



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 07:33 AM UTC

PDB ID : 2O2D / pdb_00002o2d
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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

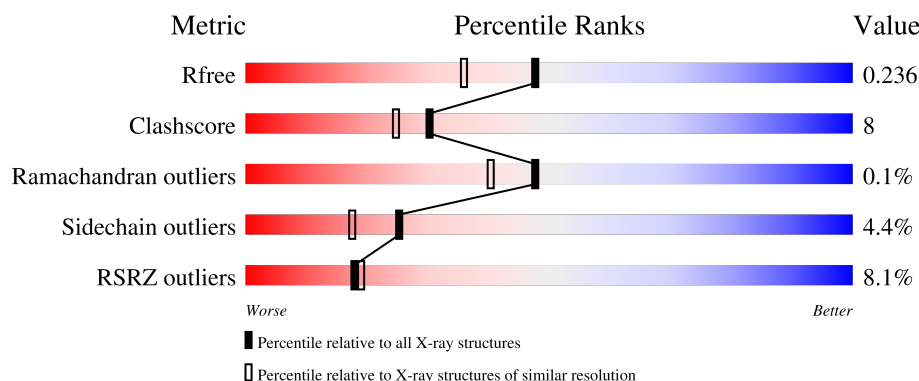
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 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	613	5% 73% 16% • 7%
1	B	613	5% 71% 18% • 7%
1	C	613	12% 74% 16% • 8%

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	GOL	A	7001	-	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 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 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 (CCD ID: 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 (CCD ID: 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		

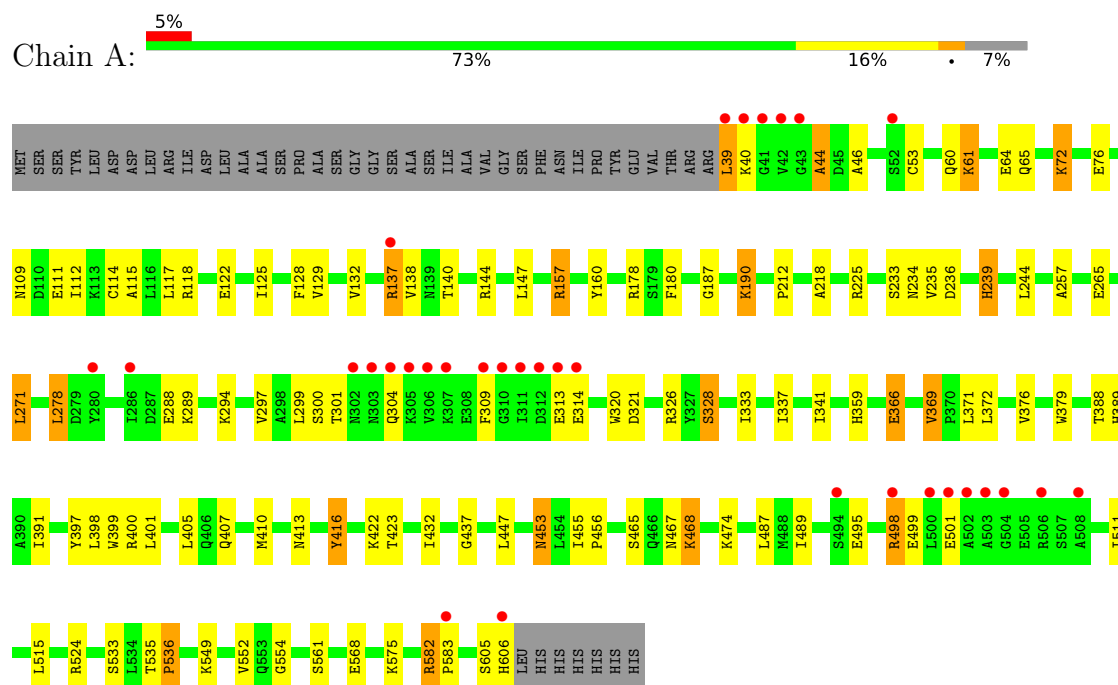
- Molecule 4 is water.

