



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:10 PM UTC

PDB ID : 8GLL / pdb_00008gll
Title : R149E variant of Citrate Synthase (CitA) in Mycobacterium tuberculosis
Authors : Pathirage, R.; Ronning, D.; Petit, C.
Deposited on : 2023-03-22
Resolution : 2.65 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

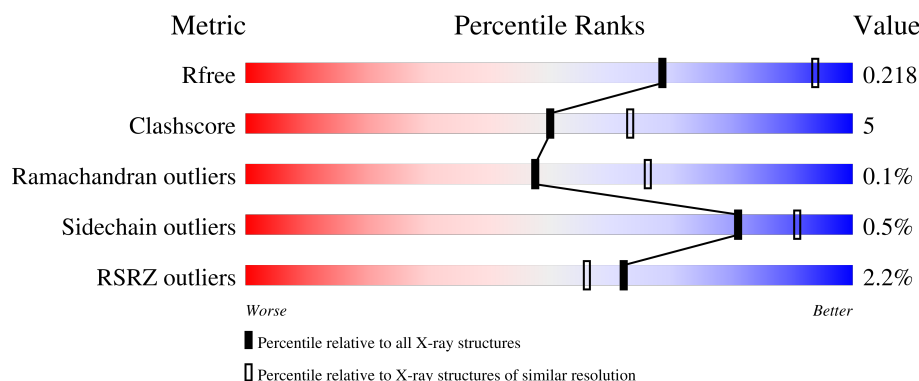
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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.



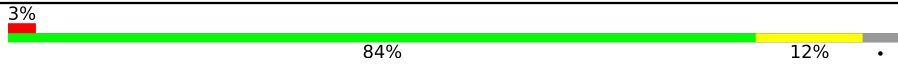
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	379	% 86% 12% .
1	B	379	3% 85% 11% .
1	C	379	% 85% 13% .
1	D	379	2% 82% 14% .
1	E	379	3% 86% 10% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	379	
1	G	379	
1	H	379	

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
3	PEG	C	404	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23209 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 citrate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	371	Total	C	N	O	S	0	0	0
			2810	1769	506	521	14			
1	B	365	Total	C	N	O	S	0	0	0
			2764	1741	499	511	13			
1	C	370	Total	C	N	O	S	0	0	0
			2800	1763	505	519	13			
1	D	365	Total	C	N	O	S	0	0	0
			2764	1741	499	511	13			
1	E	362	Total	C	N	O	S	0	0	0
			2739	1723	496	507	13			
1	F	363	Total	C	N	O	S	0	0	0
			2749	1731	497	508	13			
1	G	366	Total	C	N	O	S	0	0	0
			2769	1744	500	512	13			
1	H	367	Total	C	N	O	S	0	0	0
			2781	1752	502	514	13			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	149	GLU	ARG	engineered mutation	UNP A0A045JB88
A	374	HIS	-	expression tag	UNP A0A045JB88
A	375	HIS	-	expression tag	UNP A0A045JB88
A	376	HIS	-	expression tag	UNP A0A045JB88
A	377	HIS	-	expression tag	UNP A0A045JB88
A	378	HIS	-	expression tag	UNP A0A045JB88
A	379	HIS	-	expression tag	UNP A0A045JB88
B	149	GLU	ARG	engineered mutation	UNP A0A045JB88
B	374	HIS	-	expression tag	UNP A0A045JB88
B	375	HIS	-	expression tag	UNP A0A045JB88
B	376	HIS	-	expression tag	UNP A0A045JB88
B	377	HIS	-	expression tag	UNP A0A045JB88
B	378	HIS	-	expression tag	UNP A0A045JB88

Continued on next page...

Continued from previous page...

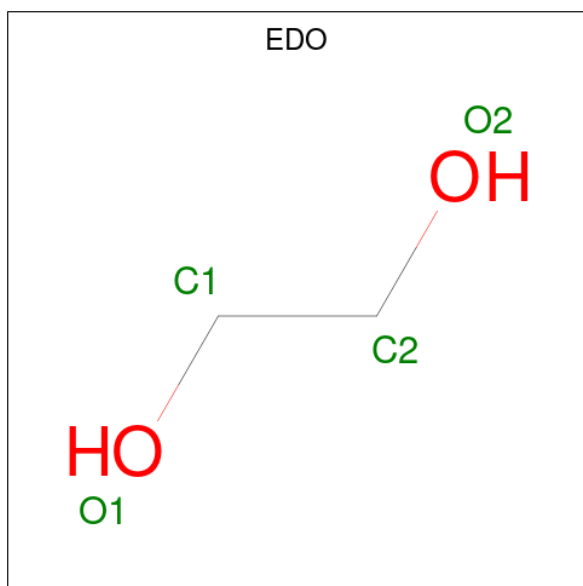
Chain	Residue	Modelled	Actual	Comment	Reference
B	379	HIS	-	expression tag	UNP A0A045JB88
C	149	GLU	ARG	engineered mutation	UNP A0A045JB88
C	374	HIS	-	expression tag	UNP A0A045JB88
C	375	HIS	-	expression tag	UNP A0A045JB88
C	376	HIS	-	expression tag	UNP A0A045JB88
C	377	HIS	-	expression tag	UNP A0A045JB88
C	378	HIS	-	expression tag	UNP A0A045JB88
C	379	HIS	-	expression tag	UNP A0A045JB88
D	149	GLU	ARG	engineered mutation	UNP A0A045JB88
D	374	HIS	-	expression tag	UNP A0A045JB88
D	375	HIS	-	expression tag	UNP A0A045JB88
D	376	HIS	-	expression tag	UNP A0A045JB88
D	377	HIS	-	expression tag	UNP A0A045JB88
D	378	HIS	-	expression tag	UNP A0A045JB88
D	379	HIS	-	expression tag	UNP A0A045JB88
E	149	GLU	ARG	engineered mutation	UNP A0A045JB88
E	374	HIS	-	expression tag	UNP A0A045JB88
E	375	HIS	-	expression tag	UNP A0A045JB88
E	376	HIS	-	expression tag	UNP A0A045JB88
E	377	HIS	-	expression tag	UNP A0A045JB88
E	378	HIS	-	expression tag	UNP A0A045JB88
E	379	HIS	-	expression tag	UNP A0A045JB88
F	149	GLU	ARG	engineered mutation	UNP A0A045JB88
F	374	HIS	-	expression tag	UNP A0A045JB88
F	375	HIS	-	expression tag	UNP A0A045JB88
F	376	HIS	-	expression tag	UNP A0A045JB88
F	377	HIS	-	expression tag	UNP A0A045JB88
F	378	HIS	-	expression tag	UNP A0A045JB88
F	379	HIS	-	expression tag	UNP A0A045JB88
G	149	GLU	ARG	engineered mutation	UNP A0A045JB88
G	374	HIS	-	expression tag	UNP A0A045JB88
G	375	HIS	-	expression tag	UNP A0A045JB88
G	376	HIS	-	expression tag	UNP A0A045JB88
G	377	HIS	-	expression tag	UNP A0A045JB88
G	378	HIS	-	expression tag	UNP A0A045JB88
G	379	HIS	-	expression tag	UNP A0A045JB88
H	149	GLU	ARG	engineered mutation	UNP A0A045JB88
H	374	HIS	-	expression tag	UNP A0A045JB88
H	375	HIS	-	expression tag	UNP A0A045JB88
H	376	HIS	-	expression tag	UNP A0A045JB88
H	377	HIS	-	expression tag	UNP A0A045JB88
H	378	HIS	-	expression tag	UNP A0A045JB88

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	379	HIS	-	expression tag	UNP A0A045JB88

