wwPDB X-ray Structure Validation Summary Report (i)

Dec 5, 2023 – 02:36 am GMT

PDB ID	:	2UXQ
Title	:	Isocitrate dehydrogenase from the psychrophilic bacterium Desulfotalea psychrophila: biochemical properties and crystal structure analysis
Authors	:	Fedoy, A.-E.; Yang, N.; Martinez, A.; Leiros, H.-K.S.; Steen, I.H.
Deposited on	:	2007-03-29
Resolution	:	1.75 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:

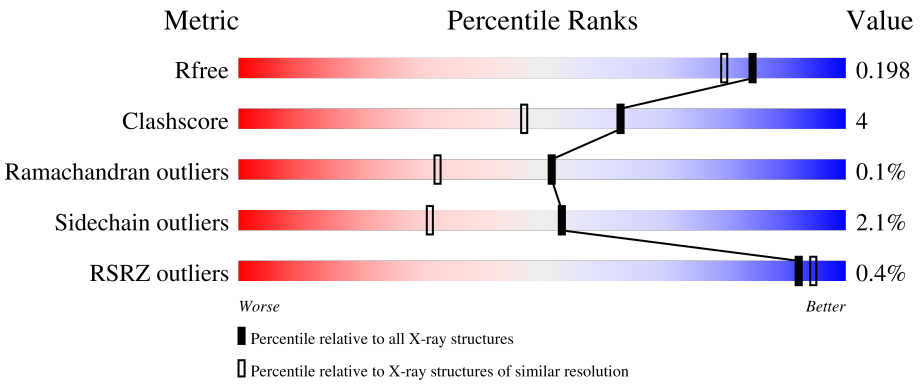
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	402	90% 7% •
1	B	402	91% 7% •
1	C	402	% 85% 12% • •
1	D	402	86% 11% •

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	GOL	D	1405	-	-	X	-

2 Entry composition (i)

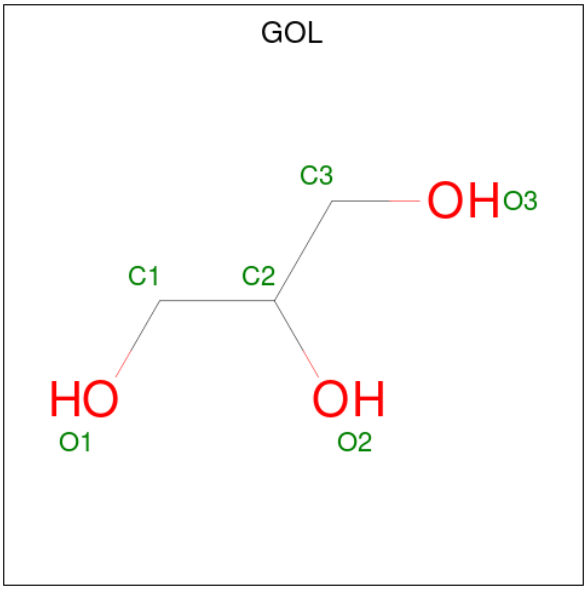
There are 6 unique types of molecules in this entry. The entry contains 15038 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ISOCITRATE DEHYDROGENASE NATIVE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	402	3234	2061	538	613	22	49	4	0
1	B	401	3242	2066	539	614	23	42	5	0
1	C	402	3271	2085	545	618	23	66	7	0
1	D	402	3243	2067	539	615	22	65	5	0

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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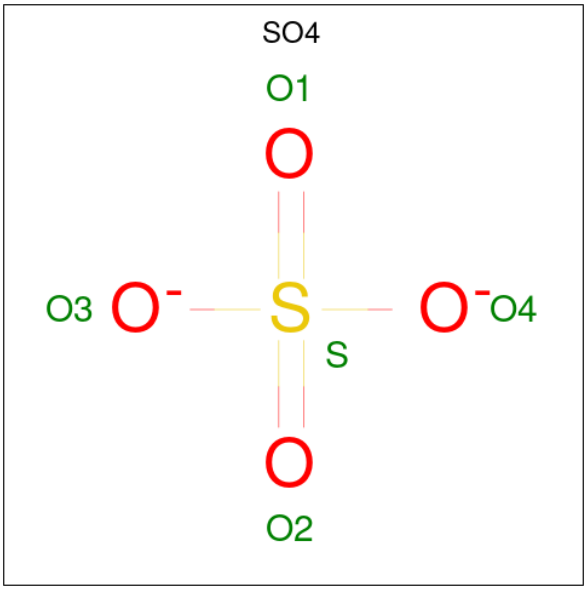
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	6	3	3	0	0
2	B	1	6	3	3	0	0
2	C	1	6	3	3	0	0
2	C	1	6	3	3	0	0
2	C	1	6	3	3	0	0
2	D	1	6	3	3	0	0
2	D	1	6	3	3	0	0
2	D	1	6	3	3	0	0

