



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:17 PM UTC

PDB ID : 6EDW / pdb_00006edw
Title : Crystal structure of Mycobacterium tuberculosis ICL2 in the apo form
Authors : Bashiri, G.; Bhusal, R.; Leung, I.
Deposited on : 2018-08-12
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

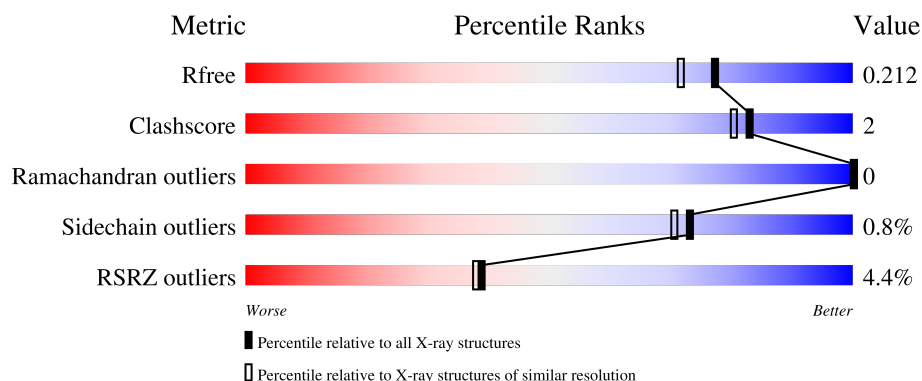
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 $\leq 5\%$. 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	786	5% 89% 5% 6%
1	B	786	2% 90% 5% 5%
1	C	786	6% 87% 5% 8%
1	D	786	4% 88% 6% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 26840 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 lyase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	742	Total	C	N	O	S	0	6	0
			5877	3709	1052	1094	22			
1	B	746	Total	C	N	O	S	0	5	0
			5885	3714	1050	1099	22			
1	C	724	Total	C	N	O	S	0	5	0
			5710	3607	1020	1061	22			
1	D	741	Total	C	N	O	S	0	6	0
			5863	3700	1053	1088	22			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q8VJU4
A	-18	GLY	-	expression tag	UNP Q8VJU4
A	-17	SER	-	expression tag	UNP Q8VJU4
A	-16	SER	-	expression tag	UNP Q8VJU4
A	-15	HIS	-	expression tag	UNP Q8VJU4
A	-14	HIS	-	expression tag	UNP Q8VJU4
A	-13	HIS	-	expression tag	UNP Q8VJU4
A	-12	HIS	-	expression tag	UNP Q8VJU4
A	-11	HIS	-	expression tag	UNP Q8VJU4
A	-10	HIS	-	expression tag	UNP Q8VJU4
A	-9	SER	-	expression tag	UNP Q8VJU4
A	-8	SER	-	expression tag	UNP Q8VJU4
A	-7	GLY	-	expression tag	UNP Q8VJU4
A	-6	LEU	-	expression tag	UNP Q8VJU4
A	-5	VAL	-	expression tag	UNP Q8VJU4
A	-4	PRO	-	expression tag	UNP Q8VJU4
A	-3	ARG	-	expression tag	UNP Q8VJU4
A	-2	GLY	-	expression tag	UNP Q8VJU4
A	-1	SER	-	expression tag	UNP Q8VJU4
A	0	HIS	-	expression tag	UNP Q8VJU4
B	-19	MET	-	initiating methionine	UNP Q8VJU4

