



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:04 PM GMT

PDB ID : 2O2D
Title : Crystal structure of phosphoglucose isomerase from Trypanosoma brucei complexed with citrate
Authors : Arsenieva, D.; Mazock, G.H.; Appavu, B.L.; Jeffery, C.J.
Deposited on : 2006-11-29
Resolution : 1.90 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>

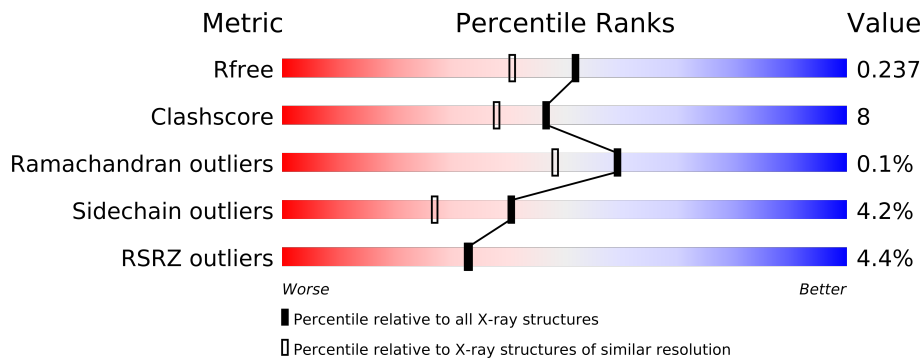
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.90 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}	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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	613	
1	B	613	
1	C	613	

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	5001	-	X
2	CIT	B	5002	-	X
3	GOL	A	7001	X	X
3	GOL	B	7002	X	-
3	GOL	C	7003	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14574 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.

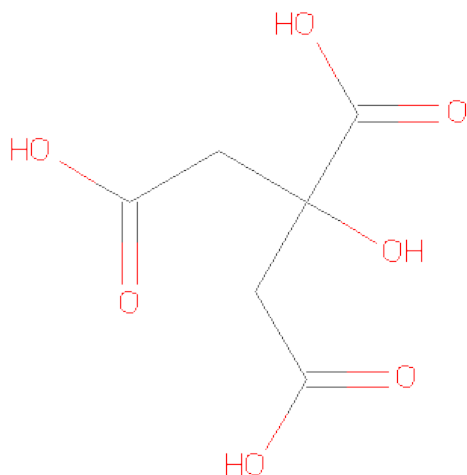
- Molecule 1 is a protein called Glucose-6-phosphate isomerase, glycosomal.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	568	Total	C	N	O	S	0	0	0
			4477	2846	786	830	15			
1	B	569	Total	C	N	O	S	0	0	0
			4488	2852	790	831	15			
1	C	561	Total	C	N	O	S	0	0	0
			4432	2818	778	821	15			

There are 21 discrepancies between the modelled and reference sequences:

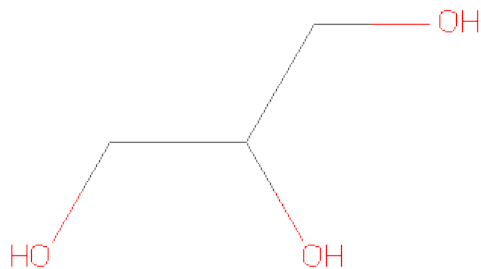
Chain	Residue	Modelled	Actual	Comment	Reference
A	77	THR	ALA	CONFLICT	UNP P13377
A	608	HIS	-	EXPRESSION TAG	UNP P13377
A	609	HIS	-	EXPRESSION TAG	UNP P13377
A	610	HIS	-	EXPRESSION TAG	UNP P13377
A	611	HIS	-	EXPRESSION TAG	UNP P13377
A	612	HIS	-	EXPRESSION TAG	UNP P13377
A	613	HIS	-	EXPRESSION TAG	UNP P13377
B	77	THR	ALA	CONFLICT	UNP P13377
B	608	HIS	-	EXPRESSION TAG	UNP P13377
B	609	HIS	-	EXPRESSION TAG	UNP P13377
B	610	HIS	-	EXPRESSION TAG	UNP P13377
B	611	HIS	-	EXPRESSION TAG	UNP P13377
B	612	HIS	-	EXPRESSION TAG	UNP P13377
B	613	HIS	-	EXPRESSION TAG	UNP P13377
C	77	THR	ALA	CONFLICT	UNP P13377
C	608	HIS	-	EXPRESSION TAG	UNP P13377
C	609	HIS	-	EXPRESSION TAG	UNP P13377
C	610	HIS	-	EXPRESSION TAG	UNP P13377
C	611	HIS	-	EXPRESSION TAG	UNP P13377
C	612	HIS	-	EXPRESSION TAG	UNP P13377
C	613	HIS	-	EXPRESSION TAG	UNP P13377

- 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		
2	B	1	Total	C	O	0	0
			13	6	7		
2	C	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 4 is water.

