Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:45 AM 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 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

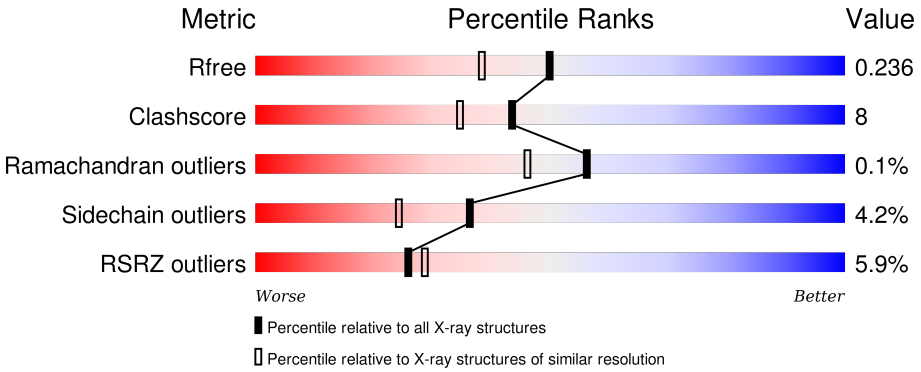
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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. 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 <=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% 75% 15% • 7%
1	B	613	5% 73% 17% • 7%
1	C	613	7% 76% 15% • 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
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 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.

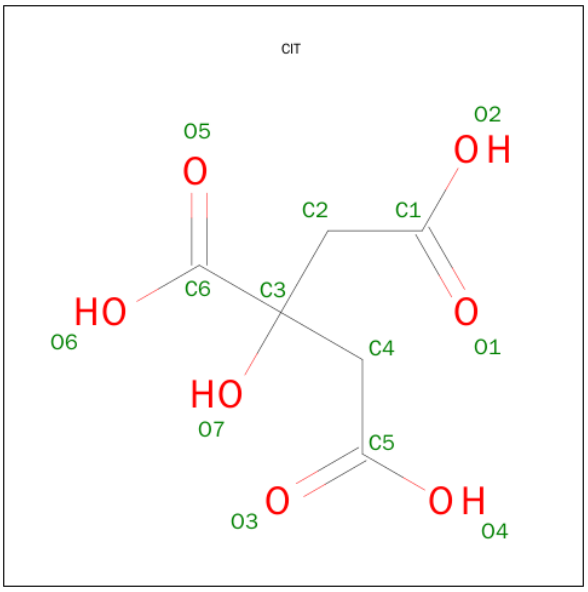
- Molecule 1 is a protein called Glucose-6-phosphate isomerase, glycosomal.

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:

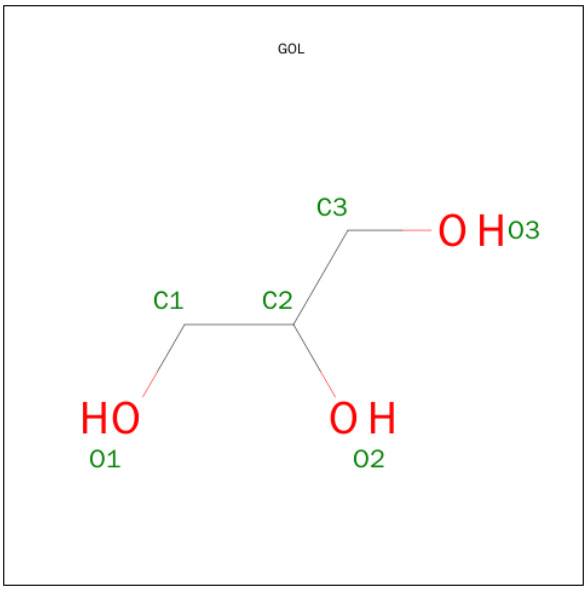
Chain	Residue	Modelled	Actual	Comment	Reference
A	77	THR	ALA	CONFLICT	UNP P13377
A	608	HIS	-	EXPRESSION TAG	UNP P13377
A	609	HIS	-	EXPRESSION TAG	UNP P13377
A	610	HIS	-	EXPRESSION TAG	UNP P13377
A	611	HIS	-	EXPRESSION TAG	UNP P13377
A	612	HIS	-	EXPRESSION TAG	UNP P13377
A	613	HIS	-	EXPRESSION TAG	UNP 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 (three-letter code: CIT) (formula: $C_6H_8O_7$).