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



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

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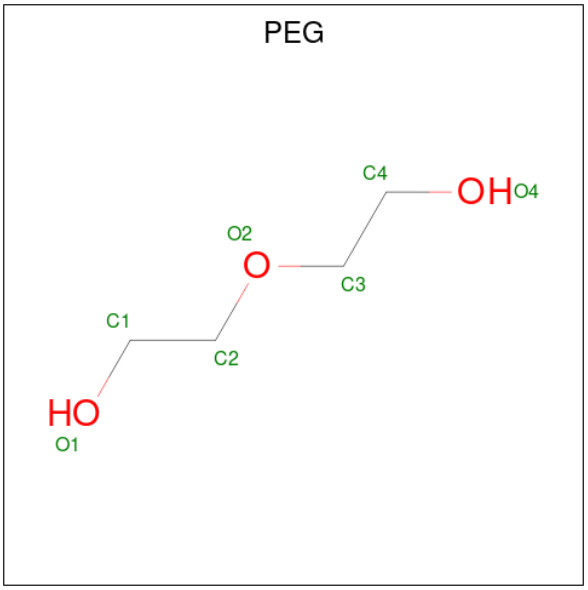
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 10 8 2	0	1
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 14 8 6	0	1

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	B	1	7	4	3	0	0
			Total	C	O		
5	B	1	7	4	3	0	0
			Total	C	O		
5	C	1	7	4	3	0	0
			Total	C	O		
5	C	1	14	8	6	0	1

- Molecule 6 is water.

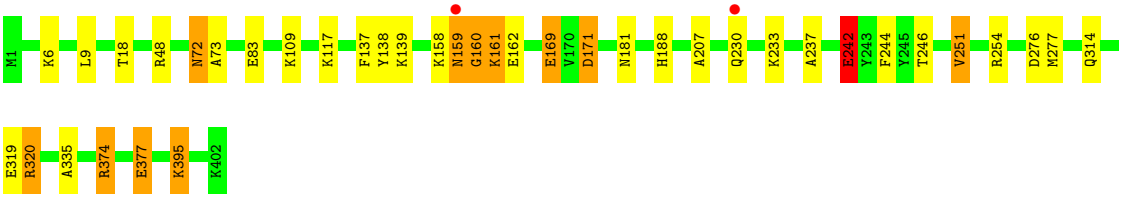
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	473	473	473	0	0
			Total	O		
6	B	513	513	513	0	0
			Total	O		
6	C	445	445	445	0	0
			Total	O		
6	D	452	452	452	0	0

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.

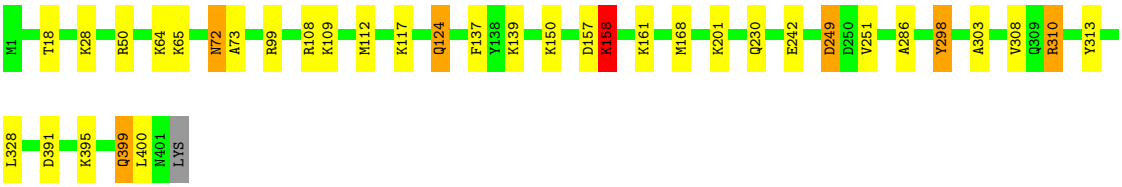
• Molecule 1: ISOCITRATE DEHYDROGENASE NATIVE

Chain A:



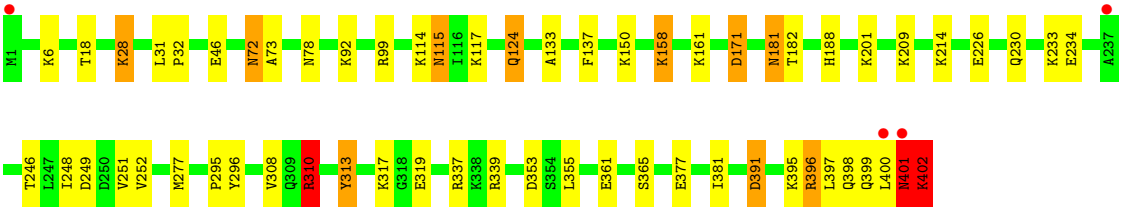
• Molecule 1: ISOCITRATE DEHYDROGENASE NATIVE