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		

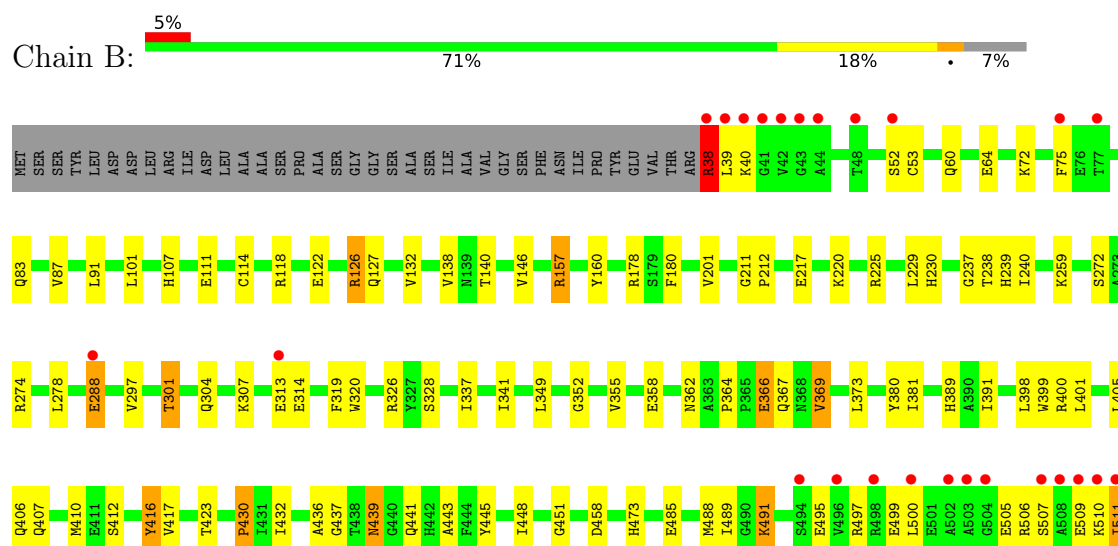
3 Residue-property plots [i](#)

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

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

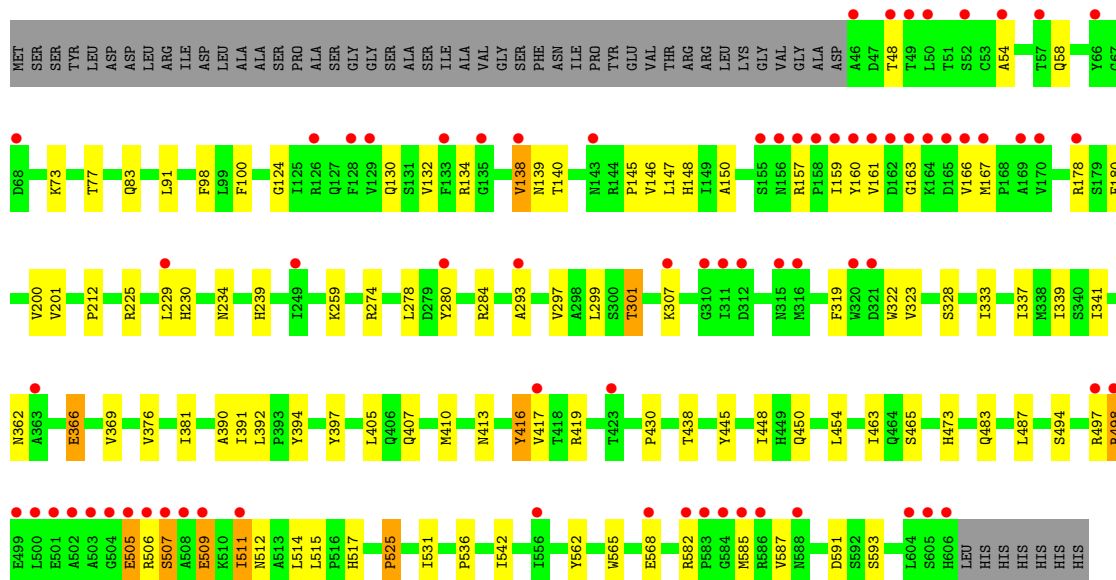
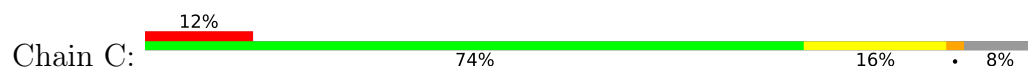