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

- 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 6 3 3	0	0

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

- Molecule 4 is water.

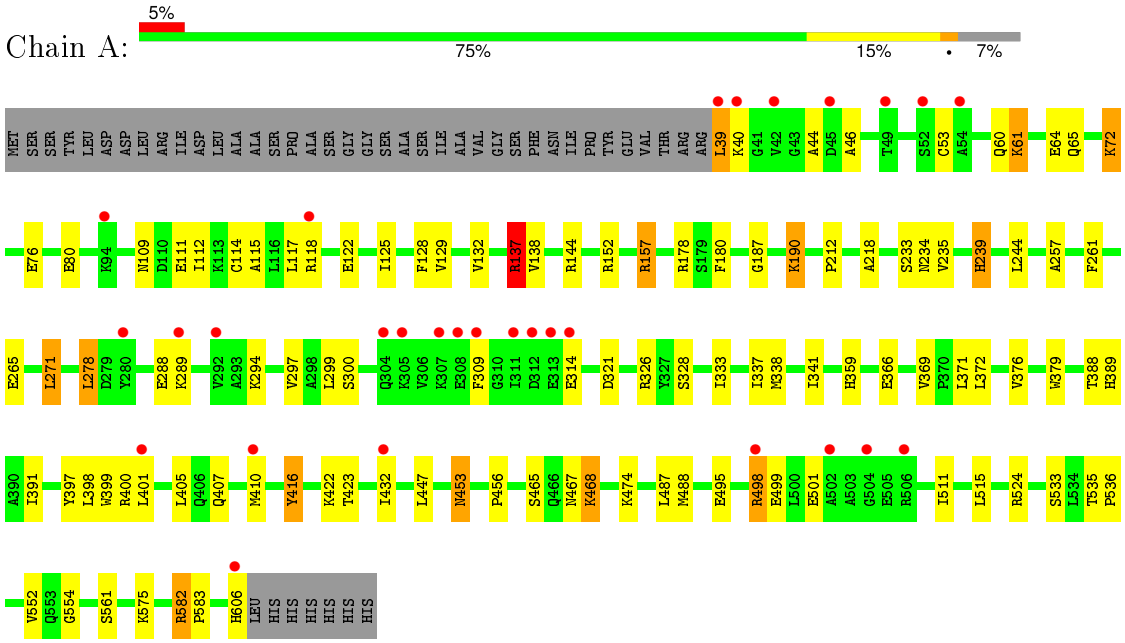
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	380	Total O 380 380	0	0
4	B	421	Total O 421 421	0	0
4	C	319	Total O 319 319	0	0

3 Residue-property plots (i)

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.

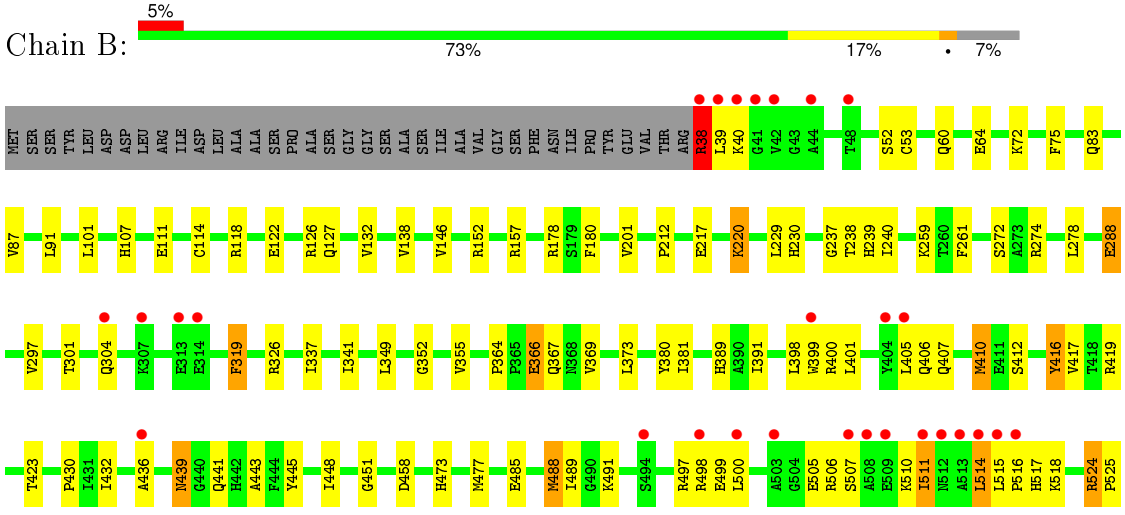
- Molecule 1: Glucose-6-phosphate isomerase, glycosomal

