



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 07:03 PM GMT

PDB ID : 1HQS
Title : CRYSTAL STRUCTURE OF ISOCITRATE DEHYDROGENASE FROM
BACILLUS SUBTILIS
Authors : Singh, S.K.; Matsuno, K.; LaPorte, D.C.; Banaszak, L.J.
Deposited on : 2000-12-19
Resolution : 1.55 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

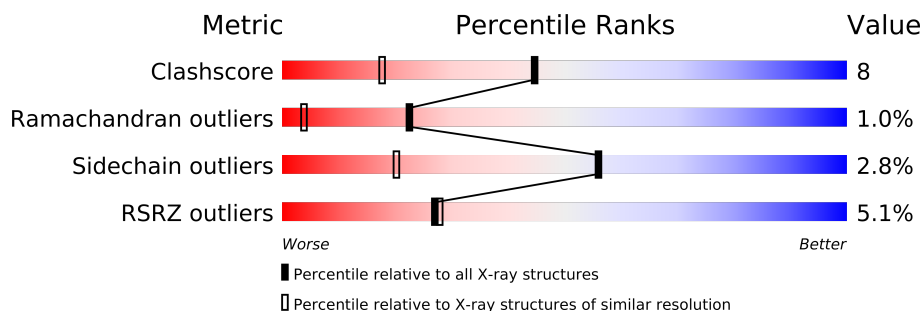
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.55 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))
Clashscore	79885	1249 (1.58-1.54)
Ramachandran outliers	78287	1212 (1.58-1.54)
Sidechain outliers	78261	1210 (1.58-1.54)
RSRZ outliers	66119	1117 (1.58-1.54)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	423	
1	B	423	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	CIT	A	425	X	-
3	PGO	A	901	-	X
3	PGO	A	902	-	X
3	PGO	B	903	-	X
3	PGO	B	904	-	X
3	PGO	B	905	-	X
4	PGR	A	906	-	X
4	PGR	A	907	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7445 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

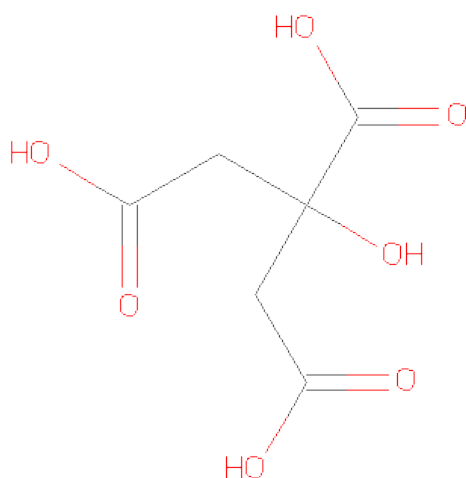
- Molecule 1 is a protein called ISOCITRATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	423	Total	C	N	O	S	10	15	0
			3396	2160	568	657	11			
1	B	423	Total	C	N	O	S	0	13	0
			3380	2147	562	658	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	118	CME	CYS	MODIFIED RESIDUE	UNP P39126
B	118	CME	CYS	MODIFIED RESIDUE	UNP P39126

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: C₆H₈O₇).



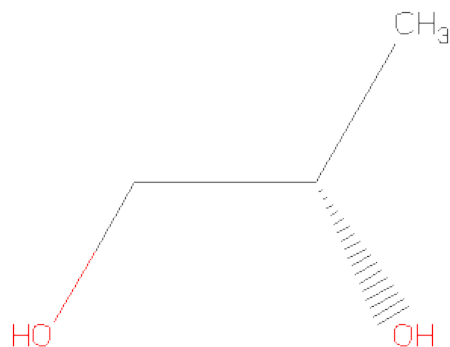
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		