- Molecule 1: Glucose-6-phosphate isomerase, glycosomal





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



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 40.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.2 (40.00-1.90) 97.3 (40.00-1.90)	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 , 0.236	Depositor DCC
R_{free} test set	6570 reflections (5.04%)	wwPDB-VP
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 , 31.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
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
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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	0.66	1/4575 (0.0%)	1.13	20/6192 (0.3%)
1	B	0.72	1/4586 (0.0%)	1.15	18/6206 (0.3%)
1	C	0.65	1/4530 (0.0%)	1.13	16/6132 (0.3%)
All	All	0.68	3/13691 (0.0%)	1.14	54/18530 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	369	VAL	CA-CB	10.49	1.59	1.54
1	C	369	VAL	CA-CB	9.61	1.58	1.54
1	A	369	VAL	CA-CB	9.25	1.59	1.54

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	605	SER	N-CA-C	8.15	120.08	111.03
1	C	507	SER	N-CA-C	7.97	120.60	110.24
1	A	301	THR	N-CA-C	-7.19	105.03	113.88
1	B	301	THR	N-CA-C	-7.15	104.82	113.97
1	A	140	THR	N-CA-C	7.00	118.91	111.28
1	A	568	GLU	N-CA-C	6.96	118.95	111.36
1	C	147	LEU	N-CA-C	6.90	118.99	109.54
1	A	147	LEU	N-CA-C	6.85	118.66	110.44
1	C	568	GLU	N-CA-C	6.80	118.78	111.36
1	C	505	GLU	N-CA-C	6.68	120.18	110.42
1	A	225	ARG	N-CA-C	6.49	119.18	111.71
1	B	437	GLY	N-CA-C	-6.48	103.78	112.14
1	C	301	THR	N-CA-C	-6.42	105.98	113.88
1	C	225	ARG	N-CA-C	6.36	120.13	112.38
1	C	410	MET	N-CA-C	6.35	118.20	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	489	ILE	N-CA-C	6.35	117.13	110.72
1	A	410	MET	N-CA-C	6.29	118.14	111.28
1	C	139	ASN	N-CA-C	-6.28	100.19	109.62
1	A	160	TYR	N-CA-C	6.26	119.45	109.24
1	A	413	ASN	N-CA-C	6.20	120.55	112.92
1	C	525	PRO	N-CA-C	6.09	120.54	111.41
1	B	225	ARG	N-CA-C	6.04	119.75	112.38
1	C	140	THR	N-CA-C	6.03	118.65	111.71
1	A	320	TRP	N-CA-C	6.02	118.99	110.14
1	C	328	SER	N-CA-C	5.97	120.73	113.38
1	B	140	THR	N-CA-C	5.94	118.54	111.71
1	B	568	GLU	N-CA-C	5.88	117.77	111.36
1	B	160	TYR	N-CA-C	5.71	119.12	109.76
1	C	160	TYR	N-CA-C	5.62	117.69	108.52
1	B	320	TRP	N-CA-C	5.61	118.39	110.14
1	A	455	ILE	N-CA-C	5.60	113.69	108.15
1	A	304	GLN	N-CA-C	5.49	117.34	111.36
1	A	328	SER	N-CA-C	5.47	120.07	113.17
1	A	236	ASP	N-CA-C	-5.37	101.69	109.59
1	C	413	ASN	N-CA-C	5.36	119.51	112.92
1	C	376	VAL	N-CA-C	-5.34	105.32	110.72
1	B	525	PRO	CB-CA-C	-5.32	103.98	110.95
1	C	450	GLN	N-CA-C	5.30	120.42	112.94
1	B	38	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	B	362	ASN	N-CA-C	5.28	120.38	113.88
1	A	44	ALA	N-CA-C	-5.26	101.98	110.14
1	C	419	ARG	NE-CZ-NH2	5.25	123.93	119.20
1	B	328	SER	N-CA-C	5.22	119.80	113.38
1	B	313	GLU	N-CA-C	5.22	116.97	111.28
1	A	157	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	A	437	GLY	N-CA-C	-5.18	105.67	112.82
1	A	549	LYS	N-CA-C	-5.18	105.55	111.14
1	B	430	PRO	CB-CA-C	-5.13	103.16	110.75
1	B	506	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	A	137	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	B	537	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	B	211	GLY	CA-C-N	5.01	124.45	119.24
1	B	211	GLY	C-N-CA	5.01	124.45	119.24
1	B	497	ARG	NE-CZ-NH2	5.01	123.71	119.20

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	4477	0	4456	83	0
1	B	4488	0	4469	88	0
1	C	4432	0	4408	66	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	225	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 8.