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

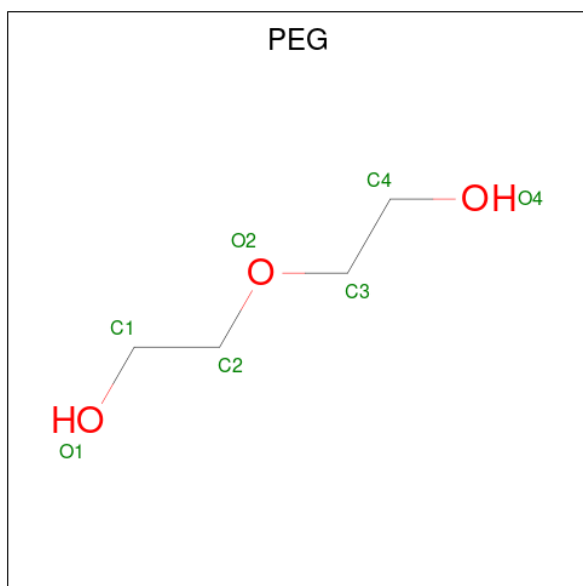
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total 4	C 2	O 2	0	0
2	E	1	Total 4	C 2	O 2	0	0
2	E	1	Total 4	C 2	O 2	0	0
2	F	1	Total 4	C 2	O 2	0	0
2	F	1	Total 4	C 2	O 2	0	0
2	F	1	Total 4	C 2	O 2	0	0
2	F	1	Total 4	C 2	O 2	0	0
2	G	1	Total 4	C 2	O 2	0	0
2	G	1	Total 4	C 2	O 2	0	0
2	G	1	Total 4	C 2	O 2	0	0
2	G	1	Total 4	C 2	O 2	0	0
2	G	1	Total 4	C 2	O 2	0	0
2	H	1	Total 4	C 2	O 2	0	0
2	H	1	Total 4	C 2	O 2	0	0
2	H	1	Total 4	C 2	O 2	0	0
2	H	1	Total 4	C 2	O 2	0	0
2	H	1	Total 4	C 2	O 2	0	0
2	H	1	Total 4	C 2	O 2	0	0
2	H	1	Total 4	C 2	O 2	0	0
2	H	1	Total 4	C 2	O 2	0	0
2	H	1	Total 4	C 2	O 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



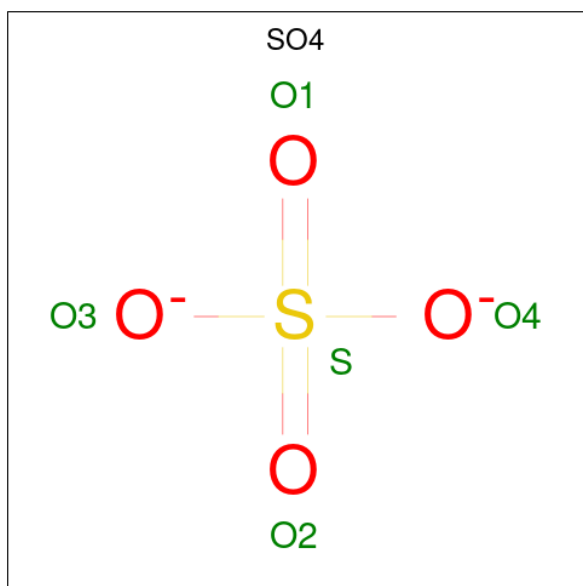
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		
3	D	1	Total	C	O	0	0
			7	4	3		
3	D	1	Total	C	O	0	0
			7	4	3		
3	D	1	Total	C	O	0	0
			7	4	3		
3	D	1	Total	C	O	0	0
			7	4	3		
3	E	1	Total	C	O	0	0
			7	4	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

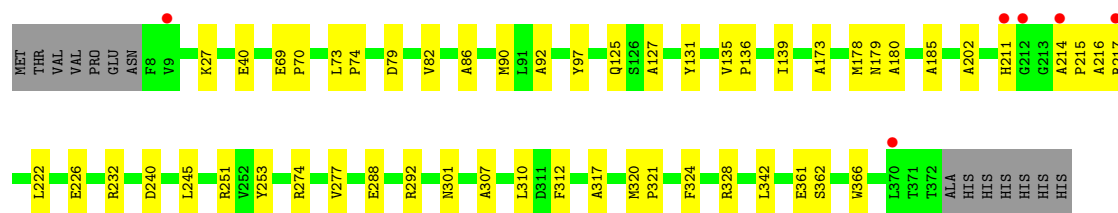
Continued on next page...

Continued from previous page...

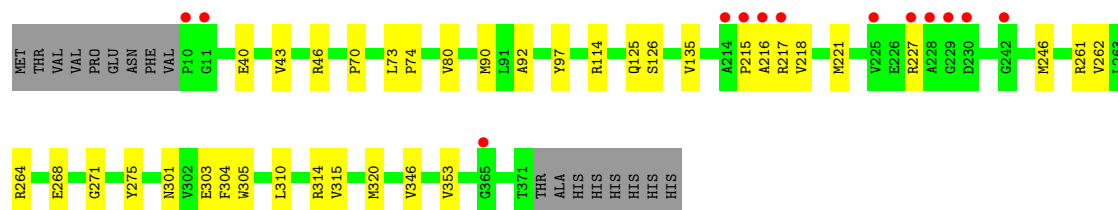
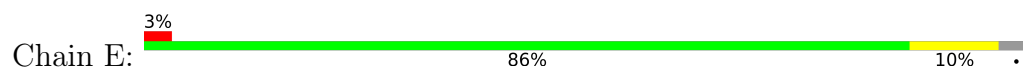
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

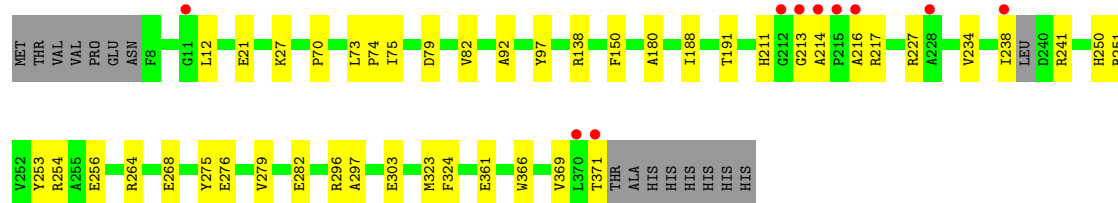
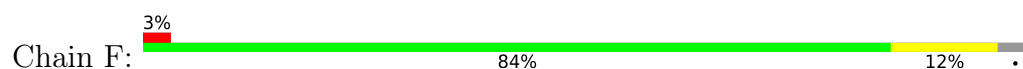
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	86	Total	O	0	0
			86	86		
5	B	59	Total	O	0	0
			59	59		
5	C	106	Total	O	0	0
			106	106		
5	D	93	Total	O	0	0
			93	93		
5	E	54	Total	O	0	0
			54	54		
5	F	47	Total	O	0	0
			47	47		
5	G	46	Total	O	0	0
			46	46		
5	H	90	Total	O	0	0
			90	90		



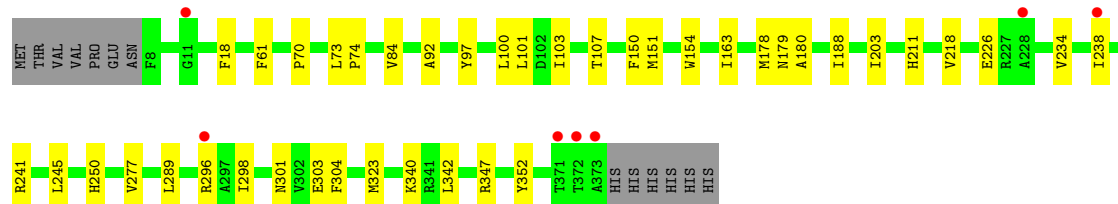
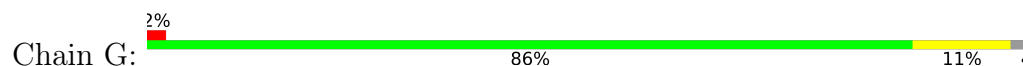
• Molecule 1: citrate synthase



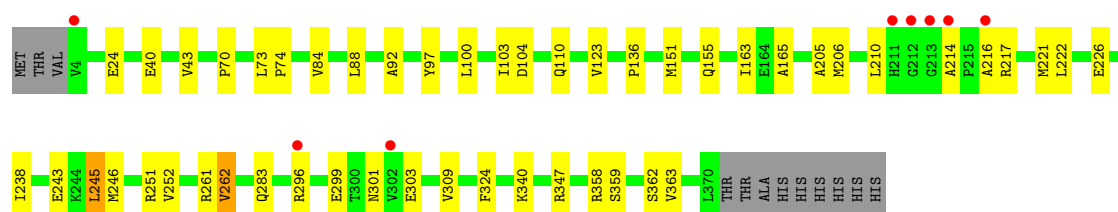
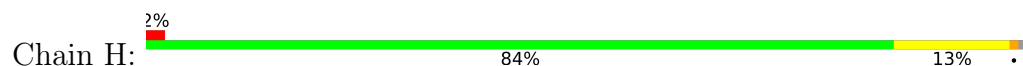
• Molecule 1: citrate synthase



• Molecule 1: citrate synthase



• Molecule 1: citrate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.93Å 129.68Å 270.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.53 – 2.65 47.53 – 2.65	Depositor EDS
% Data completeness (in resolution range)	97.4 (47.53-2.65) 92.9 (47.53-2.65)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158:000	Depositor
R, R_{free}	0.190 , 0.244 (Not available) , 0.218	Depositor DCC
R_{free} test set	2000 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	42.2	Xtriage
Anisotropy	0.452	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23209	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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: SO4, EDO, PEG