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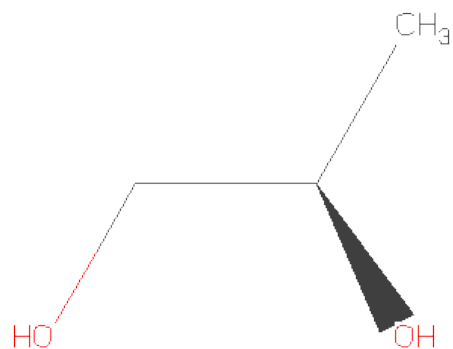
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	2	0
			13	6	7		

- Molecule 3 is S-1,2-PROPANEDIOL (three-letter code: PGO) (formula: $C_3H_8O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			5	3	2		
3	A	1	Total	C	O	0	0
			5	3	2		
3	B	1	Total	C	O	0	0
			5	3	2		
3	B	1	Total	C	O	0	0
			5	3	2		
3	B	1	Total	C	O	0	0
			5	3	2		

- Molecule 4 is R-1,2-PROPANEDIOL (three-letter code: PGR) (formula: $C_3H_8O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			5	3	2		
4	A	1	Total	C	O	0	0
			5	3	2		

- Molecule 5 is water.

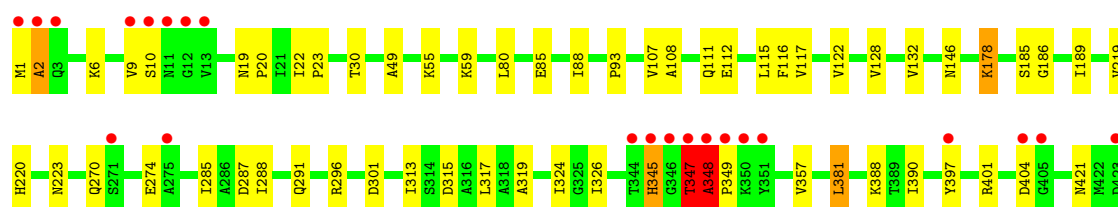
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	309	Total	O	0	0
			309	309		
5	B	299	Total	O	0	0
			299	299		

3 Residue-property plots

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

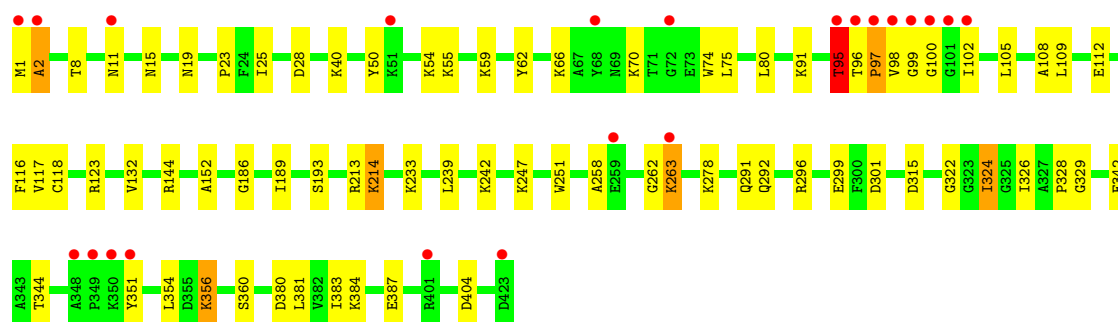
• Molecule 1: ISOCITRATE DEHYDROGENASE

Chain A: 



• Molecule 1: ISOCITRATE DEHYDROGENASE

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.69Å 73.29Å 80.90Å 90.00° 109.48° 90.00°	Depositor
Resolution (Å)	20.00 – 1.55 19.72 – 1.50	Depositor EDS
% Data completeness (in resolution range)	92.9 (20.00-1.55) 88.5 (19.72-1.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 1.50Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.202 , 0.249 0.208 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	18.4	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 48.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 114794 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7445	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGO, CME, PGR, CIT