All (225) 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:A:468:LYS:HE2	1:A:468:LYS:CA	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:A:582:ARG:HB3	1:A:582:ARG:NH1	1.76	1.00
1:B:514:LEU:HD12	1:B:518:LYS:HD2	1.40	1.00
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:HE2	1:A:468:LYS:N	1.90	0.85
1:C:497:ARG:HD2	1:C:498:ARG:NH1	1.92	0.85
1:C:498:ARG:HD3	1:C:498:ARG:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:585:MET:HE2	1:C:587:VAL:HG12	1.69	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:366:GLU:H	1:B:366:GLU:CD	2.02	0.67
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:B:600:MET:HE1	1:C:100:PHE:CD2	2.31	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:HA	1:A:468:LYS:NZ	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: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:366:GLU:CD	1:A:366:GLU:H	2.07	0.62
1:A:498:ARG:HB2	1:A:498:ARG:NH1	2.15	0.62
1:C:166:VAL:HG23	1:C:167:MET:HE2	1.82	0.62
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:B:600:MET:HE1	1:C:100:PHE:CE2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:150:ALA:HB1	1:C:167:MET:HE1	1.85	0.59
1:A:498:ARG:HH11	1:A:498:ARG:CG	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:498:ARG:HH11	1:A:498:ARG:HG3	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:337:ILE:O	1:B:341:ILE:HG12	2.05	0.56
1:B:604:LEU:HD12	1:C:463:ILE:CD1	2.34	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:B:416:TYR:CE1	4:C:7314:HOH:O	2.54	0.53
1:C:391:ILE:HG21	1:C:405:LEU:HD12	1.90	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:A:53:CYS:SG	1:A:122:GLU:CD	2.92	0.52
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:A:467:ASN:C	1:A:468:LYS:HE2	2.35	0.52
1:C:157:ARG:CZ	1:C:159:ILE:HD11	2.39	0.52
1:C:366:GLU:CD	1:C:366:GLU:H	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ASN:H	1:A:239:HIS:HD2	1.59	0.50
1:B:529:LEU:HD13	1:B:545:MET:HE1	1.93	0.50
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:161:VAL:C	1:C:163:GLY:H	2.19	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:132:VAL:HG22	1:C:138:VAL:HG21	1.93	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: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:114:CYS:O	1:A:118:ARG:HG2	2.13	0.49
1:A:495:GLU:HA	1:A:498:ARG:CD	2.42	0.49
1:B:326:ARG:HB3	1:B:407:GLN:HG2	1.94	0.49
1:C:416:TYR:HD1	1:C:417:VAL:HG13	1.78	0.49
1:C:585:MET:HE2	1:C:587:VAL:CG1	2.41	0.49
1:A:53:CYS:SG	1:A:122:GLU:OE2	2.71	0.49
1:B:515:LEU:HB2	1:B:516:PRO:HD3	1.94	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:B:436:ALA:O	1:B:439:ASN:HB2	2.14	0.48
1:C:498:ARG:HD3	1:C:498:ARG:H	1.78	0.48
1:A:190:LYS:O	1:A:294:LYS:HE3	2.14	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: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:B:473:HIS:HD2	4:C:7016:HOH:O	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:VAL:HG21	1:C:339:ILE:HG21	1.98	0.45
1:A:60:GLN:O	1:A:64:GLU:HG3	2.16	0.45
1:A:180:PHE:CZ	1:A:297:VAL:HG11	2.52	0.45
1:A:398:LEU:HD13	1:A:401:LEU:HD22	1.98	0.45
1:C:465:SER:HB2	1:C:473:HIS:CD2	2.52	0.45
1:A:128:PHE:O	1:A:132:VAL:HG23	2.16	0.45
1:A:218:ALA:HA	1:A:397:TYR:HB3	1.99	0.45
1:A:498:ARG:NH1	1:A:498:ARG:CB	2.79	0.45
1:A:554:GLY:HA3	1:A:561:SER:OG	2.17	0.45
1:B:518:LYS:HE3	1:C:565:TRP:CE3	2.52	0.45
1:B:38:ARG:HE	1:B:38:ARG:HB2	1.62	0.45
1:B:91:LEU:HA	1:B:355:VAL:HG11	1.99	0.45
1:C:178:ARG:HG2	1:C:178:ARG:HH11	1.82	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:B:570:GLY:HA3	1:C:483:GLN:NE2	2.32	0.44
1:C:392:LEU:HD13	1:C:445:TYR:CZ	2.52	0.44
1:B:400:ARG:HD2	1:B:400:ARG:HA	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:B:146:VAL:HG21	1:B:562:TYR:CD2	2.53	0.43
1:C:494:SER:O	1:C:498:ARG:NE	2.51	0.43
1:C:509:GLU:N	1:C:509:GLU:CD	2.76	0.43
1:B:217:GLU:OE1	1:B:220:LYS:NZ	2.51	0.43
1:C:531:ILE:HD13	1:C:542:ILE:HD11	2.00	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:398:LEU:HD22	1:B:401:LEU:HD22	2.01	0.43
1:B:412:SER:O	1:B:561:SER:HA	2.19	0.43
1:C:280:TYR:OH	1:C:284:ARG:NH1	2.51	0.43
1:B:485:GLU:O	1:B:489:ILE:HG12	2.19	0.43
1:C:146:VAL:HG11	1:C:562:TYR:CE1	2.54	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:B:75:PHE:CE2	1:B:488:MET:HE1	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:458:ASP:OD1	1:B:527:ASN:HB2	2.18	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:536:PRO:HD2	4:A:7301:HOH:O	2.20	0.42
1:A:583:PRO:HG3	1:A:606:HIS:CD2	2.54	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:349:LEU:HA	1:B:536:PRO:O	2.20	0.42
1:B:380:TYR:CE1	1:B:525:PRO:HG3	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:A:487:LEU:HB3	1:A:524:ARG:HB2	2.02	0.41
1:B:554:GLY:HA3	1:B:561:SER:OG	2.19	0.41
1:A:371:LEU:HD12	1:A:552:VAL:HG11	2.03	0.41
1:B:180:PHE:CZ	1:B:297:VAL:HG11	2.55	0.41
1:B:157:ARG:HH12	1:B:358:GLU:CD	2.27	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:423:THR:HG22	4:B:7197:HOH:O	2.21	0.41
1:A:447:LEU:HD21	1:A:453:ASN:HD22	1.85	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:111:GLU:HG3	4:A:7123:HOH:O	2.19	0.41
1:B:439:ASN:HD21	1:C:234:ASN:HB2	1.85	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: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:514:LEU:HD22	1:B:514:LEU:HA	1.87	0.41
1:C:509:GLU:CD	1:C:509:GLU:H	2.29	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:372:LEU:O	1:A:376:VAL:HG23	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:LYS:CE	1:A:468:LYS:N	2.71	0.40
1:B:352:GLY:HA3	1:B:537:ARG:O	2.21	0.40
1:A:72:LYS:O	1:A:76:GLU:HG3	2.21	0.40
1:A:328:SER:O	1:A:333:ILE:HB	2.22	0.40
1:B:575:LYS:HB3	1:B:575:LYS:NZ	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	566/613 (92%)	547 (97%)	19 (3%)	0	100	100
1	B	567/613 (92%)	548 (97%)	18 (3%)	1 (0%)	43	36
1	C	559/613 (91%)	539 (96%)	20 (4%)	0	100	100
All	All	1692/1839 (92%)	1634 (97%)	57 (3%)	1 (0%)	48	40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	439	ASN