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	0.08	0/2873	0.23	0/3912
1	B	0.08	0/2827	0.22	0/3851
1	C	0.10	0/2864	0.25	0/3903
1	D	0.09	0/2827	0.22	0/3851
1	E	0.08	0/2801	0.20	0/3814
1	F	0.09	0/2811	0.22	0/3827
1	G	0.08	0/2832	0.22	0/3858
1	H	0.09	0/2845	0.22	0/3876
All	All	0.09	0/22680	0.22	0/30892

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2810	0	2782	31	0
1	B	2764	0	2735	30	0
1	C	2800	0	2768	33	0
1	D	2764	0	2735	36	0
1	E	2739	0	2711	28	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2749	0	2716	34	0
1	G	2769	0	2740	28	0
1	H	2781	0	2749	41	0
2	A	40	0	60	6	0
2	B	20	0	30	6	0
2	C	56	0	84	6	0
2	D	64	0	96	6	0
2	E	44	0	66	6	0
2	F	16	0	24	0	0
2	G	20	0	30	3	0
2	H	40	0	60	6	0
3	A	7	0	10	0	0
3	B	7	0	10	2	0
3	C	14	0	20	5	0
3	D	35	0	50	6	0
3	E	7	0	10	1	0
3	H	7	0	10	1	0
4	A	15	0	0	0	0
4	B	5	0	0	0	0
4	C	15	0	0	0	0
4	E	15	0	0	0	0
4	F	10	0	0	0	0
4	G	5	0	0	0	0
4	H	10	0	0	0	0
5	A	86	0	0	1	0
5	B	59	0	0	0	0
5	C	106	0	0	2	0
5	D	93	0	0	1	0
5	E	54	0	0	2	0
5	F	47	0	0	3	0
5	G	46	0	0	0	0
5	H	90	0	0	3	0
All	All	23209	0	22496	241	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 (241) 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:206:MET:HG2	1:B:325:THR:HG22	1.66	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:125:GLN:HG2	2:E:412:EDO:H12	1.69	0.75
1:F:256:GLU:OE2	1:F:264:ARG:NH2	2.22	0.72
1:H:100:LEU:HD22	1:H:340:LYS:HD2	1.69	0.72
1:E:90:MET:HE3	1:F:75:ILE:HG23	1.71	0.72
1:B:232:ARG:NH2	1:B:288:GLU:OE2	2.23	0.72
1:F:323:MET:HE2	1:F:323:MET:HA	1.72	0.72
1:G:226:GLU:HG2	1:G:277:VAL:HG21	1.73	0.71
1:H:40:GLU:OE2	1:H:261:ARG:NH1	2.24	0.70
1:C:125:GLN:HG2	2:C:405:EDO:H12	1.74	0.69
1:A:188:ILE:HG12	1:B:205:ALA:HB2	1.74	0.69
1:G:101:LEU:HD11	1:H:210:LEU:HG	1.73	0.69
1:E:301:ASN:HA	3:E:401:PEG:H32	1.75	0.68
1:H:216:ALA:H	1:H:303:GLU:HB3	1.60	0.67
1:F:70:PRO:HB2	1:G:70:PRO:HB2	1.77	0.65
1:A:101:LEU:HD11	1:B:210:LEU:HB2	1.78	0.65
1:H:238:ILE:HG23	1:H:243:GLU:HG3	1.79	0.65
1:D:328:ARG:HH12	3:D:402:PEG:H42	1.62	0.64
1:A:301:ASN:HA	2:A:401:EDO:H11	1.81	0.63
1:F:79:ASP:HB3	1:F:82:VAL:HG22	1.80	0.62
1:G:154:TRP:HE1	2:G:403:EDO:H12	1.63	0.62
1:A:257:ASP:HB2	2:A:401:EDO:H22	1.81	0.61
1:G:238:ILE:HD13	1:G:241:ARG:HH21	1.66	0.59
1:D:274:ARG:HD3	2:D:403:EDO:H11	1.83	0.59
1:E:114:ARG:HH22	2:E:406:EDO:H22	1.66	0.59
1:B:310:LEU:HD13	1:B:320:MET:HG2	1.83	0.59
1:H:358:ARG:HH11	1:H:363:VAL:HG12	1.68	0.59
2:A:408:EDO:H22	1:D:69:GLU:HB2	1.85	0.58
1:C:43:VAL:HG12	2:C:409:EDO:H22	1.86	0.58
1:D:125:GLN:HG2	3:D:405:PEG:H22	1.85	0.58
1:F:264:ARG:NH1	1:F:282:GLU:OE2	2.37	0.57
1:A:70:PRO:HB2	1:D:70:PRO:HB2	1.86	0.56
1:F:217:ARG:NH1	5:F:603:HOH:O	2.39	0.56
1:G:18:PHE:HB3	2:G:404:EDO:H12	1.87	0.56
1:H:100:LEU:HD23	1:H:103:ILE:HD11	1.86	0.56
1:D:179:ASN:HB3	3:D:402:PEG:H21	1.87	0.56
1:A:347:ARG:NH2	2:B:401:EDO:O2	2.37	0.55
1:D:226:GLU:HG2	1:D:277:VAL:HG11	1.88	0.55
1:D:312:PHE:HB2	2:D:403:EDO:H21	1.88	0.55
1:H:110:GLN:NE2	5:H:503:HOH:O	2.39	0.55
1:E:271:GLY:HA2	2:E:411:EDO:H11	1.89	0.55
1:E:46:ARG:HB2	1:F:371:THR:HG23	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:296:ARG:HA	1:H:296:ARG:NE	2.21	0.55
1:E:217:ARG:HA	1:E:217:ARG:NE	2.21	0.54
1:D:342:LEU:HD13	2:D:404:EDO:H21	1.89	0.54
1:H:296:ARG:NH2	5:H:506:HOH:O	2.41	0.54
1:A:254:ARG:HB3	2:A:411:EDO:H11	1.90	0.54
1:G:151:MET:HG3	1:G:163:ILE:HG12	1.89	0.54
1:E:43:VAL:HG11	1:E:262:VAL:HG13	1.90	0.54
1:E:70:PRO:HB2	1:H:70:PRO:HB2	1.90	0.54
1:F:138:ARG:NH1	5:F:602:HOH:O	2.37	0.54
1:G:342:LEU:HD22	2:G:404:EDO:H11	1.90	0.54
1:G:100:LEU:HD22	1:G:340:LYS:HD2	1.91	0.54
1:F:238:ILE:HD12	1:F:238:ILE:H	1.73	0.53
1:D:73:LEU:HD12	1:D:74:PRO:HD2	1.89	0.53
1:C:274:ARG:H	3:C:404:PEG:H31	1.72	0.53
1:B:73:LEU:HD12	1:B:74:PRO:HD2	1.90	0.53
1:C:92:ALA:HA	1:C:97:TYR:HB2	1.89	0.53
1:D:92:ALA:HA	1:D:97:TYR:HB2	1.90	0.53
1:G:289:LEU:HB3	1:G:298:ILE:HD13	1.91	0.53
1:B:84:VAL:HG11	1:B:123:VAL:HG23	1.90	0.53
1:A:88:LEU:HD11	1:A:119:ALA:HB2	1.91	0.52
1:H:155:GLN:HG2	3:H:405:PEG:H31	1.91	0.52
1:E:135:VAL:H	2:E:412:EDO:H22	1.75	0.52
1:F:251:ARG:HD2	1:F:297:ALA:HB3	1.92	0.52
1:C:261:ARG:NH2	5:C:504:HOH:O	2.40	0.52
1:G:92:ALA:HA	1:G:97:TYR:HB2	1.91	0.51
1:B:81:ARG:HB2	2:B:403:EDO:H22	1.93	0.51
1:E:310:LEU:HD13	1:E:320:MET:HG2	1.93	0.51
1:F:27:LYS:HA	1:F:253:TYR:CD2	2.46	0.50
1:B:92:ALA:HA	1:B:97:TYR:HB2	1.93	0.50
1:B:367:GLU:HG2	1:B:368:ARG:HG2	1.92	0.50
1:D:301:ASN:ND2	5:D:513:HOH:O	2.44	0.50
1:E:218:VAL:HG11	1:E:304:PHE:HD1	1.76	0.50
1:G:150:PHE:CE1	1:G:323:MET:HE1	2.47	0.50
1:H:221:MET:HE1	1:H:245:LEU:HD13	1.93	0.50
1:F:180:ALA:HB3	1:F:211:HIS:HD2	1.75	0.50
1:C:114:ARG:HG3	2:C:401:EDO:H22	1.93	0.50
1:H:165:ALA:HB1	1:H:309:VAL:HG13	1.93	0.50
1:C:84:VAL:HG12	1:C:203:ILE:HD13	1.93	0.49
1:D:180:ALA:HB3	1:D:211:HIS:HD2	1.77	0.49
1:D:136:PRO:HD2	1:D:139:ILE:HD12	1.94	0.49
1:E:268:GLU:HB2	1:E:275:TYR:CZ	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:275:TYR:O	1:F:279:VAL:HG23	2.11	0.49
1:A:73:LEU:HD12	1:A:74:PRO:HD2	1.94	0.49
1:F:73:LEU:HD12	1:F:74:PRO:HD2	1.94	0.49
1:F:238:ILE:HG13	1:F:241:ARG:NH2	2.28	0.49
1:H:206:MET:HE3	1:H:324:PHE:HD2	1.78	0.49
1:A:217:ARG:CZ	1:A:217:ARG:HA	2.43	0.49
1:D:131:TYR:HB2	2:D:416:EDO:H12	1.95	0.49
1:B:80:VAL:HG13	1:B:126:SER:HB3	1.93	0.48
1:C:251:ARG:HD2	1:C:254:ARG:O	2.12	0.48
1:F:296:ARG:NH2	5:F:605:HOH:O	2.46	0.48
1:F:303:GLU:OE1	1:F:303:GLU:N	2.44	0.48
1:G:234:VAL:O	1:G:238:ILE:HG12	2.13	0.48
1:A:215:PRO:HG2	1:A:320:MET:HB3	1.96	0.48
1:H:73:LEU:HD12	1:H:74:PRO:HD2	1.95	0.48
1:F:92:ALA:HA	1:F:97:TYR:HB2	1.94	0.48
1:D:79:ASP:HB3	1:D:82:VAL:HB	1.95	0.48
1:F:366:TRP:O	1:F:369:VAL:HG12	2.14	0.48
1:G:73:LEU:HD12	1:G:74:PRO:HD2	1.96	0.48
1:C:250:HIS:HE1	1:C:296:ARG:HE	1.61	0.48
1:C:290:ARG:NH1	1:C:298:ILE:O	2.47	0.48
1:F:251:ARG:HH21	1:F:254:ARG:HA	1.78	0.48
1:E:73:LEU:HD12	1:E:74:PRO:HD2	1.96	0.47
1:G:218:VAL:HG11	1:G:304:PHE:HD1	1.78	0.47
1:D:185:ALA:HB2	1:D:202:ALA:HB2	1.95	0.47
1:F:150:PHE:CZ	1:F:323:MET:HE1	2.50	0.47
1:C:272:ALA:HB1	3:C:404:PEG:H32	1.96	0.47
1:A:205:ALA:HB2	1:B:188:ILE:HG12	1.95	0.47
1:A:275:TYR:O	1:A:279:VAL:HG23	2.15	0.47
1:A:238:ILE:HG23	1:A:243:GLU:HB2	1.96	0.47
