



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:20 PM GMT

PDB ID : 4OLC
Title : Carbamate kinase from Giardia lamblia thiocarbamoylated by disulfiram on Cys242
Authors : Lim, K.; Herzberg, O.
Deposited on : 2014-01-23
Resolution : 2.60 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

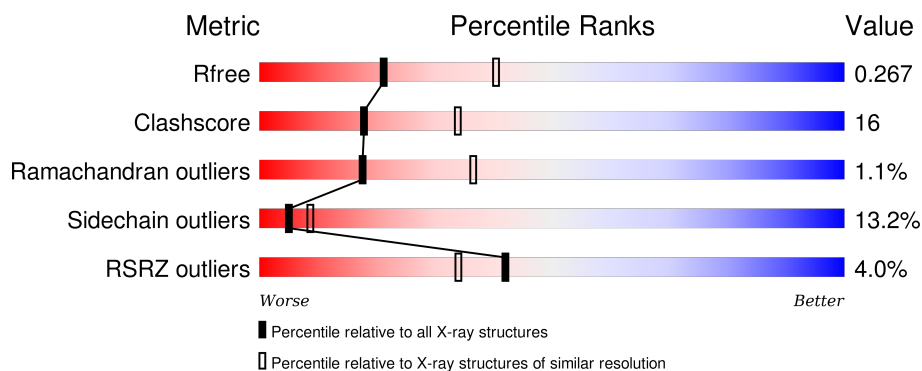
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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 $\leq 5\%$. 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	317	<div> <div>4%</div> <div>61% 30% 6% .</div> </div>
1	B	317	<div> <div>3%</div> <div>63% 28% 6% .</div> </div>
1	C	317	<div> <div>3%</div> <div>67% 26% . .</div> </div>
1	D	317	<div> <div>6%</div> <div>59% 33% 5% .</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DCD	A	402	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9525 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.

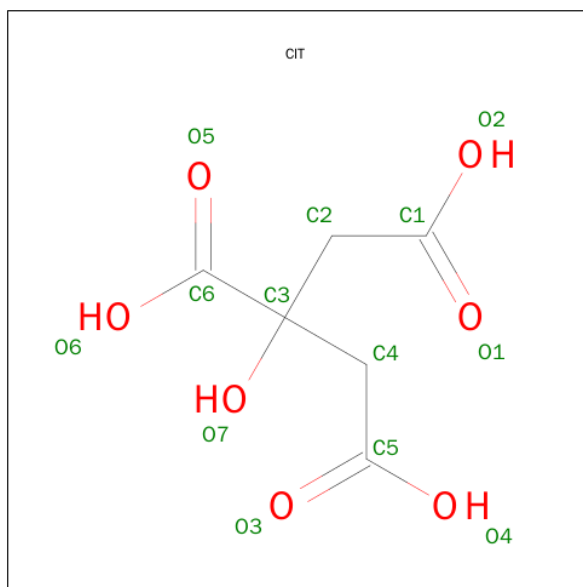
- Molecule 1 is a protein called Carbamate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	0	0
			2296	1439	397	442	18			
1	B	308	Total	C	N	O	S	0	0	0
			2296	1439	397	442	18			
1	C	308	Total	C	N	O	S	0	0	0
			2296	1439	397	442	18			
1	D	308	Total	C	N	O	S	0	0	0
			2296	1439	397	442	18			

There are 4 discrepancies between the modelled and reference sequences:

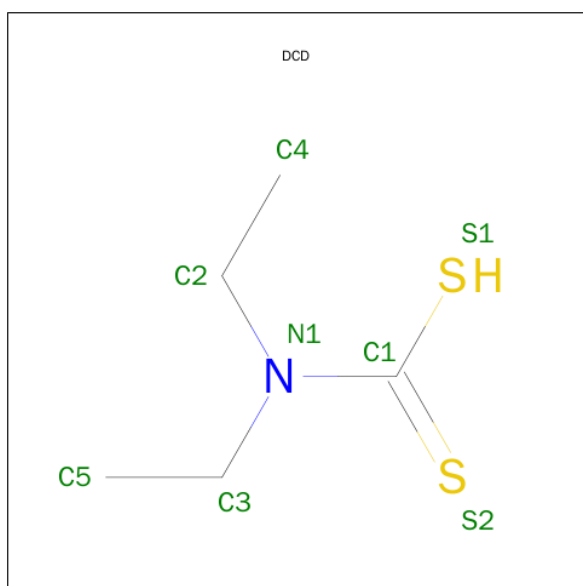
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	CLONING ARTIFACT	UNP A8BB85
B	0	GLY	-	CLONING ARTIFACT	UNP A8BB85
C	0	GLY	-	CLONING ARTIFACT	UNP A8BB85
D	0	GLY	-	CLONING ARTIFACT	UNP A8BB85