Chain B:



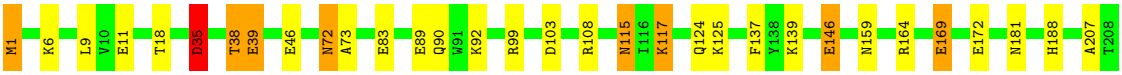
• Molecule 1: ISOCITRATE DEHYDROGENASE NATIVE

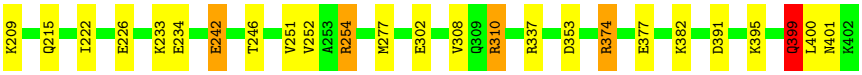
Chain C:



• Molecule 1: ISOCITRATE DEHYDROGENASE NATIVE

Chain D:




K209
Q215
I222
E226
K233
E234
E242
T246
V251
V252
A253
R254
M277
E302
V308
Q309
R310
R337
D353
R374
E377
K382
D391
K395
Q399
L400
N401
K402

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	59.32Å 73.28Å 126.41Å 98.90° 98.98° 113.88°	Depositor
Resolution (Å)	20.00 – 1.75 53.21 – 1.75	Depositor EDS
% Data completeness (in resolution range)	86.3 (20.00-1.75) 86.3 (53.21-1.75)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.17 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.146 , 0.189 0.158 , 0.198	Depositor DCC
R_{free} test set	3243 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å^2)	17.6	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 70.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,h+k+l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15038	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, SO4, GOL, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	1.59	21/3299 (0.6%)	1.74	33/4455 (0.7%)
1	B	1.40	14/3307 (0.4%)	1.06	14/4465 (0.3%)
1	C	1.46	28/3336 (0.8%)	1.66	39/4504 (0.9%)
1	D	1.80	25/3308 (0.8%)	1.63	36/4468 (0.8%)
All	All	1.57	88/13250 (0.7%)	1.55	122/17892 (0.7%)

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	A	0	7
1	B	0	3
1	C	0	3
1	D	0	6
All	All	0	19

The worst 5 of 88 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	377	GLU	CD-OE2	-36.05	0.85	1.25
1	D	399	GLN	CG-CD	-34.22	0.72	1.51
1	D	169	GLU	CD-OE2	-32.34	0.90	1.25
1	A	242	GLU	CG-CD	31.39	1.99	1.51
1	A	395	LYS	CE-NZ	30.79	2.26	1.49

The worst 5 of 122 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	320	ARG	NE-CZ-NH1	-66.17	87.22	120.30
1	D	374	ARG	NE-CZ-NH2	-47.27	96.66	120.30
1	D	374	ARG	NE-CZ-NH1	45.70	143.15	120.30
1	C	310	ARG	NE-CZ-NH2	-45.58	97.51	120.30
1	C	310	ARG	NE-CZ-NH1	43.81	142.21	120.30

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	160	GLY	Mainchain,Peptide
1	A	169	GLU	Sidechain
1	A	171	ASP	Sidechain
1	A	242	GLU	Sidechain
1	A	374	ARG	Sidechain

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	3234	0	3209	23	0
1	B	3242	0	3217	23	0
1	C	3271	0	3250	35	0
1	D	3243	0	3216	37	0
2	A	18	0	24	0	0
2	B	6	0	8	1	0
2	C	18	0	24	0	0
2	D	18	0	24	5	0
3	A	5	0	0	1	0
3	B	30	0	0	3	0
3	C	10	0	0	1	0
3	D	10	0	0	1	0
4	A	1	0	0	0	0
5	A	14	0	20	0	0
5	B	14	0	20	1	0
5	C	21	0	30	1	0
6	A	473	0	0	10	2
6	B	513	0	0	12	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	445	0	0	7	0
6	D	452	0	0	7	0
All	All	15038	0	13042	109	2

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 109 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:254:ARG:HD2	6:A:2326:HOH:O	1.50	1.10
1:D:99[A]:ARG:HH12	2:D:1405:GOL:H12	1.13	1.06
1:C:277[B]:MET:HG3	1:D:252[B]:VAL:HG22	1.35	1.06
5:B:1409:PEG:O4	6:B:2512:HOH:O	1.83	0.93
1:C:28:LYS:CD	1:C:28:LYS:NZ	2.34	0.89

All (2) 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)
6:A:2372:HOH:O	6:B:2511:HOH:O[1_445]	1.95	0.25
6:A:2086:HOH:O	6:B:2480:HOH:O[1_545]	2.11	0.09