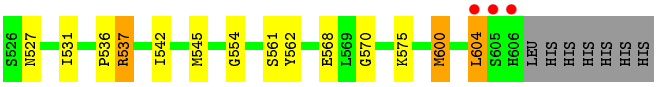
Chain A:



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

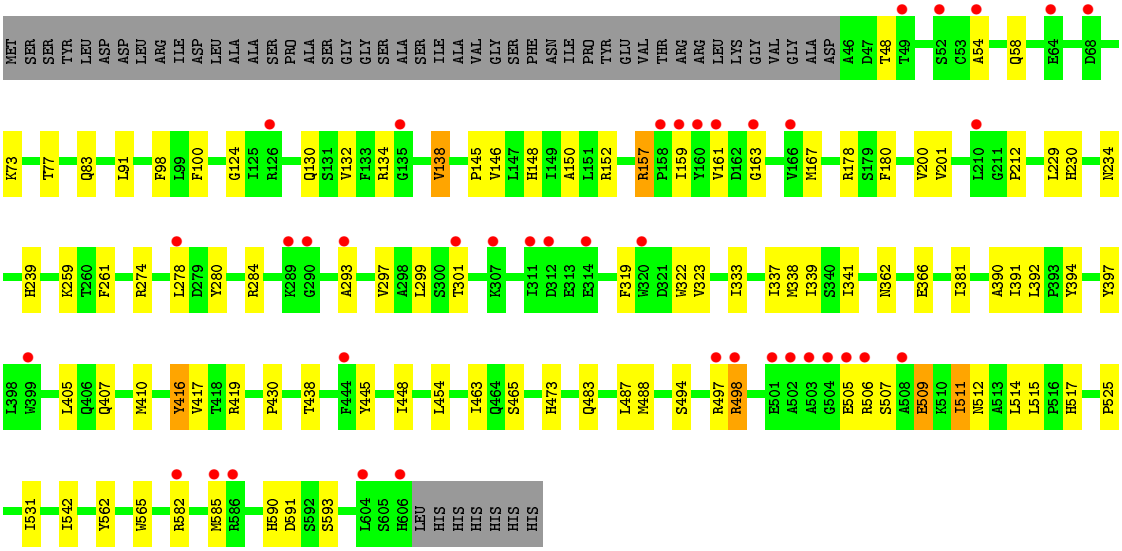
Chain B:





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

Chain C:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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	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)	0.36 , 37.5	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[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.59	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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 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	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

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 (218) 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: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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:ARG:NH1	1:A:498:ARG:HB2	2.15	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 (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%)	52 42
1	C	559/613 (91%)	539 (96%)	20 (4%)	0	100 100
All	All	1692/1839 (92%)	1634 (97%)	57 (3%)	1 (0%)	56 46

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%)	457 (95%)	25 (5%)	29 17
1	B	483/519 (93%)	463 (96%)	20 (4%)	37 25
1	C	478/519 (92%)	463 (97%)	15 (3%)	47 37
All	All	1443/1557 (93%)	1383 (96%)	60 (4%)	36 24