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

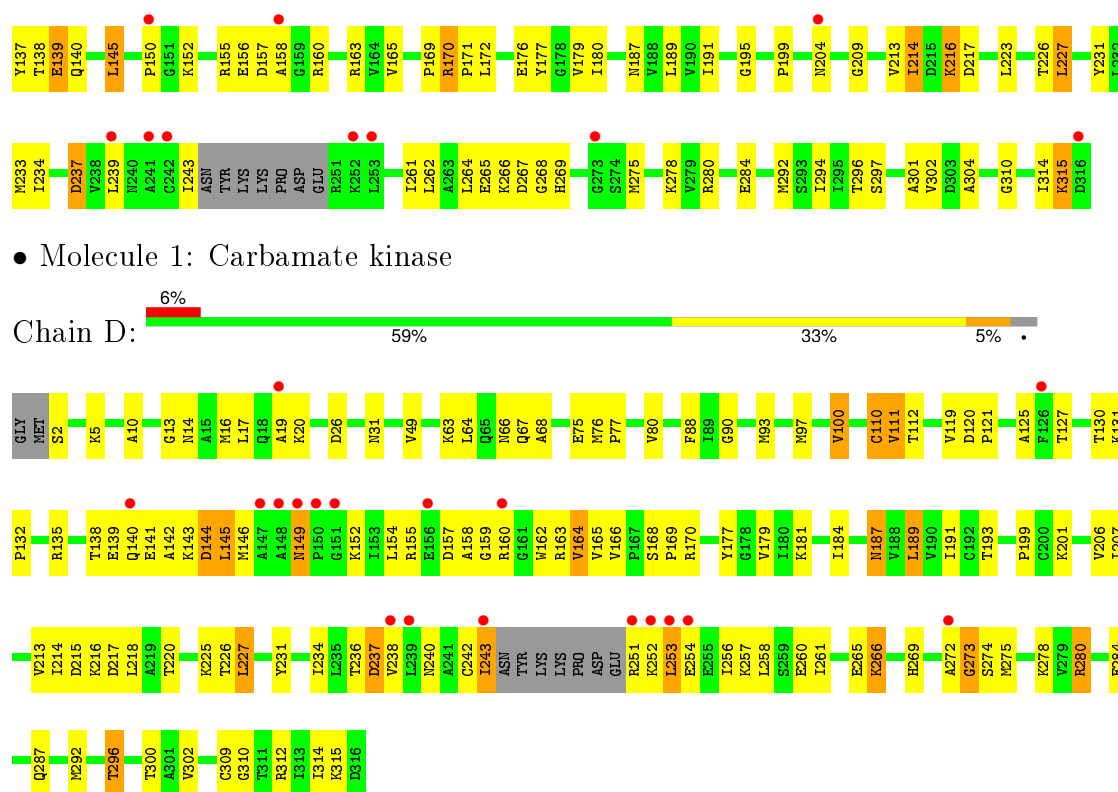
- Molecule 3 is DIETHYLCARBAMODITHIOIC ACID (three-letter code: DCD) (formula: $C_5H_{11}NS_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	S	0	0
			8	5	1	2		
3	B	1	Total	C	N	S	0	0
			8	5	1	2		
3	C	1	Total	C	N	S	0	0
			8	5	1	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	57	Total	O	0	0
			57	57		
4	B	73	Total	O	0	0
			73	73		
4	C	71	Total	O	0	0
			71	71		
4	D	64	Total	O	0	0
			64	64		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.30Å 98.18Å 102.67Å 90.00° 107.57° 90.00°	Depositor
Resolution (Å)	49.00 – 2.60 43.88 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.00-2.60) 95.1 (43.88-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.08 (at 2.61Å)	Xtriage
Refinement program	Phenix	Depositor
R, R_{free}	0.206 , 0.274 0.204 , 0.267	Depositor DCC
R_{free} test set	2013 reflections (5.43%)	DCC
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.726	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 37.6	EDS
Estimated twinning fraction	0.005 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 40453 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9525	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.28 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.8050e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DCD, 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	0.42	0/2325	0.60	0/3141
1	B	0.44	0/2325	0.60	0/3141
1	C	0.44	0/2325	0.61	0/3141
1	D	0.42	0/2325	0.59	0/3141
All	All	0.43	0/9300	0.60	0/12564

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2296	0	2359	86	0
1	B	2296	0	2358	69	0
1	C	2296	0	2359	68	0
1	D	2296	0	2359	85	0
2	A	13	0	5	1	0
2	B	13	0	5	3	0
2	C	13	0	5	1	0
2	D	13	0	5	2	0
3	A	8	0	11	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	8	0	10	0	0
3	C	8	0	11	3	0
4	A	57	0	0	5	0
4	B	73	0	0	2	0
4	C	71	0	0	2	0
4	D	64	0	0	4	0
All	All	9525	0	9487	296	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 16.