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	404/402 (100%)	390 (96%)	14 (4%)	0	100 100
1	B	405/402 (101%)	393 (97%)	12 (3%)	0	100 100
1	C	408/402 (102%)	396 (97%)	11 (3%)	1 (0%)	47 29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	405/402 (101%)	392 (97%)	13 (3%)	0	100	100
All	All	1622/1608 (101%)	1571 (97%)	50 (3%)	1 (0%)	51	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	401	ASN

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	345/341 (101%)	340 (99%)	5 (1%)	67	52
1	B	346/341 (102%)	339 (98%)	7 (2%)	55	34
1	C	349/341 (102%)	341 (98%)	8 (2%)	50	28
1	D	346/341 (102%)	337 (97%)	9 (3%)	46	23
All	All	1386/1364 (102%)	1357 (98%)	29 (2%)	53	31

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	137	PHE
1	D	310	ARG
1	C	310	ARG
1	D	115	ASN
1	C	308	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	200	GLN
1	D	177	GLN
1	C	115	ASN

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Mol	Chain	Res	Type
1	D	159	ASN
1	C	90	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 29 ligands modelled in this entry, 1 is monoatomic - leaving 28 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	GOL	C	1404	-	5,5,5	0.53	0	5,5,5	0.58	0
5	PEG	C	1408	-	6,6,6	0.40	0	5,5,5	0.30	0
2	GOL	D	1403	-	5,5,5	0.50	0	5,5,5	1.48	0
3	SO4	A	1406	-	4,4,4	0.36	0	6,6,6	1.29	1 (16%)
2	GOL	D	1405	-	5,5,5	0.35	0	5,5,5	0.68	0
3	SO4	B	1403	-	4,4,4	0.24	0	6,6,6	0.38	0
5	PEG	B	1409	-	6,6,6	0.52	0	5,5,5	0.63	0
2	GOL	A	1405	-	5,5,5	0.26	0	5,5,5	0.42	0
5	PEG	C	1409[A]	-	6,6,6	0.34	0	5,5,5	0.20	0
5	PEG	A	1408[B]	-	6,6,6	0.45	0	5,5,5	0.42	0
5	PEG	B	1408	-	6,6,6	0.38	0	5,5,5	0.43	0
3	SO4	C	1406	-	4,4,4	0.32	0	6,6,6	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GOL	B	1402	-	5,5,5	0.58	0	5,5,5	0.44	0
3	SO4	D	1406	-	4,4,4	0.23	0	6,6,6	0.36	0
2	GOL	C	1403	-	5,5,5	0.32	0	5,5,5	0.50	0
3	SO4	B	1407[A]	-	4,4,4	0.28	0	6,6,6	0.54	0
3	SO4	B	1406	-	4,4,4	0.23	0	6,6,6	0.75	0
2	GOL	A	1404	-	5,5,5	0.69	0	5,5,5	1.40	1 (20%)
3	SO4	C	1407	-	4,4,4	0.21	0	6,6,6	0.66	0
5	PEG	C	1409[B]	-	6,6,6	0.52	0	5,5,5	0.23	0
3	SO4	B	1405	-	4,4,4	0.25	0	6,6,6	0.41	0
3	SO4	D	1407	-	4,4,4	0.18	0	6,6,6	0.40	0
3	SO4	B	1404	-	4,4,4	0.32	0	6,6,6	0.40	0
2	GOL	A	1403	-	5,5,5	0.57	0	5,5,5	1.60	2 (40%)
5	PEG	A	1408[A]	-	6,6,6	0.40	0	5,5,5	0.18	0
2	GOL	D	1404	-	5,5,5	0.49	0	5,5,5	0.54	0
3	SO4	B	1407[B]	-	4,4,4	0.26	0	6,6,6	0.62	0
2	GOL	C	1405	-	5,5,5	0.48	0	5,5,5	0.82	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	GOL	C	1404	-	-	0/4/4/4	-
5	PEG	C	1408	-	-	1/4/4/4	-
2	GOL	D	1403	-	-	0/4/4/4	-
5	PEG	A	1408[B]	-	-	4/4/4/4	-
5	PEG	A	1408[A]	-	-	2/4/4/4	-
5	PEG	B	1408	-	-	3/4/4/4	-
2	GOL	B	1402	-	-	3/4/4/4	-
2	GOL	A	1404	-	-	4/4/4/4	-
2	GOL	D	1405	-	-	1/4/4/4	-
5	PEG	C	1409[B]	-	-	2/4/4/4	-
5	PEG	B	1409	-	-	3/4/4/4	-
5	PEG	C	1409[A]	-	-	3/4/4/4	-
2	GOL	A	1405	-	-	4/4/4/4	-
2	GOL	D	1404	-	-	0/4/4/4	-
2	GOL	A	1403	-	-	2/4/4/4	-
2	GOL	C	1403	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	C	1405	-	-	3/4/4/4	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1403	GOL	O1-C1-C2	-2.56	97.92	110.20
2	A	1404	GOL	O1-C1-C2	2.34	121.42	110.20
2	A	1403	GOL	O3-C3-C2	-2.32	99.09	110.20
3	A	1406	SO4	O3-S-O1	2.24	120.99	109.31