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	0.46	0/3449	0.73	3/4665 (0.1%)
1	B	0.48	0/3423	0.68	1/4632 (0.0%)
All	All	0.47	0/6872	0.71	4/9297 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	347	THR	N-CA-C	9.29	136.10	111.00
1	A	348	ALA	N-CA-C	-8.49	88.07	111.00
1	A	186	GLY	N-CA-C	-6.70	96.36	113.10
1	B	186	GLY	N-CA-C	-5.89	98.38	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3396	0	3386	54	0
1	B	3380	0	3360	71	0
2	A	13	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	13	0	3	0	0
3	A	10	0	16	1	0
3	B	15	0	24	7	0
4	A	10	0	16	6	0
5	A	309	0	0	6	0
5	B	299	0	0	13	0
All	All	7445	0	6809	116	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (116) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:288[A]:ILE:HD11	4:A:907:PGR:H32	1.18	1.18
1:B:1:MET:HB3	5:B:1297:HOH:O	1.44	1.17
1:A:288[A]:ILE:CD1	4:A:907:PGR:H32	1.81	1.11
1:B:40[B]:LYS:CE	5:B:1243:HOH:O	2.08	1.01
1:B:40[B]:LYS:HE3	5:B:1243:HOH:O	1.59	1.01
1:A:347:THR:HB	1:A:349:PRO:HD3	1.42	0.98
1:B:70:LYS:HD2	5:B:1477:HOH:O	1.67	0.93
1:A:288[A]:ILE:CD1	4:A:907:PGR:C3	2.51	0.88
1:B:96[B]:THR:HG23	1:B:102:ILE:HD11	1.56	0.86
1:A:108:ALA:O	1:A:112[B]:GLU:HG2	1.81	0.81
1:A:288[A]:ILE:HD11	4:A:907:PGR:C3	2.07	0.78
1:B:213:ARG:HD2	1:B:301:ASP:OD2	1.83	0.78
1:A:288[A]:ILE:HD12	4:A:907:PGR:C3	2.17	0.74
1:A:348:ALA:H	1:A:349:PRO:HD3	1.52	0.74
1:B:351:TYR:CD2	1:B:356:LYS:HD2	2.23	0.74
1:B:296:ARG:HB3	1:B:299:GLU:HG3	1.71	0.72
1:B:351:TYR:HA	1:B:354:LEU:HD12	1.72	0.72
1:A:9:VAL:HG11	5:A:1568:HOH:O	1.91	0.71
1:A:288[A]:ILE:HD12	4:A:907:PGR:H33	1.74	0.70
1:A:347:THR:HB	1:A:349:PRO:CD	2.18	0.70
1:B:95[B]:THR:HB	1:B:96[B]:THR:HG22	1.75	0.68
1:B:28:ASP:OD1	1:B:95[B]:THR:HG23	1.93	0.68
1:A:80:LEU:HD22	1:A:112[A]:GLU:HG2	1.75	0.67
3:B:905:PGO:H11	5:B:1579:HOH:O	1.95	0.66
1:B:291[B]:GLN:OE1	5:B:1344:HOH:O	2.14	0.65
1:B:251:TRP:CE2	3:B:904:PGO:H2	2.32	0.65
1:A:30:THR:HB	1:A:357:VAL:HG21	1.79	0.64
1:B:40[B]:LYS:HE2	5:B:1243:HOH:O	1.81	0.64