1:A:347:ARG:HH21	2:B:401:EDO:HO2	1.62	0.47
1:D:222:LEU:O	1:D:226:GLU:HG3	2.14	0.47
1:D:232:ARG:NH1	1:D:288:GLU:OE1	2.45	0.47
1:E:227:ARG:NH2	5:E:509:HOH:O	2.47	0.47
1:B:293:ARG:HH21	1:B:298:ILE:HD11	1.79	0.47
1:C:84:VAL:HG21	1:C:123:VAL:HG23	1.96	0.47
1:H:104:ASP:HB3	2:H:411:EDO:H22	1.97	0.47
1:C:73:LEU:HD12	1:C:74:PRO:HD2	1.97	0.47
1:D:127:ALA:HA	3:D:408:PEG:H11	1.96	0.47
1:C:312:PHE:HB2	3:C:404:PEG:H42	1.98	0.46
1:D:251:ARG:HH21	3:D:413:PEG:H11	1.80	0.46
1:E:80:VAL:HG13	1:E:126:SER:HB3	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:415:EDO:H21	1:D:178:MET:H	1.80	0.46
2:E:406:EDO:H11	1:H:136:PRO:HA	1.95	0.46
1:H:251:ARG:HE	2:H:408:EDO:H21	1.80	0.46
1:C:40:GLU:OE1	1:C:261:ARG:NH1	2.48	0.46
1:C:236:LYS:NZ	5:C:507:HOH:O	2.48	0.46
1:E:92:ALA:HA	1:E:97:TYR:HB2	1.97	0.46
1:B:70:PRO:HB2	1:C:70:PRO:HB2	1.97	0.46
1:C:215:PRO:HG2	1:C:320:MET:HB3	1.98	0.46
1:G:352:TYR:CG	1:H:24:GLU:HB2	2.51	0.46
1:H:301:ASN:HA	2:H:410:EDO:H21	1.98	0.46
1:C:218:VAL:HG11	1:C:304:PHE:HD1	1.81	0.46
1:E:264:ARG:HG3	1:E:305:TRP:CZ2	2.51	0.46
1:E:215:PRO:HA	1:E:303:GLU:HB3	1.97	0.46
1:A:344:LYS:HD3	1:B:11:GLY:HA3	1.98	0.45
1:H:151:MET:HG3	1:H:163:ILE:HG12	1.98	0.45
1:B:161:ARG:NH1	1:B:270:LEU:O	2.50	0.45
1:B:338:GLU:HG2	3:B:402:PEG:H21	1.98	0.45
1:H:43:VAL:HG11	1:H:262:VAL:HG13	1.99	0.45
1:F:213:GLY:HA3	1:F:324:PHE:CE2	2.52	0.45
1:D:321:PRO:HG2	2:D:411:EDO:H21	1.98	0.45
1:F:250:HIS:HB2	1:F:296:ARG:NH2	2.32	0.45
1:D:274:ARG:HB2	2:D:403:EDO:H22	1.99	0.44
1:F:268:GLU:HB2	1:F:275:TYR:CZ	2.52	0.44
1:G:180:ALA:HB3	1:G:211:HIS:CD2	2.52	0.44
1:A:92:ALA:HA	1:A:97:TYR:HB2	1.98	0.44
1:B:321:PRO:HB2	2:B:403:EDO:H21	1.99	0.44
1:D:86:ALA:O	1:D:90:MET:HG3	2.18	0.44
1:E:216:ALA:H	1:E:303:GLU:HB3	1.82	0.44
1:D:240:ASP:CG	1:D:292:ARG:HH22	2.26	0.44
1:A:151:MET:HG3	1:A:163:ILE:HG12	2.00	0.44
1:E:217:ARG:HA	1:E:217:ARG:CZ	2.47	0.44
1:F:238:ILE:HG13	1:F:241:ARG:HH22	1.82	0.44
1:H:299:GLU:HB2	2:H:410:EDO:H12	2.00	0.44
1:C:287:SER:O	1:C:291:GLU:HB2	2.17	0.44
1:G:150:PHE:HE1	1:G:323:MET:HE1	1.83	0.44
1:B:347:ARG:O	1:B:347:ARG:HG3	2.17	0.43
1:D:216:ALA:HB1	1:D:317:ALA:HB1	2.00	0.43
1:G:103:ILE:HB	1:G:107:THR:HB	1.99	0.43
1:B:275:TYR:O	1:B:279:VAL:HG23	2.18	0.43
1:C:6:GLU:N	1:C:6:GLU:OE1	2.51	0.43
1:D:135:VAL:H	3:D:405:PEG:H11	1.81	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215:PRO:HB2	1:D:307:ALA:HB2	2.00	0.43
1:A:40:GLU:OE1	1:A:261:ARG:NH1	2.51	0.43
1:B:251:ARG:HH11	2:B:404:EDO:H21	1.82	0.43
1:A:235:VAL:HG13	1:A:245:LEU:HD11	1.99	0.43
1:A:296:ARG:NH1	5:A:514:HOH:O	2.51	0.43
1:E:43:VAL:HG21	1:E:262:VAL:HG11	2.00	0.43
1:E:221:MET:HE1	1:E:246:MET:H	1.83	0.43
1:H:252:VAL:HB	2:H:410:EDO:H22	2.01	0.43
1:C:151:MET:HG3	1:C:163:ILE:HG12	2.00	0.43
1:C:344:LYS:HA	1:C:344:LYS:HD2	1.87	0.43
1:F:214:ALA:O	1:F:216:ALA:N	2.50	0.43
1:B:224:GLU:OE2	1:B:227:ARG:NH2	2.46	0.43
1:B:342:LEU:HD13	3:B:402:PEG:H22	2.00	0.43
1:H:222:LEU:O	1:H:226:GLU:HG3	2.19	0.43
1:G:178:MET:O	1:H:347:ARG:HD3	2.19	0.43
1:H:84:VAL:HG21	1:H:123:VAL:HG22	2.00	0.43
1:F:361:GLU:HG3	1:F:366:TRP:NE1	2.33	0.42
1:H:104:ASP:C	1:H:340:LYS:HZ3	2.26	0.42
1:B:72:PRO:HD2	1:C:72:PRO:HD2	2.00	0.42
1:D:27:LYS:HA	1:D:253:TYR:CD2	2.55	0.42
1:D:310:LEU:HD13	1:D:320:MET:HG2	2.01	0.42
1:A:33:ARG:HG2	1:A:38:ASP:HA	2.01	0.42
1:E:70:PRO:HD2	2:E:410:EDO:H22	2.01	0.42
1:E:346:VAL:HG13	1:F:12:LEU:HD12	2.00	0.42
1:A:217:ARG:HA	1:A:217:ARG:NE	2.34	0.42
1:F:188:ILE:O	1:F:191:THR:OG1	2.34	0.42
1:G:245:LEU:HD12	1:G:245:LEU:HA	1.76	0.42
1:B:321:PRO:O	1:B:325:THR:HG23	2.20	0.42
1:C:135:VAL:H	2:C:405:EDO:H22	1.84	0.42
1:F:234:VAL:O	1:F:238:ILE:HD12	2.19	0.42
1:H:283:GLN:HE21	1:H:283:GLN:HB2	1.67	0.42
1:B:293:ARG:NH2	1:B:296:ARG:HH11	2.17	0.42
1:D:245:LEU:HD23	1:D:245:LEU:HA	1.91	0.42
1:E:314:ARG:NH2	5:E:512:HOH:O	2.52	0.42
1:G:61:PHE:CD2	1:H:363:VAL:HG21	2.55	0.42
1:A:138:ARG:HG2	2:A:409:EDO:H22	2.01	0.42
1:A:264:ARG:HG3	1:A:305:TRP:CZ2	2.55	0.42
1:G:179:ASN:HA	1:H:347:ARG:HD3	2.02	0.42
1:C:63:SER:O	1:C:109:ARG:NH2	2.47	0.42
1:C:339:GLN:O	2:C:402:EDO:O2	2.38	0.41
1:H:283:GLN:NE2	2:H:406:EDO:O1	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:ARG:HA	1:C:328:ARG:HD3	1.76	0.41
1:H:92:ALA:HA	1:H:97:TYR:HB2	2.01	0.41
1:A:27:LYS:HA	1:A:253:TYR:CD2	2.55	0.41
1:B:58:ASP:OD2	1:B:109:ARG:NH2	2.52	0.41
1:E:353:VAL:HG23	1:F:21:GLU:HG2	2.03	0.41
1:G:347:ARG:NH2	5:H:515:HOH:O	2.53	0.41
1:B:227:ARG:HB3	1:F:227:ARG:HE	1.84	0.41
1:C:311:ASP:OD2	3:C:404:PEG:O4	2.38	0.41
1:D:361:GLU:HA	1:D:366:TRP:CD1	2.56	0.41
1:B:52:VAL:HG21	1:B:171:VAL:HG22	2.03	0.41
1:H:214:ALA:O	1:H:303:GLU:HG2	2.21	0.41
1:A:104:ASP:OD2	1:A:104:ASP:N	2.46	0.41
1:A:216:ALA:H	1:A:303:GLU:HB3	1.86	0.41
1:G:188:ILE:HG12	1:H:205:ALA:HB2	2.02	0.41
1:D:173:ALA:HB1	1:D:324:PHE:CE1	2.56	0.41
1:G:301:ASN:HB3	1:G:303:GLU:OE1	2.21	0.41
1:H:359:SER:O	1:H:362:SER:OG	2.32	0.41
1:H:362:SER:H	1:H:362:SER:HG	1.66	0.41
1:A:95:TRP:HE1	2:A:402:EDO:H12	1.86	0.41
1:A:303:GLU:N	1:A:303:GLU:OE2	2.54	0.41
1:D:362:SER:O	1:D:362:SER:OG	2.37	0.41
1:C:162:HIS:CD2	1:C:313:ALA:HA	2.56	0.40
1:C:274:ARG:HB2	3:C:404:PEG:C4	2.51	0.40
1:G:250:HIS:HB3	1:G:296:ARG:NH2	2.36	0.40
1:A:58:ASP:OD2	1:A:109:ARG:NH2	2.54	0.40
1:G:84:VAL:HG13	1:G:203:ILE:HD13	2.01	0.40
1:H:243:GLU:H	1:H:243:GLU:HG2	1.72	0.40
1:C:27:LYS:HA	1:C:253:TYR:CD2	2.57	0.40
1:C:46:ARG:HE	1:C:46:ARG:HB2	1.70	0.40
1:D:214:ALA:O	1:D:217:ARG:NE	2.37	0.40
1:H:88:LEU:HD23	1:H:88:LEU:HA	1.97	0.40
1:E:40:GLU:OE1	1:E:261:ARG:NH1	2.54	0.40
1:F:276:GLU:CD	1:F:276:GLU:H	2.29	0.40
1:B:251:ARG:HD3	2:B:404:EDO:H21	2.04	0.40
1:H:217:ARG:HG3	1:H:246:MET:HE2	2.02	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	367/379 (97%)	359 (98%)	7 (2%)	1 (0%)	36	52
1	B	363/379 (96%)	349 (96%)	14 (4%)	0	100	100
1	C	368/379 (97%)	354 (96%)	12 (3%)	2 (0%)	24	39
1	D	363/379 (96%)	353 (97%)	10 (3%)	0	100	100
1	E	360/379 (95%)	350 (97%)	10 (3%)	0	100	100
1	F	359/379 (95%)	350 (98%)	9 (2%)	0	100	100
1	G	364/379 (96%)	354 (97%)	10 (3%)	0	100	100
1	H	365/379 (96%)	354 (97%)	11 (3%)	0	100	100
All	All	2909/3032 (96%)	2823 (97%)	83 (3%)	3 (0%)	48	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	7	ASN
1	C	255	ALA
1	A	2	THR

