



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:49 PM UTC

PDB ID : 3O8J / pdb_00003o8j
Title : Crystal structure of 2-methylcitrate synthase (PrpC) from *Salmonella typhimurium*
Authors : Chittori, S.; Savithri, H.S.; Murthy, M.R.N.
Deposited on : 2010-08-03
Resolution : 2.41 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:

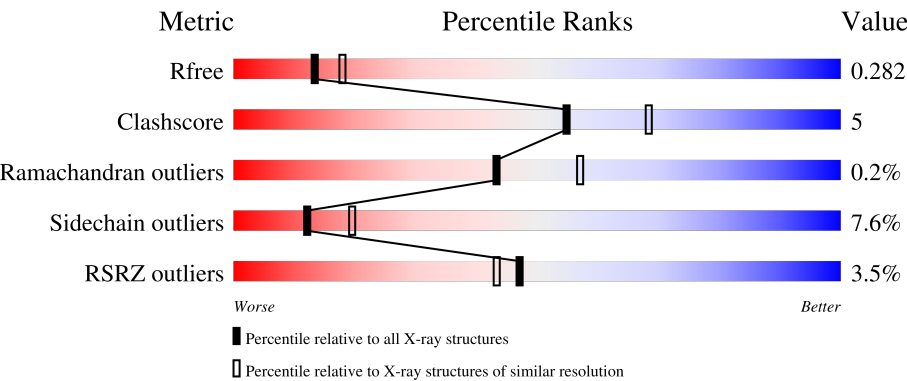
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.41 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	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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	404	0% 79%10%10%
1	B	404	3% 75%13%10%
1	C	404	5% 77%10%11%
1	D	404	5% 74%13%11%
1	E	404	2% 76%11%10%

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Mol	Chain	Length	Quality of chain
1	F	404	2% 77% 11% • 10%
1	G	404	4% 76% 14% • 10%
1	H	404	% 78% 11% • 10%
1	I	404	2% 75% 13% • 10%
1	J	404	4% 76% 12% • 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 29229 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 2-methylcitrate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	364	Total	C	N	O	S	0	0	0
			2808	1775	494	526	13			
1	B	364	Total	C	N	O	S	0	0	0
			2799	1769	492	526	12			
1	C	360	Total	C	N	O	S	0	0	0
			2769	1750	486	521	12			
1	D	358	Total	C	N	O	S	0	0	0
			2764	1746	486	519	13			
1	E	364	Total	C	N	O	S	0	0	0
			2813	1780	494	526	13			
1	F	364	Total	C	N	O	S	0	0	0
			2816	1781	491	532	12			
1	G	364	Total	C	N	O	S	0	0	0
			2801	1773	492	523	13			
1	H	362	Total	C	N	O	S	0	0	0
			2801	1772	491	525	13			
1	I	362	Total	C	N	O	S	0	0	0
			2799	1769	492	525	13			
1	J	362	Total	C	N	O	S	0	0	0
			2815	1780	494	528	13			

There are 150 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	MET	-	expression tag	UNP Q56063
A	-13	ARG	-	expression tag	UNP Q56063
A	-12	GLY	-	expression tag	UNP Q56063
A	-11	SER	-	expression tag	UNP Q56063
A	-10	HIS	-	expression tag	UNP Q56063
A	-9	HIS	-	expression tag	UNP Q56063
A	-8	HIS	-	expression tag	UNP Q56063
A	-7	HIS	-	expression tag	UNP Q56063
A	-6	HIS	-	expression tag	UNP Q56063

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP Q56063
A	-4	GLY	-	expression tag	UNP Q56063
A	-3	MET	-	expression tag	UNP Q56063
A	-2	ALA	-	expression tag	UNP Q56063
A	-1	SER	-	expression tag	UNP Q56063
A	0	HIS	-	expression tag	UNP Q56063
B	-14	MET	-	expression tag	UNP Q56063
B	-13	ARG	-	expression tag	UNP Q56063
B	-12	GLY	-	expression tag	UNP Q56063
B	-11	SER	-	expression tag	UNP Q56063
B	-10	HIS	-	expression tag	UNP Q56063
B	-9	HIS	-	expression tag	UNP Q56063
B	-8	HIS	-	expression tag	UNP Q56063
B	-7	HIS	-	expression tag	UNP Q56063
B	-6	HIS	-	expression tag	UNP Q56063
B	-5	HIS	-	expression tag	UNP Q56063
B	-4	GLY	-	expression tag	UNP Q56063
B	-3	MET	-	expression tag	UNP Q56063
B	-2	ALA	-	expression tag	UNP Q56063
B	-1	SER	-	expression tag	UNP Q56063
B	0	HIS	-	expression tag	UNP Q56063
C	-14	MET	-	expression tag	UNP Q56063
C	-13	ARG	-	expression tag	UNP Q56063
C	-12	GLY	-	expression tag	UNP Q56063
C	-11	SER	-	expression tag	UNP Q56063
C	-10	HIS	-	expression tag	UNP Q56063
C	-9	HIS	-	expression tag	UNP Q56063
C	-8	HIS	-	expression tag	UNP Q56063
C	-7	HIS	-	expression tag	UNP Q56063
C	-6	HIS	-	expression tag	UNP Q56063
C	-5	HIS	-	expression tag	UNP Q56063
C	-4	GLY	-	expression tag	UNP Q56063
C	-3	MET	-	expression tag	UNP Q56063
C	-2	ALA	-	expression tag	UNP Q56063
C	-1	SER	-	expression tag	UNP Q56063
C	0	HIS	-	expression tag	UNP Q56063
D	-14	MET	-	expression tag	UNP Q56063
D	-13	ARG	-	expression tag	UNP Q56063
D	-12	GLY	-	expression tag	UNP Q56063
D	-11	SER	-	expression tag	UNP Q56063
D	-10	HIS	-	expression tag	UNP Q56063
D	-9	HIS	-	expression tag	UNP Q56063

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-8	HIS	-	expression tag	UNP Q56063
D	-7	HIS	-	expression tag	UNP Q56063
D	-6	HIS	-	expression tag	UNP Q56063
D	-5	HIS	-	expression tag	UNP Q56063
D	-4	GLY	-	expression tag	UNP Q56063
D	-3	MET	-	expression tag	UNP Q56063
D	-2	ALA	-	expression tag	UNP Q56063
D	-1	SER	-	expression tag	UNP Q56063
D	0	HIS	-	expression tag	UNP Q56063
E	-14	MET	-	expression tag	UNP Q56063
E	-13	ARG	-	expression tag	UNP Q56063
E	-12	GLY	-	expression tag	UNP Q56063
E	-11	SER	-	expression tag	UNP Q56063
E	-10	HIS	-	expression tag	UNP Q56063
E	-9	HIS	-	expression tag	UNP Q56063
E	-8	HIS	-	expression tag	UNP Q56063
E	-7	HIS	-	expression tag	UNP Q56063
E	-6	HIS	-	expression tag	UNP Q56063
E	-5	HIS	-	expression tag	UNP Q56063
E	-4	GLY	-	expression tag	UNP Q56063
E	-3	MET	-	expression tag	UNP Q56063
E	-2	ALA	-	expression tag	UNP Q56063
E	-1	SER	-	expression tag	UNP Q56063
E	0	HIS	-	expression tag	UNP Q56063
F	-14	MET	-	expression tag	UNP Q56063
F	-13	ARG	-	expression tag	UNP Q56063
F	-12	GLY	-	expression tag	UNP Q56063
F	-11	SER	-	expression tag	UNP Q56063
F	-10	HIS	-	expression tag	UNP Q56063
F	-9	HIS	-	expression tag	UNP Q56063
F	-8	HIS	-	expression tag	UNP Q56063
F	-7	HIS	-	expression tag	UNP Q56063
F	-6	HIS	-	expression tag	UNP Q56063
F	-5	HIS	-	expression tag	UNP Q56063
F	-4	GLY	-	expression tag	UNP Q56063
F	-3	MET	-	expression tag	UNP Q56063
F	-2	ALA	-	expression tag	UNP Q56063
F	-1	SER	-	expression tag	UNP Q56063
F	0	HIS	-	expression tag	UNP Q56063
G	-14	MET	-	expression tag	UNP Q56063
G	-13	ARG	-	expression tag	UNP Q56063
G	-12	GLY	-	expression tag	UNP Q56063

