wwPDB X-ray Structure Validation Summary Report (i)

Nov 5, 2023 – 11:38 PM EST

PDB ID	:	3L21
Title	:	The crystal structure of a dimeric mutant of dihydrodipicolinate synthase (DAPA, RV2753C) from Mycobacterium Tuberculosis - DHDPS-A204R
Authors	:	Evans, G.L.; Schuldt, L.; Jamerson, G.B.; Devenish, S.R.; Weiss, M.S.; Gerrard, J.A.
Deposited on	:	2009-12-14
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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

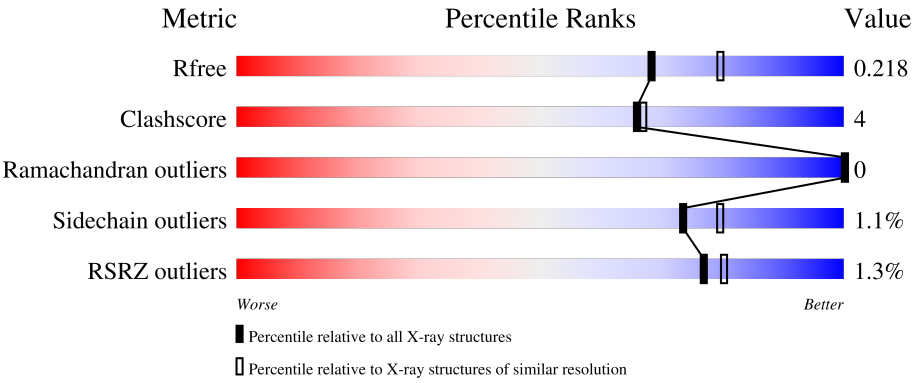
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.10 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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 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	304	89% 9%
1	B	304	88% 9%
1	C	304	90% 7%
1	D	304	91% 6%
1	E	304	3% 90% 7%

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Mol	Chain	Length	Quality of chain
1	F	304	2% 91% 6%

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	SO4	C	301	-	-	X	-
3	GOL	A	305	-	-	X	-
3	GOL	D	304	-	-	X	-
3	GOL	E	307	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 14886 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 Dihydrodipicolinate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	4	0
			2183	1363	386	424	10			
1	B	295	Total	C	N	O	S	0	5	0
			2179	1360	385	424	10			
1	C	295	Total	C	N	O	S	0	1	0
			2152	1344	382	416	10			
1	D	295	Total	C	N	O	S	0	2	0
			2157	1348	380	419	10			
1	E	295	Total	C	N	O	S	0	1	0
			2156	1346	382	418	10			
1	F	295	Total	C	N	O	S	0	3	0
			2170	1357	386	417	10			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P63945
A	-2	ALA	-	expression tag	UNP P63945
A	-1	MET	-	expression tag	UNP P63945
A	0	ALA	-	expression tag	UNP P63945
A	1	VAL	-	expression tag	UNP P63945
A	204	ARG	ALA	engineered mutation	UNP P63945
B	-3	GLY	-	expression tag	UNP P63945
B	-2	ALA	-	expression tag	UNP P63945
B	-1	MET	-	expression tag	UNP P63945
B	0	ALA	-	expression tag	UNP P63945
B	1	VAL	-	expression tag	UNP P63945
B	204	ARG	ALA	engineered mutation	UNP P63945
C	-3	GLY	-	expression tag	UNP P63945
C	-2	ALA	-	expression tag	UNP P63945
C	-1	MET	-	expression tag	UNP P63945
C	0	ALA	-	expression tag	UNP P63945
C	1	VAL	-	expression tag	UNP P63945