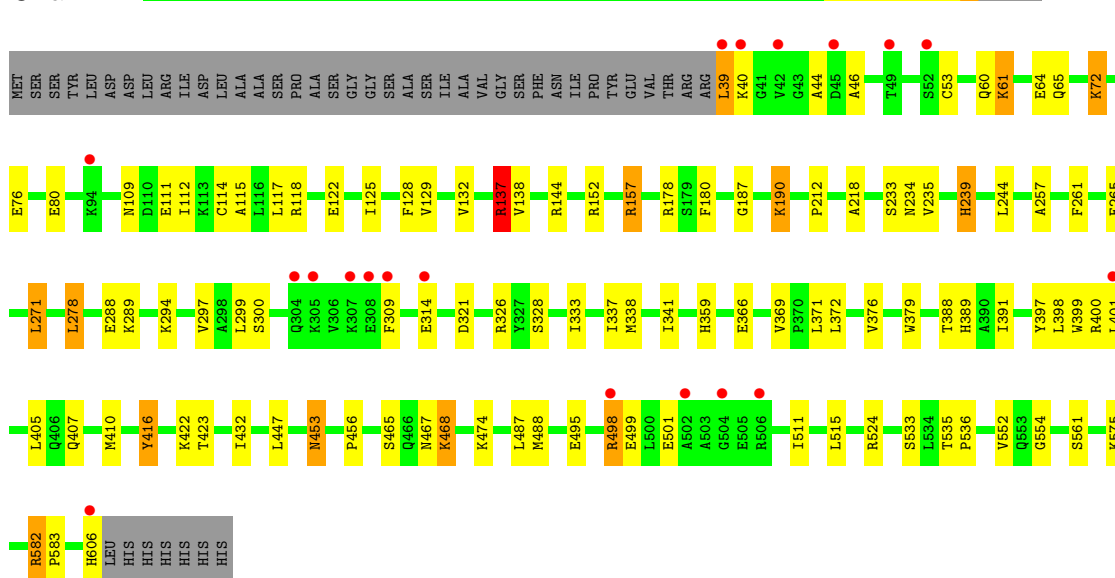
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	380	Total	O	0	0
			380	380		
4	B	421	Total	O	0	0
			421	421		
4	C	319	Total	O	0	0
			319	319		

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.

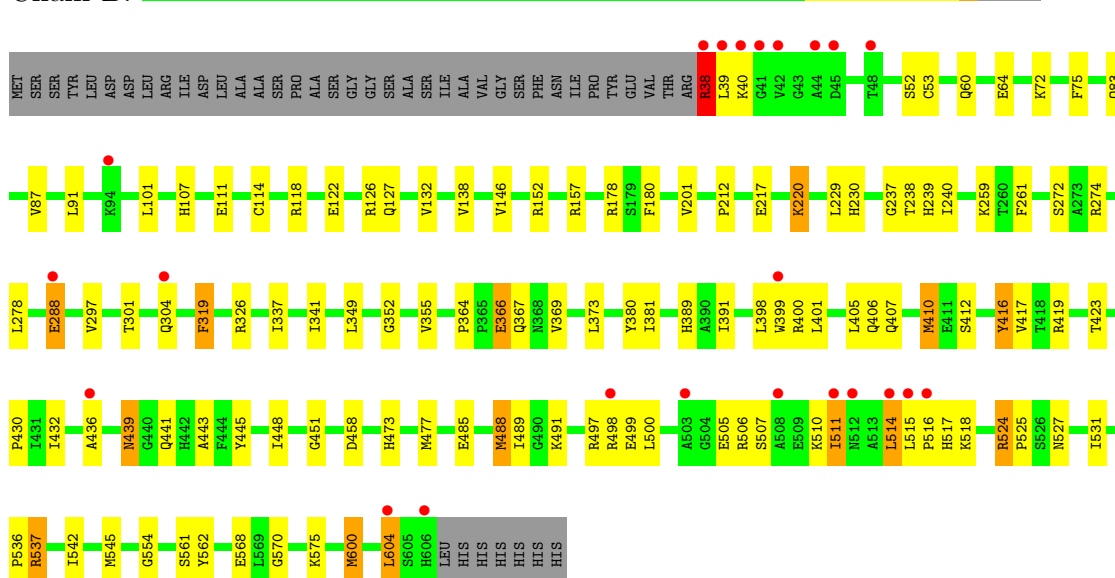
- Molecule 1: Glucose-6-phosphate isomerase, glycosomal

Chain A:



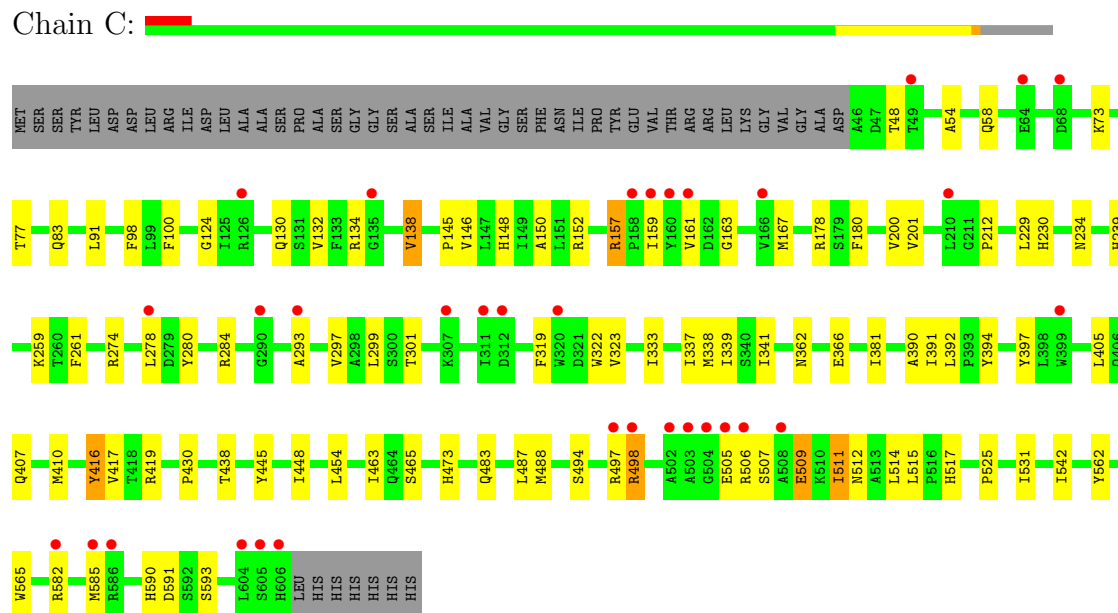
- Molecule 1: Glucose-6-phosphate isomerase, glycosomal