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	482/519 (93%)	458 (95%)	24 (5%)	22	14
1	B	483/519 (93%)	460 (95%)	23 (5%)	23	15
1	C	478/519 (92%)	462 (97%)	16 (3%)	33	26
All	All	1443/1557 (93%)	1380 (96%)	63 (4%)	25	17

All (63) 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	157	ARG
1	A	190	LYS
1	A	212	PRO
1	A	239	HIS
1	A	244	LEU
1	A	271	LEU
1	A	278	LEU
1	A	289	LYS
1	A	300	SER
1	A	313	GLU
1	A	366	GLU
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	536	PRO
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	126	ARG
1	B	157	ARG
1	B	212	PRO
1	B	229	LEU
1	B	239	HIS
1	B	288	GLU

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Mol	Chain	Res	Type
1	B	304	GLN
1	B	307	LYS
1	B	314	GLU
1	B	366	GLU
1	B	416	TYR
1	B	491	LYS
1	B	495	GLU
1	B	509	GLU
1	B	510	LYS
1	B	511	ILE
1	B	514	LEU
1	B	575	LYS
1	B	604	LEU
1	C	48	THR
1	C	83	GLN
1	C	138	VAL
1	C	212	PRO
1	C	229	LEU
1	C	239	HIS
1	C	307	LYS
1	C	366	GLU
1	C	416	TYR
1	C	498	ARG
1	C	505	GLU
1	C	509	GLU
1	C	511	ILE
1	C	515	LEU
1	C	536	PRO
1	C	582	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	143	ASN
1	A	171	ASN
1	A	199	HIS
1	A	239	HIS
1	A	302	ASN
1	A	359	HIS
1	A	396	GLN
1	A	453	ASN