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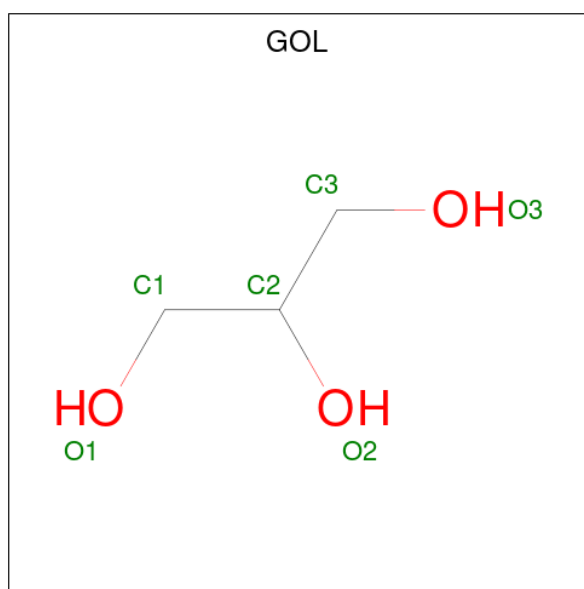
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP Q8VJU4
B	-17	SER	-	expression tag	UNP Q8VJU4
B	-16	SER	-	expression tag	UNP Q8VJU4
B	-15	HIS	-	expression tag	UNP Q8VJU4
B	-14	HIS	-	expression tag	UNP Q8VJU4
B	-13	HIS	-	expression tag	UNP Q8VJU4
B	-12	HIS	-	expression tag	UNP Q8VJU4
B	-11	HIS	-	expression tag	UNP Q8VJU4
B	-10	HIS	-	expression tag	UNP Q8VJU4
B	-9	SER	-	expression tag	UNP Q8VJU4
B	-8	SER	-	expression tag	UNP Q8VJU4
B	-7	GLY	-	expression tag	UNP Q8VJU4
B	-6	LEU	-	expression tag	UNP Q8VJU4
B	-5	VAL	-	expression tag	UNP Q8VJU4
B	-4	PRO	-	expression tag	UNP Q8VJU4
B	-3	ARG	-	expression tag	UNP Q8VJU4
B	-2	GLY	-	expression tag	UNP Q8VJU4
B	-1	SER	-	expression tag	UNP Q8VJU4
B	0	HIS	-	expression tag	UNP Q8VJU4
C	-19	MET	-	initiating methionine	UNP Q8VJU4
C	-18	GLY	-	expression tag	UNP Q8VJU4
C	-17	SER	-	expression tag	UNP Q8VJU4
C	-16	SER	-	expression tag	UNP Q8VJU4
C	-15	HIS	-	expression tag	UNP Q8VJU4
C	-14	HIS	-	expression tag	UNP Q8VJU4
C	-13	HIS	-	expression tag	UNP Q8VJU4
C	-12	HIS	-	expression tag	UNP Q8VJU4
C	-11	HIS	-	expression tag	UNP Q8VJU4
C	-10	HIS	-	expression tag	UNP Q8VJU4
C	-9	SER	-	expression tag	UNP Q8VJU4
C	-8	SER	-	expression tag	UNP Q8VJU4
C	-7	GLY	-	expression tag	UNP Q8VJU4
C	-6	LEU	-	expression tag	UNP Q8VJU4
C	-5	VAL	-	expression tag	UNP Q8VJU4
C	-4	PRO	-	expression tag	UNP Q8VJU4
C	-3	ARG	-	expression tag	UNP Q8VJU4
C	-2	GLY	-	expression tag	UNP Q8VJU4
C	-1	SER	-	expression tag	UNP Q8VJU4
C	0	HIS	-	expression tag	UNP Q8VJU4
D	-19	MET	-	initiating methionine	UNP Q8VJU4
D	-18	GLY	-	expression tag	UNP Q8VJU4
D	-17	SER	-	expression tag	UNP Q8VJU4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP Q8VJU4
D	-15	HIS	-	expression tag	UNP Q8VJU4
D	-14	HIS	-	expression tag	UNP Q8VJU4
D	-13	HIS	-	expression tag	UNP Q8VJU4
D	-12	HIS	-	expression tag	UNP Q8VJU4
D	-11	HIS	-	expression tag	UNP Q8VJU4
D	-10	HIS	-	expression tag	UNP Q8VJU4
D	-9	SER	-	expression tag	UNP Q8VJU4
D	-8	SER	-	expression tag	UNP Q8VJU4
D	-7	GLY	-	expression tag	UNP Q8VJU4
D	-6	LEU	-	expression tag	UNP Q8VJU4
D	-5	VAL	-	expression tag	UNP Q8VJU4
D	-4	PRO	-	expression tag	UNP Q8VJU4
D	-3	ARG	-	expression tag	UNP Q8VJU4
D	-2	GLY	-	expression tag	UNP Q8VJU4
D	-1	SER	-	expression tag	UNP Q8VJU4
D	0	HIS	-	expression tag	UNP Q8VJU4

