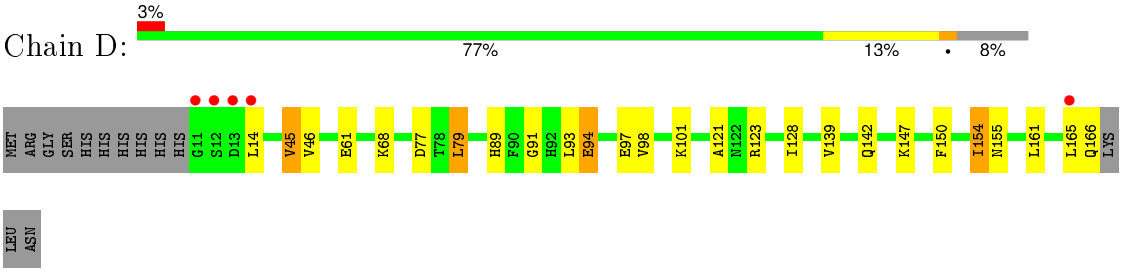
• Molecule 1: Acriflavine resistance protein B

Chain C:



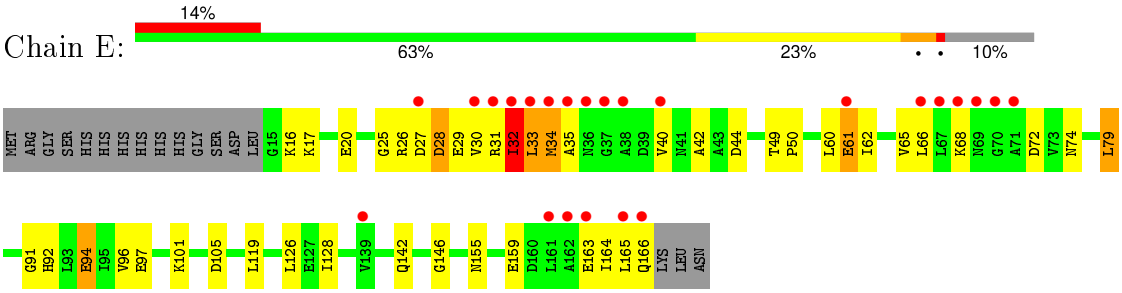
• Molecule 2: DARPIN

Chain D:



• Molecule 2: DARPIN

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	145.99Å 161.72Å 245.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.47 – 1.90 39.47 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.47-1.90) 99.4 (39.47-1.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 1.89Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.200 , 0.231 0.201 , 0.229	Depositor DCC
R_{free} test set	22550 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	29.2	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 58.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 451016 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	29010	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.90% 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, 0.375 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: GOL, DD9, D10, D12, LMT, HEX, LMU, MIY, UND, SO4, OCT, C14

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	0.37	0/8095	0.54	1/10991 (0.0%)
1	B	0.37	0/7999	0.53	0/10863
1	C	0.39	0/7999	0.55	0/10863
2	D	0.34	0/1196	0.48	0/1626
2	E	0.31	0/1170	0.46	0/1591
All	All	0.37	0/26459	0.53	1/35934 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	88	VAL	CB-CA-C	-5.61	100.75	111.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7943	0	8084	363	0
1	B	7849	0	8001	201	0
1	C	7849	0	8001	195	0
2	D	1177	0	1159	23	0
2	E	1151	0	1136	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	12	0	16	2	0
3	B	36	0	48	11	0
3	C	24	0	32	5	0
3	D	12	8	16	0	0
3	E	6	0	8	1	0
4	A	140	0	184	33	0
4	B	105	0	138	17	0
4	C	35	0	46	1	0
5	A	16	36	36	0	0
5	C	40	90	90	1	0
6	A	10	22	22	1	0
6	B	20	44	44	1	0
6	C	30	66	66	0	0
7	A	6	14	14	0	0
7	B	12	28	28	0	0
7	C	12	28	28	0	0
8	A	12	26	26	8	0
8	B	12	26	26	1	0
8	C	24	52	52	1	0
9	B	33	27	26	2	0
10	B	14	30	30	2	0
11	B	35	46	45	3	0
12	C	9	20	20	0	0
13	C	5	0	0	0	0
14	C	11	24	24	0	0
15	A	540	0	0	15	0
15	B	531	0	0	16	0
15	C	583	0	0	18	0
15	D	87	0	0	4	0
15	E	42	0	0	1	0
All	All	28423	587	27446	841	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 16.