All (296) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:ILE:HG13	1:B:269:HIS:HB3	1.51	0.93
1:D:296:THR:HG23	1:D:310:GLY:HA3	1.52	0.89
1:B:11:LEU:O	1:B:216:LYS:HE3	1.78	0.84
1:D:19:ALA:O	1:D:20:LYS:HG2	1.83	0.79
1:B:258:LEU:HD21	1:B:287:GLN:HG2	1.65	0.77
1:A:138:THR:HG21	1:A:140:GLN:OE1	1.84	0.76
1:D:243:ILE:HD11	1:D:269:HIS:HB3	1.67	0.76
1:A:55:ASN:HB2	1:A:195:GLY:HA3	1.68	0.75
1:B:138:THR:HB	1:B:141:GLU:HB2	1.69	0.74
1:C:233:MET:HG2	1:C:294:ILE:HB	1.69	0.74
1:A:296:THR:HG21	1:A:304:ALA:HB2	1.67	0.74
1:A:237:ASP:O	3:A:402:DCD:S2	2.46	0.74
1:B:20:LYS:NZ	1:B:160:ARG:HB3	2.02	0.73
1:A:138:THR:HG22	1:A:140:GLN:H	1.53	0.72
1:A:243:ILE:HG21	1:A:269:HIS:CD2	2.25	0.72
1:A:243:ILE:HG12	1:A:269:HIS:HB3	1.71	0.71
1:C:55:ASN:HB2	1:C:195:GLY:HA3	1.73	0.71
1:A:13:GLY:O	1:A:15:ALA:N	2.24	0.70
1:D:142:ALA:O	1:D:146:MET:HB2	1.92	0.70
1:B:90:GLY:HA3	1:B:112:THR:HG21	1.72	0.70
1:D:252:LYS:HE2	1:D:254:GLU:OE2	1.92	0.70
1:D:2:SER:N	1:D:187:ASN:HD21	1.88	0.70
1:A:233:MET:HG2	1:A:294:ILE:HB	1.74	0.69
1:A:239:LEU:HD21	3:A:402:DCD:H4C2	1.72	0.69
1:D:170:ARG:NH2	1:D:284:GLU:OE2	2.26	0.69
1:B:199:PRO:HG3	1:B:214:ILE:HD12	1.74	0.69
1:D:216:LYS:NZ	4:D:518:HOH:O	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:158:ALA:C	1:D:160:ARG:H	1.97	0.69
1:A:283:ILE:O	1:A:287:GLN:HB2	1.93	0.68
1:D:234:ILE:HG21	1:D:278:LYS:HG2	1.75	0.68
1:C:237:ASP:O	3:C:402:DCD:S2	2.51	0.68
1:D:90:GLY:HA3	1:D:112:THR:HG21	1.75	0.68
1:A:243:ILE:HG21	1:A:269:HIS:HD2	1.59	0.67
1:A:215:ASP:HB3	1:A:218:LEU:HD12	1.77	0.67
1:C:11:LEU:O	1:C:216:LYS:NZ	2.28	0.67
1:C:243:ILE:HD11	1:C:264:LEU:HD13	1.77	0.66
1:A:90:GLY:HA3	1:A:112:THR:HG21	1.76	0.66
1:A:149:ASN:HB3	1:A:152:LYS:HB2	1.77	0.66
1:B:49:VAL:HB	1:B:189:LEU:HD22	1.77	0.65
1:A:256:ILE:HG12	1:A:257:LYS:H	1.60	0.65
1:A:14:ASN:ND2	4:A:549:HOH:O	2.30	0.65
1:B:93:MET:HB3	1:B:191:ILE:HD13	1.78	0.65
1:C:231:TYR:HE2	1:C:292:MET:HE2	1.61	0.65
1:B:13:GLY:N	2:B:402:CIT:H41	2.11	0.65
1:A:2:SER:N	1:A:187:ASN:HD21	1.95	0.64
1:B:201:LYS:HE3	1:B:203:GLU:CD	2.18	0.64
1:B:233:MET:HE3	1:B:235:LEU:HD21	1.78	0.64
1:B:20:LYS:HZ3	1:B:160:ARG:HB3	1.61	0.64
1:C:296:THR:CG2	1:C:310:GLY:HA3	2.28	0.64
1:A:146:MET:HG2	1:A:152:LYS:O	1.99	0.63
1:B:96:ALA:O	1:B:100:VAL:HG23	1.98	0.63
1:C:111:VAL:HG13	1:D:179:VAL:HG21	1.80	0.63
1:A:179:VAL:HG11	1:B:111:VAL:HG21	1.80	0.63
1:A:292:MET:HE2	1:A:294:ILE:HD11	1.80	0.63
1:A:55:ASN:HB2	1:A:195:GLY:CA	2.29	0.62
1:B:177:TYR:CE1	1:B:226:THR:HG22	2.34	0.62
1:D:177:TYR:CE1	1:D:226:THR:HG22	2.35	0.62
1:C:130:THR:C	1:C:165:VAL:HG13	2.20	0.62
1:A:111:VAL:HG21	1:B:179:VAL:HG11	1.81	0.62
1:C:55:ASN:HB2	1:C:195:GLY:CA	2.30	0.62
1:C:296:THR:HG21	1:C:304:ALA:HB2	1.82	0.62
1:A:189:LEU:HD12	1:A:189:LEU:C	2.20	0.62
1:D:243:ILE:HG22	1:D:251:ARG:N	2.15	0.61
1:C:138:THR:HG22	1:C:140:GLN:H	1.66	0.61
1:C:296:THR:HG22	1:C:310:GLY:HA3	1.83	0.61
1:D:296:THR:HG23	1:D:310:GLY:CA	2.26	0.61
1:A:256:ILE:HG12	1:A:257:LYS:N	2.15	0.61
1:B:53:SER:HB3	1:B:93:MET:HE1	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:ILE:HG23	1:C:269:HIS:HB3	1.82	0.61
1:C:216:LYS:HE3	1:C:217:ASP:OD1	2.01	0.60
1:C:170:ARG:NH2	1:C:284:GLU:OE1	2.34	0.60
1:A:179:VAL:HG11	1:B:111:VAL:CG2	2.30	0.60
1:D:258:LEU:HD21	1:D:287:GLN:HG2	1.83	0.60
1:A:51:LEU:HD13	1:A:93:MET:CE	2.32	0.59
1:C:57:PRO:HD3	2:C:401:CIT:O1	2.02	0.59
1:B:56:GLY:O	1:B:133:VAL:HG22	2.02	0.59
1:C:90:GLY:HA3	1:C:112:THR:HG21	1.83	0.59
1:D:216:LYS:HE3	1:D:217:ASP:OD1	2.03	0.59
1:B:13:GLY:H	2:B:402:CIT:H41	1.68	0.59
1:A:51:LEU:HD13	1:A:93:MET:HE3	1.84	0.59
1:C:169:PRO:HD2	1:C:213:VAL:O	2.01	0.59
1:A:13:GLY:C	1:A:15:ALA:H	2.06	0.59
1:A:292:MET:CE	1:A:294:ILE:HD11	2.33	0.59
1:B:139:GLU:O	1:B:143:LYS:HG3	2.02	0.58
1:B:148:ALA:O	1:B:150:PRO:HD3	2.03	0.58
1:B:296:THR:HG23	1:B:310:GLY:CA	2.33	0.58
1:B:264:LEU:O	1:B:269:HIS:HB2	2.03	0.58
1:D:138:THR:OG1	1:D:141:GLU:HB2	2.04	0.57
1:D:280:ARG:O	1:D:284:GLU:HG3	2.05	0.57
1:C:231:TYR:CE2	1:C:292:MET:HE2	2.38	0.57
1:A:16:MET:C	1:A:17:LEU:HD12	2.24	0.57
1:B:10:ALA:HB1	1:B:216:LYS:HE2	1.86	0.57
1:A:96:ALA:O	1:A:100:VAL:HG23	2.04	0.57
1:B:233:MET:HE1	1:B:301:ALA:HB1	1.86	0.57
1:D:140:GLN:HA	1:D:143:LYS:HZ3	1.69	0.57
1:B:221:SER:HB2	1:B:281:ALA:HB1	1.85	0.57
1:C:239:LEU:HD11	3:C:402:DCD:S2	2.45	0.56
4:A:520:HOH:O	1:B:135:ARG:HD2	2.06	0.56
1:D:63:LYS:O	1:D:63:LYS:HD2	2.06	0.56
1:C:179:VAL:HG11	1:D:111:VAL:CG1	2.36	0.56