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

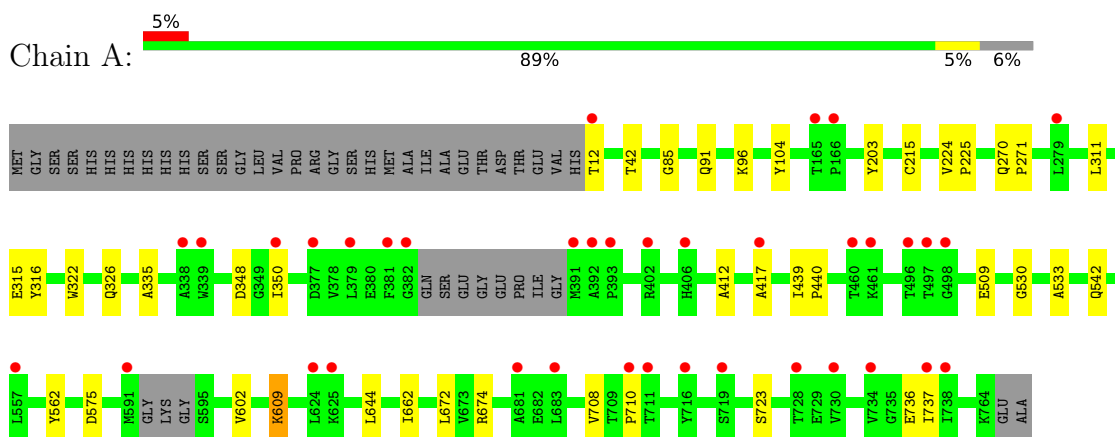
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	804	Total	O	0	0
			804	804		
4	B	986	Total	O	0	0
			986	986		
4	C	791	Total	O	0	0
			791	791		
4	D	887	Total	O	0	0
			887	887		

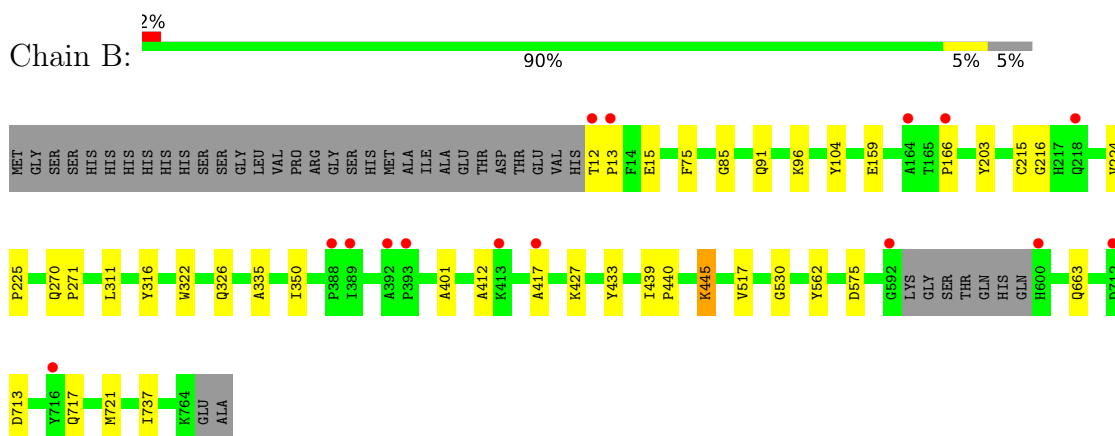
3 Residue-property plots [i](#)

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.