The worst 5 of 841 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:A:1040:ILE:CA	1:A:1041:GLU:HB2	1.68	1.18
1:B:414:GLU:HG3	1:B:977:MET:CE	1.76	1.16
1:A:1038:GLU:CB	1:A:1039:ASP:HA	1.74	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:94:GLU:N	2:D:94:GLU:OE2	1.82	1.12
1:A:971:ARG:HG3	1:A:971:ARG:HH11	0.99	1.11

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	1042/1057 (99%)	986 (95%)	40 (4%)	16 (2%)	13 3
1	B	1031/1057 (98%)	1004 (97%)	22 (2%)	5 (0%)	34 21
1	C	1031/1057 (98%)	1002 (97%)	26 (2%)	3 (0%)	46 35
2	D	154/169 (91%)	152 (99%)	2 (1%)	0	100 100
2	E	150/169 (89%)	145 (97%)	2 (1%)	3 (2%)	9 2
All	All	3408/3509 (97%)	3289 (96%)	92 (3%)	27 (1%)	24 11

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	538	THR
1	A	539	GLY
1	A	673	GLU
1	A	677	ALA
1	A	1036	LYS

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	850/863 (98%)	783 (92%)	67 (8%)	15 6
1	B	839/863 (97%)	785 (94%)	54 (6%)	22 10
1	C	839/863 (97%)	791 (94%)	48 (6%)	25 13
2	D	120/132 (91%)	114 (95%)	6 (5%)	30 18
2	E	117/132 (89%)	107 (92%)	10 (8%)	13 5
All	All	2765/2853 (97%)	2580 (93%)	185 (7%)	20 9

5 of 185 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	365	THR
1	B	748	THR
2	D	61	GLU
1	B	399	VAL
1	B	574	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1042	HIS
1	B	274	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