1:C:266:LYS:C	1:C:268:GLY:H	2.10	0.56
1:D:231:TYR:HE2	1:D:292:MET:HE2	1.70	0.55
1:B:139:GLU:OE2	1:B:143:LYS:NZ	2.38	0.55
1:D:49:VAL:HB	1:D:189:LEU:HD22	1.87	0.55
1:C:187:ASN:ND2	4:C:2053:HOH:O	2.40	0.55
1:D:177:TYR:CE1	1:D:227:LEU:HD13	2.41	0.55
1:C:234:ILE:HG21	1:C:278:LYS:HD3	1.89	0.55
1:A:177:TYR:CE1	1:A:226:THR:HG22	2.42	0.55
1:B:253:LEU:HG	1:B:256:ILE:HD13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:312:ARG:NH2	4:D:562:HOH:O	2.40	0.55
1:D:10:ALA:HB2	1:D:220:THR:HG21	1.88	0.54
1:A:86:GLN:NE2	1:A:197:GLY:HA2	2.23	0.54
1:B:243:ILE:CG1	1:B:269:HIS:HB3	2.29	0.54
1:C:55:ASN:O	1:C:59:VAL:HG12	2.08	0.54
1:A:88:PHE:CD1	1:B:80:VAL:HG13	2.43	0.54
1:C:2:SER:N	1:C:187:ASN:OD1	2.40	0.54
1:D:145:LEU:HD11	1:D:152:LYS:HZ3	1.73	0.54
1:B:277:PRO:HG2	4:B:528:HOH:O	2.08	0.54
1:D:258:LEU:HD21	1:D:287:GLN:CG	2.38	0.54
1:A:256:ILE:HD13	1:A:261:ILE:HB	1.90	0.53
1:D:237:ASP:N	1:D:237:ASP:OD1	2.41	0.53
1:B:272:ALA:O	1:B:273:GLY:O	2.26	0.53
1:A:18:GLN:HB2	1:A:21:GLU:OE2	2.08	0.53
1:D:240:ASN:ND2	1:D:253:LEU:O	2.40	0.53
1:D:256:ILE:HD11	1:D:260:GLU:HG2	1.89	0.53
2:D:401:CIT:O7	2:D:401:CIT:O1	2.26	0.53
1:A:236:THR:HG23	1:A:238:VAL:O	2.09	0.53
1:A:239:LEU:HD12	1:A:239:LEU:H	1.74	0.53
1:D:177:TYR:HE1	1:D:227:LEU:HD13	1.74	0.53
1:D:2:SER:N	1:D:187:ASN:ND2	2.57	0.52
1:B:283:ILE:O	1:B:287:GLN:HG3	2.09	0.52
1:B:255:GLU:OE2	1:B:312:ARG:NH1	2.43	0.52
1:C:72:VAL:HG11	1:D:68:ALA:HB2	1.90	0.52
1:A:41:LYS:HB3	1:A:302:VAL:HG11	1.91	0.51
1:C:296:THR:HG21	1:C:304:ALA:CB	2.39	0.51
1:D:67:GLN:HA	1:D:75:GLU:OE2	2.10	0.51
1:A:270:PHE:HB3	1:A:275:MET:HB3	1.91	0.51
1:C:179:VAL:HG11	1:D:111:VAL:HG11	1.93	0.51
1:A:189:LEU:CD1	1:A:189:LEU:C	2.78	0.51
1:B:296:THR:HG23	1:B:310:GLY:HA2	1.92	0.51
1:C:26:ASP:O	1:C:30:LYS:HG2	2.10	0.51
2:A:401:CIT:O4	2:A:401:CIT:O7	2.29	0.51
1:A:234:ILE:HG21	1:A:278:LYS:HG2	1.93	0.51
1:D:131:LYS:HE3	1:D:213:VAL:CG1	2.41	0.51
1:A:145:LEU:O	1:A:149:ASN:HB2	2.11	0.51
1:B:138:THR:HG22	1:B:140:GLN:H	1.75	0.50
1:D:158:ALA:C	1:D:160:ARG:N	2.64	0.50
1:A:20:LYS:HG3	1:A:160:ARG:HH12	1.76	0.50
1:A:120:ASP:OD1	1:A:122:LYS:HG2	2.11	0.50
1:A:243:ILE:HD13	1:A:269:HIS:CG	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:184:ILE:HD11	1:D:227:LEU:HG	1.92	0.50
1:A:186:ASN:O	1:A:187:ASN:HB2	2.11	0.50
1:D:131:LYS:HB3	1:D:166:VAL:O	2.12	0.50
1:B:96:ALA:O	1:B:100:VAL:CG2	2.60	0.50
1:C:112:THR:HA	1:C:191:ILE:O	2.12	0.50
1:C:111:VAL:HG11	1:D:179:VAL:HG11	1.93	0.49
1:A:239:LEU:HD11	3:A:402:DCD:C4	2.42	0.49
1:D:149:ASN:HD21	1:D:152:LYS:HZ1	1.60	0.49
1:B:156:GLU:OE2	1:B:159:GLY:HA2	2.13	0.49
1:A:280:ARG:NH1	4:A:532:HOH:O	2.40	0.49
1:C:199:PRO:HG3	1:C:214:ILE:HG13	1.94	0.49
1:A:170:ARG:HH11	1:A:170:ARG:HB2	1.77	0.49
1:D:5:LYS:NZ	4:D:502:HOH:O	2.45	0.49
1:C:136:PHE:CE2	1:C:160:ARG:HB3	2.47	0.49
1:A:138:THR:H	1:A:141:GLU:HB2	1.78	0.49
1:D:154:LEU:HD23	1:D:164:VAL:HA	1.95	0.49
1:B:243:ILE:HG22	1:B:251:ARG:O	2.14	0.48
1:B:29:ARG:O	1:B:33:GLU:HG3	2.13	0.48
1:A:203:GLU:HG2	4:A:534:HOH:O	2.13	0.48
1:A:189:LEU:O	1:A:189:LEU:HD12	2.13	0.48
1:D:258:LEU:O	1:D:261:ILE:HG22	2.13	0.48
1:B:154:LEU:HG	1:B:164:VAL:HA	1.95	0.48
1:A:296:THR:HG22	1:A:310:GLY:HA2	1.95	0.48
1:B:57:PRO:HD3	2:B:402:CIT:O2	2.14	0.48
1:D:231:TYR:CE2	1:D:292:MET:HE2	2.49	0.48
1:A:203:GLU:O	1:A:204:ASN:HB2	2.13	0.48
1:A:60:GLY:CA	1:A:133:VAL:HG13	2.43	0.48
1:B:112:THR:HA	1:B:191:ILE:O	2.13	0.48
1:C:223:LEU:O	1:C:227:LEU:HB2	2.13	0.48
1:B:129:PRO:HB2	1:B:165:VAL:HG12	1.95	0.48
1:B:243:ILE:HD11	1:B:269:HIS:CG	2.50	0.47
1:C:292:MET:CE	1:C:294:ILE:HD11	2.43	0.47
1:A:264:LEU:HD23	1:A:264:LEU:N	2.29	0.47
1:D:135:ARG:HD2	1:D:135:ARG:C	2.35	0.47
1:B:197:GLY:O	1:B:199:PRO:HD3	2.14	0.47
1:B:296:THR:HG23	1:B:310:GLY:HA3	1.96	0.47
1:D:125:ALA:HB1	1:D:168:SER:H	1.79	0.47
1:A:266:LYS:C	1:A:268:GLY:H	2.17	0.47
3:A:402:DCD:H4C3	3:A:402:DCD:S2	2.54	0.47
1:C:138:THR:CG2	1:C:139:GLU:N	2.77	0.47
1:B:236:THR:OG1	1:B:237:ASP:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:MET:HB3	1:C:28:GLN:HG2	1.95	0.47
1:D:131:LYS:HA	1:D:132:PRO:HD3	1.73	0.47
1:D:139:GLU:HG3	1:D:162:TRP:HE1	1.80	0.47
1:D:97:MET:HA	1:D:100:VAL:HG23	1.97	0.47
1:A:199:PRO:HG3	1:A:214:ILE:HG13	1.97	0.46
1:D:193:THR:O	1:D:193:THR:HG22	2.15	0.46
1:A:42:ILE:HG22	1:A:47:TYR:HB2	1.97	0.46
1:A:243:ILE:HD13	1:A:269:HIS:CD2	2.50	0.46
1:A:13:GLY:C	1:A:15:ALA:N	2.64	0.46
1:A:111:VAL:CG2	1:B:179:VAL:HG11	2.45	0.46
1:C:280:ARG:O	1:C:284:GLU:HG3	2.16	0.46