Chain B:



- Molecule 1: Glucose-6-phosphate isomerase, glycosomal

Chain C:



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	124.20Å 217.39Å 126.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.90 49.93 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.2 (40.00-1.90) 97.4 (49.93-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.82 (at 1.90Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.213 , 0.236 0.215 , 0.237	Depositor DCC
R_{free} test set	6569 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	17.8	Xtriage
Anisotropy	0.371	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 21.8	EDS
Estimated twinning fraction	0.048 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.033 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 130390 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14574	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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: GOL, 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	0.59	0/4575	0.76	5/6192 (0.1%)
1	B	0.66	0/4586	0.84	12/6206 (0.2%)
1	C	0.58	0/4530	0.76	6/6132 (0.1%)
All	All	0.61	0/13691	0.79	23/18530 (0.1%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	38	ARG	NE-CZ-NH2	7.32	123.96	120.30
1	C	419	ARG	NE-CZ-NH2	7.25	123.93	120.30
1	A	157	ARG	NE-CZ-NH2	7.17	123.89	120.30
1	B	506	ARG	NE-CZ-NH2	7.00	123.80	120.30
1	A	137	ARG	NE-CZ-NH2	7.00	123.80	120.30
1	B	537	ARG	NE-CZ-NH2	6.83	123.71	120.30
1	B	497	ARG	NE-CZ-NH2	6.82	123.71	120.30
1	B	498	ARG	NE-CZ-NH2	6.41	123.50	120.30
1	B	524	ARG	NE-CZ-NH2	6.41	123.50	120.30
1	B	419	ARG	NE-CZ-NH2	6.19	123.39	120.30
1	B	410	MET	CG-SD-CE	6.12	109.99	100.20
1	C	488	MET	CG-SD-CE	6.04	109.86	100.20
1	C	585	MET	CG-SD-CE	6.00	109.80	100.20
1	C	410	MET	CG-SD-CE	5.82	109.51	100.20
1	B	488	MET	CG-SD-CE	5.82	109.51	100.20
1	A	338	MET	CG-SD-CE	5.78	109.44	100.20
1	B	545	MET	CG-SD-CE	5.67	109.27	100.20
1	A	410	MET	CG-SD-CE	5.63	109.21	100.20
1	C	338	MET	CG-SD-CE	5.62	109.19	100.20
1	A	488	MET	CG-SD-CE	5.56	109.09	100.20
1	C	515	LEU	CA-CB-CG	5.41	127.75	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	477	MET	CG-SD-CE	5.39	108.82	100.20
1	B	319	PHE	CB-CA-C	5.22	120.83	110.40

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	4477	0	4456	83	0
1	B	4488	0	4469	86	0
1	C	4432	0	4408	61	0
2	A	13	0	5	0	0
2	B	13	0	5	0	0
2	C	13	0	5	0	0
3	A	6	0	4	0	0
3	B	6	0	4	0	0
3	C	6	0	4	0	0
4	A	380	0	0	7	0
4	B	421	0	0	12	0
4	C	319	0	0	8	0
All	All	14574	0	13360	218	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 (218) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:468:LYS:CA	1:A:468:LYS:HE2	1.35	1.47
1:A:468:LYS:CE	1:A:468:LYS:HA	1.53	1.34
1:B:514:LEU:CD1	1:B:518:LYS:HD2	1.78	1.12
1:A:582:ARG:HH11	1:A:582:ARG:HB3	1.20	1.01
1:B:514:LEU:HD12	1:B:518:LYS:HD2	1.40	1.00
1:A:582:ARG:HB3	1:A:582:ARG:NH1	1.76	1.00