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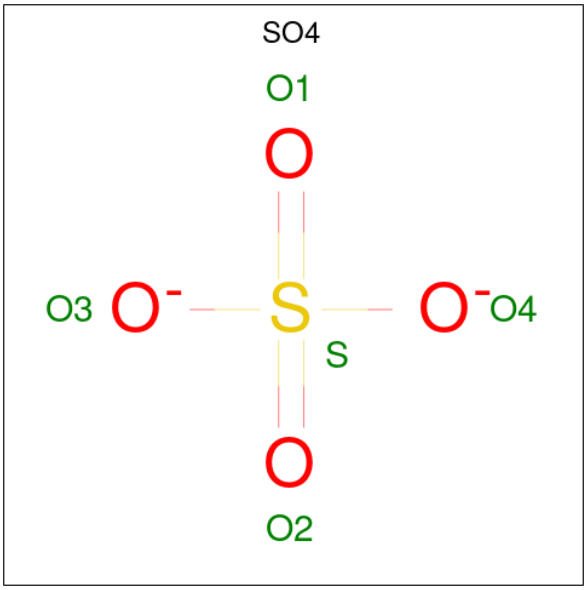
Chain	Residue	Modelled	Actual	Comment	Reference
C	204	ARG	ALA	engineered mutation	UNP P63945
D	-3	GLY	-	expression tag	UNP P63945
D	-2	ALA	-	expression tag	UNP P63945
D	-1	MET	-	expression tag	UNP P63945
D	0	ALA	-	expression tag	UNP P63945
D	1	VAL	-	expression tag	UNP P63945
D	204	ARG	ALA	engineered mutation	UNP P63945
E	-3	GLY	-	expression tag	UNP P63945
E	-2	ALA	-	expression tag	UNP P63945
E	-1	MET	-	expression tag	UNP P63945
E	0	ALA	-	expression tag	UNP P63945
E	1	VAL	-	expression tag	UNP P63945
E	204	ARG	ALA	engineered mutation	UNP P63945
F	-3	GLY	-	expression tag	UNP P63945
F	-2	ALA	-	expression tag	UNP P63945
F	-1	MET	-	expression tag	UNP P63945
F	0	ALA	-	expression tag	UNP P63945
F	1	VAL	-	expression tag	UNP P63945
F	204	ARG	ALA	engineered mutation	UNP P63945

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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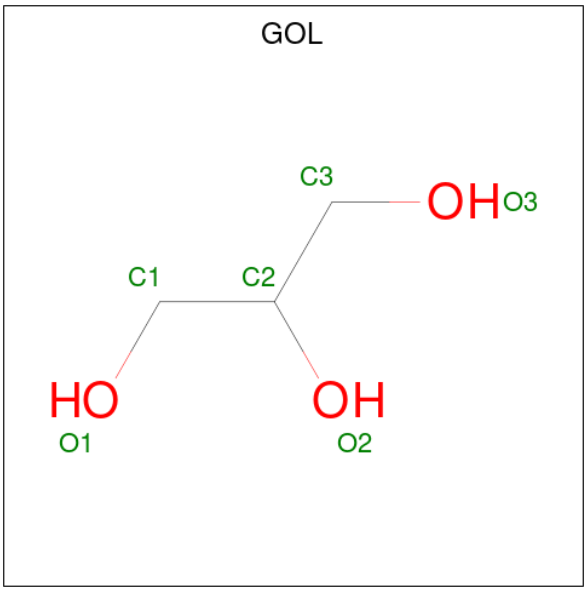
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0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

- 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 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
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

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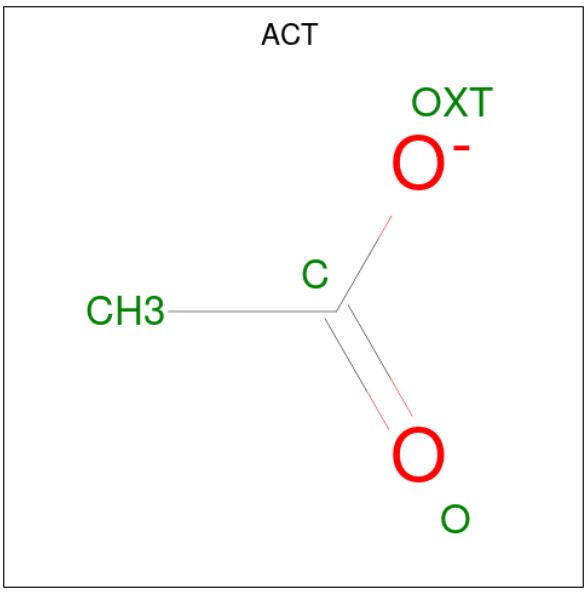
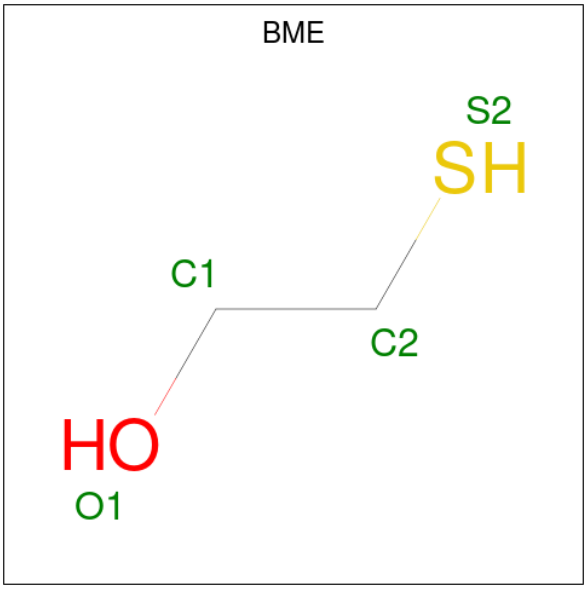
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