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 molecules 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	-	3,12,12	2.30	2 (66%)	3,17,17	2.94	2 (66%)
3	GOL	A	7001	-	5,5,5	4.78	5 (100%)	5,5,5	5.60	3 (60%)
2	CIT	B	5002	-	3,12,12	2.41	2 (66%)	3,17,17	3.10	2 (66%)
3	GOL	B	7002	-	5,5,5	4.62	5 (100%)	5,5,5	5.54	3 (60%)
2	CIT	C	5003	-	3,12,12	2.08	2 (66%)	3,17,17	2.94	2 (66%)
3	GOL	C	7003	-	5,5,5	4.78	5 (100%)	5,5,5	5.55	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	-	-	0/6/16/16	0/0/0/0
3	GOL	A	7001	-	-	0/4/4/4	0/0/0/0
2	CIT	B	5002	-	-	0/6/16/16	0/0/0/0
3	GOL	B	7002	-	-	0/4/4/4	0/0/0/0
2	CIT	C	5003	-	-	0/6/16/16	0/0/0/0
3	GOL	C	7003	-	-	0/4/4/4	0/0/0/0

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	7003	GOL	C3-C2	-8.18	1.21	1.52
3	A	7001	GOL	C3-C2	-7.83	1.22	1.52
3	B	7002	GOL	C3-C2	-7.75	1.22	1.52
3	A	7001	GOL	C1-C2	-3.57	1.38	1.52
3	C	7003	GOL	C1-C2	-3.41	1.39	1.52
3	B	7002	GOL	C1-C2	-3.17	1.40	1.52
3	B	7002	GOL	O2-C2	-3.12	1.34	1.43
3	C	7003	GOL	O2-C2	-3.05	1.34	1.43
2	B	5002	CIT	C4-C3	-3.02	1.50	1.54
3	A	7001	GOL	O2-C2	-2.47	1.36	1.43
2	A	5001	CIT	C4-C3	-2.42	1.51	1.54
2	C	5003	CIT	C4-C3	-2.31	1.51	1.54
2	B	5002	CIT	O7-C3	2.10	1.46	1.43
2	C	5003	CIT	O7-C3	2.41	1.47	1.43
2	A	5001	CIT	O7-C3	2.57	1.47	1.43
3	B	7002	GOL	O3-C3	2.97	1.55	1.42
3	C	7003	GOL	O3-C3	3.10	1.55	1.42
3	A	7001	GOL	O3-C3	3.34	1.56	1.42
3	C	7003	GOL	O1-C1	4.12	1.60	1.42
3	B	7002	GOL	O1-C1	4.23	1.60	1.42
3	A	7001	GOL	O1-C1	4.79	1.63	1.42

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	5002	CIT	C3-C4-C5	2.92	119.63	114.96
3	C	7003	GOL	O1-C1-C2	3.14	125.40	110.18
2	C	5003	CIT	C3-C2-C1	3.25	120.15	114.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	5001	CIT	C3-C4-C5	3.25	120.16	114.96
3	A	7001	GOL	O1-C1-C2	3.41	126.70	110.18
3	B	7002	GOL	O1-C1-C2	3.46	126.96	110.18
2	C	5003	CIT	C3-C4-C5	3.64	120.78	114.96
2	A	5001	CIT	C3-C2-C1	3.74	120.94	114.96
2	B	5002	CIT	C3-C2-C1	4.33	121.88	114.96
3	B	7002	GOL	O2-C2-C3	6.01	136.21	108.65
3	A	7001	GOL	O2-C2-C3	6.15	136.86	108.65
3	C	7003	GOL	O2-C2-C3	6.43	138.14	108.65
3	C	7003	GOL	O3-C3-C2	10.10	159.15	110.18
3	B	7002	GOL	O3-C3-C2	10.22	159.75	110.18
3	A	7001	GOL	O3-C3-C2	10.34	160.31	110.18

There are no chirality outliers.

There are no torsion outliers.