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:271:LEU:CD1	1:A:309:PHE:HE1	1.81	0.94
1:B:511:ILE:O	1:B:515:LEU:HG	1.74	0.88
1:B:52:SER:HB2	4:B:7397:HOH:O	1.73	0.87
1:A:468:LYS:N	1:A:468:LYS:HE2	1.90	0.85
1:C:497:ARG:HD2	1:C:498:ARG:NH1	1.92	0.85
1:C:498:ARG:N	1:C:498:ARG:HD3	1.92	0.83
1:B:491:LYS:HE2	1:B:499:GLU:OE1	1.78	0.83
1:B:114:CYS:SG	1:B:118:ARG:NH2	2.53	0.81
1:A:61:LYS:HD3	1:A:65:GLN:NE2	1.95	0.80
1:A:468:LYS:CA	1:A:468:LYS:CE	2.25	0.80
1:B:514:LEU:HD13	1:B:518:LYS:HD2	1.62	0.80
1:A:187:GLY:O	1:A:190:LYS:HE2	1.83	0.77
1:A:271:LEU:CD1	1:A:309:PHE:CE1	2.67	0.77
1:A:271:LEU:HD12	1:A:309:PHE:CE1	2.20	0.76
1:A:271:LEU:HD12	1:A:309:PHE:HE1	1.50	0.75
1:A:39:LEU:HD21	1:A:416:TYR:HB2	1.68	0.74
1:B:126:ARG:HH12	1:B:127:GLN:NE2	1.85	0.74
1:A:495:GLU:HA	1:A:498:ARG:HD2	1.71	0.72
1:C:54:ALA:O	1:C:58:GLN:HG3	1.90	0.72
1:A:498:ARG:HG2	1:A:499:GLU:N	2.04	0.71
1:C:301:THR:HG22	1:C:319:PHE:O	1.94	0.68
1:B:514:LEU:HD13	1:B:518:LYS:CG	2.24	0.68
1:C:381:ILE:HD11	1:C:430:PRO:HG3	1.76	0.68
1:C:145:PRO:HG2	1:C:322:TRP:HB3	1.75	0.68
1:A:468:LYS:HE2	1:A:468:LYS:HA	0.70	0.68
1:B:514:LEU:HD13	1:B:518:LYS:CD	2.25	0.66
1:C:507:SER:HB2	1:C:509:GLU:OE2	1.95	0.66
1:B:505:GLU:OE2	1:B:507:SER:HB3	1.96	0.66
1:B:514:LEU:CD1	1:B:518:LYS:CD	2.66	0.66
1:C:507:SER:O	1:C:511:ILE:HG23	1.97	0.65
1:C:454:LEU:HD11	1:C:525:PRO:HD2	1.79	0.65
1:A:468:LYS:NZ	1:A:468:LYS:HA	2.11	0.65
1:A:109:ASN:OD1	1:A:112:ILE:HG13	1.97	0.64
1:A:359:HIS:CE1	1:A:369:VAL:H	2.16	0.64
1:C:73:LYS:HZ3	1:C:77:THR:HG21	1.63	0.63
1:A:132:VAL:HG22	1:A:138:VAL:HG21	1.80	0.63
1:B:366:GLU:H	1:B:366:GLU:CD	2.02	0.63
1:B:132:VAL:HG22	1:B:138:VAL:HG21	1.82	0.62
4:B:7048:HOH:O	1:C:473:HIS:HD2	1.81	0.62
1:A:359:HIS:HE1	1:A:369:VAL:H	1.43	0.62
1:B:278:LEU:HD22	1:B:288:GLU:OE1	2.00	0.62
1:A:498:ARG:NH1	1:A:498:ARG:HB2	2.15	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:60:GLN:O	1:B:64:GLU:HG3	2.00	0.62
1:C:157:ARG:NH1	1:C:159:ILE:HD11	2.14	0.62
1:B:399:TRP:CZ3	1:B:400:ARG:HD3	2.35	0.61
1:A:314:GLU:HG2	4:A:7366:HOH:O	2.00	0.60
1:A:44:ALA:HB3	1:A:423:THR:HG23	1.83	0.59
1:A:498:ARG:CG	1:A:498:ARG:HH11	2.17	0.58
1:B:568:GLU:HG2	4:B:7127:HOH:O	2.02	0.58
1:A:233:SER:H	1:A:239:HIS:CD2	2.21	0.58
1:A:366:GLU:CD	1:A:366:GLU:H	2.07	0.58
1:A:498:ARG:HG3	1:A:498:ARG:HH11	1.69	0.57
1:C:157:ARG:NH1	1:C:159:ILE:CD1	2.67	0.57
1:B:417:VAL:HG22	4:B:7278:HOH:O	2.05	0.57
1:B:126:ARG:NH1	1:B:127:GLN:NE2	2.53	0.56
1:B:604:LEU:HD12	1:C:463:ILE:CD1	2.34	0.56
1:B:337:ILE:O	1:B:341:ILE:HG12	2.05	0.56
1:B:391:ILE:HG21	1:B:405:LEU:HD12	1.88	0.56
1:B:517:HIS:HA	1:C:417:VAL:HG21	1.87	0.56
1:B:364:PRO:HB2	1:B:366:GLU:OE2	2.06	0.55
1:B:500:LEU:HB3	1:B:511:ILE:HD13	1.89	0.55
1:C:73:LYS:O	1:C:77:THR:HG23	2.07	0.55
1:A:233:SER:H	1:A:239:HIS:HD2	1.53	0.55
1:A:326:ARG:HB3	1:A:407:GLN:HG2	1.89	0.54
1:A:422:LYS:HE2	4:A:7288:HOH:O	2.06	0.54
1:A:46:ALA:HA	1:A:423:THR:OG1	2.08	0.54
1:C:391:ILE:HG21	1:C:405:LEU:HD12	1.90	0.53
1:B:416:TYR:CE1	4:C:7314:HOH:O	2.54	0.53
1:A:53:CYS:SG	1:A:122:GLU:HG2	2.48	0.53
1:C:362:ASN:HB2	4:C:7276:HOH:O	2.08	0.53
1:B:514:LEU:HD13	1:B:518:LYS:HG3	1.91	0.53
1:B:111:GLU:HG3	4:B:7098:HOH:O	2.08	0.53
1:A:61:LYS:HD3	1:A:65:GLN:HE22	1.70	0.53
1:B:301:THR:HG22	1:B:319:PHE:O	2.09	0.53
1:B:443:ALA:HA	1:C:407:GLN:HG3	1.89	0.53
1:B:381:ILE:HD11	1:B:430:PRO:HG3	1.90	0.52
1:C:293:ALA:HA	4:C:7277:HOH:O	2.10	0.52
1:A:235:VAL:HB	1:A:265:GLU:HG3	1.91	0.52
1:C:157:ARG:CZ	1:C:159:ILE:HD11	2.39	0.52
1:C:73:LYS:NZ	1:C:77:THR:HG21	2.25	0.51
1:A:465:SER:HB3	1:A:468:LYS:HE3	1.91	0.51
1:B:406:GLN:O	1:B:410:MET:HB2	2.10	0.51
1:B:448:ILE:O	1:B:524:ARG:HD3	2.11	0.51
1:A:234:ASN:H	1:A:239:HIS:HD2	1.59	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:83:GLN:HG3	4:B:7292:HOH:O	2.11	0.50
1:B:417:VAL:HG21	1:C:517:HIS:HA	1.92	0.50
1:C:337:ILE:O	1:C:341:ILE:HG12	2.12	0.50
1:A:112:ILE:HD13	1:A:379:TRP:CZ2	2.46	0.50
1:C:259:LYS:HE3	1:C:323:VAL:O	2.12	0.50
1:C:299:LEU:HD13	1:C:333:ILE:HA	1.94	0.50
1:C:132:VAL:HG22	1:C:138:VAL:HG21	1.93	0.50
1:A:337:ILE:O	1:A:341:ILE:HG12	2.12	0.50
1:B:514:LEU:O	1:B:518:LYS:HG3	2.11	0.49
1:A:391:ILE:HG21	1:A:405:LEU:HD12	1.94	0.49
1:A:495:GLU:HA	1:A:498:ARG:CD	2.42	0.49
1:A:114:CYS:O	1:A:118:ARG:HG2	2.13	0.49
1:C:416:TYR:HD1	1:C:417:VAL:HG13	1.78	0.49
1:B:326:ARG:HB3	1:B:407:GLN:HG2	1.94	0.49
1:B:515:LEU:HB2	1:B:516:PRO:HD3	1.94	0.49
1:A:53:CYS:SG	1:A:122:GLU:OE2	2.71	0.49
1:C:180:PHE:CZ	1:C:297:VAL:HG11	2.48	0.49
1:C:124:GLY:HA2	4:C:7208:HOH:O	2.12	0.48
1:A:53:CYS:SG	1:A:122:GLU:CG	3.01	0.48
1:A:144:ARG:HD3	1:A:321:ASP:O	2.14	0.48
1:C:498:ARG:H	1:C:498:ARG:HD3	1.78	0.48
1:A:53:CYS:SG	1:A:122:GLU:CD	2.92	0.48
1:B:436:ALA:O	1:B:439:ASN:HB2	2.14	0.48
1:A:190:LYS:O	1:A:294:LYS:HE3	2.14	0.47
1:B:600:MET:HE1	1:C:100:PHE:CD2	2.49	0.47
1:B:53:CYS:SG	1:B:122:GLU:HG2	2.54	0.47