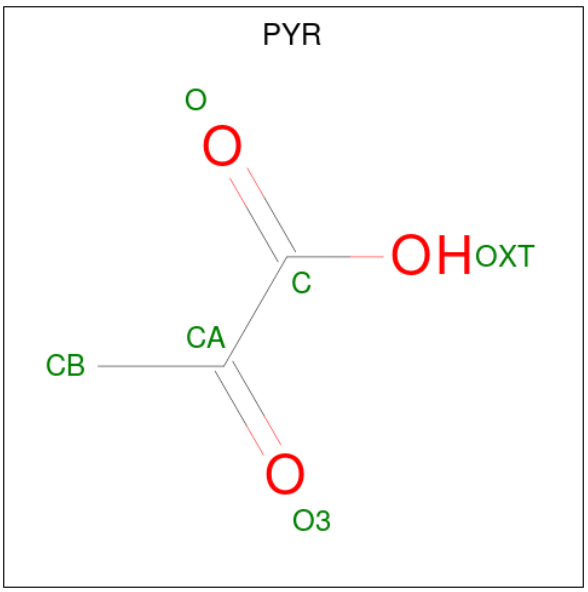
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0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

- Molecule 5 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).



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

- Molecule 6 is PYRUVIC ACID (three-letter code: PYR) (formula: $C_3H_4O_3$).



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

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	2	Total Cl 2 2	0	0
7	E	1	Total Cl 1 1	0	0

- Molecule 8 is water.

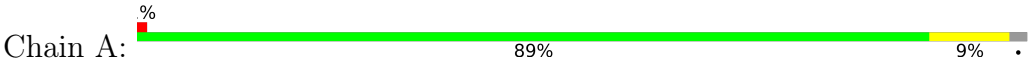
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	340	Total O 340 340	0	0
8	B	274	Total O 274 274	0	0
8	C	246	Total O 246 246	0	0
8	D	263	Total O 263 263	0	0
8	E	248	Total O 248 248	0	0
8	F	225	Total O 225 225	0	0

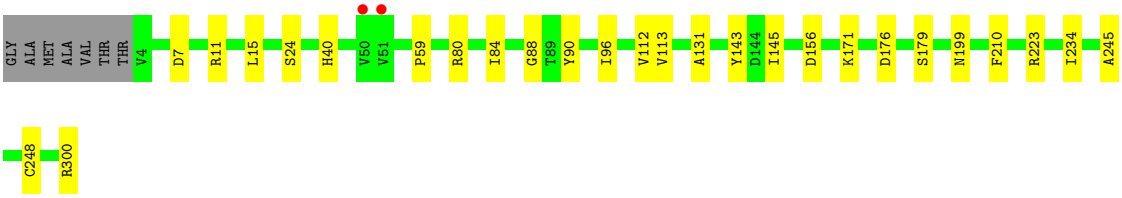
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Dihydrodipicolinate synthase

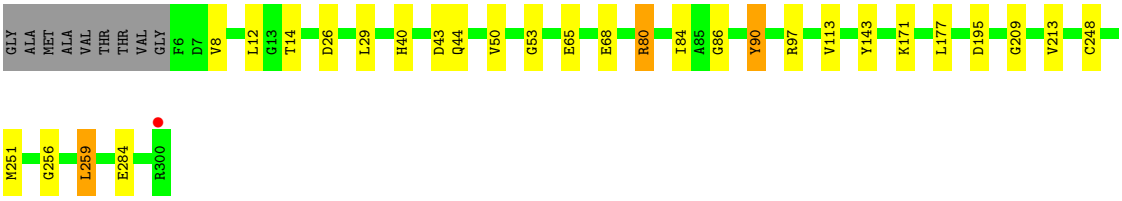
Chain A:





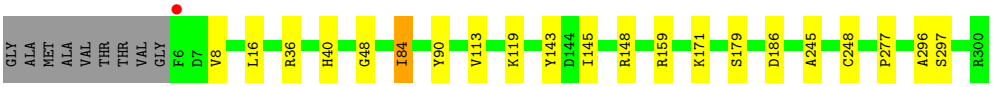
• Molecule 1: Dihydrodipicolinate synthase

Chain B:



• Molecule 1: Dihydrodipicolinate synthase

Chain C:

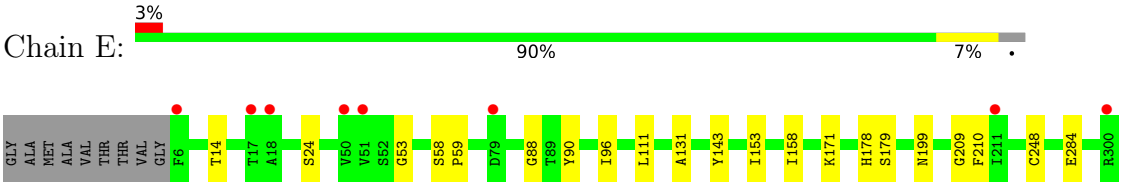


• Molecule 1: Dihydrodipicolinate synthase

Chain D:

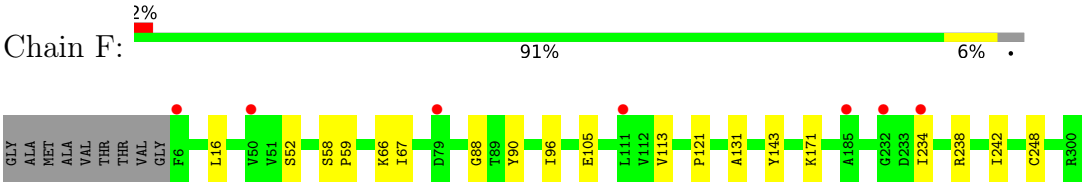
• Molecule 1: Dihydrodipicolinate synthase

Chain E:



• Molecule 1: Dihydrodipicolinate synthase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	188.83Å 188.83Å 130.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.51 – 2.10 28.51 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.5 (28.51-2.10) 98.5 (28.51-2.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.44 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.178 , 0.204 0.192 , 0.218	Depositor DCC
R_{free} test set	4198 reflections (2.70%)	wwPDB-VP
Wilson B-factor (Å^2)	22.1	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 38.8	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	0.94	EDS
Total number of atoms	14886	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: KPI, PYR, BME, SO4, CME, GOL, CL, ACT

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	0.78	1/2194 (0.0%)	0.79	0/2986
1	B	0.74	0/2190	0.74	0/2981
1	C	0.67	0/2160	0.75	0/2940
1	D	0.67	0/2165	0.75	1/2950 (0.0%)
1	E	0.61	0/2164	0.71	0/2946
1	F	0.63	0/2181	0.72	0/2969
All	All	0.69	1/13054 (0.0%)	0.74	1/17772 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	112	VAL	CB-CG2	5.12	1.63	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	144	ASP	CB-CG-OD1	5.78	123.50	118.30

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	2183	0	2202	26	0
1	B	2179	0	2190	26	1
1	C	2152	0	2169	16	0
1	D	2157	0	2172	13	0
1	E	2156	0	2173	15	0
1	F	2170	0	2200	11	0
2	A	15	0	0	1	0
2	B	15	0	0	0	0
2	C	15	0	0	2	0
2	D	10	0	0	0	0
2	E	15	0	0	0	0
2	F	10	0	0	0	0
3	A	24	0	32	8	0
3	B	36	0	48	7	0
3	C	30	0	40	3	0
3	D	24	0	32	5	0
3	E	18	0	24	8	0
3	F	24	0	32	4	0
4	A	12	0	9	1	0
4	B	16	0	12	0	0
4	C	4	0	3	0	0
4	E	8	0	4	0	0
4	F	4	0	1	0	0
5	A	4	0	6	1	0
6	B	6	0	0	0	0
7	D	2	0	0	0	0
7	E	1	0	0	0	0
8	A	340	0	0	6	0
8	B	274	0	0	4	0
8	C	246	0	0	2	0
8	D	263	0	0	0	0
8	E	248	0	0	0	0
8	F	225	0	0	2	0
All	All	14886	0	13349	106	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 106 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195[A]:ASP:OD2	8:B:1806:HOH:O	1.53	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:121:PRO:HB2	3:D:304:GOL:H12	1.30	1.11
3:F:305:GOL:H11	8:F:1696:HOH:O	1.58	1.02
1:B:43[B]:ASP:OD1	1:B:80[B]:ARG:NH2	2.00	0.94
1:C:148:ARG:HG2	1:D:119:LYS:HE3	1.50	0.92

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:GLU:OE2	1:B:195[B]:ASP:OD2[4_464]	2.16	0.04