1:A:64:LEU:HD13	1:B:72:VAL:HG12	1.98	0.46
1:B:184:ILE:HD11	1:B:227:LEU:HG	1.97	0.46
1:D:112:THR:HA	1:D:191:ILE:O	2.16	0.46
1:B:26:ASP:OD1	1:B:29:ARG:NH2	2.48	0.46
1:B:20:LYS:HZ1	1:B:160:ARG:HB3	1.80	0.46
1:D:131:LYS:HE3	1:D:213:VAL:HG11	1.98	0.46
1:D:236:THR:HG23	1:D:238:VAL:H	1.81	0.46
1:A:43:HIS:NE2	1:A:106:GLU:OE1	2.30	0.46
1:C:239:LEU:N	1:C:239:LEU:HD12	2.31	0.46
1:D:13:GLY:H	2:D:401:CIT:C5	2.29	0.46
1:D:215:ASP:OD1	1:D:218:LEU:HG	2.16	0.46
1:C:80:VAL:HG13	1:D:88:PHE:CD1	2.51	0.46
1:D:243:ILE:HD11	1:D:269:HIS:CB	2.44	0.45
1:B:17:LEU:HD12	1:B:17:LEU:HA	1.71	0.45
3:A:402:DCD:H5C2	3:A:402:DCD:H2C2	1.72	0.45
1:C:292:MET:HE1	1:C:294:ILE:HD11	1.97	0.45
1:A:111:VAL:HG12	1:B:176:GLU:HG2	1.98	0.45
1:C:155:ARG:NH1	4:C:2018:HOH:O	2.31	0.45
1:A:304:ALA:HA	1:A:309:CYS:O	2.17	0.45
1:D:149:ASN:HD21	1:D:152:LYS:NZ	2.14	0.45
1:A:136:PHE:HA	1:A:162:TRP:O	2.17	0.44
1:C:14:ASN:N	1:C:14:ASN:OD1	2.47	0.44
1:D:76:MET:HA	1:D:77:PRO:HD3	1.84	0.44
1:A:243:ILE:HD11	1:A:264:LEU:HD13	1.99	0.44
1:A:11:LEU:CD2	1:A:235:LEU:HD12	2.48	0.44
1:C:111:VAL:CG1	1:D:179:VAL:HG11	2.48	0.44
1:D:132:PRO:HB2	1:D:163:ARG:NH2	2.32	0.44
1:C:79:HIS:ND1	1:C:209:GLY:HA3	2.33	0.44
1:D:120:ASP:OD1	1:D:121:PRO:HD2	2.17	0.44
1:B:121:PRO:HG3	1:B:201:LYS:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:ALA:HB1	1:D:168:SER:N	2.33	0.44
1:C:18:GLN:HB2	1:C:21:GLU:CD	2.38	0.44
1:D:158:ALA:O	1:D:160:ARG:N	2.51	0.43
1:D:266:LYS:HA	1:D:266:LYS:HD3	1.80	0.43
1:D:110:CYS:HB2	1:D:189:LEU:HB3	2.00	0.43
1:D:16:MET:C	1:D:31:ASN:HD22	2.20	0.43
1:B:16:MET:O	1:B:31:ASN:ND2	2.49	0.43
1:A:131:LYS:HB2	1:A:168:SER:HB2	1.99	0.43
1:A:296:THR:HB	1:A:300:THR:OG1	2.19	0.43
1:B:262:LEU:O	1:B:266:LYS:HG2	2.19	0.43
1:D:146:MET:CE	1:D:154:LEU:HB2	2.48	0.43
1:C:177:TYR:CE1	1:C:226:THR:HG22	2.54	0.43
1:A:167:PRO:C	1:A:169:PRO:HD3	2.39	0.43
1:C:138:THR:HG22	1:C:140:GLN:N	2.30	0.43
1:D:120:ASP:HA	1:D:121:PRO:HD3	1.88	0.43
1:D:199:PRO:HG3	1:D:214:ILE:HG13	2.01	0.43
1:D:140:GLN:O	1:D:144:ASP:OD1	2.37	0.42
1:C:176:GLU:HG2	1:D:111:VAL:HG12	2.01	0.42
1:A:60:GLY:HA3	1:A:133:VAL:HG13	2.01	0.42
1:D:300:THR:HB	1:D:309:CYS:SG	2.59	0.42
1:B:294:ILE:HG21	1:B:304:ALA:HB1	2.01	0.42
1:C:280:ARG:HA	1:C:280:ARG:HD2	1.68	0.42
1:B:79:HIS:HB3	1:B:210:VAL:O	2.19	0.42
1:A:139:GLU:HG2	1:A:162:TRP:NE1	2.34	0.42
3:C:402:DCD:H2C2	3:C:402:DCD:H5C2	1.77	0.42
1:B:203:GLU:HA	4:B:567:HOH:O	2.19	0.42
1:C:296:THR:HG21	1:C:310:GLY:HA3	2.00	0.42
1:D:272:ALA:O	1:D:273:GLY:O	2.38	0.42
1:D:142:ALA:HB1	1:D:154:LEU:HD13	2.02	0.42
1:B:258:LEU:O	1:B:262:LEU:HB2	2.20	0.41
1:C:266:LYS:C	1:C:268:GLY:N	2.72	0.41
1:C:18:GLN:HA	1:C:18:GLN:OE1	2.20	0.41
1:D:216:LYS:HE3	1:D:217:ASP:CG	2.41	0.41
1:D:201:LYS:O	1:D:207:ILE:HA	2.20	0.41
1:D:119:VAL:HB	1:D:169:PRO:HB2	2.01	0.41
1:A:239:LEU:HD11	3:A:402:DCD:H4C1	2.02	0.41
1:A:181:LYS:NZ	1:A:185:ASP:OD2	2.52	0.41
1:B:30:LYS:O	1:B:34:ILE:HG13	2.20	0.41
1:C:265:GLU:OE2	1:C:280:ARG:NH1	2.54	0.41
1:D:181:LYS:HD3	1:D:227:LEU:HD12	2.02	0.41
1:C:93:MET:HE1	1:C:191:ILE:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:ILE:HD11	1:C:301:ALA:HB1	2.02	0.41
1:B:136:PHE:HE2	1:B:157:ASP:HB3	1.86	0.41
1:A:122:LYS:HE2	1:A:122:LYS:HB3	1.91	0.41
1:A:66:ASN:O	1:A:75:GLU:HB2	2.19	0.41
1:A:138:THR:HG22	1:A:139:GLU:N	2.35	0.41
1:C:176:GLU:O	1:C:180:ILE:HG13	2.21	0.41
1:A:129:PRO:CB	1:A:165:VAL:HG12	2.50	0.41
1:A:23:GLY:O	4:A:509:HOH:O	2.22	0.41
1:C:296:THR:HG22	1:C:310:GLY:CA	2.49	0.40
1:B:55:ASN:CG	1:B:195:GLY:HA3	2.41	0.40
1:A:91:TYR:CD1	1:B:198:ILE:HD13	2.56	0.40
1:D:66:ASN:ND2	4:D:523:HOH:O	2.53	0.40
1:C:314:ILE:HG22	1:C:315:LYS:O	2.21	0.40
1:A:36:ALA:HB1	1:A:100:VAL:HG21	2.03	0.40
1:A:126:PHE:HA	1:A:167:PRO:HB3	2.02	0.40
1:C:137:TYR:CE2	1:C:145:LEU:HD21	2.56	0.40
1:C:171:PRO:HG3	1:C:214:ILE:CG2	2.51	0.40
1:C:88:PHE:CD1	1:D:80:VAL:HG13	2.56	0.40
1:C:129:PRO:CB	1:C:165:VAL:HG12	2.51	0.40
1:D:236:THR:OG1	1:D:237:ASP:N	2.54	0.40
1:C:24:ASP:OD2	1:C:27:THR:HB	2.20	0.40
1:C:216:LYS:HE3	1:C:217:ASP:CG	2.42	0.40
1:C:17:LEU:HA	1:C:17:LEU:HD12	1.89	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	304/317 (96%)	283 (93%)	19 (6%)	2 (1%)	26 51
1	B	304/317 (96%)	287 (94%)	12 (4%)	5 (2%)	12 24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	304/317 (96%)	274 (90%)	26 (9%)	4 (1%)	15	30
1	D	304/317 (96%)	275 (90%)	27 (9%)	2 (1%)	26	51
All	All	1216/1268 (96%)	1119 (92%)	84 (7%)	13 (1%)	17	36