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	284/291 (98%)	281 (99%)	3 (1%)	65	80
1	B	278/291 (96%)	275 (99%)	3 (1%)	65	80

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	282/291 (97%)	280 (99%)	2 (1%)	76	86
1	D	278/291 (96%)	277 (100%)	1 (0%)	84	93
1	E	275/291 (94%)	274 (100%)	1 (0%)	84	93
1	F	276/291 (95%)	276 (100%)	0	100	100
1	G	278/291 (96%)	278 (100%)	0	100	100
1	H	280/291 (96%)	278 (99%)	2 (1%)	76	86
All	All	2231/2328 (96%)	2219 (100%)	12 (0%)	81	91

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	7	ASN
1	A	8	PHE
1	B	144	SER
1	B	251	ARG
1	B	346	VAL
1	C	4	VAL
1	C	21	GLU
1	D	40	GLU
1	E	315	VAL
1	H	245	LEU
1	H	262	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	76	HIS
1	A	132	GLN
1	B	45	GLN
1	B	76	HIS
1	B	283	GLN
1	C	7	ASN
1	D	76	HIS
1	D	301	ASN
1	E	45	GLN
1	E	76	HIS
1	F	60	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	76	HIS
1	G	137	GLN
1	H	60	ASN
1	H	76	HIS
1	H	132	GLN
1	H	283	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](#)