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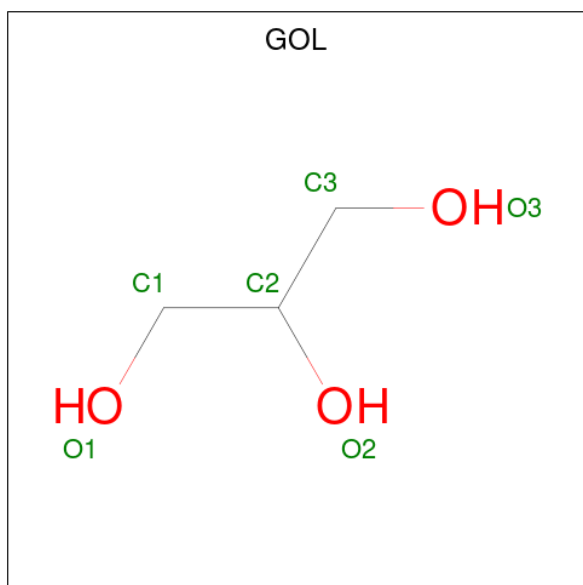
Chain	Residue	Modelled	Actual	Comment	Reference
G	-11	SER	-	expression tag	UNP Q56063
G	-10	HIS	-	expression tag	UNP Q56063
G	-9	HIS	-	expression tag	UNP Q56063
G	-8	HIS	-	expression tag	UNP Q56063
G	-7	HIS	-	expression tag	UNP Q56063
G	-6	HIS	-	expression tag	UNP Q56063
G	-5	HIS	-	expression tag	UNP Q56063
G	-4	GLY	-	expression tag	UNP Q56063
G	-3	MET	-	expression tag	UNP Q56063
G	-2	ALA	-	expression tag	UNP Q56063
G	-1	SER	-	expression tag	UNP Q56063
G	0	HIS	-	expression tag	UNP Q56063
H	-14	MET	-	expression tag	UNP Q56063
H	-13	ARG	-	expression tag	UNP Q56063
H	-12	GLY	-	expression tag	UNP Q56063
H	-11	SER	-	expression tag	UNP Q56063
H	-10	HIS	-	expression tag	UNP Q56063
H	-9	HIS	-	expression tag	UNP Q56063
H	-8	HIS	-	expression tag	UNP Q56063
H	-7	HIS	-	expression tag	UNP Q56063
H	-6	HIS	-	expression tag	UNP Q56063
H	-5	HIS	-	expression tag	UNP Q56063
H	-4	GLY	-	expression tag	UNP Q56063
H	-3	MET	-	expression tag	UNP Q56063
H	-2	ALA	-	expression tag	UNP Q56063
H	-1	SER	-	expression tag	UNP Q56063
H	0	HIS	-	expression tag	UNP Q56063
I	-14	MET	-	expression tag	UNP Q56063
I	-13	ARG	-	expression tag	UNP Q56063
I	-12	GLY	-	expression tag	UNP Q56063
I	-11	SER	-	expression tag	UNP Q56063
I	-10	HIS	-	expression tag	UNP Q56063
I	-9	HIS	-	expression tag	UNP Q56063
I	-8	HIS	-	expression tag	UNP Q56063
I	-7	HIS	-	expression tag	UNP Q56063
I	-6	HIS	-	expression tag	UNP Q56063
I	-5	HIS	-	expression tag	UNP Q56063
I	-4	GLY	-	expression tag	UNP Q56063
I	-3	MET	-	expression tag	UNP Q56063
I	-2	ALA	-	expression tag	UNP Q56063
I	-1	SER	-	expression tag	UNP Q56063
I	0	HIS	-	expression tag	UNP Q56063

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-14	MET	-	expression tag	UNP Q56063
J	-13	ARG	-	expression tag	UNP Q56063
J	-12	GLY	-	expression tag	UNP Q56063
J	-11	SER	-	expression tag	UNP Q56063
J	-10	HIS	-	expression tag	UNP Q56063
J	-9	HIS	-	expression tag	UNP Q56063
J	-8	HIS	-	expression tag	UNP Q56063
J	-7	HIS	-	expression tag	UNP Q56063
J	-6	HIS	-	expression tag	UNP Q56063
J	-5	HIS	-	expression tag	UNP Q56063
J	-4	GLY	-	expression tag	UNP Q56063
J	-3	MET	-	expression tag	UNP Q56063
J	-2	ALA	-	expression tag	UNP Q56063
J	-1	SER	-	expression tag	UNP Q56063
J	0	HIS	-	expression tag	UNP Q56063

- 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	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		

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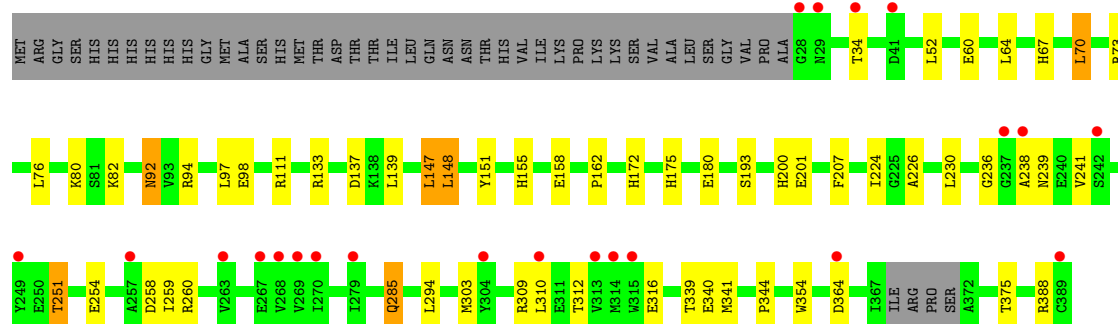
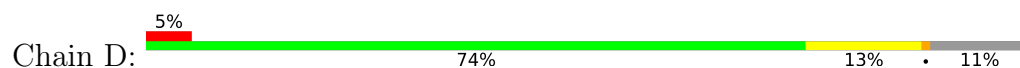
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		
2	I	1	Total	C	O	0	0
			6	3	3		
2	J	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is water.

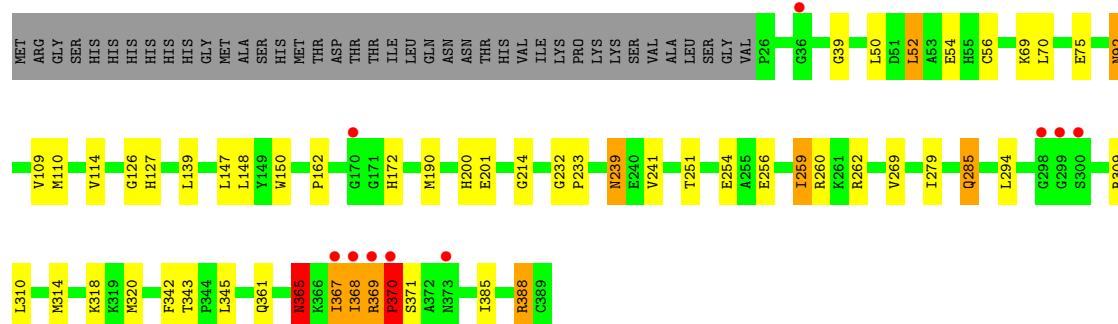
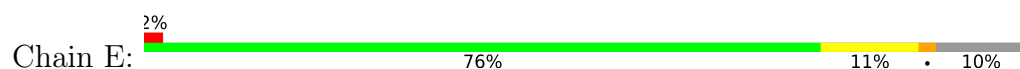
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	145	Total	O	0	0
			145	145		
3	B	119	Total	O	0	0
			119	119		
3	C	84	Total	O	0	0
			84	84		
3	D	96	Total	O	0	0
			96	96		
3	E	146	Total	O	0	0
			146	146		
3	F	113	Total	O	0	0
			113	113		
3	G	106	Total	O	0	0
			106	106		
3	H	126	Total	O	0	0
			126	126		
3	I	131	Total	O	0	0
			131	131		
3	J	112	Total	O	0	0
			112	112		



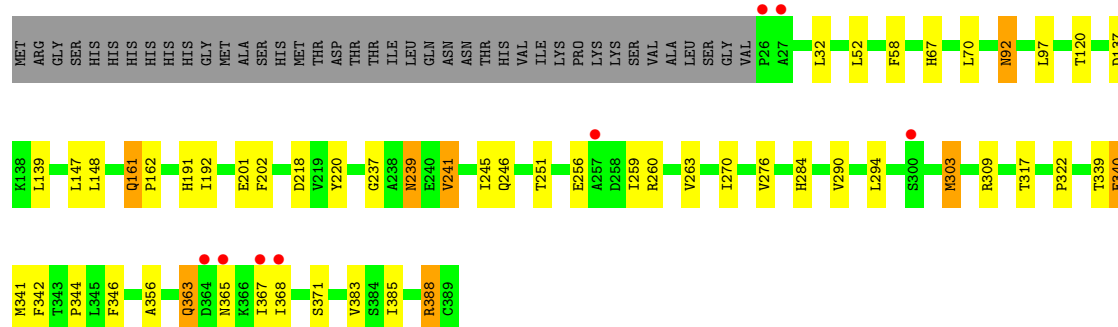
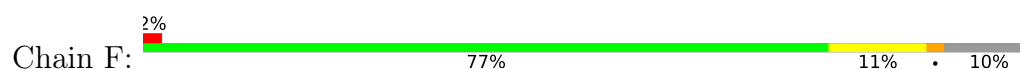
- Molecule 1: 2-methylcitrate synthase