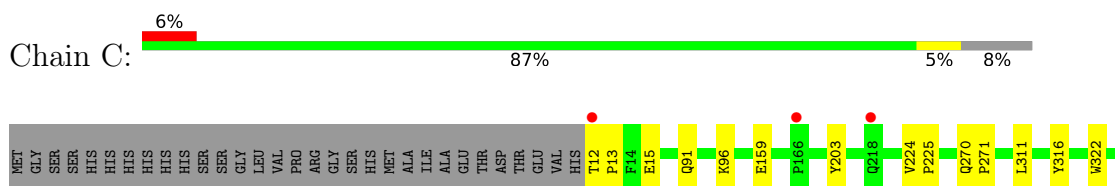
• Molecule 1: Isocitrate lyase 2

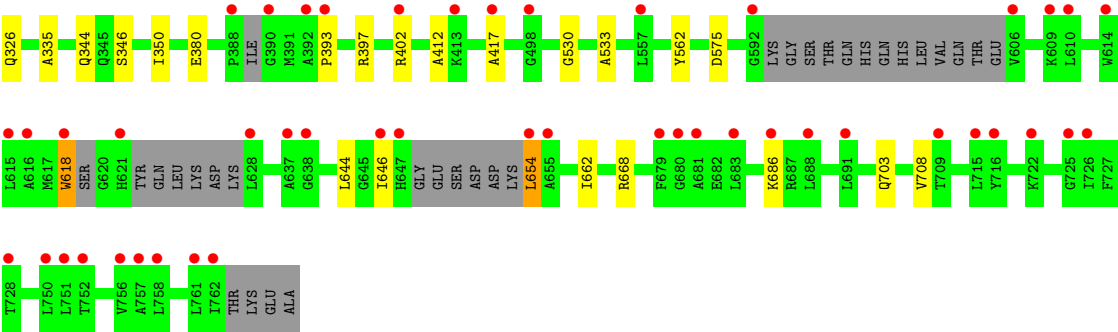


• Molecule 1: Isocitrate lyase 2

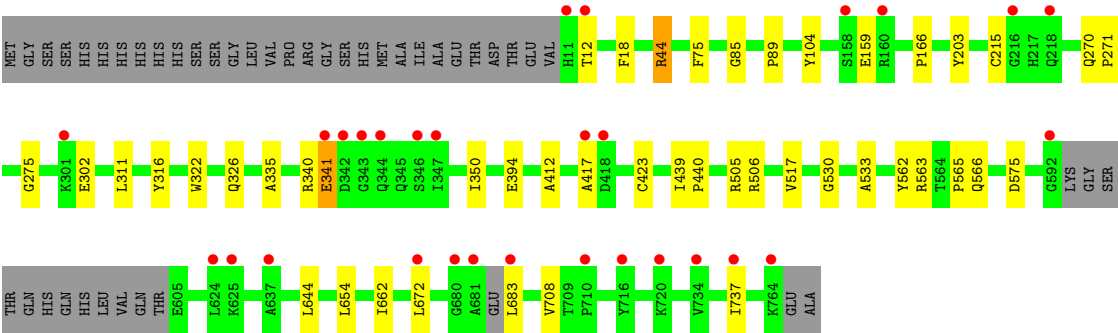
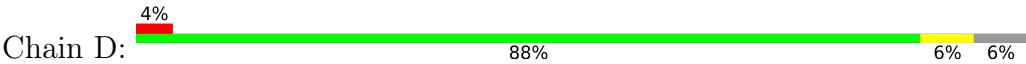


• Molecule 1: Isocitrate lyase 2





● Molecule 1: Isocitrate lyase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.82Å 136.08Å 138.92Å 90.00° 99.59° 90.00°	Depositor
Resolution (Å)	48.32 – 1.80 48.32 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.32-1.80) 99.9 (48.32-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.168 , 0.203 0.181 , 0.212	Depositor DCC
R_{free} test set	16234 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	21.9	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	26840	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: MG, GOL, CSX

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	0.62	0/6011	0.87	0/8136
1	B	0.62	0/6014	0.87	1/8142 (0.0%)
1	C	0.62	0/5833	0.87	0/7893
1	D	0.64	1/5992 (0.0%)	0.88	1/8108 (0.0%)
All	All	0.62	1/23850 (0.0%)	0.87	2/32279 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	565	PRO	C-O	-5.93	1.16	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	445	LYS	CB-CG-CD	5.70	124.41	111.30
1	D	341	GLU	CB-CG-CD	5.53	122.00	112.60

There are no chirality outliers.

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	5877	0	5797	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5885	0	5796	30	0
1	C	5710	0	5618	33	0
1	D	5863	0	5778	45	0
2	A	12	0	16	0	0
2	C	12	0	16	1	0
2	D	6	0	8	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	804	0	0	4	0
4	B	986	0	0	5	0
4	C	791	0	0	4	0
4	D	887	0	0	6	0
All	All	26840	0	23029	111	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 2.