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	297/304 (98%)	291 (98%)	6 (2%)	0	100	100
1	B	296/304 (97%)	287 (97%)	9 (3%)	0	100	100
1	C	292/304 (96%)	286 (98%)	6 (2%)	0	100	100
1	D	293/304 (96%)	286 (98%)	7 (2%)	0	100	100
1	E	292/304 (96%)	289 (99%)	3 (1%)	0	100	100
1	F	294/304 (97%)	287 (98%)	7 (2%)	0	100	100
All	All	1764/1824 (97%)	1726 (98%)	38 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	220/220 (100%)	218 (99%)	2 (1%)	78 84
1	B	219/220 (100%)	215 (98%)	4 (2%)	59 65
1	C	215/220 (98%)	211 (98%)	4 (2%)	57 63
1	D	216/220 (98%)	214 (99%)	2 (1%)	78 84
1	E	216/220 (98%)	214 (99%)	2 (1%)	78 84
1	F	218/220 (99%)	217 (100%)	1 (0%)	88 92
All	All	1304/1320 (99%)	1289 (99%)	15 (1%)	73 77

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	84	ILE
1	E	90	TYR
1	C	90	TYR
1	F	90	TYR
1	D	201	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	178	HIS
1	D	182	GLN
1	E	44	GLN
1	B	249	ASN
1	A	44	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)

12 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	KPI	E	171	1	11,13,14	1.13	0	10,15,17	1.80	2 (20%)
1	KPI	C	171	1	11,13,14	0.86	0	10,15,17	1.76	4 (40%)
1	KPI	A	171	1	11,13,14	1.34	2 (18%)	10,15,17	1.35	2 (20%)
1	KPI	F	171	1	11,13,14	0.90	0	10,15,17	1.61	2 (20%)
1	CME	F	248	1	8,9,10	0.78	0	5,9,11	1.83	2 (40%)
1	CME	A	248	1	8,9,10	0.69	0	5,9,11	1.55	0
1	CME	C	248	1	8,9,10	0.63	0	5,9,11	1.43	0
1	KPI	B	171	1	11,13,14	0.91	0	10,15,17	1.71	4 (40%)
1	CME	E	248	1	8,9,10	0.79	0	5,9,11	1.95	2 (40%)
1	KPI	D	171	1	11,13,14	0.89	0	10,15,17	1.66	3 (30%)
1	CME	B	248	1	8,9,10	0.86	0	5,9,11	1.39	1 (20%)
1	CME	D	248	1	8,9,10	0.83	0	5,9,11	1.69	2 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KPI	E	171	1	-	0/13/14/16	-
1	KPI	C	171	1	-	0/13/14/16	-
1	KPI	A	171	1	-	0/13/14/16	-
1	KPI	F	171	1	-	0/13/14/16	-
1	CME	F	248	1	-	2/5/8/10	-
1	CME	A	248	1	-	1/5/8/10	-
1	CME	C	248	1	-	1/5/8/10	-
1	KPI	B	171	1	-	0/13/14/16	-
1	CME	E	248	1	-	2/5/8/10	-
1	KPI	D	171	1	-	1/13/14/16	-
1	CME	B	248	1	-	0/5/8/10	-
1	CME	D	248	1	-	0/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	171	KPI	CB-CA	2.41	1.56	1.53
1	A	171	KPI	O1-CX2	-2.37	1.23	1.30

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	171	KPI	C1-CX1-CX2	3.75	121.81	118.17
1	E	171	KPI	CE-NZ-CX1	2.84	129.44	121.70
1	E	248	CME	CB-SG-SD	2.83	111.15	103.82
1	C	171	KPI	CE-NZ-CX1	2.68	128.99	121.70
1	D	248	CME	CE-SD-SG	2.67	115.77	103.45

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	248	CME	SD-CE-CZ-OH
1	E	248	CME	SD-CE-CZ-OH
1	F	248	CME	CZ-CE-SD-SG
1	F	248	CME	SD-CE-CZ-OH
1	D	171	KPI	CG-CD-CE-NZ