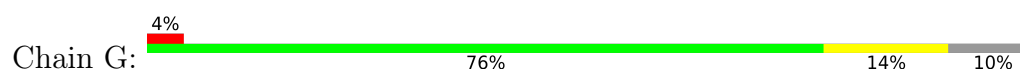
- Molecule 1: 2-methylcitrate synthase

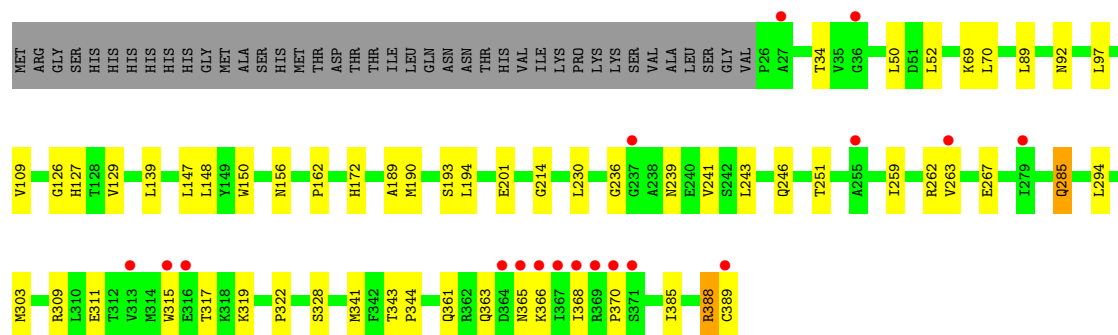


- Molecule 1: 2-methylcitrate synthase

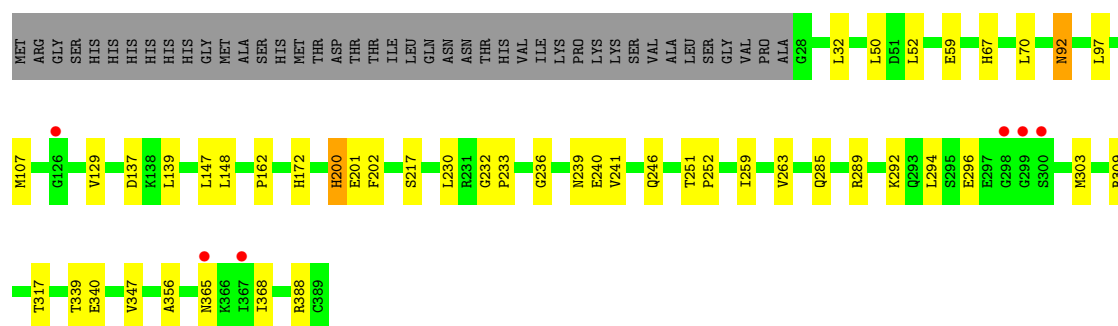
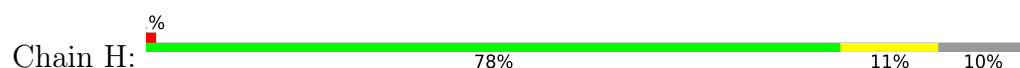


- Molecule 1: 2-methylcitrate synthase

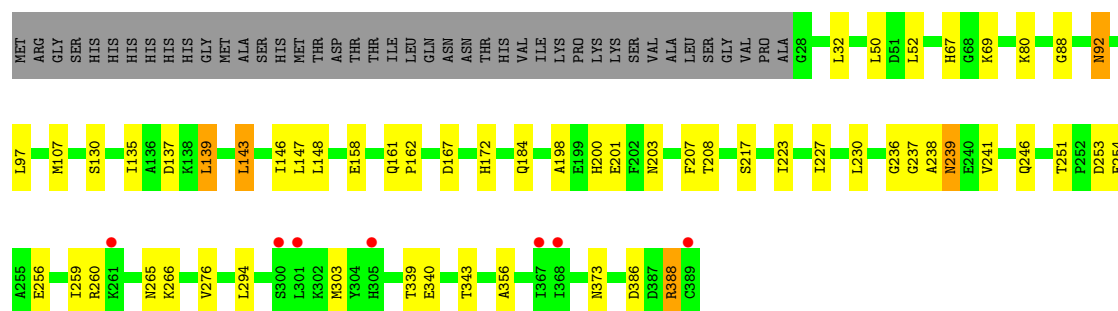
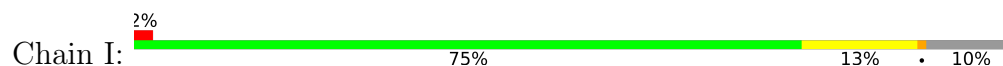




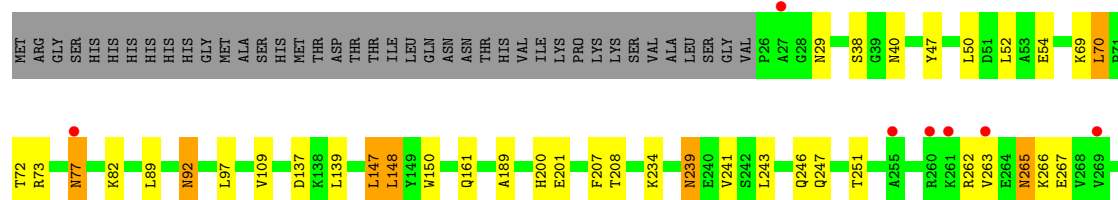
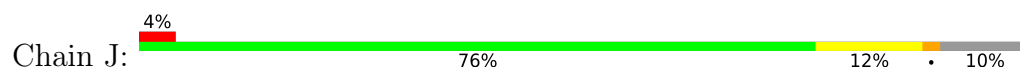
• Molecule 1: 2-methylcitrate synthase

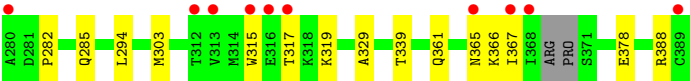


• Molecule 1: 2-methylcitrate synthase



• Molecule 1: 2-methylcitrate synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	92.07Å 118.16Å 120.66Å 60.84° 67.77° 81.92°	Depositor
Resolution (Å)	50.00 – 2.41 50.00 – 2.41	Depositor EDS
% Data completeness (in resolution range)	91.0 (50.00-2.41) 91.4 (50.00-2.41)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.09 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.218 , 0.282 0.220 , 0.282	Depositor DCC
R_{free} test set	7257 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	29229	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.64% 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

5.1 Standard geometry

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

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	0.57	0/2876	0.88	3/3907 (0.1%)
1	B	0.56	0/2867	0.87	0/3894
1	C	0.50	0/2836	0.88	2/3852 (0.1%)
1	D	0.50	0/2829	0.86	0/3840
1	E	0.56	0/2881	0.92	4/3912 (0.1%)
1	F	0.56	0/2884	0.88	0/3919
1	G	0.56	0/2869	0.90	2/3898 (0.1%)
1	H	0.57	0/2868	0.88	0/3895
1	I	0.55	0/2866	0.89	1/3892 (0.0%)
1	J	0.55	0/2881	0.89	3/3907 (0.1%)
All	All	0.55	0/28657	0.88	15/38916 (0.0%)

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	E	0	1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	365	ASN	N-CA-C	8.78	123.39	108.02
1	E	369	ARG	CA-C-N	8.40	130.34	119.84
1	E	369	ARG	C-N-CA	8.40	130.34	119.84
1	C	232	GLY	CA-C-N	7.11	127.10	119.28
1	C	232	GLY	C-N-CA	7.11	127.10	119.28
1	J	89	LEU	CA-C-N	6.10	126.11	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	89	LEU	C-N-CA	6.10	126.11	119.89
1	G	89	LEU	CA-C-N	6.03	126.05	119.90
1	G	89	LEU	C-N-CA	6.03	126.05	119.90
1	A	385	ILE	N-CA-C	5.99	117.45	110.62
1	E	370	PRO	N-CA-C	5.97	124.78	112.47
1	J	365	ASN	N-CA-C	5.59	117.28	110.41
1	A	369	ARG	CA-C-N	-5.57	114.85	120.31
1	A	369	ARG	C-N-CA	-5.57	114.85	120.31
1	I	198	ALA	N-CA-C	5.23	117.73	111.71