1:B:108:ALA:O	1:B:112:GLU:HG3	1.97	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:62:TYR:HE1	1:B:66:LYS:HE2	1.63	0.63
1:A:30:THR:HG21	1:A:357:VAL:HG11	1.82	0.62
1:B:247[B]:LYS:HE3	5:B:1532:HOH:O	2.01	0.61
1:A:93:PRO:HD3	5:A:1500:HOH:O	2.00	0.60
1:B:97[B]:PRO:HG2	1:B:100:GLY:O	2.01	0.60
1:A:23:PRO:HA	1:A:59:LYS:O	2.02	0.60
1:A:223:ASN:HB3	1:B:98:VAL:HG22	1.84	0.59
1:A:22[B]:ILE:HD12	1:A:88:ILE:HD11	1.85	0.59
1:B:1:MET:HG2	1:B:2:ALA:H	1.67	0.58
5:A:1105:HOH:O	3:B:903:PGO:H12	2.02	0.58
1:B:50:TYR:CD2	1:B:54:LYS:HD2	2.37	0.58
1:A:347:THR:HA	5:A:1287:HOH:O	2.03	0.58
1:B:251:TRP:CZ2	3:B:904:PGO:H2	2.39	0.58
1:A:348:ALA:N	1:A:349:PRO:CD	2.67	0.57
1:A:270:GLN:O	1:A:274:GLU:HG2	2.05	0.56
1:B:326:ILE:HG22	1:B:360:SER:HB2	1.88	0.56
1:B:118[B]:CME:OH	1:B:118[B]:CME:SG	2.64	0.56
1:A:189:ILE:CD1	1:B:189:ILE:CD1	2.84	0.54
1:A:348:ALA:H	1:A:349:PRO:CD	2.20	0.54
1:A:348:ALA:N	1:A:349:PRO:HD3	2.21	0.54
1:B:322:GLY:HA2	5:B:1138:HOH:O	2.08	0.54
1:A:189:ILE:HD13	1:B:189:ILE:CD1	2.37	0.54
1:A:219:VAL:HG11	1:A:313:ILE:HD11	1.91	0.53
1:B:96[B]:THR:CG2	1:B:102:ILE:HD11	2.34	0.53
1:B:118[B]:CME:HB2	1:B:144:ARG:HB3	1.90	0.52
1:A:189:ILE:HD13	1:B:189:ILE:HD13	1.92	0.52
1:A:319:ALA:HB2	1:B:291[B]:GLN:HG2	1.92	0.52
1:B:351:TYR:CE2	1:B:356:LYS:HD2	2.45	0.51
1:B:263:LYS:HD3	1:B:263:LYS:N	2.26	0.51
1:B:263:LYS:CE	1:B:263:LYS:H	2.25	0.50
1:B:23:PRO:HA	1:B:59:LYS:O	2.11	0.50
1:A:401:ARG:CZ	5:A:1549:HOH:O	2.60	0.50
1:B:118[A]:CME:HZ3	1:B:329:GLY:HA3	1.92	0.50
1:A:178:LYS:HB2	1:A:178:LYS:HZ3	1.76	0.49
1:B:258:ALA:HA	1:B:262:GLY:O	2.12	0.48
1:B:62:TYR:CE1	1:B:66:LYS:HE2	2.47	0.48
1:A:326:ILE:HG12	3:A:901:PGO:H32	1.96	0.48
1:A:88:ILE:O	1:A:88:ILE:HG13	2.13	0.48
1:B:383:ILE:O	1:B:387:GLU:HG3	2.14	0.47
1:B:263:LYS:CD	1:B:263:LYS:N	2.78	0.46
1:A:20:PRO:HD2	1:A:55:LYS:O	2.15	0.46
1:A:107:VAL:O	1:A:111[B]:GLN:HG3	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:116:PHE:CD1	1:B:117:VAL:HG23	2.50	0.46
1:A:19:ASN:HA	1:A:55:LYS:O	2.14	0.46
1:A:388[A]:LYS:HE2	5:A:1166:HOH:O	2.15	0.46