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	248	CME	2	0
1	C	248	CME	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 58 ligands modelled in this entry, 3 are monoatomic - leaving 55 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GOL	F	307	-	5,5,5	0.39	0	5,5,5	0.33	0
3	GOL	D	305	-	5,5,5	0.36	0	5,5,5	0.29	0
3	GOL	B	312	-	5,5,5	0.39	0	5,5,5	0.55	0
3	GOL	E	307	-	5,5,5	0.46	0	5,5,5	0.97	0
3	GOL	F	304	-	5,5,5	0.50	0	5,5,5	0.39	0
5	BME	A	312	-	3,3,3	0.31	0	1,2,2	0.36	0
2	SO4	D	302	-	4,4,4	0.13	0	6,6,6	0.20	0
3	GOL	A	306	-	5,5,5	0.41	0	5,5,5	0.29	0
3	GOL	B	304	-	5,5,5	0.44	0	5,5,5	1.04	0
3	GOL	A	310	-	5,5,5	0.45	0	5,5,5	0.45	0
4	ACT	B	310	-	3,3,3	0.78	0	3,3,3	1.41	0
4	ACT	A	307	-	3,3,3	0.83	0	3,3,3	1.90	2 (66%)
4	ACT	B	311	-	3,3,3	0.77	0	3,3,3	1.74	1 (33%)
2	SO4	C	303	-	4,4,4	0.12	0	6,6,6	0.17	0
2	SO4	F	302	-	4,4,4	0.13	0	6,6,6	0.12	0
2	SO4	E	301	-	4,4,4	0.43	0	6,6,6	0.24	0
4	ACT	A	308	-	3,3,3	0.74	0	3,3,3	1.33	0
4	ACT	E	306	-	3,3,3	0.64	0	3,3,3	1.68	1 (33%)
3	GOL	F	306	-	5,5,5	0.39	0	5,5,5	0.43	0
2	SO4	E	302	-	4,4,4	0.12	0	6,6,6	0.34	0
2	SO4	A	304	-	4,4,4	0.15	0	6,6,6	0.24	0
2	SO4	F	301	-	4,4,4	0.29	0	6,6,6	0.41	0
3	GOL	A	311	-	5,5,5	0.33	0	5,5,5	0.75	0
3	GOL	C	306	-	5,5,5	0.32	0	5,5,5	0.37	0
3	GOL	C	307	-	5,5,5	0.37	0	5,5,5	0.38	0
3	GOL	D	304	-	5,5,5	0.74	0	5,5,5	1.16	1 (20%)
3	GOL	B	306	-	5,5,5	0.52	0	5,5,5	0.44	0
2	SO4	C	301	-	4,4,4	0.45	0	6,6,6	0.68	0
4	ACT	C	308	-	3,3,3	0.75	0	3,3,3	1.44	1 (33%)
2	SO4	E	303	-	4,4,4	0.12	0	6,6,6	0.12	0
2	SO4	A	303	-	4,4,4	0.19	0	6,6,6	0.25	0
2	SO4	C	302	-	4,4,4	0.12	0	6,6,6	0.17	0
4	ACT	B	308	-	3,3,3	0.80	0	3,3,3	1.30	0
3	GOL	D	303	-	5,5,5	0.32	0	5,5,5	0.65	0
3	GOL	B	309	-	5,5,5	0.42	0	5,5,5	0.43	0
2	SO4	A	302	-	4,4,4	0.23	0	6,6,6	0.51	0
3	GOL	C	304	-	5,5,5	0.29	0	5,5,5	0.24	0
3	GOL	C	309	-	5,5,5	0.40	0	5,5,5	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	F	305	-	5,5,5	0.37	0	5,5,5	0.39	0
2	SO4	B	301	-	4,4,4	0.13	0	6,6,6	0.20	0
3	GOL	C	305	-	5,5,5	0.34	0	5,5,5	0.32	0
3	GOL	D	306	-	5,5,5	0.24	0	5,5,5	0.61	0
2	SO4	B	302	-	4,4,4	0.33	0	6,6,6	0.15	0
3	GOL	E	308	-	5,5,5	0.45	0	5,5,5	0.74	0
4	ACT	F	303	-	3,3,3	0.83	0	3,3,3	1.39	0
3	GOL	B	305	-	5,5,5	0.43	0	5,5,5	0.77	0
3	GOL	B	314	-	5,5,5	0.50	0	5,5,5	1.53	1 (20%)
4	ACT	E	305	-	3,3,3	0.73	0	3,3,3	1.48	0
4	ACT	B	307	-	3,3,3	0.70	0	3,3,3	1.34	0
3	GOL	E	304	-	5,5,5	0.33	0	5,5,5	0.36	0
4	ACT	A	309	-	3,3,3	0.83	0	3,3,3	1.48	0
2	SO4	B	303	-	4,4,4	0.17	0	6,6,6	0.21	0
2	SO4	D	301	-	4,4,4	0.17	0	6,6,6	0.19	0
6	PYR	B	313	-	5,5,5	2.87	3 (60%)	3,6,6	1.26	0
3	GOL	A	305	-	5,5,5	0.59	0	5,5,5	0.63	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	F	307	-	-	4/4/4/4	-
3	GOL	D	305	-	-	2/4/4/4	-
3	GOL	B	312	-	-	4/4/4/4	-
3	GOL	E	307	-	-	1/4/4/4	-
3	GOL	F	304	-	-	2/4/4/4	-
5	BME	A	312	-	-	0/1/1/1	-
3	GOL	A	306	-	-	4/4/4/4	-
3	GOL	B	304	-	-	2/4/4/4	-
3	GOL	A	310	-	-	2/4/4/4	-
3	GOL	F	306	-	-	4/4/4/4	-
3	GOL	C	307	-	-	1/4/4/4	-
3	GOL	A	311	-	-	2/4/4/4	-
3	GOL	C	306	-	-	2/4/4/4	-
3	GOL	D	304	-	-	3/4/4/4	-
3	GOL	B	306	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	D	303	-	-	4/4/4/4	-
3	GOL	B	309	-	-	2/4/4/4	-
3	GOL	C	304	-	-	4/4/4/4	-
3	GOL	C	309	-	-	2/4/4/4	-
3	GOL	F	305	-	-	0/4/4/4	-
3	GOL	C	305	-	-	0/4/4/4	-
3	GOL	D	306	-	-	4/4/4/4	-
3	GOL	E	308	-	-	2/4/4/4	-
3	GOL	B	305	-	-	4/4/4/4	-
3	GOL	B	314	-	-	4/4/4/4	-
3	GOL	E	304	-	-	2/4/4/4	-
6	PYR	B	313	-	-	2/4/4/4	-
3	GOL	A	305	-	-	2/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	313	PYR	CA-C	-3.89	1.40	1.54
6	B	313	PYR	O-C	3.74	1.32	1.22
6	B	313	PYR	O3-CA	3.46	1.30	1.23