51 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GOL	A	1101	-	5,5,5	0.26	0	5,5,5	0.57	0
4	LMT	A	1102	-	36,36,36	1.15	3 (8%)	47,47,47	1.48	9 (19%)
4	LMT	A	1103	-	36,36,36	1.16	3 (8%)	47,47,47	1.14	2 (4%)
4	LMT	A	1104	-	36,36,36	1.20	3 (8%)	47,47,47	1.12	4 (8%)
5	OCT	A	1105	-	7,7,7	0.34	0	6,6,6	0.80	0
5	OCT	A	1106	-	7,7,7	0.22	0	6,6,6	0.61	0
6	D10	A	1107	-	9,9,9	0.25	0	8,8,8	0.70	0
7	HEX	A	1108	-	5,5,5	0.23	0	4,4,4	0.68	0
4	LMT	A	1109	-	36,36,36	1.11	3 (8%)	47,47,47	1.54	11 (23%)
3	GOL	A	1110	-	5,5,5	0.35	0	5,5,5	0.67	0
8	D12	A	1111	-	11,11,11	0.42	0	10,10,10	1.10	0
3	GOL	B	1101	-	5,5,5	0.29	0	5,5,5	0.32	0
3	GOL	B	1102	-	5,5,5	0.37	0	5,5,5	0.30	0
9	MIY	B	1103	-	35,36,36	3.28	17 (48%)	40,58,58	2.28	14 (35%)
4	LMT	B	1104	-	36,36,36	1.13	3 (8%)	47,47,47	1.26	4 (8%)
6	D10	B	1105	-	9,9,9	0.35	0	8,8,8	0.90	0
8	D12	B	1106	-	11,11,11	0.22	0	10,10,10	0.73	0
6	D10	B	1107	-	9,9,9	0.31	0	8,8,8	0.95	0
7	HEX	B	1108	-	5,5,5	0.25	0	4,4,4	0.60	0
10	C14	B	1109	-	13,13,13	0.27	0	12,12,12	0.93	0
4	LMT	B	1110	-	36,36,36	1.20	3 (8%)	47,47,47	1.38	7 (14%)
4	LMT	B	1111	-	36,36,36	1.17	3 (8%)	47,47,47	1.05	3 (6%)
7	HEX	B	1112	-	5,5,5	0.20	0	4,4,4	0.52	0
3	GOL	B	1113	-	5,5,5	0.33	0	5,5,5	0.53	0
11	LMU	B	1114	-	36,36,36	1.13	4 (11%)	47,47,47	2.37	14 (29%)
3	GOL	B	1115	-	5,5,5	0.33	0	5,5,5	0.33	0
3	GOL	B	1116	-	5,5,5	0.36	0	5,5,5	0.12	0
3	GOL	B	1117	-	5,5,5	0.45	0	5,5,5	0.38	0
3	GOL	C	1101	-	5,5,5	0.24	0	5,5,5	0.50	0
4	LMT	C	1102	-	36,36,36	1.15	3 (8%)	47,47,47	1.07	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	OCT	C	1103	-	7,7,7	0.29	0	6,6,6	0.76	0
8	D12	C	1104	-	11,11,11	0.27	0	10,10,10	0.79	0
5	OCT	C	1105	-	7,7,7	0.30	0	6,6,6	1.15	1 (16%)
5	OCT	C	1106	-	7,7,7	0.24	0	6,6,6	0.64	0
6	D10	C	1107	-	9,9,9	0.37	0	8,8,8	1.00	0
8	D12	C	1108	-	11,11,11	0.39	0	10,10,10	1.10	1 (10%)
6	D10	C	1109	-	9,9,9	0.26	0	8,8,8	0.80	0
7	HEX	C	1110	-	5,5,5	0.24	0	4,4,4	0.70	0
12	DD9	C	1111	-	8,8,8	0.23	0	7,7,7	0.75	0
5	OCT	C	1112	-	7,7,7	0.24	0	6,6,6	0.74	0
7	HEX	C	1113	-	5,5,5	0.20	0	4,4,4	0.49	0
3	GOL	C	1114	-	5,5,5	0.28	0	5,5,5	0.33	0
3	GOL	C	1115	-	5,5,5	0.46	0	5,5,5	0.69	0
5	OCT	C	1116	-	7,7,7	0.30	0	6,6,6	0.86	0
3	GOL	C	1117	-	5,5,5	0.48	0	5,5,5	0.44	0
13	SO4	C	1118	-	4,4,4	0.28	0	6,6,6	0.13	0
14	UND	C	1119	-	10,10,10	0.24	0	9,9,9	0.73	0
6	D10	C	1120	-	9,9,9	0.24	0	8,8,8	0.71	0
3	GOL	D	201	-	5,5,5	0.30	0	5,5,5	0.33	0
3	GOL	D	202	-	5,5,5	0.31	0	5,5,5	0.42	0
3	GOL	E	201	-	5,5,5	0.29	0	5,5,5	0.28	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	1101	-	-	0/4/4/4	0/0/0/0
4	LMT	A	1102	-	-	0/21/61/61	0/2/2/2
4	LMT	A	1103	-	-	0/21/61/61	0/2/2/2
4	LMT	A	1104	-	-	0/21/61/61	0/2/2/2
5	OCT	A	1105	-	-	0/5/5/5	0/0/0/0
5	OCT	A	1106	-	-	0/5/5/5	0/0/0/0
6	D10	A	1107	-	-	0/7/7/7	0/0/0/0
7	HEX	A	1108	-	-	0/3/3/3	0/0/0/0
4	LMT	A	1109	-	-	0/21/61/61	0/2/2/2
3	GOL	A	1110	-	-	0/4/4/4	0/0/0/0
8	D12	A	1111	-	-	0/9/9/9	0/0/0/0
3	GOL	B	1101	-	-	0/4/4/4	0/0/0/0
3	GOL	B	1102	-	-	0/4/4/4	0/0/0/0
9	MIY	B	1103	-	-	0/12/70/70	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LMT	B	1104	-	-	0/21/61/61	0/2/2/2
6	D10	B	1105	-	-	0/7/7/7	0/0/0/0
8	D12	B	1106	-	-	0/9/9/9	0/0/0/0
6	D10	B	1107	-	-	0/7/7/7	0/0/0/0
7	HEX	B	1108	-	-	0/3/3/3	0/0/0/0
10	C14	B	1109	-	-	0/11/11/11	0/0/0/0
4	LMT	B	1110	-	-	0/21/61/61	0/2/2/2
4	LMT	B	1111	-	-	0/21/61/61	0/2/2/2
7	HEX	B	1112	-	-	0/3/3/3	0/0/0/0
3	GOL	B	1113	-	-	0/4/4/4	0/0/0/0
11	LMU	B	1114	-	-	0/21/61/61	0/2/2/2
3	GOL	B	1115	-	-	0/4/4/4	0/0/0/0
3	GOL	B	1116	-	-	0/4/4/4	0/0/0/0
3	GOL	B	1117	-	-	0/4/4/4	0/0/0/0
3	GOL	C	1101	-	-	0/4/4/4	0/0/0/0
4	LMT	C	1102	-	-	0/21/61/61	0/2/2/2
5	OCT	C	1103	-	-	0/5/5/5	0/0/0/0
8	D12	C	1104	-	-	0/9/9/9	0/0/0/0
5	OCT	C	1105	-	-	0/5/5/5	0/0/0/0
5	OCT	C	1106	-	-	0/5/5/5	0/0/0/0
6	D10	C	1107	-	-	0/7/7/7	0/0/0/0
8	D12	C	1108	-	-	0/9/9/9	0/0/0/0
6	D10	C	1109	-	-	0/7/7/7	0/0/0/0
7	HEX	C	1110	-	-	0/3/3/3	0/0/0/0
12	DD9	C	1111	-	-	0/6/6/6	0/0/0/0
5	OCT	C	1112	-	-	0/5/5/5	0/0/0/0
7	HEX	C	1113	-	-	0/3/3/3	0/0/0/0
3	GOL	C	1114	-	-	0/4/4/4	0/0/0/0
3	GOL	C	1115	-	-	0/4/4/4	0/0/0/0
5	OCT	C	1116	-	-	0/5/5/5	0/0/0/0
3	GOL	C	1117	-	-	0/4/4/4	0/0/0/0
13	SO4	C	1118	-	-	0/0/0/0	0/0/0/0
14	UND	C	1119	-	-	0/8/8/8	0/0/0/0
6	D10	C	1120	-	-	0/7/7/7	0/0/0/0
3	GOL	D	201	-	-	0/4/4/4	0/0/0/0
3	GOL	D	202	-	-	0/4/4/4	0/0/0/0
3	GOL	E	201	-	-	0/4/4/4	0/0/0/0