1:A:287:ASP:HB2	1:B:315:ASP:OD1	2.16	0.46
1:A:178:LYS:HD2	1:B:152:ALA:O	2.15	0.45
1:B:214:LYS:HA	1:B:214:LYS:HE3	1.98	0.45
1:B:1:MET:HG2	1:B:2:ALA:N	2.32	0.45
1:A:185[B]:SER:HB3	1:B:193:SER:HB3	1.98	0.45
1:B:263:LYS:CD	1:B:263:LYS:H	2.29	0.45
1:B:380:ASP:O	1:B:384:LYS:HG2	2.17	0.45
1:A:49:ALA:HB2	1:A:381:LEU:HD22	1.98	0.44
1:B:351:TYR:HA	1:B:354:LEU:CD1	2.45	0.44
1:A:291:GLN:NE2	1:B:324:ILE:HG22	2.32	0.44
1:B:91:LYS:HE3	1:B:342:GLU:OE2	2.17	0.44
1:B:278:LYS:HE3	5:B:1401:HOH:O	2.16	0.44
1:A:132:VAL:HA	1:B:132:VAL:HA	1.99	0.44
1:B:263:LYS:HE2	1:B:263:LYS:HB2	1.75	0.43
1:B:80:LEU:HD21	1:B:109:LEU:HD23	2.00	0.43
1:A:128:VAL:HG23	1:A:390:ILE:HG21	1.99	0.43
1:A:347:THR:HB	1:A:348:ALA:H	1.44	0.43
1:A:388[A]:LYS:HD2	1:A:421:ASN:HB3	1.99	0.43
1:B:233:LYS:NZ	5:B:1440:HOH:O	2.40	0.43
1:B:118[A]:CME:OH	1:B:344:THR:HG22	2.18	0.43
1:B:74:TRP:CZ3	1:B:95[B]:THR:HG21	2.54	0.43
1:A:315:ASP:O	1:B:291[B]:GLN:HG2	2.18	0.43
1:B:351:TYR:HD2	1:B:356:LYS:HD2	1.78	0.43
1:B:8:THR:CG2	1:B:15:ASN:HB2	2.48	0.43
1:B:123:ARG:HG2	3:B:905:PGO:H12	2.00	0.42
1:B:324:ILE:HG13	1:B:324:ILE:H	1.29	0.42
1:A:115:LEU:O	1:A:146:ASN:HB3	2.19	0.42
1:B:292:GLN:NE2	5:B:1133:HOH:O	2.44	0.42
1:A:122:VAL:HG11	1:A:317:LEU:HB3	2.01	0.42
1:A:220:HIS:O	1:A:285:ILE:HA	2.20	0.42
1:A:116:PHE:CD1	1:A:117:VAL:HG23	2.55	0.41
1:A:347:THR:O	1:A:348:ALA:HB3	2.20	0.41
1:B:19:ASN:HA	1:B:55:LYS:O	2.20	0.41
1:B:8:THR:HG22	1:B:15:ASN:HB2	2.02	0.41
1:A:324:ILE:HG23	1:A:345[B]:HIS:HA	2.02	0.41
1:B:123:ARG:HD3	3:B:905:PGO:H12	2.03	0.41
1:B:15:ASN:ND2	5:B:1551:HOH:O	2.54	0.41
1:A:1:MET:O	1:A:2:ALA:O	2.38	0.40
1:B:95[B]:THR:OG1	1:B:105:LEU:HD12	2.22	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:328:PRO:HG3	3:B:905:PGO:H32	2.04	0.40
1:A:397:TYR:O	1:A:401:ARG:HG2	2.21	0.40
1:B:25:ILE:HB	1:B:91:LYS:HB2	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	435/423 (103%)	417 (96%)	13 (3%)	5 (1%)	21	3
1	B	432/423 (102%)	413 (96%)	13 (3%)	6 (1%)	16	2
All	All	867/846 (102%)	830 (96%)	26 (3%)	11 (1%)	22	2