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	314	GOL	C3-C2-C1	-3.04	99.88	111.70
4	A	307	ACT	OXT-C-O	-2.55	112.64	122.05
4	B	311	ACT	OXT-C-O	-2.29	113.61	122.05
3	D	304	GOL	O2-C2-C1	-2.25	99.22	109.12
4	E	306	ACT	OXT-C-CH3	2.11	123.92	115.18

There are no chirality outliers.

5 of 69 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	305	GOL	C1-C2-C3-O3
3	A	306	GOL	O1-C1-C2-C3
3	A	306	GOL	C1-C2-C3-O3
3	A	310	GOL	O1-C1-C2-C3
3	B	306	GOL	C1-C2-C3-O3

There are no ring outliers.

20 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	307	GOL	1	0
3	B	312	GOL	1	0
3	E	307	GOL	6	0
5	A	312	BME	1	0
3	B	304	GOL	1	0
4	A	308	ACT	1	0
3	F	306	GOL	2	0
2	A	304	SO4	1	0
3	A	311	GOL	1	0
3	C	306	GOL	1	0
3	D	304	GOL	4	0
3	B	306	GOL	2	0
2	C	301	SO4	2	0
3	F	305	GOL	1	0
3	C	305	GOL	2	0
3	D	306	GOL	1	0
3	E	308	GOL	2	0
3	B	305	GOL	1	0
3	B	314	GOL	2	0
3	A	305	GOL	7	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	295/304 (97%)	-0.39	2 (0%)	87	89	10, 16, 24, 35	3 (1%)
1	B	293/304 (96%)	-0.27	1 (0%)	94	94	10, 18, 29, 42	5 (1%)
1	C	293/304 (96%)	-0.18	1 (0%)	94	94	16, 23, 33, 40	4 (1%)
1	D	293/304 (96%)	-0.20	4 (1%)	75	78	13, 21, 31, 39	5 (1%)
1	E	293/304 (96%)	-0.04	8 (2%)	54	60	15, 23, 33, 44	7 (2%)
1	F	293/304 (96%)	0.11	7 (2%)	59	64	16, 27, 39, 48	4 (1%)
All	All	1760/1824 (96%)	-0.16	23 (1%)	77	80	10, 22, 33, 48	28 (1%)

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	232	GLY	2.9
1	E	50	VAL	2.9
1	E	6	PHE	2.9
1	C	6	PHE	2.8
1	F	234	ILE	2.7