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Mol	Chain	Res	Type
1	A	472	HIS
1	A	606	HIS
1	B	127	GLN
1	B	367	GLN
1	B	439	ASN
1	B	466	GLN
1	B	473	HIS
1	B	580	GLN
1	C	302	ASN
1	C	453	ASN
1	C	473	HIS
1	C	606	HIS

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](#)

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	$\# Z > 2$
3	GOL	A	7001	-	5,5,5	4.76	5 (100%)	5,5,5	6.03	3 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	B	7002	-	5,5,5	4.59	5 (100%)	5,5,5	5.96	3 (60%)
2	CIT	A	5001	-	12,12,12	2.72	8 (66%)	17,17,17	2.10	7 (41%)
3	GOL	C	7003	-	5,5,5	4.75	5 (100%)	5,5,5	5.98	3 (60%)
2	CIT	C	5003	-	12,12,12	2.53	8 (66%)	17,17,17	2.15	7 (41%)
2	CIT	B	5002	-	12,12,12	2.68	7 (58%)	17,17,17	2.14	7 (41%)

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
3	GOL	A	7001	-	-	1/4/4/4	-
3	GOL	B	7002	-	-	4/4/4/4	-
2	CIT	A	5001	-	-	0/16/16/16	-
3	GOL	C	7003	-	-	3/4/4/4	-
2	CIT	C	5003	-	-	0/16/16/16	-
2	CIT	B	5002	-	-	2/16/16/16	-

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	7003	GOL	C3-C2	-8.06	1.21	1.51
3	A	7001	GOL	C3-C2	-7.71	1.22	1.51
3	B	7002	GOL	C3-C2	-7.63	1.22	1.51
2	A	5001	CIT	C3-C6	5.30	1.59	1.53
3	A	7001	GOL	O1-C1	4.90	1.63	1.42
2	C	5003	CIT	C3-C6	4.83	1.58	1.53
2	B	5002	CIT	C3-C6	4.70	1.58	1.53
3	B	7002	GOL	O1-C1	4.33	1.60	1.42
3	C	7003	GOL	O1-C1	4.22	1.60	1.42
2	A	5001	CIT	O5-C6	3.64	1.33	1.22
2	B	5002	CIT	O3-C5	3.61	1.33	1.22
2	C	5003	CIT	O3-C5	3.52	1.33	1.22
2	A	5001	CIT	O3-C5	3.51	1.33	1.22
2	B	5002	CIT	O5-C6	3.50	1.33	1.22
3	A	7001	GOL	C1-C2	-3.44	1.38	1.51
3	A	7001	GOL	O3-C3	3.41	1.56	1.42
2	C	5003	CIT	O5-C6	3.36	1.32	1.22
3	C	7003	GOL	C1-C2	-3.28	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	7002	GOL	O2-C2	-3.17	1.34	1.43
3	C	7003	GOL	O3-C3	3.17	1.55	1.42
2	B	5002	CIT	C4-C3	-3.10	1.50	1.54
3	C	7003	GOL	O2-C2	-3.09	1.34	1.43
3	B	7002	GOL	C1-C2	-3.04	1.40	1.51
3	B	7002	GOL	O3-C3	3.04	1.55	1.42
2	B	5002	CIT	C2-C3	3.03	1.57	1.54
2	A	5001	CIT	C2-C3	2.88	1.57	1.54
2	A	5001	CIT	O4-C5	-2.72	1.21	1.30
2	B	5002	CIT	O4-C5	-2.70	1.21	1.30
2	A	5001	CIT	O1-C1	2.60	1.30	1.22
2	C	5003	CIT	O4-C5	-2.55	1.22	1.30
3	A	7001	GOL	O2-C2	-2.50	1.36	1.43
2	B	5002	CIT	O1-C1	2.47	1.30	1.22
2	C	5003	CIT	O1-C1	2.45	1.30	1.22
2	A	5001	CIT	C4-C3	-2.36	1.51	1.54
2	C	5003	CIT	C2-C3	2.27	1.56	1.54
2	C	5003	CIT	C4-C3	-2.23	1.51	1.54
2	A	5001	CIT	O7-C3	2.14	1.47	1.43
2	C	5003	CIT	O7-C3	2.00	1.47	1.43