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ALA
1	A	345[A]	HIS
1	A	345[B]	HIS
1	B	95[A]	THR
1	B	95[B]	THR
1	B	97[A]	PRO
1	B	97[B]	PRO
1	B	2	ALA
1	A	347	THR
1	A	348	ALA
1	B	99	GLY

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	357/343 (104%)	349 (98%)	8 (2%)	64	31
1	B	355/343 (104%)	342 (96%)	13 (4%)	45	12
All	All	712/686 (104%)	691 (97%)	21 (3%)	56	19

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	10	SER
1	A	85	GLU
1	A	178	LYS
1	A	296	ARG
1	A	301	ASP
1	A	381	LEU
1	A	404	ASP
1	B	11[A]	ASN
1	B	11[B]	ASN
1	B	75	LEU
1	B	95[A]	THR
1	B	95[B]	THR
1	B	214	LYS
1	B	239	LEU
1	B	242	LYS
1	B	263	LYS
1	B	324	ILE
1	B	356	LYS
1	B	381	LEU
1	B	404	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	GLN
1	A	291	GLN
1	A	376	ASN
1	B	3	GLN
1	B	172	ASN
1	B	292	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	CME	A	118	1	9,9,10	6.20	3 (33%)	7,9,11	5.32	2 (28%)
1	CME	B	118[A]	1	9,9,10	6.16	3 (33%)	7,9,11	5.00	3 (42%)
1	CME	B	118[B]	1	9,9,10	6.18	3 (33%)	7,9,11	4.85	2 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CME	A	118	1	-	0/6/8/10	0/0/0/0
1	CME	B	118[A]	1	-	0/6/8/10	0/0/0/0
1	CME	B	118[B]	1	-	0/6/8/10	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	118	CME	O-C	18.30	1.24	1.11
1	B	118[B]	CME	O-C	18.23	1.24	1.11
1	B	118[A]	CME	O-C	18.16	1.23	1.11
1	A	118	CME	CA-C	2.52	1.53	1.48
1	B	118[B]	CME	CA-C	2.50	1.52	1.48
1	B	118[A]	CME	CA-C	2.30	1.52	1.48
1	B	118[A]	CME	OH-CZ	-2.16	1.30	1.42
1	B	118[B]	CME	OH-CZ	-2.11	1.30	1.42
1	A	118	CME	OH-CZ	-2.04	1.31	1.42

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	CME	C-CA-N	-13.74	100.11	113.83
1	B	118[A]	CME	C-CA-N	-12.84	101.00	113.83
1	B	118[B]	CME	C-CA-N	-12.59	101.26	113.83
1	B	118[B]	CME	OH-CZ-CE	2.27	120.74	110.86
1	B	118[A]	CME	OH-CZ-CE	2.24	120.61	110.86
1	A	118	CME	OH-CZ-CE	2.22	120.52	110.86
1	B	118[A]	CME	CB-CA-N	2.16	113.93	110.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

9 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	CIT	A	425	-	12,12,12	5.97	9 (75%)	17,17,17	3.90	11 (64%)
3	PGO	A	901	-	4,4,4	1.71	1 (25%)	4,4,4	2.34	3 (75%)
3	PGO	A	902	-	4,4,4	2.59	1 (25%)	4,4,4	1.40	0
4	PGR	A	906	-	4,4,4	1.72	1 (25%)	4,4,4	2.34	3 (75%)
4	PGR	A	907	-	4,4,4	1.71	1 (25%)	4,4,4	2.35	3 (75%)
2	CIT	B	825	-	12,12,12	8.01	7 (58%)	17,17,17	4.15	12 (70%)
3	PGO	B	903	-	4,4,4	1.46	1 (25%)	4,4,4	3.45	1 (25%)
3	PGO	B	904	-	4,4,4	1.69	1 (25%)	4,4,4	2.36	3 (75%)
3	PGO	B	905	-	4,4,4	4.85	1 (25%)	4,4,4	2.37	1 (25%)