1:B:389:HIS:HB3	1:B:432:ILE:HD13	1.95	0.47
1:A:278:LEU:HG	1:A:288:GLU:OE1	2.14	0.47
1:A:467:ASN:C	1:A:468:LYS:HE2	2.35	0.47
1:C:366:GLU:CD	1:C:366:GLU:H	2.18	0.47
1:B:240:ILE:HD13	1:B:272:SER:HB2	1.96	0.47
1:A:299:LEU:HD13	1:A:333:ILE:HA	1.97	0.47
1:A:125:ILE:O	1:A:129:VAL:HG23	2.15	0.46
1:C:390:ALA:HB1	1:C:392:LEU:HD21	1.97	0.46
1:A:389:HIS:HB3	1:A:432:ILE:HD13	1.97	0.46
1:C:394:TYR:HE2	1:C:438:THR:HG22	1.79	0.46
1:B:373:LEU:HG	4:B:7034:HOH:O	2.15	0.46
1:B:237:GLY:HA3	4:C:7044:HOH:O	2.15	0.46
1:B:238:THR:HG23	1:C:397:TYR:CZ	2.50	0.46
1:B:604:LEU:HD12	1:C:463:ILE:HD13	1.98	0.45
1:C:161:VAL:C	1:C:163:GLY:H	2.19	0.45
1:B:473:HIS:HD2	4:C:7016:HOH:O	1.99	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:200:VAL:HG21	1:C:339:ILE:HG21	1.98	0.45
1:C:465:SER:HB2	1:C:473:HIS:CD2	2.52	0.45
1:A:180:PHE:CZ	1:A:297:VAL:HG11	2.52	0.45
1:A:60:GLN:O	1:A:64:GLU:HG3	2.16	0.45
1:A:398:LEU:HD13	1:A:401:LEU:HD22	1.98	0.45
1:A:128:PHE:O	1:A:132:VAL:HG23	2.16	0.45
1:A:498:ARG:NH1	1:A:498:ARG:CB	2.79	0.45
1:A:218:ALA:HA	1:A:397:TYR:HB3	1.99	0.45
1:B:518:LYS:HE3	1:C:565:TRP:CE3	2.52	0.45
1:A:554:GLY:HA3	1:A:561:SER:OG	2.17	0.45
1:B:38:ARG:HB2	1:B:38:ARG:HE	1.62	0.45
1:C:178:ARG:HH11	1:C:178:ARG:HG2	1.82	0.45
1:B:91:LEU:HA	1:B:355:VAL:HG11	1.99	0.45
1:B:87:VAL:HG22	1:B:367:GLN:NE2	2.32	0.45
1:B:201:VAL:HG22	1:B:230:HIS:HB2	1.99	0.44
1:C:150:ALA:HB1	1:C:167:MET:HE1	2.00	0.44
1:C:392:LEU:HD13	1:C:445:TYR:CZ	2.52	0.44
1:B:570:GLY:HA3	1:C:483:GLN:NE2	2.32	0.44
1:B:400:ARG:HA	1:B:400:ARG:HD2	1.79	0.44
1:C:591:ASP:OD1	1:C:593:SER:HB3	2.18	0.44
1:C:274:ARG:O	1:C:278:LEU:HG	2.18	0.44
1:A:498:ARG:CB	1:A:498:ARG:CZ	2.96	0.44
1:A:257:ALA:HB2	1:A:299:LEU:HD12	2.00	0.43
1:A:388:THR:O	1:A:456:PRO:HD2	2.18	0.43
1:C:494:SER:O	1:C:498:ARG:NE	2.51	0.43
1:B:146:VAL:HG21	1:B:562:TYR:CD2	2.53	0.43
1:C:531:ILE:HD13	1:C:542:ILE:HD11	2.00	0.43
1:B:217:GLU:OE1	1:B:220:LYS:NZ	2.51	0.43
1:A:495:GLU:CA	1:A:498:ARG:HD2	2.44	0.43
1:C:148:HIS:N	4:C:7107:HOH:O	2.52	0.43
1:B:412:SER:O	1:B:561:SER:HA	2.19	0.43
1:B:398:LEU:HD22	1:B:401:LEU:HD22	2.01	0.43
1:C:280:TYR:OH	1:C:284:ARG:NH1	2.51	0.43
1:C:146:VAL:HG11	1:C:562:TYR:CE1	2.54	0.43
1:B:485:GLU:O	1:B:489:ILE:HG12	2.19	0.43
1:B:107:HIS:HB3	4:B:7093:HOH:O	2.19	0.43
1:A:178:ARG:NH2	4:A:7379:HOH:O	2.51	0.43
1:C:511:ILE:HG13	1:C:512:ASN:N	2.31	0.43
1:A:137:ARG:NH1	1:B:178:ARG:HD3	2.34	0.42
1:B:101:LEU:HD22	1:B:369:VAL:HG13	2.00	0.42
1:B:441:GLN:HA	1:B:445:TYR:CG	2.53	0.42
1:A:498:ARG:NH1	1:A:498:ARG:CG	2.77	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:458:ASP:OD1	1:B:527:ASN:HB2	2.18	0.42
1:B:600:MET:HB3	1:B:600:MET:HE3	1.56	0.42
1:C:130:GLN:O	1:C:134:ARG:HG3	2.18	0.42
1:A:399:TRP:CZ3	1:A:400:ARG:HD3	2.55	0.42
1:A:511:ILE:O	1:A:515:LEU:HB2	2.19	0.42
1:B:500:LEU:CB	1:B:511:ILE:HD13	2.48	0.42
1:C:91:LEU:HG	1:C:98:PHE:HA	2.01	0.42
1:A:115:ALA:HB1	4:A:7354:HOH:O	2.20	0.42
1:A:583:PRO:HG3	1:A:606:HIS:CD2	2.54	0.42
1:A:536:PRO:HD2	4:A:7301:HOH:O	2.20	0.42
1:C:201:VAL:HG22	1:C:230:HIS:HB2	2.02	0.42
1:A:39:LEU:HD11	1:A:416:TYR:CD2	2.55	0.42
1:B:259:LYS:HG3	1:B:319:PHE:CE2	2.55	0.42
1:B:410:MET:HA	4:B:7003:HOH:O	2.20	0.42
1:C:394:TYR:CE2	1:C:438:THR:HG22	2.55	0.42
1:B:380:TYR:CE1	1:B:525:PRO:HG3	2.55	0.42
1:B:349:LEU:HA	1:B:536:PRO:O	2.20	0.42
1:B:554:GLY:HA3	1:B:561:SER:OG	2.19	0.41
1:A:487:LEU:HB3	1:A:524:ARG:HB2	2.02	0.41
1:B:180:PHE:CZ	1:B:297:VAL:HG11	2.55	0.41
1:A:371:LEU:HD12	1:A:552:VAL:HG11	2.03	0.41
1:B:423:THR:HG22	4:B:7197:HOH:O	2.21	0.41
1:A:533:SER:OG	1:A:535:THR:HG23	2.20	0.41
1:B:75:PHE:CE2	1:B:488:MET:SD	3.14	0.41
1:B:274:ARG:O	1:B:278:LEU:HG	2.21	0.41
1:B:367:GLN:NE2	4:B:7419:HOH:O	2.54	0.41
1:A:447:LEU:HD21	1:A:453:ASN:HD22	1.85	0.41
1:B:439:ASN:HD21	1:C:234:ASN:HB2	1.85	0.41
1:A:111:GLU:HG3	4:A:7123:HOH:O	2.19	0.41
1:B:451:GLY:HA3	4:B:7253:HOH:O	2.20	0.41
1:B:531:ILE:HD13	1:B:542:ILE:HD11	2.03	0.41
1:C:448:ILE:HG22	1:C:487:LEU:HD21	2.03	0.41
1:B:514:LEU:HA	1:B:514:LEU:HD22	1.87	0.41
1:A:117:LEU:HD13	1:A:366:GLU:HG3	2.03	0.41
1:A:137:ARG:NH2	4:A:7269:HOH:O	2.53	0.41
1:B:416:TYR:HE1	4:C:7314:HOH:O	1.99	0.40
1:C:506:ARG:NH2	1:C:514:LEU:HD13	2.36	0.40
1:A:468:LYS:N	1:A:468:LYS:CE	2.71	0.40
1:B:352:GLY:HA3	1:B:537:ARG:O	2.21	0.40
1:A:372:LEU:O	1:A:376:VAL:HG23	2.20	0.40
1:A:328:SER:O	1:A:333:ILE:HB	2.22	0.40
1:A:72:LYS:O	1:A:76:GLU:HG3	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:575:LYS:NZ	1:B:575:LYS:HB3	2.36	0.40
1:B:485:GLU:OE2	1:C:590:HIS:ND1	2.55	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	566/613 (92%)	547 (97%)	19 (3%)	0	100	100
1	B	567/613 (92%)	548 (97%)	18 (3%)	1 (0%)	56	44
1	C	559/613 (91%)	539 (96%)	20 (4%)	0	100	100
All	All	1692/1839 (92%)	1634 (97%)	57 (3%)	1 (0%)	59	48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	439	ASN