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	365	ASN	Peptide

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	2808	0	2703	25	0
1	B	2799	0	2679	41	0
1	C	2769	0	2653	23	0
1	D	2764	0	2653	29	0
1	E	2813	0	2726	34	0
1	F	2816	0	2713	28	0
1	G	2801	0	2696	25	0
1	H	2801	0	2705	23	0
1	I	2799	0	2701	29	0
1	J	2815	0	2745	25	0
2	A	6	0	8	0	0
2	B	6	0	8	1	0
2	C	6	0	8	1	0
2	E	12	0	16	1	0
2	F	12	0	16	0	0
2	G	6	0	8	0	0
2	H	6	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	6	0	8	2	0
2	J	6	0	8	0	0
3	A	145	0	0	1	0
3	B	119	0	0	1	0
3	C	84	0	0	2	0
3	D	96	0	0	0	0
3	E	146	0	0	0	0
3	F	113	0	0	1	0
3	G	106	0	0	1	0
3	H	126	0	0	4	0
3	I	131	0	0	1	0
3	J	112	0	0	2	0
All	All	29229	0	27062	265	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 5.

All (265) 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:G:243:LEU:HD12	1:G:303:MET:HE1	1.35	1.06
1:E:361:GLN:HE21	1:E:365:ASN:HB2	1.29	0.95
1:B:186:TRP:HA	1:B:335:MET:HE2	1.56	0.87
1:F:58:PHE:H	1:F:191:HIS:HD2	1.22	0.87
1:C:207:PHE:HE2	1:D:207:PHE:HE2	1.22	0.86
1:A:230:LEU:O	1:A:236:GLY:HA3	1.76	0.85
1:G:243:LEU:CD1	1:G:303:MET:HE1	2.06	0.84
1:E:361:GLN:HE21	1:E:365:ASN:CB	1.92	0.81
1:B:186:TRP:HA	1:B:335:MET:CE	2.12	0.80
1:E:369:ARG:N	1:E:370:PRO:HD2	1.95	0.80
1:B:189:ALA:HB3	1:B:335:MET:HE1	1.66	0.77
1:E:214:GLY:HA3	1:E:367:ILE:HD11	1.65	0.77
1:G:246:GLN:HE21	1:G:303:MET:HE2	1.48	0.77
1:G:263:VAL:HG11	1:G:317:THR:HG21	1.67	0.77
1:F:58:PHE:H	1:F:191:HIS:CD2	2.03	0.76
1:A:207:PHE:HE2	1:B:207:PHE:HE2	1.32	0.76
1:E:368:ILE:C	1:E:370:PRO:HD2	2.12	0.75
1:B:317:THR:HG22	1:B:318:LYS:HG3	1.68	0.74
1:H:263:VAL:HG11	1:H:317:THR:CG2	2.19	0.71
1:E:361:GLN:O	1:E:365:ASN:HB3	1.91	0.70
1:B:250:GLU:CD	1:B:250:GLU:H	1.97	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:ARG:NH2	1:D:316:GLU:OE1	2.25	0.70
1:E:361:GLN:NE2	1:E:365:ASN:HB2	2.06	0.69
1:B:189:ALA:HB3	1:B:335:MET:CE	2.22	0.68
1:I:266:LYS:HA	3:I:1047:HOH:O	1.93	0.68
1:A:207:PHE:CE2	1:B:207:PHE:HE2	2.11	0.68
1:A:369:ARG:HH11	1:A:369:ARG:CG	2.06	0.67
1:E:92:ASN:H	1:E:92:ASN:HD22	1.41	0.67
1:G:285:GLN:H	1:G:285:GLN:HE21	1.42	0.67
1:H:263:VAL:HG11	1:H:317:THR:HG21	1.76	0.67
1:A:207:PHE:HE2	1:B:207:PHE:CE2	2.13	0.66
1:C:161:GLN:HE21	1:C:163:GLU:HB2	1.61	0.66
1:A:161:GLN:HE21	1:A:163:GLU:H	1.45	0.65
1:F:161:GLN:HE21	1:F:162:PRO:HD2	1.61	0.65
1:H:162:PRO:O	1:H:172:HIS:HE1	1.80	0.65
1:C:241:VAL:HA	1:C:244:GLU:HG2	1.80	0.64
1:I:139:LEU:O	1:I:143:LEU:HD13	1.98	0.64
1:B:92:ASN:HD21	1:B:120:THR:HG21	1.61	0.64
1:C:207:PHE:CE2	1:D:207:PHE:HE2	2.10	0.63
1:H:32:LEU:HD21	1:H:356:ALA:HB1	1.79	0.63
1:G:366:LYS:HD3	1:G:368:ILE:CB	2.29	0.63
1:D:162:PRO:O	1:D:172:HIS:HE1	1.83	0.62
1:G:370:PRO:HB2	1:H:202:PHE:HB3	1.82	0.62
1:J:189:ALA:HB2	1:J:294:LEU:HD11	1.83	0.61
1:E:361:GLN:NE2	1:E:365:ASN:CB	2.63	0.61
1:A:251:THR:HG23	1:A:254:GLU:H	1.66	0.60
1:A:368:ILE:O	1:A:369:ARG:HG2	2.01	0.60
1:I:162:PRO:O	1:I:172:HIS:HE1	1.83	0.60
1:I:92:ASN:HD22	1:I:92:ASN:H	1.49	0.60
1:J:246:GLN:HE21	1:J:303:MET:HE2	1.66	0.60
1:D:238:ALA:O	1:D:241:VAL:HG22	2.02	0.59
1:G:361:GLN:HE22	1:G:366:LYS:H	1.48	0.59
1:I:67:HIS:HE1	1:I:137:ASP:OD2	1.84	0.59
1:G:315:TRP:O	1:G:319:LYS:HA	2.03	0.59
1:B:246:GLN:HE21	1:B:303:MET:HE3	1.69	0.58
1:H:309:ARG:HD3	3:H:789:HOH:O	2.03	0.58
1:C:207:PHE:HE2	1:D:207:PHE:CE2	2.12	0.58
1:J:247:GLN:HG3	1:J:303:MET:HE3	1.85	0.58
1:E:368:ILE:HG22	1:E:370:PRO:CD	2.33	0.58
1:B:84:LYS:NZ	1:B:167:ASP:OD1	2.37	0.57
1:B:186:TRP:O	1:B:335:MET:HE1	2.05	0.57
1:F:363:GLN:HE21	1:F:363:GLN:HA	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:TYR:O	1:C:155:HIS:HB2	2.05	0.56
1:F:263:VAL:HG11	1:F:317:THR:CG2	2.35	0.56
1:C:255:ALA:HB1	1:C:310:LEU:HD21	1.88	0.56
1:E:262:ARG:HG2	2:E:408:GOL:H2	1.88	0.56
1:E:368:ILE:HG22	1:E:370:PRO:HD2	1.88	0.56
1:B:186:TRP:CA	1:B:335:MET:HE2	2.33	0.55
1:H:285:GLN:HG3	1:H:289:ARG:NH2	2.22	0.54
1:A:160:ILE:HD12	1:A:176:LEU:HD22	1.90	0.54
1:A:341:MET:HA	1:A:344:PRO:HG2	1.90	0.54
1:D:230:LEU:O	1:D:236:GLY:HA3	2.06	0.54
1:G:361:GLN:NE2	1:G:366:LYS:H	2.06	0.54
1:G:311:GLU:HG3	1:G:322:PRO:HG3	1.90	0.53
1:B:67:HIS:HE1	1:B:137:ASP:OD2	1.90	0.53
1:B:162:PRO:O	1:B:172:HIS:HE1	1.91	0.53
1:C:246:GLN:HE21	1:C:303:MET:HE3	1.73	0.53
1:E:251:THR:HG23	1:E:254:GLU:H	1.72	0.53
1:H:200:HIS:ND1	2:H:404:GOL:H12	2.22	0.53
1:H:252:PRO:HB2	1:H:309:ARG:NH1	2.24	0.53