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	CIT	A	425	-	-	0/16/16/16	0/0/0/0
3	PGO	A	901	-	-	0/2/2/2	0/0/0/0
3	PGO	A	902	-	-	0/2/2/2	0/0/0/0
4	PGR	A	906	-	-	0/2/2/2	0/0/0/0
4	PGR	A	907	-	-	0/2/2/2	0/0/0/0
2	CIT	B	825	-	-	0/16/16/16	0/0/0/0
3	PGO	B	903	-	-	0/2/2/2	0/0/0/0
3	PGO	B	904	-	-	0/2/2/2	0/0/0/0
3	PGO	B	905	-	-	0/2/2/2	0/0/0/0

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	825	CIT	C4-C3	-23.41	1.22	1.53
2	A	425	CIT	C4-C3	-17.67	1.30	1.53
3	B	905	PGO	C1-C2	9.59	1.74	1.51
2	B	825	CIT	O7-C3	8.05	1.61	1.43
2	B	825	CIT	O3-C5	7.86	1.50	1.22
2	B	825	CIT	C2-C3	-5.89	1.45	1.53
2	A	425	CIT	O5-C6	5.70	1.41	1.22
2	A	425	CIT	O3-C5	5.56	1.42	1.22
2	B	825	CIT	O5-C6	5.50	1.41	1.22
3	A	902	PGO	C1-C2	5.12	1.63	1.51
2	B	825	CIT	C3-C6	-4.10	1.48	1.53
2	A	425	CIT	O7-C3	3.44	1.50	1.43
2	A	425	CIT	C2-C3	3.34	1.58	1.53
4	A	906	PGR	C1-C2	3.28	1.58	1.51
3	A	901	PGO	C1-C2	3.26	1.58	1.51
4	A	907	PGR	C1-C2	3.25	1.58	1.51
3	B	904	PGO	C1-C2	3.23	1.58	1.51
2	A	425	CIT	O4-C5	-3.17	1.19	1.30
3	B	903	PGO	C1-C2	2.86	1.57	1.51
2	B	825	CIT	C4-C5	-2.69	1.41	1.50
2	A	425	CIT	O6-C6	2.54	1.39	1.30
2	A	425	CIT	C4-C5	-2.24	1.42	1.50
2	A	425	CIT	C3-C6	-2.22	1.50	1.53