101 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	EDO	D	420	-	3,3,3	0.43	0	2,2,2	0.37	0
2	EDO	D	415	-	3,3,3	0.43	0	2,2,2	0.37	0
3	PEG	D	413	-	6,6,6	0.49	0	5,5,5	0.22	0
2	EDO	D	409	-	3,3,3	0.44	0	2,2,2	0.36	0
2	EDO	C	416	-	3,3,3	0.43	0	2,2,2	0.38	0
2	EDO	C	411	-	3,3,3	0.44	0	2,2,2	0.32	0
3	PEG	D	408	-	6,6,6	0.49	0	5,5,5	0.25	0
4	SO4	E	414	-	4,4,4	0.24	0	6,6,6	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	D	403	-	3,3,3	0.40	0	2,2,2	0.39	0
2	EDO	C	403	-	3,3,3	0.42	0	2,2,2	0.39	0
2	EDO	H	411	-	3,3,3	0.43	0	2,2,2	0.37	0
2	EDO	D	404	-	3,3,3	0.46	0	2,2,2	0.24	0
2	EDO	H	409	-	3,3,3	0.42	0	2,2,2	0.39	0
2	EDO	A	403	-	3,3,3	0.44	0	2,2,2	0.32	0
2	EDO	G	403	-	3,3,3	0.42	0	2,2,2	0.37	0
3	PEG	D	407	-	6,6,6	0.50	0	5,5,5	0.27	0
2	EDO	H	407	-	3,3,3	0.43	0	2,2,2	0.35	0
2	EDO	D	412	-	3,3,3	0.43	0	2,2,2	0.38	0
2	EDO	D	414	-	3,3,3	0.43	0	2,2,2	0.36	0
4	SO4	E	413	-	4,4,4	0.23	0	6,6,6	0.06	0
2	EDO	E	406	-	3,3,3	0.44	0	2,2,2	0.32	0
2	EDO	C	415	-	3,3,3	0.42	0	2,2,2	0.38	0
2	EDO	H	408	-	3,3,3	0.44	0	2,2,2	0.35	0
3	PEG	C	407	-	6,6,6	0.50	0	5,5,5	0.23	0
2	EDO	C	413	-	3,3,3	0.43	0	2,2,2	0.38	0
2	EDO	E	402	-	3,3,3	0.43	0	2,2,2	0.37	0
2	EDO	A	410	-	3,3,3	0.44	0	2,2,2	0.31	0
4	SO4	H	412	-	4,4,4	0.24	0	6,6,6	0.07	0
2	EDO	A	411	-	3,3,3	0.42	0	2,2,2	0.41	0
2	EDO	D	418	-	3,3,3	0.42	0	2,2,2	0.37	0
2	EDO	A	405	-	3,3,3	0.43	0	2,2,2	0.37	0
4	SO4	F	406	-	4,4,4	0.24	0	6,6,6	0.08	0
4	SO4	A	414	-	4,4,4	0.23	0	6,6,6	0.08	0
2	EDO	E	405	-	3,3,3	0.44	0	2,2,2	0.33	0
2	EDO	B	404	-	3,3,3	0.43	0	2,2,2	0.37	0
2	EDO	F	403	-	3,3,3	0.43	0	2,2,2	0.39	0
2	EDO	A	409	-	3,3,3	0.44	0	2,2,2	0.37	0
2	EDO	A	407	-	3,3,3	0.42	0	2,2,2	0.38	0
2	EDO	E	409	-	3,3,3	0.44	0	2,2,2	0.31	0
2	EDO	E	411	-	3,3,3	0.43	0	2,2,2	0.35	0
2	EDO	D	406	-	3,3,3	0.43	0	2,2,2	0.37	0
3	PEG	B	402	-	6,6,6	0.50	0	5,5,5	0.22	0
4	SO4	B	407	-	4,4,4	0.24	0	6,6,6	0.08	0
4	SO4	C	418	-	4,4,4	0.24	0	6,6,6	0.07	0
2	EDO	D	401	-	3,3,3	0.44	0	2,2,2	0.32	0
2	EDO	H	404	-	3,3,3	0.43	0	2,2,2	0.34	0
3	PEG	D	405	-	6,6,6	0.51	0	5,5,5	0.22	0
4	SO4	A	413	-	4,4,4	0.23	0	6,6,6	0.08	0
4	SO4	F	405	-	4,4,4	0.23	0	6,6,6	0.11	0
2	EDO	E	408	-	3,3,3	0.43	0	2,2,2	0.31	0
2	EDO	F	402	-	3,3,3	0.43	0	2,2,2	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	H	403	-	3,3,3	0.43	0	2,2,2	0.39	0
3	PEG	H	405	-	6,6,6	0.50	0	5,5,5	0.23	0
2	EDO	B	406	-	3,3,3	0.44	0	2,2,2	0.30	0
2	EDO	E	407	-	3,3,3	0.43	0	2,2,2	0.32	0
2	EDO	B	403	-	3,3,3	0.42	0	2,2,2	0.34	0
2	EDO	G	404	-	3,3,3	0.43	0	2,2,2	0.37	0
4	SO4	H	413	-	4,4,4	0.24	0	6,6,6	0.08	0
2	EDO	E	412	-	3,3,3	0.42	0	2,2,2	0.35	0
2	EDO	A	402	-	3,3,3	0.43	0	2,2,2	0.32	0
4	SO4	A	412	-	4,4,4	0.25	0	6,6,6	0.06	0
3	PEG	E	401	-	6,6,6	0.50	0	5,5,5	0.24	0
2	EDO	C	406	-	3,3,3	0.43	0	2,2,2	0.37	0
2	EDO	H	410	-	3,3,3	0.43	0	2,2,2	0.31	0
2	EDO	D	417	-	3,3,3	0.42	0	2,2,2	0.38	0
2	EDO	C	405	-	3,3,3	0.42	0	2,2,2	0.32	0
2	EDO	C	408	-	3,3,3	0.42	0	2,2,2	0.41	0
2	EDO	E	410	-	3,3,3	0.44	0	2,2,2	0.36	0
2	EDO	H	406	-	3,3,3	0.44	0	2,2,2	0.34	0
2	EDO	C	401	-	3,3,3	0.43	0	2,2,2	0.36	0
2	EDO	C	410	-	3,3,3	0.43	0	2,2,2	0.37	0
2	EDO	E	403	-	3,3,3	0.43	0	2,2,2	0.34	0
4	SO4	C	417	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	C	419	-	4,4,4	0.23	0	6,6,6	0.07	0
4	SO4	E	415	-	4,4,4	0.24	0	6,6,6	0.08	0
2	EDO	C	402	-	3,3,3	0.42	0	2,2,2	0.38	0
2	EDO	D	416	-	3,3,3	0.44	0	2,2,2	0.33	0
2	EDO	A	408	-	3,3,3	0.44	0	2,2,2	0.28	0
3	PEG	D	402	-	6,6,6	0.49	0	5,5,5	0.32	0
2	EDO	B	401	-	3,3,3	0.44	0	2,2,2	0.36	0
2	EDO	C	409	-	3,3,3	0.43	0	2,2,2	0.37	0
2	EDO	F	401	-	3,3,3	0.43	0	2,2,2	0.29	0
2	EDO	D	410	-	3,3,3	0.43	0	2,2,2	0.34	0
2	EDO	A	404	-	3,3,3	0.42	0	2,2,2	0.37	0
2	EDO	D	411	-	3,3,3	0.43	0	2,2,2	0.38	0
3	PEG	C	404	-	6,6,6	0.51	0	5,5,5	0.29	0