1:A:369:ARG:CG	1:A:369:ARG:NH1	2.69	0.53
1:I:256:GLU:O	1:I:260:ARG:HG2	2.08	0.53
1:E:162:PRO:O	1:E:172:HIS:HE1	1.91	0.53
1:G:162:PRO:O	1:G:172:HIS:HE1	1.92	0.52
1:I:139:LEU:HD23	1:I:223:ILE:HD12	1.90	0.52
1:J:92:ASN:H	1:J:92:ASN:HD22	1.58	0.52
1:C:385:ILE:HD12	1:D:73:ARG:HE	1.75	0.52
1:H:246:GLN:HE21	1:H:303:MET:HE2	1.74	0.52
1:A:369:ARG:HH11	1:A:369:ARG:HG3	1.73	0.52
1:C:57:GLU:HB3	1:C:191:HIS:CE1	2.45	0.52
1:F:346:PHE:HD1	1:F:346:PHE:O	1.92	0.51
1:A:263:VAL:HG11	1:A:317:THR:HG21	1.92	0.51
1:B:160:ILE:HD12	1:B:176:LEU:HD22	1.91	0.51
1:B:200:HIS:ND1	2:B:410:GOL:H2	2.25	0.51
1:D:64:LEU:HB2	1:D:70:LEU:HD13	1.92	0.51
1:I:230:LEU:O	1:I:236:GLY:HA3	2.10	0.51
1:C:360:GLU:HA	1:C:363:GLN:HE21	1.76	0.51
1:D:76:LEU:O	1:D:80:LYS:HG3	2.10	0.51
1:F:341:MET:HA	1:F:344:PRO:HG2	1.92	0.51
1:B:303:MET:HG2	1:B:330:VAL:HG22	1.93	0.51
1:A:243:LEU:HD12	1:A:303:MET:HE1	1.92	0.51
1:F:263:VAL:HG11	1:F:317:THR:HG21	1.93	0.51
1:I:203:ASN:HB3	2:I:405:GOL:H11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:VAL:HG21	1:C:270:ILE:HD12	1.93	0.51
1:J:147:LEU:HD13	1:J:148:LEU:HD13	1.93	0.51
1:C:285:GLN:H	1:C:285:GLN:HE21	1.59	0.50
1:C:311:GLU:HG3	1:C:322:PRO:HG3	1.93	0.50
1:F:67:HIS:HE1	1:F:137:ASP:OD2	1.93	0.50
2:C:401:GOL:H2	3:C:569:HOH:O	2.12	0.50
1:J:82:LYS:NZ	1:J:137:ASP:OD2	2.42	0.50
1:J:109:VAL:HG21	1:J:150:TRP:CD2	2.47	0.50
1:H:263:VAL:HG11	1:H:317:THR:HG22	1.93	0.50
1:E:92:ASN:HD22	1:E:92:ASN:N	2.10	0.50
1:D:226:ALA:HB1	1:D:354:TRP:CE2	2.47	0.50
1:I:246:GLN:HE21	1:I:303:MET:HE2	1.77	0.50
1:J:263:VAL:HG11	1:J:317:THR:CG2	2.41	0.50
1:E:318:LYS:HB3	1:E:320:MET:HE3	1.94	0.49
1:J:40:ASN:HB2	3:J:461:HOH:O	2.12	0.49
1:E:259:ILE:HG21	1:E:310:LEU:HD22	1.95	0.49
1:B:109:VAL:HG21	1:B:150:TRP:CD2	2.46	0.49
1:F:284:HIS:CE1	1:F:322:PRO:HG2	2.47	0.49
1:H:67:HIS:HE1	1:H:137:ASP:OD2	1.94	0.49
1:I:388:ARG:HB2	1:J:72:THR:HG22	1.94	0.49
1:A:263:VAL:HG11	1:A:317:THR:CG2	2.43	0.49
1:G:230:LEU:O	1:G:236:GLY:HA3	2.12	0.49
1:D:341:MET:HA	1:D:344:PRO:HG2	1.94	0.49
1:E:110:MET:O	1:E:114:VAL:HG23	2.12	0.49
1:F:92:ASN:HD21	1:F:120:THR:HG21	1.78	0.49
1:G:190:MET:O	1:G:194:LEU:HG	2.13	0.49
1:H:246:GLN:NE2	1:H:303:MET:HE2	2.28	0.49
1:B:253:ASP:OD1	1:B:309:ARG:NH2	2.45	0.48
1:G:214:GLY:HA2	1:G:365:ASN:OD1	2.13	0.48
1:A:92:ASN:HD21	1:A:120:THR:HG21	1.78	0.48
1:H:240:GLU:HG2	1:H:339:THR:HG22	1.94	0.48
1:B:184:GLN:NE2	3:B:1072:HOH:O	2.47	0.48
1:J:265:ASN:O	1:J:266:LYS:HB2	2.14	0.48
1:A:256:GLU:OE1	1:A:309:ARG:NE	2.39	0.48
1:I:67:HIS:CE1	1:I:137:ASP:OD2	2.66	0.48
1:G:243:LEU:HD12	1:G:303:MET:CE	2.25	0.48
1:E:285:GLN:H	1:E:285:GLN:HE21	1.62	0.48
1:I:203:ASN:ND2	2:I:405:GOL:H31	2.28	0.48
1:J:239:ASN:N	1:J:239:ASN:HD22	2.11	0.47
1:E:109:VAL:HG21	1:E:150:TRP:CD2	2.50	0.47
1:B:230:LEU:O	1:B:236:GLY:HA3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:ILE:HD12	1:B:262:ARG:HD2	1.97	0.47
1:F:340:GLU:H	1:F:340:GLU:HG3	1.54	0.47
1:G:341:MET:HA	1:G:344:PRO:HG2	1.96	0.47
1:G:385:ILE:O	1:G:388:ARG:HG2	2.15	0.47
1:C:129:VAL:HG23	3:C:611:HOH:O	2.14	0.47
1:E:190:MET:HE1	1:E:345:LEU:HD22	1.97	0.47
1:I:386:ASP:CG	1:J:73:ARG:HH21	2.22	0.46
1:C:230:LEU:O	1:C:236:GLY:HA3	2.16	0.46
1:E:369:ARG:N	1:E:370:PRO:CD	2.75	0.46
1:F:92:ASN:H	1:F:92:ASN:HD22	1.62	0.46
1:F:256:GLU:OE2	1:F:260:ARG:NH1	2.48	0.46
1:I:246:GLN:NE2	1:I:303:MET:HE2	2.31	0.46
1:J:315:TRP:O	1:J:319:LYS:HA	2.16	0.46
1:D:82:LYS:NZ	1:D:137:ASP:OD2	2.45	0.46
1:E:239:ASN:HD21	1:E:342:PHE:HB3	1.79	0.46
1:B:186:TRP:HA	1:B:335:MET:HE1	1.96	0.46
1:D:67:HIS:CD2	1:D:133:ARG:HD3	2.51	0.46
1:E:269:VAL:HG11	1:E:314:MET:HE3	1.98	0.46
1:A:76:LEU:O	1:A:80:LYS:HG3	2.16	0.46
1:H:59:GLU:OE1	1:H:59:GLU:N	2.49	0.46
1:I:32:LEU:HD21	1:I:356:ALA:HB1	1.97	0.46
1:B:34:THR:HG21	1:B:37:LYS:NZ	2.32	0.45
1:B:256:GLU:OE2	1:B:260:ARG:NH1	2.49	0.45
1:D:94:ARG:O	1:D:98:GLU:HG3	2.17	0.45
1:H:92:ASN:H	1:H:92:ASN:HD22	1.63	0.45
1:I:251:THR:HG23	1:I:254:GLU:H	1.80	0.45
1:E:269:VAL:HG21	1:E:314:MET:CE	2.47	0.45
1:I:208:THR:HG23	1:J:208:THR:HG23	1.98	0.45
1:D:251:THR:HG23	1:D:254:GLU:CB	2.47	0.45
1:B:139:LEU:HD23	1:B:223:ILE:CD1	2.46	0.45
1:B:239:ASN:N	1:B:239:ASN:HD22	2.15	0.45
1:B:294:LEU:HD21	1:B:335:MET:HE3	1.97	0.45
1:H:230:LEU:O	1:H:236:GLY:HA3	2.17	0.45
1:D:162:PRO:O	1:D:172:HIS:CE1	2.66	0.45
1:I:135:ILE:HG22	1:I:139:LEU:HD22	1.98	0.45