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	825	CIT	O7-C3-C4	-13.23	82.55	109.22
2	A	425	CIT	C3-C4-C5	8.28	133.83	113.77
2	A	425	CIT	O7-C3-C4	-7.83	93.44	109.22
3	B	903	PGO	O1-C1-C2	6.62	125.43	110.60
2	B	825	CIT	C4-C3-C6	6.55	125.28	110.12
2	A	425	CIT	O4-C5-C4	4.67	131.06	114.63
2	A	425	CIT	O2-C1-O1	4.66	135.14	123.30
3	B	905	PGO	O1-C1-C2	4.59	120.89	110.60
2	B	825	CIT	O4-C5-C4	4.05	128.91	114.63
2	A	425	CIT	O7-C3-C2	-3.97	101.22	109.22
2	A	425	CIT	O6-C6-C3	3.39	117.82	112.89
2	A	425	CIT	O1-C1-C2	-3.37	112.07	122.74
2	A	425	CIT	O4-C5-O3	-3.33	114.82	123.30
2	A	425	CIT	C4-C3-C2	3.28	117.14	109.52
2	A	425	CIT	C4-C3-C6	3.20	117.53	110.12
2	B	825	CIT	O2-C1-O1	2.92	130.74	123.30
2	B	825	CIT	O3-C5-C4	-2.91	113.54	122.74
2	A	425	CIT	O3-C5-C4	-2.75	114.02	122.74
4	A	906	PGR	C3-C2-C1	-2.68	103.79	112.41
4	A	907	PGR	C3-C2-C1	-2.68	103.80	112.41
3	A	901	PGO	C3-C2-C1	-2.66	103.86	112.41
4	A	906	PGR	O1-C1-C2	-2.65	104.67	110.60
4	A	907	PGR	O1-C1-C2	-2.65	104.67	110.60
3	B	904	PGO	C3-C2-C1	-2.65	103.90	112.41
3	B	904	PGO	O1-C1-C2	-2.64	104.69	110.60
3	A	901	PGO	O1-C1-C2	-2.58	104.81	110.60
2	B	825	CIT	O4-C5-O3	-2.49	116.97	123.30
2	B	825	CIT	O1-C1-C2	-2.44	115.01	122.74
2	B	825	CIT	C3-C4-C5	2.43	119.66	113.77
3	B	904	PGO	O2-C2-C1	-2.43	101.02	109.63
2	B	825	CIT	C4-C3-C2	2.42	115.15	109.52
3	A	901	PGO	O2-C2-C1	-2.38	101.18	109.63
2	B	825	CIT	C3-C2-C1	2.33	119.42	113.77
4	A	907	PGR	O2-C2-C1	-2.26	101.64	109.63
4	A	906	PGR	O2-C2-C1	-2.25	101.65	109.63
2	B	825	CIT	O7-C3-C2	2.21	113.68	109.22
2	B	825	CIT	O7-C3-C6	-2.09	105.94	108.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	423/423 (100%)	0.28	22 (5%) 26 27	10, 20, 39, 54	3 (0%)
1	B	423/423 (100%)	0.27	22 (5%) 26 27	10, 20, 38, 65	0
All	All	846/846 (100%)	0.28	44 (5%) 27 27	10, 20, 39, 65	3 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	10.0
1	A	347	THR	9.8
1	B	2	ALA	6.8
1	B	96[A]	THR	6.7
1	A	1	MET	6.6
1	B	102	ILE	6.5
1	A	423	ASP	6.2
1	B	98	VAL	6.2
1	A	2	ALA	5.9
1	A	350	LYS	5.4
1	A	346[A]	GLY	5.3
1	B	97[A]	PRO	4.9
1	B	100	GLY	4.9
1	A	3	GLN	4.6
1	B	351	TYR	4.3
1	A	348	ALA	4.3
1	A	11	ASN	4.0
1	A	351	TYR	3.9
1	B	101	GLY	3.8
1	A	12	GLY	3.7
1	B	350	LYS	3.6
1	A	9	VAL	3.5
1	A	349	PRO	3.5
1	B	423	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	95[A]	THR	3.2
1	A	344	THR	3.2
1	A	13	VAL	3.1
1	B	99	GLY	3.1
1	B	68	TYR	3.0
1	B	72	GLY	2.9
1	B	51	LYS	2.8
1	B	263	LYS	2.7
1	A	345[A]	HIS	2.6
1	B	11[A]	ASN	2.5
1	A	271	SER	2.4
1	B	349	PRO	2.4
1	A	397	TYR	2.4
1	B	259	GLU	2.4
1	A	405	GLY	2.3
1	A	275	ALA	2.2
1	A	404	ASP	2.2
1	B	401	ARG	2.2
1	B	348	ALA	2.1
1	A	10	SER	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	CME	B	118[A]	10/11	0.14	4.36	10,14,21,27	10
1	CME	B	118[B]	10/11	0.14	4.26	14,20,28,31	10
1	CME	A	118	10/11	0.10	0.07	12,14,34,37	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	PGR	A	906	5/5	0.26	21.22	47,48,50,52	0
3	PGO	B	904	5/5	0.28	21.20	47,48,49,51	0
4	PGR	A	907	5/5	0.25	9.84	42,46,46,49	0
3	PGO	B	905	5/5	0.16	5.17	32,33,35,38	0
3	PGO	B	903	5/5	0.28	4.31	39,40,41,42	0
3	PGO	A	901	5/5	0.18	4.17	34,35,36,38	0
3	PGO	A	902	5/5	0.13	3.26	38,38,39,40	0
2	CIT	A	425	13/13	0.22	1.91	30,43,52,54	0
2	CIT	B	825	13/13	0.17	0.89	37,47,49,53	2

6.5 Other polymers ⓘ

There are no such residues in this entry.