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	7001	GOL	O3-C3-C2	11.09	160.31	110.38
3	B	7002	GOL	O3-C3-C2	10.97	159.75	110.38
3	C	7003	GOL	O3-C3-C2	10.83	159.15	110.38
3	C	7003	GOL	O2-C2-C3	6.99	138.14	109.18
3	A	7001	GOL	O2-C2-C3	6.69	136.86	109.18
3	B	7002	GOL	O2-C2-C3	6.53	136.21	109.18
2	C	5003	CIT	O5-C6-C3	-4.81	112.78	122.09
2	A	5001	CIT	O5-C6-C3	-4.70	112.98	122.09
2	B	5002	CIT	O5-C6-C3	-4.61	113.16	122.09
3	B	7002	GOL	O1-C1-C2	3.68	126.96	110.38
3	A	7001	GOL	O1-C1-C2	3.63	126.70	110.38
3	C	7003	GOL	O1-C1-C2	3.34	125.40	110.38
2	C	5003	CIT	O7-C3-C2	-3.26	101.95	109.38
2	B	5002	CIT	O7-C3-C2	-3.17	102.15	109.38
2	A	5001	CIT	O7-C3-C2	-3.06	102.40	109.38
2	B	5002	CIT	C3-C2-C1	2.91	121.88	113.92
2	C	5003	CIT	O6-C6-C3	2.89	118.68	113.14
2	A	5001	CIT	O6-C6-C3	2.78	118.47	113.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5002	CIT	O6-C6-C3	2.69	118.29	113.14
2	A	5001	CIT	C3-C2-C1	2.57	120.94	113.92
2	C	5003	CIT	C3-C4-C5	2.51	120.78	113.92
2	A	5001	CIT	O2-C1-C2	2.33	121.72	114.35
2	A	5001	CIT	C3-C4-C5	2.28	120.16	113.92
2	C	5003	CIT	C3-C2-C1	2.28	120.15	113.92
2	C	5003	CIT	O2-C1-C2	2.24	121.45	114.35
2	B	5002	CIT	O2-C1-C2	2.18	121.27	114.35
2	C	5003	CIT	O3-C5-C4	-2.14	116.88	122.95
2	B	5002	CIT	C3-C4-C5	2.09	119.63	113.92
2	B	5002	CIT	O3-C5-C4	-2.08	117.05	122.95
2	A	5001	CIT	O3-C5-C4	-2.04	117.18	122.95

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	7002	GOL	C1-C2-C3-O3
3	C	7003	GOL	O1-C1-C2-C3
3	C	7003	GOL	C1-C2-C3-O3
3	B	7002	GOL	O1-C1-C2-O2
3	B	7002	GOL	O2-C2-C3-O3
3	A	7001	GOL	O1-C1-C2-O2
3	B	7002	GOL	O1-C1-C2-C3
3	C	7003	GOL	O2-C2-C3-O3
2	B	5002	CIT	O1-C1-C2-C3
2	B	5002	CIT	O2-C1-C2-C3

There are no ring outliers.

No monomer is involved in short contacts.