2	EDO	F	404	-	3,3,3	0.43	0	2,2,2	0.37	0
2	EDO	A	401	-	3,3,3	0.46	0	2,2,2	0.18	0
2	EDO	D	421	-	3,3,3	0.43	0	2,2,2	0.34	0
2	EDO	G	402	-	3,3,3	0.42	0	2,2,2	0.39	0
2	EDO	C	414	-	3,3,3	0.43	0	2,2,2	0.36	0
2	EDO	E	404	-	3,3,3	0.44	0	2,2,2	0.32	0
2	EDO	G	401	-	3,3,3	0.42	0	2,2,2	0.36	0
2	EDO	G	405	-	3,3,3	0.42	0	2,2,2	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	B	405	-	3,3,3	0.42	0	2,2,2	0.38	0
2	EDO	H	402	-	3,3,3	0.43	0	2,2,2	0.34	0
3	PEG	A	406	-	6,6,6	0.51	0	5,5,5	0.25	0
2	EDO	D	419	-	3,3,3	0.42	0	2,2,2	0.38	0
2	EDO	H	401	-	3,3,3	0.42	0	2,2,2	0.37	0
2	EDO	C	412	-	3,3,3	0.43	0	2,2,2	0.37	0
4	SO4	G	406	-	4,4,4	0.24	0	6,6,6	0.08	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	EDO	D	420	-	-	0/1/1/1	-
2	EDO	D	415	-	-	0/1/1/1	-
3	PEG	D	413	-	-	1/4/4/4	-
2	EDO	D	409	-	-	0/1/1/1	-
2	EDO	C	416	-	-	0/1/1/1	-
2	EDO	C	411	-	-	0/1/1/1	-
3	PEG	D	408	-	-	1/4/4/4	-
2	EDO	D	403	-	-	0/1/1/1	-
2	EDO	C	403	-	-	0/1/1/1	-
2	EDO	H	411	-	-	0/1/1/1	-
2	EDO	D	404	-	-	0/1/1/1	-
2	EDO	H	409	-	-	0/1/1/1	-
2	EDO	A	403	-	-	0/1/1/1	-
2	EDO	G	403	-	-	1/1/1/1	-
3	PEG	D	407	-	-	2/4/4/4	-
2	EDO	H	407	-	-	0/1/1/1	-
2	EDO	D	412	-	-	0/1/1/1	-
2	EDO	D	414	-	-	0/1/1/1	-
2	EDO	E	406	-	-	0/1/1/1	-
2	EDO	C	415	-	-	0/1/1/1	-
2	EDO	H	408	-	-	0/1/1/1	-
3	PEG	C	407	-	-	2/4/4/4	-
2	EDO	C	413	-	-	0/1/1/1	-
2	EDO	E	402	-	-	0/1/1/1	-
2	EDO	A	410	-	-	0/1/1/1	-
2	EDO	A	411	-	-	0/1/1/1	-
2	EDO	D	418	-	-	0/1/1/1	-
2	EDO	A	405	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	E	405	-	-	0/1/1/1	-
2	EDO	B	404	-	-	0/1/1/1	-
2	EDO	F	403	-	-	0/1/1/1	-
2	EDO	A	409	-	-	0/1/1/1	-
2	EDO	A	407	-	-	0/1/1/1	-
2	EDO	E	409	-	-	0/1/1/1	-
2	EDO	E	411	-	-	0/1/1/1	-
2	EDO	D	406	-	-	0/1/1/1	-
3	PEG	B	402	-	-	2/4/4/4	-
2	EDO	D	401	-	-	0/1/1/1	-
2	EDO	H	404	-	-	0/1/1/1	-
3	PEG	D	405	-	-	1/4/4/4	-
2	EDO	E	408	-	-	0/1/1/1	-
2	EDO	F	402	-	-	0/1/1/1	-
2	EDO	H	403	-	-	0/1/1/1	-
3	PEG	H	405	-	-	0/4/4/4	-
2	EDO	B	406	-	-	0/1/1/1	-
2	EDO	E	407	-	-	0/1/1/1	-
2	EDO	B	403	-	-	0/1/1/1	-
2	EDO	G	404	-	-	0/1/1/1	-
2	EDO	E	412	-	-	0/1/1/1	-
2	EDO	A	402	-	-	0/1/1/1	-
3	PEG	E	401	-	-	3/4/4/4	-
2	EDO	C	406	-	-	0/1/1/1	-
2	EDO	H	410	-	-	1/1/1/1	-
2	EDO	D	417	-	-	0/1/1/1	-
2	EDO	C	405	-	-	0/1/1/1	-
2	EDO	C	408	-	-	0/1/1/1	-
2	EDO	E	410	-	-	0/1/1/1	-
2	EDO	H	406	-	-	0/1/1/1	-
2	EDO	C	401	-	-	0/1/1/1	-
2	EDO	C	410	-	-	0/1/1/1	-
2	EDO	E	403	-	-	0/1/1/1	-
2	EDO	C	402	-	-	0/1/1/1	-
2	EDO	D	416	-	-	0/1/1/1	-
2	EDO	A	408	-	-	1/1/1/1	-
3	PEG	D	402	-	-	2/4/4/4	-
2	EDO	B	401	-	-	0/1/1/1	-
2	EDO	C	409	-	-	0/1/1/1	-
2	EDO	F	401	-	-	0/1/1/1	-
2	EDO	D	410	-	-	0/1/1/1	-
2	EDO	A	404	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	D	411	-	-	0/1/1/1	-
3	PEG	C	404	-	-	1/4/4/4	-
2	EDO	F	404	-	-	0/1/1/1	-
2	EDO	A	401	-	-	0/1/1/1	-
2	EDO	D	421	-	-	0/1/1/1	-
2	EDO	G	402	-	-	0/1/1/1	-
2	EDO	C	414	-	-	0/1/1/1	-
2	EDO	E	404	-	-	0/1/1/1	-
2	EDO	G	401	-	-	0/1/1/1	-
2	EDO	G	405	-	-	0/1/1/1	-
2	EDO	B	405	-	-	0/1/1/1	-
2	EDO	H	402	-	-	0/1/1/1	-
3	PEG	A	406	-	-	4/4/4/4	-
2	EDO	D	419	-	-	0/1/1/1	-
2	EDO	H	401	-	-	0/1/1/1	-
2	EDO	C	412	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	401	PEG	O2-C3-C4-O4
3	A	406	PEG	O1-C1-C2-O2
3	B	402	PEG	O2-C3-C4-O4
3	D	408	PEG	O1-C1-C2-O2
3	C	404	PEG	C4-C3-O2-C2
3	D	402	PEG	C1-C2-O2-C3
3	D	413	PEG	C1-C2-O2-C3
3	E	401	PEG	C4-C3-O2-C2
3	D	402	PEG	O2-C3-C4-O4
3	C	407	PEG	C4-C3-O2-C2
3	B	402	PEG	C1-C2-O2-C3
3	D	405	PEG	C4-C3-O2-C2
2	H	410	EDO	O1-C1-C2-O2
3	D	407	PEG	C1-C2-O2-C3
3	D	407	PEG	O1-C1-C2-O2
3	A	406	PEG	C1-C2-O2-C3
3	A	406	PEG	C4-C3-O2-C2
3	E	401	PEG	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	408	EDO	O1-C1-C2-O2
2	G	403	EDO	O1-C1-C2-O2
3	C	407	PEG	O2-C3-C4-O4
3	A	406	PEG	O2-C3-C4-O4