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, 95^{th} 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%)	0.44	29 (5%)	32	35	8, 17, 38, 52	0
1	B	569/613 (92%)	0.38	31 (5%)	29	33	7, 16, 40, 73	0
1	C	561/613 (91%)	0.62	40 (7%)	19	21	8, 21, 44, 64	0
All	All	1698/1839 (92%)	0.48	100 (5%)	26	29	7, 18, 43, 73	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	504	GLY	6.4
1	B	606	HIS	5.7
1	B	42	VAL	5.6
1	C	503	ALA	5.4
1	C	508	ALA	4.8
1	B	39	LEU	4.6
1	A	304	GLN	4.6
1	B	41	GLY	4.6
1	B	44	ALA	4.3
1	C	504	GLY	4.2
1	C	498	ARG	4.0
1	B	514	LEU	3.8
1	C	606	HIS	3.8
1	C	161	VAL	3.7
1	A	52	SER	3.7
1	C	505	GLU	3.7
1	C	585	MET	3.6
1	B	38	ARG	3.6
1	B	508	ALA	3.5
1	C	160	TYR	3.5
1	A	498	ARG	3.4
1	A	308	GLU	3.3
1	B	515	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	307	LYS	3.1
1	C	604	LEU	3.1
1	C	312	ASP	2.9
1	C	159	ILE	2.9
1	C	158	PRO	2.9
1	A	40	LYS	2.9
1	C	320	TRP	2.9
1	C	506	ARG	2.8
1	A	309	PHE	2.8
1	B	604	LEU	2.8
1	C	278	LEU	2.8
1	A	506	ARG	2.7
1	A	606	HIS	2.7
1	A	502	ALA	2.7
1	B	498	ARG	2.7
1	C	68	ASP	2.7
1	B	399	TRP	2.7
1	A	305	LYS	2.6
1	A	401	LEU	2.6
1	C	210	LEU	2.6
1	C	290	GLY	2.6
1	B	512	ASN	2.6
1	A	42	VAL	2.6
1	A	39	LEU	2.6
1	C	293	ALA	2.6
1	C	64	GLU	2.6
1	B	40	LYS	2.5
1	B	605	SER	2.5
1	B	48	THR	2.5
1	C	582	ARG	2.5
1	B	509	GLU	2.5
1	C	314	GLU	2.5
1	C	126	ARG	2.5
1	C	52	SER	2.5
1	B	405	LEU	2.5
1	C	49	THR	2.5
1	B	494	SER	2.5
1	B	516	PRO	2.5
1	C	444	PHE	2.4
1	A	54	ALA	2.4
1	B	503	ALA	2.4
1	C	502	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	304	GLN	2.4
1	B	511	ILE	2.4
1	B	307	LYS	2.4
1	B	436	ALA	2.4
1	C	399	TRP	2.3
1	C	54	ALA	2.3
1	C	163	GLY	2.3
1	C	135	GLY	2.3
1	A	49	THR	2.3
1	A	314	GLU	2.3
1	C	301	THR	2.3
1	C	166	VAL	2.3
1	C	586	ARG	2.3
1	A	45	ASP	2.2
1	C	497	ARG	2.2
1	B	507	SER	2.2
1	C	307	LYS	2.2
1	A	94	LYS	2.2
1	C	289	LYS	2.2
1	B	314	GLU	2.1
1	A	289	LYS	2.1
1	B	404	TYR	2.1
1	A	292	VAL	2.1
1	A	312	ASP	2.1
1	A	311	ILE	2.1
1	C	311	ILE	2.1
1	A	280	TYR	2.1
1	A	410	MET	2.1
1	A	118	ARG	2.1
1	B	313	GLU	2.1
1	C	501	GLU	2.0
1	A	313	GLU	2.0
1	B	500	LEU	2.0
1	B	513	ALA	2.0
1	A	432	ILE	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 carbohydrates 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. 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, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
3	GOL	A	7001	6/6	0.68	0.21	2.90	31,35,36,39	0
2	CIT	B	5002	13/13	0.79	0.19	2.80	25,30,35,37	0
2	CIT	A	5001	13/13	0.86	0.18	2.16	23,30,38,39	0
3	GOL	C	7003	6/6	0.69	0.21	1.84	32,34,35,38	0
2	CIT	C	5003	13/13	0.81	0.18	1.72	32,35,37,39	0
3	GOL	B	7002	6/6	0.87	0.15	1.22	21,25,26,28	0

6.5 Other polymers (i)

There are no such residues in this entry.