6.2 Non-standard residues in protein, DNA, RNA chains

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
1	KPI	E	171	14/15	0.94	0.20	15,19,25,27	0
1	CME	E	248	10/11	0.94	0.12	21,24,36,37	0
1	CME	B	248	10/11	0.95	0.09	23,26,38,41	0
1	KPI	F	171	14/15	0.95	0.19	18,21,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CME	F	248	10/11	0.95	0.10	21,26,43,44	0
1	KPI	D	171	14/15	0.96	0.22	8,14,22,23	0
1	CME	D	248	10/11	0.96	0.10	17,21,33,36	0
1	CME	C	248	10/11	0.96	0.10	24,26,35,36	0
1	KPI	C	171	14/15	0.97	0.19	17,19,24,27	0
1	CME	A	248	10/11	0.97	0.08	16,20,33,36	0
1	KPI	B	171	14/15	0.97	0.16	8,13,21,21	0
1	KPI	A	171	14/15	0.97	0.18	9,14,21,22	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
4	ACT	B	311	4/4	0.75	0.22	52,53,53,54	0
3	GOL	C	306	6/6	0.78	0.28	44,46,48,49	0
4	ACT	A	307	4/4	0.78	0.20	43,45,45,45	0
2	SO4	A	304	5/5	0.78	0.28	91,92,93,94	0
3	GOL	F	304	6/6	0.79	0.23	39,47,48,50	0
3	GOL	D	305	6/6	0.81	0.33	44,49,51,51	0
3	GOL	E	304	6/6	0.82	0.20	53,55,56,57	0
3	GOL	C	304	6/6	0.82	0.31	43,48,49,50	0
6	PYR	B	313	6/6	0.83	0.22	45,50,51,52	0
3	GOL	A	306	6/6	0.84	0.24	38,46,48,48	0
3	GOL	F	305	6/6	0.84	0.33	45,49,49,52	0
3	GOL	F	306	6/6	0.84	0.55	50,55,56,58	0
7	CL	D	308	1/1	0.84	0.08	55,55,55,55	0
3	GOL	A	311	6/6	0.85	0.20	25,39,42,43	0
4	ACT	A	309	4/4	0.86	0.23	32,33,34,34	0
3	GOL	E	308	6/6	0.86	0.25	39,45,47,50	0
7	CL	E	309	1/1	0.86	0.08	59,59,59,59	0
3	GOL	A	305	6/6	0.87	0.24	37,39,40,43	0
2	SO4	C	303	5/5	0.88	0.27	76,76,78,78	0
4	ACT	A	308	4/4	0.88	0.16	61,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	D	303	6/6	0.88	0.27	31,38,40,42	0
4	ACT	B	308	4/4	0.88	0.23	48,48,49,49	0
2	SO4	C	302	5/5	0.89	0.33	80,80,81,81	0
3	GOL	B	304	6/6	0.89	0.16	14,19,24,26	0
4	ACT	C	308	4/4	0.89	0.11	30,31,33,34	0
4	ACT	E	305	4/4	0.89	0.16	57,57,57,57	0
3	GOL	E	307	6/6	0.89	0.15	30,33,39,39	0
3	GOL	C	307	6/6	0.89	0.24	31,42,44,45	0
3	GOL	B	306	6/6	0.89	0.16	20,29,32,35	0
2	SO4	D	302	5/5	0.90	0.25	76,76,76,76	0
3	GOL	B	305	6/6	0.90	0.13	37,39,43,43	0
2	SO4	C	301	5/5	0.90	0.22	37,37,41,47	0
5	BME	A	312	4/4	0.90	0.15	44,47,49,49	0
2	SO4	B	301	5/5	0.90	0.19	35,36,38,38	5
3	GOL	A	310	6/6	0.90	0.30	32,38,41,43	0
2	SO4	B	303	5/5	0.90	0.26	71,73,73,74	0
4	ACT	F	303	4/4	0.91	0.52	23,24,24,24	4
2	SO4	B	302	5/5	0.91	0.19	46,51,52,55	0
3	GOL	B	312	6/6	0.91	0.33	33,43,45,49	0
2	SO4	A	303	5/5	0.91	0.12	62,65,66,66	0
2	SO4	E	303	5/5	0.91	0.26	92,92,92,93	0
3	GOL	F	307	6/6	0.92	0.18	36,42,42,42	0
4	ACT	B	310	4/4	0.92	0.29	54,54,54,54	0
2	SO4	F	302	5/5	0.92	0.17	85,86,87,87	0
3	GOL	C	309	6/6	0.92	0.22	33,39,42,44	0
3	GOL	D	306	6/6	0.92	0.19	28,32,35,38	0
2	SO4	F	301	5/5	0.93	0.17	43,50,52,53	0
3	GOL	C	305	6/6	0.93	0.13	36,37,39,42	0
4	ACT	E	306	4/4	0.93	0.45	16,16,17,17	4
2	SO4	E	301	5/5	0.93	0.20	30,31,32,38	0
3	GOL	D	304	6/6	0.94	0.15	24,24,26,32	0
2	SO4	E	302	5/5	0.94	0.20	50,53,55,56	0
2	SO4	A	302	5/5	0.94	0.18	49,50,53,54	0
2	SO4	D	301	5/5	0.94	0.14	84,84,85,85	0
4	ACT	B	307	4/4	0.95	0.09	28,29,29,30	0
7	CL	D	307	1/1	0.95	0.15	58,58,58,58	0
3	GOL	B	314	6/6	0.95	0.18	18,28,31,34	0
3	GOL	B	309	6/6	0.95	0.11	35,37,38,38	0

6.5 Other polymers (i)

There are no such residues in this entry.