All (111) 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:575[B]:ASP:OD1	1:D:215[B]:CSX:HB3	1.53	1.08
1:C:618:TRP:HZ3	1:C:686:LYS:O	1.37	1.06
1:C:618:TRP:CZ3	1:C:686:LYS:O	2.20	0.95
1:A:215[A]:CSX:HB3	1:C:575[A]:ASP:OD1	1.74	0.86
1:D:505[A]:ARG:HH22	1:D:506[A]:ARG:HH22	1.24	0.86
1:C:618:TRP:CH2	1:C:686:LYS:HB3	2.14	0.81
1:D:505[A]:ARG:HH22	1:D:506[A]:ARG:NH2	1.78	0.81
1:C:668:ARG:HD2	1:C:703:GLN:HG2	1.63	0.79
1:B:215[B]:CSX:HB3	1:D:575[B]:ASP:OD1	1.83	0.78
1:C:618:TRP:HH2	1:C:686:LYS:HB3	1.50	0.76
1:A:737:ILE:HD11	1:D:708:VAL:CG1	2.23	0.68
1:A:737:ILE:HD11	1:D:708:VAL:HG11	1.75	0.67
1:D:412:ALA:HB1	1:D:417:ALA:O	1.96	0.66
1:C:397:ARG:NH1	4:C:902:HOH:O	2.30	0.63
1:C:159:GLU:CD	1:D:12:THR:HG21	2.23	0.62
1:C:380:GLU:OE2	1:C:397:ARG:NH2	2.33	0.60
1:D:566:GLN:HG3	4:D:1089:HOH:O	2.03	0.59
1:B:216:GLY:N	1:D:566:GLN:HE22	2.01	0.58
1:B:575[B]:ASP:CG	1:D:215[B]:CSX:HB3	2.29	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:646:ILE:O	1:C:654:LEU:HB3	2.04	0.58
1:A:708:VAL:HA	1:A:737:ILE:HD12	1.87	0.57
1:B:427:LYS:HD3	1:B:433:TYR:CZ	2.41	0.56
1:D:505[A]:ARG:NH2	1:D:506[A]:ARG:NH2	2.51	0.56
1:C:344:GLN:NE2	4:C:907:HOH:O	2.38	0.55
1:D:505[B]:ARG:NH1	4:D:909:HOH:O	2.38	0.55
1:B:166:PRO:HA	4:B:1008:HOH:O	2.06	0.55
1:B:737:ILE:HD11	1:C:708:VAL:HB	1.89	0.55
1:A:609:LYS:HD3	4:A:1391:HOH:O	2.07	0.54
1:A:708:VAL:HA	1:A:737:ILE:CD1	2.38	0.53
1:B:663:GLN:NE2	4:B:909:HOH:O	2.36	0.53
1:B:12:THR:OG1	1:B:13:PRO:HD2	2.09	0.53
1:C:618:TRP:CH2	1:C:686:LYS:CB	2.91	0.52
1:C:12:THR:OG1	1:C:13:PRO:HD2	2.10	0.51
1:C:393:PRO:O	1:C:397:ARG:HG3	2.11	0.51
1:B:575[B]:ASP:OD1	1:D:215[B]:CSX:CB	2.43	0.51
1:C:159:GLU:HG2	1:D:12:THR:HG21	1.94	0.50
1:A:710:PRO:HG3	1:A:736:GLU:HB3	1.93	0.49
1:C:335:ALA:HB1	1:C:350:ILE:CG2	2.43	0.49
1:A:42:THR:CG2	1:D:302:GLU:HB2	2.42	0.49
1:B:322:TRP:CE2	1:B:326:GLN:HG3	2.48	0.49
4:B:1021:HOH:O	1:D:89:PRO:HB2	2.13	0.48
1:D:505[A]:ARG:NH2	4:D:923:HOH:O	2.46	0.48
1:B:75:PHE:HB2	1:B:517:VAL:HG11	1.95	0.48
1:A:602:VAL:HG23	4:A:1468:HOH:O	2.13	0.48
1:A:322:TRP:CE2	1:A:326:GLN:HG3	2.49	0.48
1:D:394:GLU:HG2	4:D:1417:HOH:O	2.14	0.47
1:B:562:TYR:CZ	1:D:530:GLY:HA3	2.49	0.47
1:D:322:TRP:CE2	1:D:326:GLN:HG3	2.49	0.47
1:A:530:GLY:HA3	1:C:562:TYR:CZ	2.50	0.47
1:A:737:ILE:HD11	1:D:708:VAL:HG13	1.96	0.47
1:B:12:THR:HG23	1:B:15:GLU:H	1.78	0.47
1:C:12:THR:HG23	1:C:15:GLU:H	1.78	0.47
1:D:166:PRO:HA	4:D:992:HOH:O	2.13	0.47
1:B:412:ALA:HB1	1:B:417:ALA:O	2.15	0.47
1:C:322:TRP:CE2	1:C:326:GLN:HG3	2.50	0.47
1:A:412:ALA:HB1	1:A:417:ALA:O	2.16	0.46
1:D:75:PHE:HB2	1:D:517:VAL:HG11	1.98	0.46
1:A:335:ALA:HB1	1:A:350:ILE:CG2	2.46	0.46
1:B:216:GLY:N	1:D:566:GLN:NE2	2.65	0.45
1:A:42:THR:HG21	1:D:302:GLU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:ASP:OD2	1:D:44:ARG:NH2	2.49	0.45
1:B:216:GLY:H	1:D:566:GLN:HE22	1.65	0.45
1:D:340:ARG:NH2	4:D:912:HOH:O	2.40	0.45
1:A:662:ILE:HD13	1:A:672:LEU:HD12	1.98	0.45
1:A:542:GLN:HG3	4:A:1409:HOH:O	2.16	0.45
1:B:401:ALA:O	4:B:901:HOH:O	2.21	0.44
1:B:530:GLY:HA3	1:D:562:TYR:CZ	2.53	0.44
1:A:270:GLN:N	1:A:271:PRO:CD	2.81	0.44
1:B:717:GLN:HG3	1:B:721:MET:HE2	2.00	0.44
1:B:311:LEU:HB3	1:B:316:TYR:CE2	2.53	0.43
1:C:270:GLN:N	1:C:271:PRO:CD	2.81	0.43
1:C:412:ALA:HB1	1:C:417:ALA:O	2.18	0.43
1:D:270:GLN:N	1:D:271:PRO:CD	2.81	0.43
2:C:802:GOL:H32	1:D:18:PHE:HA	1.99	0.43
1:C:662:ILE:C	1:C:662:ILE:HD12	2.44	0.43
1:A:562:TYR:CZ	1:C:530:GLY:HA3	2.54	0.43
1:C:350:ILE:HD13	4:C:1078:HOH:O	2.17	0.43
1:A:311:LEU:HB3	1:A:316:TYR:CE2	2.54	0.42
1:C:224:VAL:HB	1:C:225:PRO:HD2	2.01	0.42
1:B:270:GLN:N	1:B:271:PRO:CD	2.82	0.42
1:C:159:GLU:CG	1:D:12:THR:HG21	2.49	0.42
1:D:335:ALA:HB1	1:D:350:ILE:CG2	2.49	0.42
1:A:91:GLN:HG2	1:C:533:ALA:HB2	2.01	0.42
1:D:311:LEU:HB3	1:D:316:TYR:CE2	2.55	0.42
1:B:224:VAL:HB	1:B:225:PRO:HD2	2.00	0.42
1:A:224:VAL:HB	1:A:225:PRO:HD2	2.02	0.42
1:A:439:ILE:N	1:A:440:PRO:CD	2.83	0.42
1:C:644:LEU:C	1:C:644:LEU:HD13	2.45	0.41
1:D:644:LEU:C	1:D:644:LEU:HD13	2.46	0.41
1:A:85:GLY:HA2	1:A:104:TYR:O	2.21	0.41
1:A:533:ALA:HB2	1:C:91:GLN:HG2	2.01	0.41
1:D:439:ILE:N	1:D:440:PRO:CD	2.84	0.41
1:B:427:LYS:NZ	4:B:951:HOH:O	2.53	0.41
1:C:311:LEU:HB3	1:C:316:TYR:CE2	2.55	0.41
1:A:644:LEU:HD13	1:A:644:LEU:C	2.45	0.41
1:A:674:ARG:NH2	1:D:737:ILE:HD11	2.35	0.41
1:B:335:ALA:HB1	1:B:350:ILE:CG2	2.51	0.41
1:D:654:LEU:HB3	1:D:683:LEU:CD1	2.50	0.41
1:A:509:GLU:HB2	4:A:908:HOH:O	2.21	0.41
1:C:393:PRO:HB3	4:C:1473:HOH:O	2.21	0.41
1:D:85:GLY:HA2	1:D:104:TYR:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:662:ILE:C	1:D:662:ILE:HD12	2.46	0.41
1:B:439:ILE:N	1:B:440:PRO:CD	2.84	0.40
1:B:85:GLY:HA2	1:B:104:TYR:O	2.21	0.40
1:B:91:GLN:HG2	1:D:533:ALA:HB2	2.03	0.40
1:C:12:THR:HG21	1:D:159:GLU:OE1	2.20	0.40
1:A:12:THR:HG21	1:B:159:GLU:OE2	2.22	0.40
1:D:275:GLY:HA2	1:D:423:CYS:HA	2.04	0.40