1:J:262:ARG:O	1:J:267:GLU:HB2	2.16	0.45
1:I:237:GLY:O	1:I:239:ASN:N	2.50	0.45
1:C:139:LEU:HD23	1:C:223:ILE:HD13	1.99	0.45
1:J:47:TYR:CE2	1:J:70:LEU:HD22	2.52	0.44
1:B:303:MET:HE2	1:B:330:VAL:HA	1.97	0.44
1:E:39:GLY:HA3	1:E:279:ILE:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:126:GLY:O	1:G:127:HIS:HB2	2.15	0.44
1:H:309:ARG:NH2	3:H:788:HOH:O	2.49	0.44
1:I:388:ARG:H	1:I:388:ARG:HG2	1.57	0.44
1:B:232:GLY:HA2	1:B:233:PRO:HD3	1.84	0.44
1:I:107:MET:HE3	1:I:227:ILE:HG23	1.99	0.44
1:C:60:GLU:OE2	1:D:388:ARG:NH2	2.49	0.44
1:G:368:ILE:CB	3:G:1167:HOH:O	2.65	0.44
1:D:175:HIS:HA	1:D:180:GLU:O	2.18	0.44
1:E:126:GLY:O	1:E:127:HIS:HB2	2.17	0.44
1:F:371:SER:OG	3:F:1146:HOH:O	2.21	0.44
1:F:383:VAL:O	1:F:388:ARG:NH1	2.50	0.44
1:I:143:LEU:HD12	1:I:146:ILE:HD12	2.00	0.44
1:F:246:GLN:HE21	1:F:303:MET:HE3	1.83	0.44
1:J:92:ASN:ND2	3:J:651:HOH:O	2.51	0.44
1:E:269:VAL:HG21	1:E:314:MET:HE1	2.00	0.43
1:H:292:LYS:O	1:H:296:GLU:HG3	2.18	0.43
1:B:296:GLU:HA	1:B:301:LEU:HD11	2.00	0.43
1:B:186:TRP:CA	1:B:335:MET:CE	2.91	0.43
1:I:207:PHE:HE2	1:J:207:PHE:HE2	1.67	0.43
1:A:92:ASN:H	1:A:92:ASN:HD22	1.66	0.43
1:E:52:LEU:O	1:E:56:CYS:HB2	2.18	0.43
1:F:241:VAL:O	1:F:245:ILE:HG13	2.18	0.43
1:D:151:TYR:O	1:D:155:HIS:HB2	2.17	0.43
1:J:361:GLN:HE22	1:J:366:LYS:HB3	1.82	0.43
1:A:354:TRP:O	1:A:358:ILE:HG13	2.18	0.43
1:A:369:ARG:HG2	1:A:369:ARG:NH1	2.32	0.43
1:D:147:LEU:HD13	1:D:148:LEU:HD13	2.01	0.43
1:E:256:GLU:OE2	1:E:260:ARG:NH1	2.52	0.43
1:F:218:ASP:OD1	1:F:220:TYR:HB2	2.18	0.43
1:I:80:LYS:CE	1:I:167:ASP:O	2.67	0.43
1:B:233:PRO:HA	1:B:237:GLY:HA3	2.01	0.43
1:F:58:PHE:N	1:F:191:HIS:HD2	2.03	0.43
1:I:373:ASN:HB2	1:J:29:ASN:OD1	2.19	0.43
1:J:239:ASN:HD22	1:J:239:ASN:H	1.66	0.43
1:A:111:ARG:NH1	1:B:221:SER:OG	2.52	0.42
1:C:232:GLY:HA2	1:C:233:PRO:HD3	1.78	0.42
1:D:251:THR:HG23	1:D:254:GLU:HB3	1.99	0.42
1:E:69:LYS:HE2	1:E:75:GLU:OE1	2.19	0.42
1:I:92:ASN:HD22	1:I:92:ASN:N	2.16	0.42
1:F:32:LEU:HD21	1:F:356:ALA:HB1	2.01	0.42
1:F:58:PHE:N	1:F:191:HIS:CD2	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:ASN:HD22	1:D:92:ASN:H	1.66	0.42
1:A:161:GLN:HB2	3:A:424:HOH:O	2.19	0.42
1:B:166:ASP:OD2	1:B:175:HIS:ND1	2.49	0.42
1:D:64:LEU:HD13	1:D:70:LEU:HD22	2.01	0.42
1:F:237:GLY:O	1:F:241:VAL:HG12	2.19	0.42
1:A:346:PHE:HD1	1:A:346:PHE:O	2.03	0.42
1:E:385:ILE:O	1:E:388:ARG:HG2	2.20	0.41
1:C:388:ARG:NH2	1:D:60:GLU:OE2	2.44	0.41
1:D:285:GLN:HE21	1:D:285:GLN:H	1.69	0.41
1:C:82:LYS:NZ	1:C:137:ASP:OD2	2.49	0.41
1:A:57:GLU:HB3	1:A:191:HIS:CE1	2.55	0.41
1:E:232:GLY:HA2	1:E:233:PRO:HD3	1.94	0.41
1:G:262:ARG:O	1:G:267:GLU:HB2	2.21	0.41
1:J:77:ASN:C	1:J:77:ASN:HD22	2.29	0.41
1:J:243:LEU:HB2	1:J:329:ALA:HB1	2.03	0.41
1:F:263:VAL:HG11	1:F:317:THR:HG22	2.01	0.41
1:G:109:VAL:HG21	1:G:150:TRP:CD2	2.55	0.41
1:G:189:ALA:HB2	1:G:294:LEU:HD11	2.02	0.41
1:H:107:MET:HE1	1:H:347:VAL:CG2	2.50	0.41
1:C:92:ASN:HD21	1:C:120:THR:HG21	1.86	0.41
1:H:232:GLY:HA2	1:H:233:PRO:HD3	1.92	0.41
1:H:129:VAL:HG23	3:H:782:HOH:O	2.20	0.41
1:I:139:LEU:HD23	1:I:223:ILE:CD1	2.51	0.41
1:J:282:PRO:O	1:J:285:GLN:HG2	2.21	0.41
1:B:67:HIS:CE1	1:B:137:ASP:OD2	2.72	0.41
1:B:285:GLN:HG2	1:B:286:VAL:N	2.36	0.41
1:D:310:LEU:HD23	1:D:310:LEU:HA	1.86	0.41
1:F:192:ILE:HG21	1:F:290:VAL:HG21	2.03	0.41
1:G:361:GLN:C	1:G:363:GLN:H	2.29	0.41
1:B:92:ASN:HD22	1:B:92:ASN:H	1.69	0.40
1:D:111:ARG:HG3	1:D:224:ILE:HG23	2.02	0.40
1:G:156:ASN:OD1	1:I:88:GLY:HA3	2.20	0.40
1:H:172:HIS:HD2	3:H:780:HOH:O	2.04	0.40
1:D:147:LEU:HD11	1:D:341:MET:HG2	2.01	0.40
1:E:371:SER:HA	1:F:202:PHE:HB2	2.03	0.40
1:F:385:ILE:O	1:F:388:ARG:HG3	2.20	0.40
1:B:383:VAL:O	1:B:388:ARG:NH1	2.52	0.40
1:C:341:MET:HA	1:C:344:PRO:HG2	2.04	0.40
1:F:239:ASN:HD21	1:F:342:PHE:HB3	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	362/404 (90%)	350 (97%)	10 (3%)	2 (1%)	21	30
1	B	362/404 (90%)	351 (97%)	11 (3%)	0	100	100
1	C	356/404 (88%)	349 (98%)	7 (2%)	0	100	100
1	D	354/404 (88%)	346 (98%)	7 (2%)	1 (0%)	36	49
1	E	362/404 (90%)	346 (96%)	14 (4%)	2 (1%)	21	30
1	F	362/404 (90%)	355 (98%)	6 (2%)	1 (0%)	36	49
1	G	362/404 (90%)	348 (96%)	14 (4%)	0	100	100
1	H	360/404 (89%)	349 (97%)	10 (3%)	1 (0%)	36	49
1	I	360/404 (89%)	349 (97%)	10 (3%)	1 (0%)	36	49
1	J	358/404 (89%)	349 (98%)	9 (2%)	0	100	100
All	All	3598/4040 (89%)	3492 (97%)	98 (3%)	8 (0%)	43	57