There are no ring outliers.

35 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	413	PEG	1	0
3	D	408	PEG	1	0
2	D	403	EDO	3	0
2	H	411	EDO	1	0
2	D	404	EDO	1	0
2	G	403	EDO	1	0
2	E	406	EDO	2	0
2	C	415	EDO	1	0
2	H	408	EDO	1	0
2	A	411	EDO	1	0
2	B	404	EDO	2	0
2	A	409	EDO	1	0
2	E	411	EDO	1	0
3	B	402	PEG	2	0
3	D	405	PEG	2	0
3	H	405	PEG	1	0
2	B	403	EDO	2	0
2	G	404	EDO	2	0
2	E	412	EDO	2	0
2	A	402	EDO	1	0
3	E	401	PEG	1	0
2	H	410	EDO	3	0
2	C	405	EDO	2	0
2	E	410	EDO	1	0
2	H	406	EDO	1	0
2	C	401	EDO	1	0
2	C	402	EDO	1	0
2	D	416	EDO	1	0
2	A	408	EDO	1	0
3	D	402	PEG	2	0
2	B	401	EDO	2	0
2	C	409	EDO	1	0
2	D	411	EDO	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	404	PEG	5	0
2	A	401	EDO	2	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	371/379 (97%)	-0.12	3 (0%) 82 79	28, 40, 67, 116	0
1	B	365/379 (96%)	0.02	12 (3%) 49 40	28, 44, 80, 94	0
1	C	370/379 (97%)	-0.33	4 (1%) 78 75	24, 36, 58, 99	0
1	D	365/379 (96%)	-0.25	6 (1%) 70 66	23, 36, 63, 87	0
1	E	362/379 (95%)	0.04	13 (3%) 46 38	31, 47, 74, 115	0
1	F	363/379 (95%)	0.17	10 (2%) 55 48	35, 49, 84, 110	0
1	G	366/379 (96%)	0.04	7 (1%) 66 61	34, 49, 76, 92	0
1	H	367/379 (96%)	-0.15	8 (2%) 62 56	28, 40, 66, 90	0
All	All	2929/3032 (96%)	-0.07	63 (2%) 62 56	23, 43, 74, 116	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	213	GLY	4.7
1	F	215	PRO	4.1
1	F	214	ALA	4.0
1	D	211	HIS	3.9
1	H	4	VAL	3.9
1	C	5	PRO	3.9
1	F	213	GLY	3.7
1	F	216	ALA	3.7
1	E	228	ALA	3.5
1	B	214	ALA	3.3
1	C	4	VAL	3.3
1	A	2	THR	3.2
1	H	212	GLY	3.1
1	H	296	ARG	3.0
1	D	214	ALA	2.9
1	F	228	ALA	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	5	PRO	2.8
1	E	242	GLY	2.8
1	F	238	ILE	2.8
1	B	250	HIS	2.8
1	G	11	GLY	2.7
1	F	371	THR	2.7
1	D	212	GLY	2.6
1	B	216	ALA	2.6
1	D	9	VAL	2.6
1	H	213	GLY	2.6
1	G	373	ALA	2.6
1	B	212	GLY	2.5
1	E	11	GLY	2.5
1	E	229	GLY	2.5
1	F	11	GLY	2.5
1	G	228	ALA	2.5
1	F	212	GLY	2.5
1	E	225	VAL	2.5
1	E	214	ALA	2.5
1	H	302	VAL	2.4
1	B	211	HIS	2.4
1	E	365	GLY	2.4
1	H	211	HIS	2.3
1	C	7	ASN	2.3
1	B	210	LEU	2.3
1	G	371	THR	2.3
1	B	372	THR	2.3
1	E	227	ARG	2.3
1	H	216	ALA	2.2
1	G	372	THR	2.2
1	A	7	ASN	2.2
1	E	10	PRO	2.2
1	E	230	ASP	2.2
1	H	214	ALA	2.2
1	D	217	ARG	2.1
1	E	215	PRO	2.1
1	F	370	LEU	2.1
1	B	228	ALA	2.1
1	D	370	LEU	2.1
1	E	217	ARG	2.1
1	G	238	ILE	2.1
1	B	324	PHE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	295	ASP	2.0
1	B	10	PRO	2.0
1	G	296	ARG	2.0
1	B	230	ASP	2.0
1	E	216	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	EDO	A	407	4/4	0.59	0.21	70,72,75,80	0
2	EDO	E	403	4/4	0.67	0.20	57,60,68,73	0
2	EDO	A	410	4/4	0.69	0.24	43,45,55,72	0
2	EDO	E	405	4/4	0.70	0.29	52,53,57,61	0
2	EDO	F	404	4/4	0.72	0.19	54,59,66,68	0
2	EDO	G	402	4/4	0.74	0.14	57,60,60,60	0
2	EDO	F	401	4/4	0.75	0.18	52,58,63,64	0
2	EDO	A	405	4/4	0.75	0.14	60,62,63,67	0
2	EDO	D	421	4/4	0.75	0.15	52,56,64,72	0
2	EDO	E	404	4/4	0.76	0.21	52,53,56,60	0
2	EDO	D	416	4/4	0.76	0.24	41,42,59,61	0
2	EDO	G	401	4/4	0.76	0.18	55,60,61,62	0
2	EDO	E	411	4/4	0.76	0.21	62,67,68,79	0
3	PEG	C	407	7/7	0.76	0.16	50,55,63,64	0
2	EDO	G	403	4/4	0.77	0.21	55,59,64,76	0
2	EDO	C	413	4/4	0.77	0.19	52,54,55,62	0
3	PEG	D	405	7/7	0.77	0.28	33,49,57,59	0
4	SO4	C	419	5/5	0.77	0.09	96,100,115,132	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	H	408	4/4	0.78	0.17	40,49,50,53	0
2	EDO	H	406	4/4	0.78	0.21	52,54,55,71	0
3	PEG	C	404	7/7	0.79	0.31	39,47,58,68	0
2	EDO	G	405	4/4	0.79	0.12	58,59,64,68	0
2	EDO	A	404	4/4	0.79	0.20	55,62,70,76	0
3	PEG	D	413	7/7	0.79	0.19	50,52,59,62	0
4	SO4	C	418	5/5	0.79	0.16	75,81,99,104	0
2	EDO	C	401	4/4	0.79	0.23	51,54,57,69	0
2	EDO	E	409	4/4	0.80	0.17	48,55,56,60	0
2	EDO	H	409	4/4	0.80	0.14	58,59,60,68	0
2	EDO	B	404	4/4	0.81	0.16	55,57,58,66	0
2	EDO	D	406	4/4	0.81	0.23	40,45,45,50	0
2	EDO	H	407	4/4	0.82	0.18	54,56,63,66	0
3	PEG	E	401	7/7	0.82	0.29	44,51,64,65	0
2	EDO	D	401	4/4	0.82	0.18	43,48,52,58	0
2	EDO	D	414	4/4	0.82	0.15	53,53,62,73	0
2	EDO	B	405	4/4	0.83	0.20	52,55,67,70	0
2	EDO	H	403	4/4	0.83	0.17	45,51,56,58	0
2	EDO	D	415	4/4	0.83	0.25	49,53,56,58	0
3	PEG	D	408	7/7	0.83	0.24	48,55,62,65	0
2	EDO	A	401	4/4	0.83	0.25	35,39,40,42	0
2	EDO	D	420	4/4	0.83	0.14	46,47,50,52	0
2	EDO	C	402	4/4	0.83	0.30	39,40,52,57	0
2	EDO	H	410	4/4	0.83	0.27	47,49,56,58	0
4	SO4	F	406	5/5	0.83	0.16	87,92,106,118	0
4	SO4	H	413	5/5	0.83	0.20	67,76,103,106	0
2	EDO	A	409	4/4	0.84	0.16	55,59,59,60	0
2	EDO	A	408	4/4	0.84	0.21	52,55,57,59	0
2	EDO	D	417	4/4	0.84	0.21	51,52,54,56	0
2	EDO	D	418	4/4	0.84	0.24	36,46,50,55	0
2	EDO	C	410	4/4	0.84	0.14	54,55,60,66	0
2	EDO	C	411	4/4	0.84	0.19	55,55,58,65	0
2	EDO	F	403	4/4	0.84	0.15	62,67,68,71	0
2	EDO	E	412	4/4	0.85	0.29	40,44,51,60	0
2	EDO	H	411	4/4	0.85	0.12	56,59,59,61	0
4	SO4	A	414	5/5	0.85	0.13	73,81,101,104	0
2	EDO	C	408	4/4	0.85	0.12	52,55,56,64	0
2	EDO	B	406	4/4	0.85	0.17	46,55,56,57	0
2	EDO	D	411	4/4	0.85	0.25	47,52,53,57	0
2	EDO	H	402	4/4	0.85	0.17	51,54,56,57	0
2	EDO	C	403	4/4	0.86	0.23	52,53,55,57	0
2	EDO	D	409	4/4	0.86	0.14	51,52,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	A	411	4/4	0.86	0.13	51,55,56,58	0
4	SO4	E	414	5/5	0.86	0.16	69,75,85,95	0
4	SO4	E	415	5/5	0.86	0.11	82,85,100,107	0
3	PEG	A	406	7/7	0.86	0.14	47,56,62,63	0
2	EDO	D	404	4/4	0.86	0.21	39,40,51,57	0
2	EDO	E	410	4/4	0.87	0.17	52,52,54,58	0
2	EDO	C	406	4/4	0.87	0.17	49,50,52,54	0
2	EDO	E	402	4/4	0.87	0.10	59,59,63,64	0
2	EDO	C	414	4/4	0.87	0.13	49,54,54,57	0
2	EDO	C	415	4/4	0.87	0.14	32,43,47,58	0
2	EDO	B	403	4/4	0.87	0.25	42,46,51,57	0
2	EDO	E	408	4/4	0.87	0.20	43,47,49,50	0
2	EDO	D	403	4/4	0.87	0.22	37,38,42,44	0
4	SO4	B	407	5/5	0.88	0.18	74,77,83,84	0
2	EDO	C	412	4/4	0.88	0.12	48,48,56,62	0
3	PEG	D	407	7/7	0.88	0.14	50,51,60,68	0
2	EDO	D	410	4/4	0.88	0.24	47,51,52,52	0
3	PEG	B	402	7/7	0.88	0.23	51,56,60,62	0
4	SO4	F	405	5/5	0.88	0.14	51,66,87,87	0
2	EDO	H	404	4/4	0.88	0.11	49,51,57,57	0
2	EDO	E	407	4/4	0.88	0.12	47,51,53,54	0
2	EDO	C	416	4/4	0.89	0.12	54,55,56,58	0
2	EDO	B	401	4/4	0.89	0.20	34,35,43,52	0
2	EDO	H	401	4/4	0.89	0.16	57,58,59,64	0
2	EDO	A	403	4/4	0.89	0.18	43,56,57,71	0
2	EDO	E	406	4/4	0.89	0.15	49,50,52,61	0
2	EDO	C	409	4/4	0.89	0.22	46,47,49,63	0
4	SO4	G	406	5/5	0.90	0.13	63,72,86,89	0
3	PEG	D	402	7/7	0.91	0.13	36,40,51,54	0
2	EDO	C	405	4/4	0.91	0.27	37,45,47,51	0
2	EDO	A	402	4/4	0.91	0.21	39,41,47,47	0
2	EDO	G	404	4/4	0.91	0.20	54,58,62,69	0
3	PEG	H	405	7/7	0.92	0.10	46,50,53,58	0
4	SO4	A	413	5/5	0.92	0.16	58,74,78,79	0
2	EDO	F	402	4/4	0.92	0.12	51,59,62,66	0
4	SO4	H	412	5/5	0.93	0.11	44,64,73,75	0
2	EDO	D	412	4/4	0.93	0.21	39,45,54,56	0
4	SO4	C	417	5/5	0.94	0.20	51,53,75,79	0
4	SO4	E	413	5/5	0.95	0.13	50,59,67,67	0
2	EDO	D	419	4/4	0.95	0.07	43,45,47,53	0
4	SO4	A	412	5/5	0.97	0.08	50,54,58,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.