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	741/786 (94%)	734 (99%)	7 (1%)	0	100	100
1	B	745/786 (95%)	736 (99%)	9 (1%)	0	100	100
1	C	715/786 (91%)	708 (99%)	7 (1%)	0	100	100
1	D	739/786 (94%)	732 (99%)	7 (1%)	0	100	100
All	All	2940/3144 (94%)	2910 (99%)	30 (1%)	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	603/631 (96%)	598 (99%)	5 (1%)	73	70
1	B	602/631 (95%)	598 (99%)	4 (1%)	76	73
1	C	581/631 (92%)	575 (99%)	6 (1%)	68	64
1	D	598/631 (95%)	593 (99%)	5 (1%)	73	70
All	All	2384/2524 (94%)	2364 (99%)	20 (1%)	73	70

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	LYS
1	A	203	TYR
1	A	315	GLU
1	A	609	LYS
1	A	723	SER
1	B	96	LYS
1	B	203	TYR
1	B	445	LYS
1	B	713	ASP
1	C	96	LYS
1	C	203	TYR
1	C	346	SER
1	C	402	ARG
1	C	618	TRP
1	C	654	LEU
1	D	44	ARG
1	D	203	TYR
1	D	341	GLU
1	D	563	ARG
1	D	672	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	345	GLN
1	A	353	GLN
1	A	598	HIS
1	B	603	GLN
1	B	663	GLN
1	C	156	GLN
1	C	663	GLN