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	568/613 (92%)	0.37	32 (5%) 30 32	8, 17, 38, 52	0
1	B	569/613 (92%)	0.29	33 (5%) 29 30	7, 16, 40, 73	0
1	C	561/613 (91%)	0.77	72 (12%) 7 8	8, 21, 44, 64	0
All	All	1698/1839 (92%)	0.48	137 (8%) 18 19	7, 18, 43, 73	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	39	LEU	6.8
1	C	159	ILE	6.4
1	C	503	ALA	6.3
1	B	41	GLY	6.3
1	C	161	VAL	5.9
1	C	502	ALA	5.5
1	B	42	VAL	5.3
1	B	606	HIS	5.1
1	A	39	LEU	4.9
1	C	508	ALA	4.9
1	C	160	TYR	4.7
1	A	306	VAL	4.4
1	C	504	GLY	4.3
1	A	504	GLY	4.3
1	B	508	ALA	4.2
1	B	40	LYS	4.1
1	C	163	GLY	4.1
1	A	503	ALA	4.0
1	B	513	ALA	4.0
1	C	162	ASP	3.9
1	C	585	MET	3.9
1	C	158	PRO	3.9
1	B	514	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	604	LEU	3.8
1	C	164	LYS	3.8
1	C	506	ARG	3.8
1	B	604	LEU	3.7
1	C	501	GLU	3.7
1	B	38	ARG	3.6
1	B	511	ILE	3.5
1	A	502	ALA	3.5
1	C	500	LEU	3.5
1	C	165	ASP	3.5
1	A	42	VAL	3.4
1	C	505	GLU	3.4
1	A	311	ILE	3.4
1	C	586	ARG	3.4
1	B	605	SER	3.3
1	C	166	VAL	3.3
1	B	44	ALA	3.3
1	B	503	ALA	3.3
1	A	606	HIS	3.2
1	C	606	HIS	3.2
1	B	502	ALA	3.2
1	C	320	TRP	3.2
1	C	54	ALA	3.1
1	A	41	GLY	3.1
1	C	507	SER	3.1
1	C	135	GLY	3.0
1	C	498	ARG	3.0
1	B	516	PRO	3.0
1	C	48	THR	3.0
1	B	515	LEU	2.9
1	A	309	PHE	2.9
1	B	512	ASN	2.9
1	A	498	ARG	2.9
1	C	605	SER	2.9
1	A	304	GLN	2.8
1	C	280	TYR	2.8
1	A	500	LEU	2.8
1	C	68	ASP	2.8
1	B	52	SER	2.8
1	A	310	GLY	2.8
1	A	52	SER	2.7
1	B	507	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	155	SER	2.7
1	C	156	ASN	2.7
1	C	497	ARG	2.7
1	C	509	GLU	2.7
1	A	280	TYR	2.7
1	B	43	GLY	2.6
1	B	500	LEU	2.6
1	C	157	ARG	2.6
1	B	509	GLU	2.6
1	C	315	ASN	2.6
1	B	498	ARG	2.5
1	C	138	VAL	2.5
1	B	504	GLY	2.5
1	C	311	ILE	2.5
1	C	568	GLU	2.5
1	C	511	ILE	2.5
1	B	48	THR	2.5
1	C	129	VAL	2.5
1	C	584	GLY	2.4
1	C	133	PHE	2.4
1	C	316	MET	2.4
1	C	249	ILE	2.4
1	A	583	PRO	2.4
1	C	126	ARG	2.4
1	A	302	ASN	2.4
1	B	494	SER	2.4
1	C	50	LEU	2.4
1	A	40	LYS	2.4
1	C	46	ALA	2.4
1	B	496	VAL	2.4
1	A	307	LYS	2.4
1	B	510	LYS	2.4
1	C	49	THR	2.3
1	C	499	GLU	2.3
1	A	286	ILE	2.3
1	C	143	ASN	2.3
1	C	588	ASN	2.3
1	C	423	THR	2.3
1	C	310	GLY	2.3
1	C	582	ARG	2.3
1	A	314	GLU	2.3
1	C	363	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	313	GLU	2.3
1	A	501	GLU	2.2
1	C	52	SER	2.2
1	A	312	ASP	2.2
1	B	313	GLU	2.2
1	A	43	GLY	2.2
1	A	508	ALA	2.2
1	C	66	TYR	2.2
1	A	305	LYS	2.2
1	A	506	ARG	2.2
1	C	170	VAL	2.2
1	B	77	THR	2.2
1	C	229	LEU	2.2
1	C	583	PRO	2.2
1	B	75	PHE	2.2
1	C	293	ALA	2.2
1	C	178	ARG	2.2
1	C	167	MET	2.1
1	A	137	ARG	2.1
1	A	494	SER	2.1
1	C	307	LYS	2.1
1	B	288	GLU	2.1
1	C	312	ASP	2.1
1	A	303	ASN	2.0
1	C	169	ALA	2.0
1	C	321	ASP	2.0
1	C	128	PHE	2.0
1	C	556	ILE	2.0
1	C	57	THR	2.0
1	C	417	VAL	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($\text{\AA}^2$)	Q<0.9
3	GOL	A	7001	6/6	0.73	0.17	31,35,36,39	0
3	GOL	C	7003	6/6	0.73	0.18	32,34,35,38	0
2	CIT	C	5003	13/13	0.76	0.16	32,35,37,39	0
2	CIT	B	5002	13/13	0.80	0.13	25,30,35,37	0
2	CIT	A	5001	13/13	0.84	0.12	23,30,38,39	0
3	GOL	B	7002	6/6	0.87	0.12	21,25,26,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.