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	367	ILE
1	A	369	ARG
1	E	370	PRO
1	I	238	ALA
1	F	365	ASN
1	D	258	ASP
1	H	365	ASN
1	E	368	ILE

5.3.2 Protein sidechains

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	289/339 (85%)	270 (93%)	19 (7%)	15	25
1	B	285/339 (84%)	265 (93%)	20 (7%)	14	22
1	C	284/339 (84%)	264 (93%)	20 (7%)	14	22
1	D	284/339 (84%)	260 (92%)	24 (8%)	10	15
1	E	292/339 (86%)	272 (93%)	20 (7%)	14	24
1	F	292/339 (86%)	268 (92%)	24 (8%)	10	17
1	G	287/339 (85%)	264 (92%)	23 (8%)	11	18
1	H	290/339 (86%)	271 (93%)	19 (7%)	15	25
1	I	290/339 (86%)	263 (91%)	27 (9%)	8	13
1	J	296/339 (87%)	272 (92%)	24 (8%)	11	17
All	All	2889/3390 (85%)	2669 (92%)	220 (8%)	12	19

All (220) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	LEU
1	A	52	LEU
1	A	70	LEU
1	A	92	ASN
1	A	97	LEU
1	A	139	LEU
1	A	147	LEU
1	A	148	LEU
1	A	184	GLN
1	A	201	GLU
1	A	239	ASN
1	A	241	VAL
1	A	243	LEU
1	A	259	ILE
1	A	294	LEU
1	A	303	MET
1	A	316	GLU
1	A	369	ARG
1	A	388	ARG
1	B	50	LEU
1	B	52	LEU
1	B	70	LEU

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Mol	Chain	Res	Type
1	B	92	ASN
1	B	139	LEU
1	B	147	LEU
1	B	148	LEU
1	B	200	HIS
1	B	201	GLU
1	B	239	ASN
1	B	241	VAL
1	B	250	GLU
1	B	259	ILE
1	B	285	GLN
1	B	294	LEU
1	B	331	SER
1	B	340	GLU
1	B	343	THR
1	B	371	SER
1	B	384	SER
1	C	34	THR
1	C	52	LEU
1	C	54	GLU
1	C	70	LEU
1	C	92	ASN
1	C	97	LEU
1	C	125	GLU
1	C	139	LEU
1	C	147	LEU
1	C	148	LEU
1	C	201	GLU
1	C	239	ASN
1	C	241	VAL
1	C	285	GLN
1	C	294	LEU
1	C	303	MET
1	C	309	ARG
1	C	339	THR
1	C	364	ASP
1	C	385	ILE
1	D	34	THR
1	D	52	LEU
1	D	70	LEU
1	D	92	ASN
1	D	97	LEU

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Mol	Chain	Res	Type
1	D	139	LEU
1	D	147	LEU
1	D	148	LEU
1	D	158	GLU
1	D	193	SER
1	D	200	HIS
1	D	201	GLU
1	D	239	ASN
1	D	251	THR
1	D	259	ILE
1	D	285	GLN
1	D	294	LEU
1	D	303	MET
1	D	309	ARG
1	D	312	THR
1	D	339	THR
1	D	340	GLU
1	D	364	ASP
1	D	375	THR
1	E	50	LEU
1	E	52	LEU
1	E	54	GLU
1	E	70	LEU
1	E	92	ASN
1	E	139	LEU
1	E	147	LEU
1	E	148	LEU
1	E	200	HIS
1	E	201	GLU
1	E	239	ASN
1	E	241	VAL
1	E	259	ILE
1	E	285	GLN
1	E	294	LEU
1	E	309	ARG
1	E	343	THR
1	E	365	ASN
1	E	367	ILE
1	E	388	ARG
1	F	52	LEU
1	F	70	LEU
1	F	92	ASN

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Mol	Chain	Res	Type
1	F	97	LEU
1	F	139	LEU
1	F	147	LEU
1	F	148	LEU
1	F	161	GLN
1	F	201	GLU
1	F	239	ASN
1	F	241	VAL
1	F	251	THR
1	F	259	ILE
1	F	270	ILE
1	F	276	VAL
1	F	294	LEU
1	F	303	MET
1	F	309	ARG
1	F	339	THR
1	F	340	GLU
1	F	363	GLN
1	F	367	ILE
1	F	368	ILE
1	F	388	ARG
1	G	34	THR
1	G	50	LEU
1	G	52	LEU
1	G	69	LYS
1	G	70	LEU
1	G	92	ASN
1	G	97	LEU
1	G	129	VAL
1	G	139	LEU
1	G	147	LEU
1	G	148	LEU
1	G	193	SER
1	G	201	GLU
1	G	239	ASN
1	G	241	VAL
1	G	251	THR
1	G	259	ILE
1	G	285	GLN
1	G	309	ARG
1	G	328	SER
1	G	343	THR

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Mol	Chain	Res	Type
1	G	388	ARG
1	G	389	CYS
1	H	50	LEU
1	H	52	LEU
1	H	70	LEU
1	H	92	ASN
1	H	97	LEU
1	H	139	LEU
1	H	147	LEU
1	H	148	LEU
1	H	200	HIS
1	H	201	GLU
1	H	217	SER
1	H	239	ASN
1	H	241	VAL
1	H	251	THR
1	H	259	ILE
1	H	294	LEU
1	H	340	GLU
1	H	368	ILE
1	H	388	ARG
1	I	50	LEU
1	I	52	LEU
1	I	69	LYS
1	I	92	ASN
1	I	97	LEU
1	I	130	SER
1	I	139	LEU
1	I	143	LEU
1	I	147	LEU
1	I	148	LEU
1	I	158	GLU
1	I	161	GLN
1	I	184	GLN
1	I	200	HIS
1	I	201	GLU
1	I	217	SER
1	I	239	ASN
1	I	241	VAL
1	I	253	ASP
1	I	259	ILE
1	I	265	ASN

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Mol	Chain	Res	Type
1	I	276	VAL
1	I	294	LEU
1	I	339	THR
1	I	340	GLU
1	I	343	THR
1	I	388	ARG
1	J	38	SER
1	J	50	LEU
1	J	52	LEU
1	J	54	GLU
1	J	69	LYS
1	J	70	LEU
1	J	77	ASN
1	J	92	ASN
1	J	97	LEU
1	J	139	LEU
1	J	147	LEU
1	J	148	LEU
1	J	161	GLN
1	J	200	HIS
1	J	201	GLU
1	J	234	LYS
1	J	239	ASN
1	J	241	VAL
1	J	251	THR
1	J	265	ASN
1	J	339	THR
1	J	367	ILE
1	J	378	GLU
1	J	388	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	67	HIS
1	A	92	ASN
1	A	161	GLN
1	A	184	GLN
1	A	239	ASN
1	A	246	GLN
1	A	363	GLN

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Mol	Chain	Res	Type
1	A	373	ASN
1	B	55	HIS
1	B	67	HIS
1	B	92	ASN
1	B	184	GLN
1	B	239	ASN
1	B	246	GLN
1	B	265	ASN
1	B	285	GLN
1	B	333	ASN
1	B	363	GLN
1	C	43	HIS
1	C	92	ASN
1	C	161	GLN
1	C	203	ASN
1	C	239	ASN
1	C	246	GLN
1	C	265	ASN
1	C	285	GLN
1	C	305	HIS
1	C	363	GLN
1	D	67	HIS
1	D	92	ASN
1	D	239	ASN
1	D	246	GLN
1	D	247	GLN
1	D	284	HIS
1	D	285	GLN
1	D	333	ASN
1	D	363	GLN
1	D	365	ASN
1	E	67	HIS
1	E	92	ASN
1	E	172	HIS
1	E	239	ASN
1	E	246	GLN
1	E	285	GLN
1	E	363	GLN
1	F	43	HIS
1	F	67	HIS
1	F	92	ASN
1	F	161	GLN

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Mol	Chain	Res	Type
1	F	191	HIS
1	F	239	ASN
1	F	246	GLN
1	F	247	GLN
1	F	285	GLN
1	F	333	ASN
1	F	363	GLN
1	G	55	HIS
1	G	92	ASN
1	G	172	HIS
1	G	239	ASN
1	G	246	GLN
1	G	247	GLN
1	G	285	GLN
1	G	305	HIS
1	G	333	ASN
1	G	361	GLN
1	G	363	GLN
1	H	67	HIS
1	H	92	ASN
1	H	172	HIS
1	H	239	ASN
1	H	246	GLN
1	H	247	GLN
1	H	363	GLN
1	H	373	ASN
1	I	67	HIS
1	I	92	ASN
1	I	172	HIS
1	I	175	HIS
1	I	203	ASN
1	I	246	GLN
1	I	265	ASN
1	I	284	HIS
1	I	293	GLN
1	I	333	ASN
1	I	363	GLN
1	J	77	ASN
1	J	92	ASN
1	J	239	ASN
1	J	246	GLN
1	J	285	GLN