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	482/519 (93%)	457 (95%)	25 (5%)	32	19
1	B	483/519 (93%)	463 (96%)	20 (4%)	41	28
1	C	478/519 (92%)	463 (97%)	15 (3%)	52	41
All	All	1443/1557 (93%)	1383 (96%)	60 (4%)	40	27

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	40	LYS
1	A	61	LYS
1	A	72	LYS
1	A	80	GLU
1	A	137	ARG
1	A	152	ARG
1	A	157	ARG
1	A	190	LYS
1	A	212	PRO
1	A	239	HIS
1	A	244	LEU
1	A	261	PHE
1	A	271	LEU
1	A	278	LEU
1	A	289	LYS
1	A	300	SER
1	A	416	TYR
1	A	453	ASN
1	A	468	LYS
1	A	474	LYS
1	A	498	ARG
1	A	501	GLU
1	A	575	LYS
1	A	582	ARG
1	B	38	ARG
1	B	39	LEU
1	B	40	LYS
1	B	72	LYS
1	B	152	ARG
1	B	157	ARG
1	B	212	PRO
1	B	220	LYS
1	B	229	LEU
1	B	239	HIS
1	B	261	PHE
1	B	288	GLU
1	B	304	GLN
1	B	366	GLU
1	B	416	TYR
1	B	510	LYS
1	B	511	ILE