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1403	GOL	O1-C1-C2-C3
2	A	1404	GOL	O1-C1-C2-C3
2	A	1404	GOL	C1-C2-C3-O3
2	A	1405	GOL	O1-C1-C2-C3
2	B	1402	GOL	O1-C1-C2-C3

There are no ring outliers.

11 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1403	GOL	1	0
3	A	1406	SO4	1	0
2	D	1405	GOL	4	0
5	B	1409	PEG	1	0
5	C	1409[A]	PEG	1	0
3	C	1406	SO4	1	0
2	B	1402	GOL	1	0
3	B	1406	SO4	1	0
3	B	1405	SO4	1	0
3	D	1407	SO4	1	0
3	B	1407[B]	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	400:LEU	C	401:ASN	N	1.84

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	402/402 (100%)	-0.31	2 (0%) 91 93	9, 16, 25, 38	36 (8%)
1	B	401/402 (99%)	-0.40	0 100 100	10, 15, 25, 40	34 (8%)
1	C	402/402 (100%)	-0.32	4 (0%) 82 87	10, 17, 26, 45	44 (10%)
1	D	400/402 (99%)	-0.28	0 100 100	11, 18, 28, 34	37 (9%)
All	All	1605/1608 (99%)	-0.33	6 (0%) 92 94	9, 16, 26, 45	151 (9%)

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	159	ASN	3.3
1	C	400	LEU	3.3
1	C	401	ASN	3.1
1	C	1	MET	2.4
1	A	230	GLN	2.2

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GOL	C	1405	6/6	0.69	0.18	42,45,48,50	0
5	PEG	B	1409	7/7	0.69	0.23	45,47,49,51	0
2	GOL	D	1405	6/6	0.80	0.16	40,43,44,46	2
2	GOL	D	1403	6/6	0.83	0.18	30,35,38,41	0
2	GOL	A	1405	6/6	0.84	0.21	49,51,53,55	0
3	SO4	B	1405	5/5	0.85	0.23	31,33,36,38	5
5	PEG	C	1409[A]	7/7	0.86	0.45	15,24,28,29	7
5	PEG	C	1409[B]	7/7	0.86	0.45	36,37,39,39	7
2	GOL	C	1403	6/6	0.87	0.10	35,37,39,40	0
2	GOL	C	1404	6/6	0.88	0.13	22,32,34,37	0
2	GOL	A	1403	6/6	0.88	0.16	28,32,34,35	0
2	GOL	D	1404	6/6	0.89	0.11	32,35,37,39	0
5	PEG	B	1408	7/7	0.90	0.14	39,40,42,44	0
2	GOL	B	1402	6/6	0.90	0.09	27,31,33,37	0
5	PEG	C	1408	7/7	0.91	0.10	38,38,39,41	0
2	GOL	A	1404	6/6	0.93	0.10	20,24,28,32	0
5	PEG	A	1408[B]	7/7	0.94	0.17	26,27,30,31	7
5	PEG	A	1408[A]	7/7	0.94	0.17	20,21,22,23	7
3	SO4	A	1406	5/5	0.96	0.12	34,34,40,40	1
3	SO4	B	1407[A]	5/5	0.96	0.11	17,18,24,25	5
3	SO4	B	1407[B]	5/5	0.96	0.11	23,24,26,29	5
3	SO4	C	1406	5/5	0.96	0.11	27,29,32,32	5
3	SO4	C	1407	5/5	0.96	0.13	27,28,35,37	5
3	SO4	B	1404	5/5	0.96	0.10	52,53,54,55	1
3	SO4	D	1407	5/5	0.97	0.09	35,35,39,41	5
3	SO4	D	1406	5/5	0.97	0.08	36,37,38,40	4
4	MG	A	1407	1/1	0.98	0.08	40,40,40,40	0
3	SO4	B	1406	5/5	0.98	0.10	26,28,31,34	5
3	SO4	B	1403	5/5	0.99	0.09	35,38,39,40	0

6.5 Other polymers (i)

There are no such residues in this entry.