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Mol	Chain	Res	Type
1	J	363	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 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	$\# Z > 2$
2	GOL	F	411	-	5,5,5	0.36	0	5,5,5	0.67	0
2	GOL	G	403	-	5,5,5	0.43	0	5,5,5	0.46	0
2	GOL	I	405	-	5,5,5	0.39	0	5,5,5	0.65	0
2	GOL	H	404	-	5,5,5	0.31	0	5,5,5	0.34	0
2	GOL	E	408	-	5,5,5	0.35	0	5,5,5	0.34	0
2	GOL	B	410	-	5,5,5	0.28	0	5,5,5	0.42	0
2	GOL	E	402	-	5,5,5	0.37	0	5,5,5	0.17	0
2	GOL	C	401	-	5,5,5	0.41	0	5,5,5	0.38	0
2	GOL	F	407	-	5,5,5	0.35	0	5,5,5	0.47	0
2	GOL	A	409	-	5,5,5	0.37	0	5,5,5	0.21	0
2	GOL	J	406	-	5,5,5	0.35	0	5,5,5	0.39	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	F	411	-	-	4/4/4/4	-
2	GOL	G	403	-	-	2/4/4/4	-
2	GOL	I	405	-	-	0/4/4/4	-
2	GOL	H	404	-	-	0/4/4/4	-
2	GOL	E	408	-	-	4/4/4/4	-
2	GOL	B	410	-	-	2/4/4/4	-
2	GOL	E	402	-	-	2/4/4/4	-
2	GOL	C	401	-	-	3/4/4/4	-
2	GOL	F	407	-	-	0/4/4/4	-
2	GOL	A	409	-	-	2/4/4/4	-
2	GOL	J	406	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	409	GOL	O1-C1-C2-C3
2	B	410	GOL	O1-C1-C2-C3
2	E	402	GOL	O1-C1-C2-O2
2	E	402	GOL	O1-C1-C2-C3
2	E	408	GOL	C1-C2-C3-O3
2	F	411	GOL	C1-C2-C3-O3
2	C	401	GOL	O2-C2-C3-O3
2	G	403	GOL	O1-C1-C2-O2
2	C	401	GOL	C1-C2-C3-O3
2	E	408	GOL	O1-C1-C2-C3
2	F	411	GOL	O1-C1-C2-C3
2	G	403	GOL	O1-C1-C2-C3
2	J	406	GOL	C1-C2-C3-O3
2	B	410	GOL	O1-C1-C2-O2
2	E	408	GOL	O1-C1-C2-O2
2	E	408	GOL	O2-C2-C3-O3
2	A	409	GOL	O1-C1-C2-O2
2	F	411	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	J	406	GOL	O2-C2-C3-O3
2	C	401	GOL	O1-C1-C2-O2
2	F	411	GOL	O2-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	405	GOL	2	0
2	H	404	GOL	1	0
2	E	408	GOL	1	0
2	B	410	GOL	1	0
2	C	401	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 ⓘ

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, 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	364/404 (90%)	0.15	6 (1%) 70 67	22, 36, 53, 63	1 (0%)
1	B	364/404 (90%)	0.31	13 (3%) 46 42	23, 36, 63, 70	1 (0%)
1	C	360/404 (89%)	0.55	19 (5%) 32 28	27, 47, 72, 77	1 (0%)
1	D	358/404 (88%)	0.60	22 (6%) 27 23	25, 46, 74, 84	1 (0%)
1	E	364/404 (90%)	0.22	10 (2%) 56 52	24, 37, 58, 68	1 (0%)
1	F	364/404 (90%)	0.30	8 (2%) 62 59	24, 39, 57, 66	1 (0%)
1	G	364/404 (90%)	0.39	18 (4%) 35 31	23, 36, 66, 75	2 (0%)
1	H	362/404 (89%)	0.18	6 (1%) 69 66	24, 36, 54, 63	1 (0%)
1	I	362/404 (89%)	0.28	7 (1%) 66 63	23, 37, 57, 64	1 (0%)
1	J	362/404 (89%)	0.33	17 (4%) 36 32	23, 39, 70, 80	1 (0%)
All	All	3624/4040 (89%)	0.33	126 (3%) 47 43	22, 39, 66, 84	11 (0%)

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	368	ILE	5.6
1	G	370	PRO	5.5
1	G	255	ALA	4.3
1	D	257	ALA	3.9
1	H	298	GLY	3.9
1	D	237	GLY	3.8
1	G	365	ASN	3.8
1	E	370	PRO	3.8
1	G	364	ASP	3.7
1	D	267	GLU	3.7
1	J	368	ILE	3.6
1	C	41	ASP	3.6
1	A	27	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	G	315	TRP	3.5
1	F	368	ILE	3.5
1	C	42	LEU	3.5
1	F	26	PRO	3.5
1	I	367	ILE	3.5
1	B	368	ILE	3.4
1	J	280	ALA	3.4
1	E	299	GLY	3.3
1	D	315	TRP	3.3
1	J	365	ASN	3.2
1	C	370	PRO	3.1
1	F	257	ALA	3.0
1	F	365	ASN	3.0
1	D	263	VAL	3.0
1	B	389	CYS	3.0
1	C	317	THR	2.9
1	G	27	ALA	2.9
1	C	281	ASP	2.9
1	E	300	SER	2.9
1	I	300	SER	2.9
1	F	300	SER	2.9
1	G	371	SER	2.8
1	E	298	GLY	2.8
1	A	367	ILE	2.8
1	J	27	ALA	2.8
1	H	367	ILE	2.8
1	J	367	ILE	2.7
1	C	38	SER	2.7
1	C	257	ALA	2.7
1	B	303	MET	2.7
1	G	316	GLU	2.7
1	D	269	VAL	2.7
1	G	313	VAL	2.7
1	H	299	GLY	2.7
1	G	368	ILE	2.7
1	G	263	VAL	2.7
1	E	369	ARG	2.7
1	J	255	ALA	2.7
1	B	36	GLY	2.6
1	C	318	LYS	2.6
1	G	389	CYS	2.6
1	J	269	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	J	312	THR	2.6
1	B	370	PRO	2.6
1	D	279	ILE	2.6
1	D	268	VAL	2.6
1	H	300	SER	2.6
1	D	41	ASP	2.5
1	J	260	ARG	2.5
1	D	28	GLY	2.5
1	J	316	GLU	2.5
1	C	268	VAL	2.5
1	J	263	VAL	2.4
1	B	371	SER	2.4
1	G	367	ILE	2.4
1	J	315	TRP	2.4
1	D	270	ILE	2.4
1	J	389	CYS	2.4
1	B	369	ARG	2.3
1	F	367	ILE	2.3
1	I	261	LYS	2.3
1	C	269	VAL	2.3
1	D	29	ASN	2.3
1	G	36	GLY	2.3
1	B	37	LYS	2.3
1	C	307	ALA	2.3
1	H	365	ASN	2.3
1	A	38	SER	2.3
1	G	279	ILE	2.3
1	C	129	VAL	2.3
1	E	367	ILE	2.2
1	I	368	ILE	2.2
1	D	34	THR	2.2
1	A	366	LYS	2.2
1	B	255	ALA	2.2
1	D	314	MET	2.2
1	E	36	GLY	2.2
1	G	366	LYS	2.2
1	B	239	ASN	2.2
1	B	365	ASN	2.2
1	J	77	ASN	2.2
1	D	310	LEU	2.2
1	I	301	LEU	2.2
1	B	367	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	270	ILE	2.2
1	E	368	ILE	2.2
1	F	364	ASP	2.2
1	D	238	ALA	2.1
1	E	170	GLY	2.1
1	D	304	TYR	2.1
1	D	242	SER	2.1
1	G	369	ARG	2.1
1	I	305	HIS	2.1
1	F	27	ALA	2.1
1	C	260	ARG	2.1
1	D	249	TYR	2.1
1	I	389	CYS	2.1
1	A	26	PRO	2.1
1	D	313	VAL	2.1
1	J	313	VAL	2.1
1	C	323	ASN	2.1
1	G	237	GLY	2.1
1	H	126	GLY	2.1
1	J	317	THR	2.1
1	J	261	LYS	2.1
1	C	365	ASN	2.1
1	D	364	ASP	2.1
1	C	263	VAL	2.0
1	E	373	ASN	2.0
1	C	237	GLY	2.0
1	C	264	GLU	2.0
1	D	389	CYS	2.0
1	B	78	ALA	2.0

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 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(Å ²)	Q<0.9
2	GOL	C	401	6/6	0.72	0.22	64,66,67,68	0
2	GOL	F	411	6/6	0.73	0.18	53,55,56,56	0
2	GOL	F	407	6/6	0.75	0.15	63,64,64,64	0
2	GOL	E	402	6/6	0.76	0.17	59,61,62,62	0
2	GOL	I	405	6/6	0.77	0.15	53,56,57,57	0
2	GOL	J	406	6/6	0.78	0.18	61,61,62,63	0
2	GOL	B	410	6/6	0.80	0.21	57,59,60,60	0
2	GOL	G	403	6/6	0.83	0.20	56,58,60,60	0
2	GOL	H	404	6/6	0.85	0.15	49,49,50,52	0
2	GOL	A	409	6/6	0.86	0.17	54,55,55,56	0
2	GOL	E	408	6/6	0.86	0.13	65,66,66,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.