The worst 5 of 45 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	1103	MIY	C18-C1	-4.21	1.48	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	1103	MIY	C14-C9	-4.07	1.34	1.40
9	B	1103	MIY	O7-C18	-3.61	1.36	1.42
4	B	1110	LMT	C3'-C4'	-3.23	1.43	1.52
4	A	1104	LMT	C3'-C4'	-3.16	1.43	1.52

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	1103	MIY	C11-C12-C13	-6.31	114.02	120.49
4	A	1109	LMT	C1B-O5B-C5B	-4.24	105.51	113.75
11	B	1114	LMU	C1'-O5'-C5'	-3.93	106.12	113.75
9	B	1103	MIY	C18-C17-C16	-3.72	118.49	122.95
4	A	1104	LMT	C1B-O1B-C4'	-3.14	109.80	118.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

28 monomers are involved in 86 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1101	GOL	1	0
4	A	1102	LMT	6	0
4	A	1103	LMT	11	0
4	A	1104	LMT	2	0
6	A	1107	D10	1	0
4	A	1109	LMT	14	0
3	A	1110	GOL	1	0
8	A	1111	D12	8	0
3	B	1101	GOL	2	0
3	B	1102	GOL	2	0
9	B	1103	MIY	2	0
4	B	1104	LMT	4	0
6	B	1105	D10	1	0
8	B	1106	D12	1	0
10	B	1109	C14	2	0
4	B	1110	LMT	9	0
4	B	1111	LMT	4	0
3	B	1113	GOL	1	0
11	B	1114	LMU	3	0
3	B	1115	GOL	1	0
3	B	1116	GOL	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1101	GOL	1	0
4	C	1102	LMT	1	0
5	C	1103	OCT	1	0
8	C	1104	D12	1	0
3	C	1115	GOL	3	0
3	C	1117	GOL	1	0
3	E	201	GOL	1	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	1044/1057 (98%)	0.26	84 (8%)	15	17	17, 43, 87, 136	0
1	B	1033/1057 (97%)	0.10	48 (4%)	36	39	19, 41, 69, 133	0
1	C	1033/1057 (97%)	0.05	42 (4%)	41	45	20, 36, 61, 104	0
2	D	156/169 (92%)	-0.07	5 (3%)	51	54	30, 39, 66, 110	0
2	E	152/169 (89%)	0.76	24 (15%)	3	3	34, 50, 83, 106	0
All	All	3418/3509 (97%)	0.16	203 (5%)	26	29	17, 40, 75, 136	0

The worst 5 of 203 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	11	GLY	12.5
1	A	1043	SER	7.3
1	B	677	ALA	7.3
1	A	868	LEU	6.9
1	A	869	SER	6.2