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Mol	Chain	Res	Type
1	B	514	LEU
1	B	600	MET
1	B	604	LEU
1	C	48	THR
1	C	83	GLN
1	C	138	VAL
1	C	152	ARG
1	C	157	ARG
1	C	212	PRO
1	C	229	LEU
1	C	239	HIS
1	C	261	PHE
1	C	416	TYR
1	C	498	ARG
1	C	505	GLU
1	C	509	GLU
1	C	511	ILE
1	C	582	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	65	GLN
1	A	239	HIS
1	A	359	HIS
1	A	453	ASN
1	A	467	ASN
1	A	473	HIS
1	A	517	HIS
1	A	606	HIS
1	B	127	GLN
1	B	143	ASN
1	B	367	GLN
1	B	439	ASN
1	B	473	HIS
1	B	606	HIS
1	C	453	ASN
1	C	473	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

6 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	5001	-	12,12,12	2.54	6 (50%)	17,17,17	2.51	6 (35%)
3	GOL	A	7001	-	5,5,5	4.53	5 (100%)	5,5,5	5.65	3 (60%)
2	CIT	B	5002	-	12,12,12	2.50	7 (58%)	17,17,17	2.54	5 (29%)
3	GOL	B	7002	-	5,5,5	4.37	5 (100%)	5,5,5	5.59	3 (60%)
2	CIT	C	5003	-	12,12,12	2.35	6 (50%)	17,17,17	2.58	5 (29%)
3	GOL	C	7003	-	5,5,5	4.52	5 (100%)	5,5,5	5.61	3 (60%)

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	5001	-	-	0/16/16/16	0/0/0/0
3	GOL	A	7001	-	-	0/4/4/4	0/0/0/0
2	CIT	B	5002	-	-	0/16/16/16	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	7002	-	-	0/4/4/4	0/0/0/0
2	CIT	C	5003	-	-	0/16/16/16	0/0/0/0
3	GOL	C	7003	-	-	0/4/4/4	0/0/0/0

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	7003	GOL	C3-C2	-7.57	1.21	1.52
3	A	7001	GOL	C3-C2	-7.25	1.22	1.52
3	B	7002	GOL	C3-C2	-7.18	1.22	1.52
2	A	5001	CIT	C3-C6	5.24	1.59	1.53
2	C	5003	CIT	C3-C6	4.80	1.58	1.53
3	A	7001	GOL	O1-C1	4.74	1.63	1.42
2	B	5002	CIT	C3-C6	4.67	1.58	1.53
3	B	7002	GOL	O1-C1	4.19	1.60	1.42
3	C	7003	GOL	O1-C1	4.09	1.60	1.42
3	A	7001	GOL	C1-C2	-3.32	1.38	1.52
3	A	7001	GOL	O3-C3	3.31	1.56	1.42
2	A	5001	CIT	O5-C6	3.28	1.33	1.22
2	B	5002	CIT	O3-C5	3.27	1.33	1.22
2	C	5003	CIT	O3-C5	3.19	1.33	1.22
2	A	5001	CIT	O3-C5	3.17	1.33	1.22
3	C	7003	GOL	C1-C2	-3.17	1.39	1.52
2	B	5002	CIT	O5-C6	3.15	1.33	1.22
2	B	5002	CIT	C2-C3	3.08	1.57	1.53
3	C	7003	GOL	O3-C3	3.07	1.55	1.42
2	C	5003	CIT	O5-C6	3.03	1.32	1.22
3	B	7002	GOL	O2-C2	-3.01	1.34	1.43
3	B	7002	GOL	C1-C2	-2.95	1.40	1.52
3	B	7002	GOL	O3-C3	2.95	1.55	1.42
3	C	7003	GOL	O2-C2	-2.94	1.34	1.43
2	A	5001	CIT	C2-C3	2.93	1.57	1.53
2	B	5002	CIT	C4-C3	-2.68	1.50	1.53
2	A	5001	CIT	O4-C5	-2.40	1.21	1.30
3	A	7001	GOL	O2-C2	-2.38	1.36	1.43
2	B	5002	CIT	O4-C5	-2.37	1.21	1.30
2	C	5003	CIT	C2-C3	2.36	1.56	1.53
2	A	5001	CIT	O1-C1	2.33	1.30	1.22
2	C	5003	CIT	O4-C5	-2.24	1.22	1.30
2	B	5002	CIT	O1-C1	2.22	1.30	1.22
2	C	5003	CIT	O1-C1	2.20	1.30	1.22