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	19	ALA
1	D	273	GLY
1	A	14	ASN
1	B	273	GLY
1	C	267	ASP
1	A	273	GLY
1	C	204	ASN
1	B	14	ASN
1	B	272	ALA
1	C	158	ALA
1	B	56	GLY
1	C	150	PRO
1	D	159	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	249/257 (97%)	216 (87%)	33 (13%)	5	8
1	B	249/257 (97%)	217 (87%)	32 (13%)	5	9
1	C	249/257 (97%)	219 (88%)	30 (12%)	6	11
1	D	249/257 (97%)	213 (86%)	36 (14%)	4	6
All	All	996/1028 (97%)	865 (87%)	131 (13%)	5	9

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	16	MET
1	A	37	SER
1	A	51	LEU
1	A	64	LEU
1	A	67	GLN
1	A	105	ASN
1	A	110	CYS
1	A	111	VAL
1	A	130	THR
1	A	133	VAL
1	A	163	ARG
1	A	165	VAL
1	A	170	ARG
1	A	177	TYR
1	A	181	LYS
1	A	189	LEU
1	A	206	VAL
1	A	227	LEU
1	A	228	ASN
1	A	237	ASP
1	A	238	VAL
1	A	239	LEU
1	A	253	LEU
1	A	254	GLU
1	A	275	MET
1	A	280	ARG
1	A	287	GLN
1	A	293	SER
1	A	296	THR
1	A	299	SER
1	A	302	VAL
1	A	314	ILE
1	B	17	LEU
1	B	18	GLN
1	B	20	LYS
1	B	26	ASP
1	B	55	ASN
1	B	64	LEU
1	B	93	MET
1	B	100	VAL
1	B	102	CYS
1	B	110	CYS