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Mol	Chain	Res	Type
1	C	677	ASN
1	C	698	HIS
1	C	706	HIS
1	D	353	GLN
1	D	566	GLN
1	D	663	GLN
1	D	698	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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	CSX	A	215[B]	-	3,6,7	0.74	0	1,6,8	0.09	0
1	CSX	B	215[A]	-	3,6,7	0.82	0	1,6,8	1.71	0
1	CSX	D	215[B]	-	3,6,7	0.74	0	1,6,8	1.16	0
1	CSX	D	215[A]	-	3,6,7	0.61	0	1,6,8	1.74	0
1	CSX	C	215[A]	-	3,6,7	0.76	0	1,6,8	1.31	0
1	CSX	B	215[B]	-	3,6,7	0.82	0	1,6,8	0.63	0
1	CSX	A	215[A]	-	3,6,7	0.74	0	1,6,8	1.82	0
1	CSX	C	215[B]	-	3,6,7	0.77	0	1,6,8	0.07	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
1	CSX	A	215[B]	-	-	0/2/5/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSX	B	215[A]	-	-	0/2/5/7	-
1	CSX	D	215[B]	-	-	0/2/5/7	-
1	CSX	D	215[A]	-	-	0/2/5/7	-
1	CSX	C	215[A]	-	-	0/2/5/7	-
1	CSX	B	215[B]	-	-	0/2/5/7	-
1	CSX	A	215[A]	-	-	0/2/5/7	-
1	CSX	C	215[B]	-	-	0/2/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	215[B]	CSX	3	0
1	B	215[B]	CSX	1	0
1	A	215[A]	CSX	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 7 are monoatomic - leaving 5 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	D	801	-	5,5,5	0.33	0	5,5,5	0.25	0
2	GOL	C	801	-	5,5,5	0.45	0	5,5,5	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	A	801	-	5,5,5	0.28	0	5,5,5	0.42	0
2	GOL	C	802	-	5,5,5	0.29	0	5,5,5	0.41	0
2	GOL	A	802	-	5,5,5	0.36	0	5,5,5	0.59	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	D	801	-	-	0/4/4/4	-
2	GOL	C	801	-	-	0/4/4/4	-
2	GOL	A	801	-	-	0/4/4/4	-
2	GOL	C	802	-	-	2/4/4/4	-
2	GOL	A	802	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	802	GOL	C1-C2-C3-O3
2	C	802	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	802	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	741/786 (94%)	0.17	37 (4%)	34	33	10, 28, 64, 95	5 (0%)
1	B	745/786 (94%)	-0.15	15 (2%)	65	65	12, 23, 52, 86	4 (0%)
1	C	723/786 (91%)	0.16	50 (6%)	23	21	12, 25, 70, 108	4 (0%)
1	D	740/786 (94%)	-0.05	29 (3%)	43	43	11, 23, 54, 86	5 (0%)
All	All	2949/3144 (93%)	0.03	131 (4%)	39	38	10, 24, 60, 108	18 (0%)