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	7001	GOL	O3-C3-C2	10.37	160.31	109.71
3	B	7002	GOL	O3-C3-C2	10.25	159.75	109.71
3	C	7003	GOL	O3-C3-C2	10.13	159.15	109.71
2	C	5003	CIT	O5-C6-C3	-6.83	112.78	122.20
2	A	5001	CIT	O5-C6-C3	-6.69	112.98	122.20
3	C	7003	GOL	O2-C2-C3	6.57	138.14	108.22
2	B	5002	CIT	O5-C6-C3	-6.56	113.16	122.20
3	A	7001	GOL	O2-C2-C3	6.29	136.86	108.22
3	B	7002	GOL	O2-C2-C3	6.14	136.21	108.22
2	C	5003	CIT	O6-C6-C3	3.98	118.68	112.89
2	A	5001	CIT	O6-C6-C3	3.84	118.47	112.89
2	B	5002	CIT	O6-C6-C3	3.71	118.29	112.89
2	C	5003	CIT	O7-C3-C2	-3.61	101.95	109.22
3	B	7002	GOL	O1-C1-C2	3.53	126.96	109.71
2	B	5002	CIT	O7-C3-C2	-3.51	102.15	109.22
3	A	7001	GOL	O1-C1-C2	3.48	126.70	109.71
2	A	5001	CIT	O7-C3-C2	-3.38	102.40	109.22
2	B	5002	CIT	C3-C2-C1	3.35	121.88	113.77
3	C	7003	GOL	O1-C1-C2	3.22	125.40	109.71
2	A	5001	CIT	C3-C2-C1	2.96	120.94	113.77
2	C	5003	CIT	C3-C4-C5	2.89	120.78	113.77
2	A	5001	CIT	C3-C4-C5	2.64	120.16	113.77
2	C	5003	CIT	C3-C2-C1	2.63	120.15	113.77
2	B	5002	CIT	C3-C4-C5	2.42	119.63	113.77
2	A	5001	CIT	O2-C1-C2	2.01	121.72	114.63

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	568/613 (92%)	0.36	19 (3%)	44 45	8, 17, 38, 52	0
1	B	569/613 (92%)	0.32	23 (4%)	36 37	7, 16, 40, 73	0
1	C	561/613 (91%)	0.55	33 (5%)	22 22	8, 21, 44, 64	0
All	All	1698/1839 (92%)	0.41	75 (4%)	33 33	7, 18, 43, 73	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	503	ALA	6.3
1	C	504	GLY	5.7
1	B	42	VAL	5.7
1	A	504	GLY	5.4
1	B	606	HIS	5.2
1	B	41	GLY	4.9
1	B	39	LEU	4.3
1	C	606	HIS	4.2
1	A	304	GLN	4.2
1	A	498	ARG	3.7
1	B	38	ARG	3.7
1	C	508	ALA	3.7
1	C	505	GLU	3.6
1	B	44	ALA	3.5
1	C	498	ARG	3.4
1	C	161	VAL	3.3
1	B	514	LEU	3.3
1	B	508	ALA	3.3
1	A	42	VAL	3.2
1	C	160	TYR	3.1
1	A	52	SER	3.0
1	C	506	ARG	2.9
1	C	585	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	307	LYS	2.9
1	C	604	LEU	2.9
1	A	606	HIS	2.8
1	C	159	ILE	2.7
1	C	582	ARG	2.7
1	C	293	ALA	2.7
1	C	311	ILE	2.6
1	C	158	PRO	2.6
1	B	515	LEU	2.6
1	C	68	ASP	2.6
1	B	40	LYS	2.5
1	B	399	TRP	2.5
1	A	40	LYS	2.5
1	C	502	ALA	2.5
1	A	502	ALA	2.5
1	B	512	ASN	2.5
1	C	320	TRP	2.4
1	A	506	ARG	2.4
1	A	309	PHE	2.4
1	A	45	ASP	2.4
1	C	290	GLY	2.3
1	A	308	GLU	2.3
1	C	399	TRP	2.3
1	B	503	ALA	2.3
1	B	498	ARG	2.3
1	B	604	LEU	2.3
1	B	516	PRO	2.3
1	C	312	ASP	2.3
1	A	39	LEU	2.2
1	A	94	LYS	2.2
1	C	135	GLY	2.2
1	B	304	GLN	2.2
1	B	511	ILE	2.2
1	C	126	ARG	2.2
1	B	288	GLU	2.2
1	C	64	GLU	2.2
1	B	45	ASP	2.1
1	B	48	THR	2.1
1	C	166	VAL	2.1
1	C	307	LYS	2.1
1	C	605	SER	2.1
1	C	49	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	401	LEU	2.1
1	C	210	LEU	2.1
1	B	436	ALA	2.1
1	A	314	GLU	2.1
1	A	305	LYS	2.1
1	C	586	ARG	2.1
1	C	497	ARG	2.0
1	B	94	LYS	2.0
1	C	278	LEU	2.0
1	A	49	THR	2.0

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

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

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
3	GOL	A	7001	6/6	0.20	2.82	31,35,36,39	0
2	CIT	B	5002	13/13	0.18	2.78	25,30,35,37	0
2	CIT	A	5001	13/13	0.18	2.03	23,30,38,39	0
2	CIT	C	5003	13/13	0.18	1.91	32,35,37,39	0
3	GOL	C	7003	6/6	0.19	1.33	32,34,35,38	0
3	GOL	B	7002	6/6	0.14	0.68	21,25,26,28	0

6.5 Other polymers ⓘ

There are no such residues in this entry.