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Mol	Chain	Res	Type
1	B	111	VAL
1	B	133	VAL
1	B	156	GLU
1	B	163	ARG
1	B	187	ASN
1	B	189	LEU
1	B	206	VAL
1	B	216	LYS
1	B	225	LYS
1	B	227	LEU
1	B	233	MET
1	B	253	LEU
1	B	260	GLU
1	B	262	LEU
1	B	280	ARG
1	B	291	LYS
1	B	292	MET
1	B	293	SER
1	B	296	THR
1	B	299	SER
1	B	302	VAL
1	B	314	ILE
1	C	2	SER
1	C	5	LYS
1	C	14	ASN
1	C	17	LEU
1	C	48	LYS
1	C	51	LEU
1	C	64	LEU
1	C	67	GLN
1	C	72	VAL
1	C	100	VAL
1	C	130	THR
1	C	139	GLU
1	C	145	LEU
1	C	152	LYS
1	C	156	GLU
1	C	157	ASP
1	C	163	ARG
1	C	170	ARG
1	C	172	LEU
1	C	189	LEU

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Mol	Chain	Res	Type
1	C	214	ILE
1	C	216	LYS
1	C	227	LEU
1	C	237	ASP
1	C	261	ILE
1	C	262	LEU
1	C	275	MET
1	C	297	SER
1	C	302	VAL
1	C	315	LYS
1	D	14	ASN
1	D	17	LEU
1	D	26	ASP
1	D	64	LEU
1	D	93	MET
1	D	100	VAL
1	D	110	CYS
1	D	111	VAL
1	D	127	THR
1	D	130	THR
1	D	144	ASP
1	D	145	LEU
1	D	149	ASN
1	D	155	ARG
1	D	157	ASP
1	D	164	VAL
1	D	165	VAL
1	D	187	ASN
1	D	189	LEU
1	D	206	VAL
1	D	225	LYS
1	D	227	LEU
1	D	237	ASP
1	D	242	CYS
1	D	243	ILE
1	D	253	LEU
1	D	257	LYS
1	D	265	GLU
1	D	266	LYS
1	D	274	SER
1	D	275	MET
1	D	280	ARG