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	618	TRP	6.0
1	C	654	LEU	5.6
1	D	592	GLY	5.5
1	D	681	ALA	5.1
1	B	592	GLY	5.1
1	C	616	ALA	4.4
1	B	389	ILE	4.1
1	A	381	PHE	4.0
1	D	683	LEU	3.9
1	A	734	VAL	3.8
1	B	716	TYR	3.6
1	A	496	THR	3.6
1	D	347	ILE	3.5
1	C	683	LEU	3.5
1	B	393	PRO	3.4
1	C	393	PRO	3.4
1	A	393	PRO	3.4
1	C	761	LEU	3.4
1	B	13	PRO	3.3
1	A	737	ILE	3.2
1	D	737	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	628	LEU	3.2
1	C	679	PHE	3.1
1	B	12	THR	3.1
1	D	11	HIS	3.1
1	C	592	GLY	3.1
1	C	758	LEU	3.0
1	D	672	LEU	3.0
1	C	402	ARG	3.0
1	C	762	ILE	3.0
1	A	716	TYR	2.9
1	A	12	THR	2.9
1	C	615	LEU	2.9
1	C	757	ALA	2.9
1	A	417	ALA	2.8
1	C	12	THR	2.8
1	C	166	PRO	2.8
1	C	392	ALA	2.8
1	C	637	ALA	2.8
1	C	688	LEU	2.8
1	C	606	VAL	2.8
1	C	691	LEU	2.8
1	D	734	VAL	2.8
1	C	609	LYS	2.7
1	C	646	ILE	2.7
1	A	166	PRO	2.7
1	A	710	PRO	2.7
1	A	379	LEU	2.7
1	D	346	SER	2.7
1	B	600	HIS	2.7
1	D	637	ALA	2.6
1	A	497	THR	2.6
1	A	557	LEU	2.6
1	C	750	LEU	2.6
1	A	402	ARG	2.6
1	A	728	THR	2.6
1	D	680	GLY	2.6
1	A	730	VAL	2.6
1	D	341	GLU	2.6
1	C	388	PRO	2.5
1	C	716	TYR	2.5
1	C	680	GLY	2.5
1	D	417	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	621	HIS	2.5
1	D	12	THR	2.5
1	A	624	LEU	2.4
1	A	591	MET	2.4
1	A	350	ILE	2.4
1	C	752	THR	2.4
1	A	382	GLY	2.4
1	D	218	GLN	2.4
1	C	751	LEU	2.4
1	B	392	ALA	2.4
1	B	417	ALA	2.4
1	C	498	GLY	2.4
1	C	655	ALA	2.4
1	B	166	PRO	2.4
1	A	391	MET	2.4
1	C	722	LYS	2.4
1	A	392	ALA	2.3
1	D	216	GLY	2.3
1	A	377	ASP	2.3
1	D	710	PRO	2.3
1	A	683	LEU	2.3
1	C	715	LEU	2.3
1	A	625	LYS	2.3
1	D	625	LYS	2.3
1	A	338	ALA	2.3
1	A	498	GLY	2.3
1	C	726	ILE	2.3
1	B	218	GLN	2.3
1	C	647	HIS	2.3
1	C	557	LEU	2.3
1	B	388	PRO	2.2
1	C	681	ALA	2.2
1	D	342	ASP	2.2
1	A	406	HIS	2.2
1	C	686	LYS	2.2
1	C	417	ALA	2.2
1	D	716	TYR	2.2
1	A	165	THR	2.2
1	A	711	THR	2.2
1	B	712	ASP	2.2
1	C	413	LYS	2.2
1	D	764	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	719	SER	2.2
1	A	738	ILE	2.1
1	C	728	THR	2.1
1	C	638	GLY	2.1
1	D	343	GLY	2.1
1	D	301	LYS	2.1
1	B	164	ALA	2.1
1	C	390	GLY	2.1
1	A	461	LYS	2.1
1	A	279	LEU	2.1
1	D	344	GLN	2.1
1	D	418	ASP	2.1
1	C	614	TRP	2.1
1	C	756	VAL	2.1
1	C	218	GLN	2.1
1	C	610	LEU	2.1
1	D	624	LEU	2.1
1	A	681	ALA	2.1
1	B	413	LYS	2.0
1	D	720	LYS	2.0
1	A	460	THR	2.0
1	C	709	THR	2.0
1	A	339	TRP	2.0
1	D	158	SER	2.0
1	C	725	GLY	2.0
1	D	160	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CSX	C	215[A]	7/8	0.88	0.11	40,41,47,50	4
1	CSX	C	215[B]	7/8	0.88	0.11	33,37,40,50	4
1	CSX	A	215[A]	7/8	0.90	0.13	26,38,44,52	4
1	CSX	A	215[B]	7/8	0.90	0.13	29,31,38,38	4
1	CSX	B	215[A]	7/8	0.91	0.11	25,32,39,42	4
1	CSX	B	215[B]	7/8	0.91	0.11	24,29,33,34	4
1	CSX	D	215[A]	7/8	0.91	0.11	28,34,39,39	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	CSX	D	215[B]	7/8	0.91	0.11	28,34,39,39	4

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	MG	A	804	1/1	0.87	0.26	30,30,30,30	0
2	GOL	C	801	6/6	0.89	0.13	34,51,60,61	0
3	MG	C	804	1/1	0.91	0.27	30,30,30,30	0
3	MG	D	803	1/1	0.93	0.19	30,30,30,30	0
2	GOL	A	802	6/6	0.94	0.09	25,37,38,43	0
2	GOL	A	801	6/6	0.95	0.09	25,40,41,45	0
2	GOL	D	801	6/6	0.96	0.08	25,36,39,49	0
2	GOL	C	802	6/6	0.96	0.08	24,31,37,40	0
3	MG	A	803	1/1	0.98	0.09	21,21,21,21	0
3	MG	C	803	1/1	0.98	0.11	21,21,21,21	0
3	MG	D	802	1/1	0.99	0.06	23,23,23,23	0
3	MG	B	801	1/1	0.99	0.06	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.