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	OCT	C	1112	8/8	0.38	0.32	14.01	79,97,102,103	0
3	GOL	C	1115	6/6	0.92	0.20	10.04	30,39,51,52	0
6	D10	C	1107	10/10	0.74	0.28	9.47	72,92,96,99	0
4	LMT	A	1109	35/35	0.74	0.34	8.41	70,95,104,105	0
7	HEX	B	1108	6/6	0.79	0.22	7.84	66,79,87,87	0
3	GOL	B	1117	6/6	0.86	0.27	6.47	55,55,64,75	0
3	GOL	D	202	6/6	0.77	0.17	6.41	53,69,83,88	0
7	HEX	B	1112	6/6	0.51	0.24	5.86	79,96,103,103	0
3	GOL	B	1101	6/6	0.90	0.14	5.24	34,41,52,58	0
3	GOL	C	1117	6/6	0.75	0.29	5.14	41,53,58,61	0
3	GOL	D	201	6/6	0.92	0.10	5.06	55,60,64,71	0
3	GOL	B	1113	6/6	0.90	0.18	4.98	56,64,67,68	0
6	D10	A	1107	10/10	0.42	0.25	4.63	75,92,106,108	0
4	LMT	B	1111	35/35	0.65	0.34	4.39	78,120,130,131	0
4	LMT	A	1102	35/35	0.84	0.17	4.36	50,71,95,101	0
5	OCT	C	1106	8/8	0.58	0.19	4.22	73,88,101,101	0
3	GOL	C	1114	6/6	0.82	0.18	4.03	59,67,69,70	0
7	HEX	C	1113	6/6	0.73	0.27	3.82	71,89,105,105	0
10	C14	B	1109	14/14	0.77	0.18	3.70	70,87,106,109	0
3	GOL	B	1116	6/6	0.91	0.19	3.51	67,75,82,87	0
6	D10	C	1120	10/10	0.62	0.21	3.22	72,94,116,116	0
3	GOL	A	1101	6/6	0.91	0.13	3.16	38,47,54,58	0
11	LMU	B	1114	35/35	0.71	0.24	2.99	76,100,115,118	0
14	UND	C	1119	11/11	0.64	0.31	2.88	64,98,118,118	0
12	DD9	C	1111	9/9	0.76	0.20	2.87	56,80,98,101	0
4	LMT	B	1104	35/35	0.89	0.20	2.81	53,68,98,99	0
6	D10	B	1107	10/10	0.69	0.19	2.75	64,94,113,113	0
3	GOL	B	1102	6/6	0.91	0.12	2.67	40,58,64,69	0
5	OCT	A	1105	8/8	0.69	0.30	2.43	73,89,93,94	0
4	LMT	B	1110	35/35	0.67	0.31	2.36	65,121,126,129	0
3	GOL	B	1115	6/6	0.74	0.19	2.23	56,68,71,72	0
3	GOL	C	1101	6/6	0.89	0.17	2.04	50,57,69,74	0
3	GOL	A	1110	6/6	0.94	0.13	2.01	28,40,54,56	0
7	HEX	C	1110	6/6	0.73	0.17	1.99	77,93,98,98	0
8	D12	C	1108	12/12	0.82	0.22	1.88	40,63,90,90	0
7	HEX	A	1108	6/6	0.76	0.18	1.87	89,110,112,112	0
4	LMT	A	1104	35/35	0.90	0.13	1.62	51,74,104,108	0
9	MIY	B	1103	33/33	0.86	0.16	1.15	52,74,112,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	GOL	E	201	6/6	0.89	0.14	0.97	56,59,64,68	0
8	D12	A	1111	12/12	0.88	0.13	0.93	53,73,98,98	0
4	LMT	A	1103	35/35	0.71	0.24	0.81	68,88,105,106	0
5	OCT	C	1116	8/8	0.80	0.15	0.65	61,75,84,85	0
8	D12	C	1104	12/12	0.67	0.14	0.58	68,85,98,99	0
5	OCT	C	1103	8/8	0.90	0.10	0.55	65,80,84,86	0
4	LMT	C	1102	35/35	0.94	0.12	0.15	50,64,79,80	0
5	OCT	C	1105	8/8	0.81	0.14	-0.21	67,83,101,105	0
6	D10	B	1105	10/10	0.82	0.19	-	69,85,88,88	0
5	OCT	A	1106	8/8	0.80	0.18	-	66,82,86,86	0
13	SO4	C	1118	5/5	0.99	0.11	-	62,67,76,78	0
6	D10	C	1109	10/10	0.64	0.34	-	73,90,102,102	0
8	D12	B	1106	12/12	0.66	0.25	-	74,92,108,109	0

6.5 Other polymers

There are no such residues in this entry.