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Mol	Chain	Res	Type
1	D	296	THR
1	D	302	VAL
1	D	314	ILE
1	D	315	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

7 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	401	-	3,12,12	1.35	0	3,17,17	3.46	2 (66%)
3	DCD	A	402	-	6,7,7	0.85	0	6,8,8	0.67	0
3	DCD	B	401	1	6,7,7	0.92	0	6,8,8	0.99	1 (16%)
2	CIT	B	402	-	3,12,12	0.94	0	3,17,17	0.63	0
2	CIT	C	401	-	3,12,12	1.16	0	3,17,17	2.39	1 (33%)
3	DCD	C	402	-	6,7,7	0.81	0	6,8,8	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CIT	D	401	-	3,12,12	1.24	0	3,17,17	3.71	2 (66%)

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	401	-	-	0/6/16/16	0/0/0/0
3	DCD	A	402	-	-	0/8/8/8	0/0/0/0
3	DCD	B	401	1	-	0/8/8/8	0/0/0/0
2	CIT	B	402	-	-	0/6/16/16	0/0/0/0
2	CIT	C	401	-	-	0/6/16/16	0/0/0/0
3	DCD	C	402	-	-	0/8/8/8	0/0/0/0
2	CIT	D	401	-	-	0/6/16/16	0/0/0/0

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	CIT	C3-C4-C5	-5.39	106.34	114.96
2	D	401	CIT	C3-C4-C5	-5.26	106.54	114.96
2	C	401	CIT	C3-C4-C5	-3.99	108.58	114.96
2	D	401	CIT	C3-C2-C1	-3.54	109.30	114.96
2	A	401	CIT	C3-C2-C1	-2.61	110.79	114.96
3	B	401	DCD	S2-C1-N1	-2.38	119.14	123.74

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	CIT	1	0
3	A	402	DCD	6	0
2	B	402	CIT	3	0
2	C	401	CIT	1	0
3	C	402	DCD	3	0
2	D	401	CIT	2	0

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	308/317 (97%)	-0.10	12 (3%) 43 35	22, 38, 83, 95	0
1	B	308/317 (97%)	-0.33	9 (2%) 55 48	19, 33, 68, 84	0
1	C	308/317 (97%)	-0.18	10 (3%) 51 44	20, 37, 71, 87	0
1	D	308/317 (97%)	-0.11	18 (5%) 26 20	21, 38, 84, 104	0
All	All	1232/1268 (97%)	-0.18	49 (3%) 42 34	19, 37, 78, 104	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	140	GLN	5.1
1	C	158	ALA	4.6
1	D	147	ALA	4.6
1	D	238	VAL	4.6
1	D	150	PRO	4.4
1	D	148	ALA	4.3
1	A	150	PRO	4.2
1	D	251	ARG	4.1
1	A	157	ASP	3.9
1	D	140	GLN	3.5
1	D	239	LEU	3.5
1	D	149	ASN	3.5
1	D	151	GLY	3.4
1	D	253	LEU	3.3
1	B	158	ALA	3.3
1	D	252	LYS	3.2
1	C	253	LEU	3.2
1	A	151	GLY	3.1
1	D	160	ARG	2.9
1	A	241	ALA	2.9
1	A	239	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	240	ASN	2.8
1	A	271	ALA	2.7
1	B	144	ASP	2.7
1	C	239	LEU	2.6
1	C	242	CYS	2.6
1	B	148	ALA	2.6
1	C	252	LYS	2.5
1	B	142	ALA	2.5
1	A	136	PHE	2.5
1	D	272	ALA	2.5
1	C	273	GLY	2.4
1	A	161	GLY	2.4
1	C	241	ALA	2.4
1	A	159	GLY	2.4
1	C	316	ASP	2.3
1	C	150	PRO	2.3
1	B	242	CYS	2.2
1	D	254	GLU	2.2
1	B	157	ASP	2.2
1	C	204	ASN	2.2
1	A	238	VAL	2.2
1	B	238	VAL	2.1
1	B	252	LYS	2.1
1	D	243	ILE	2.1
1	D	156	GLU	2.1
1	D	126	PHE	2.0
1	B	147	ALA	2.0
1	D	19	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no 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, 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	LLDF	B-factors(Å ²)	Q<0.9
2	CIT	C	401	13/13	0.90	0.20	1.84	38,45,50,50	0
2	CIT	D	401	13/13	0.85	0.20	1.22	40,51,58,66	0
2	CIT	B	402	13/13	0.89	0.20	0.82	39,46,50,53	0
2	CIT	A	401	13/13	0.87	0.19	-0.06	39,53,62,68	0
3	DCD	C	402	8/8	0.79	0.16	-0.55	59,75,80,89	0
3	DCD	B	401	8/8	0.59	0.26	-	49,88,97,113	0
3	DCD	A	402	8/8	0.51	0.21	-	67,80,88,93	0

6.5 Other polymers

There are no such residues in this entry.