Full wwPDB X-ray Structure Validation Report (i)

Sep 10, 2023 – 06:58 PM EDT

PDB ID	:	4JZ9
Title	:	Carbamate kinase from Giardia lamblia bound to citric acid
Authors	:	Lim, K.; Herzberg, O.
Deposited on	:	2013-04-02
Resolution	:	2.40 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 (i) 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 (i)) were used in the production of this report:

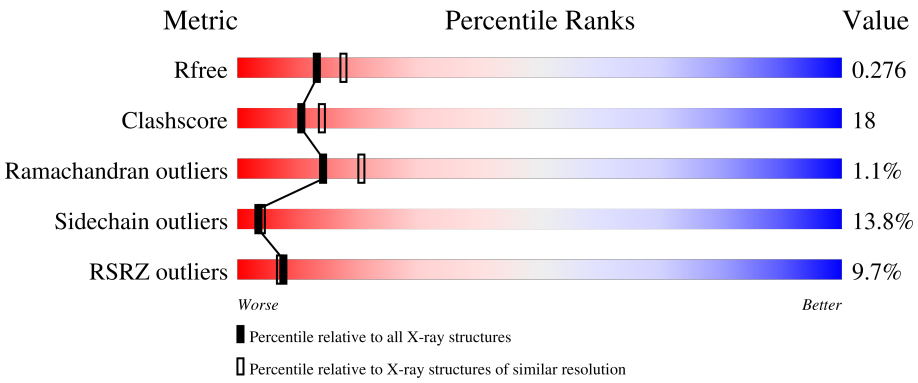
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.40 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 <=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	13% 61% 30% 8% •
1	B	317	8% 66% 28% • •
1	C	317	10% 63% 29% 7%
1	D	317	8% 62% 31% 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9791 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.

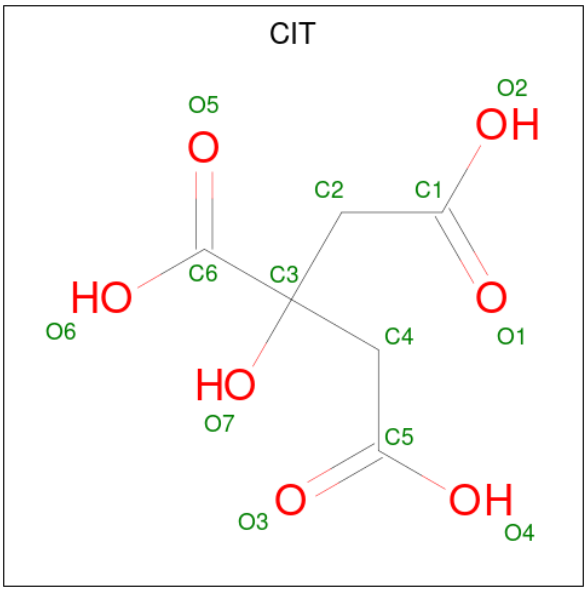
- Molecule 1 is a protein called Carbamate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	316	2366	1483	408	456	19	0	0	0
1	B	316	2366	1483	408	456	19	0	0	0
1	C	316	2366	1483	408	456	19	0	0	0
1	D	316	2366	1483	408	456	19	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

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

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

- Molecule 3 is water.

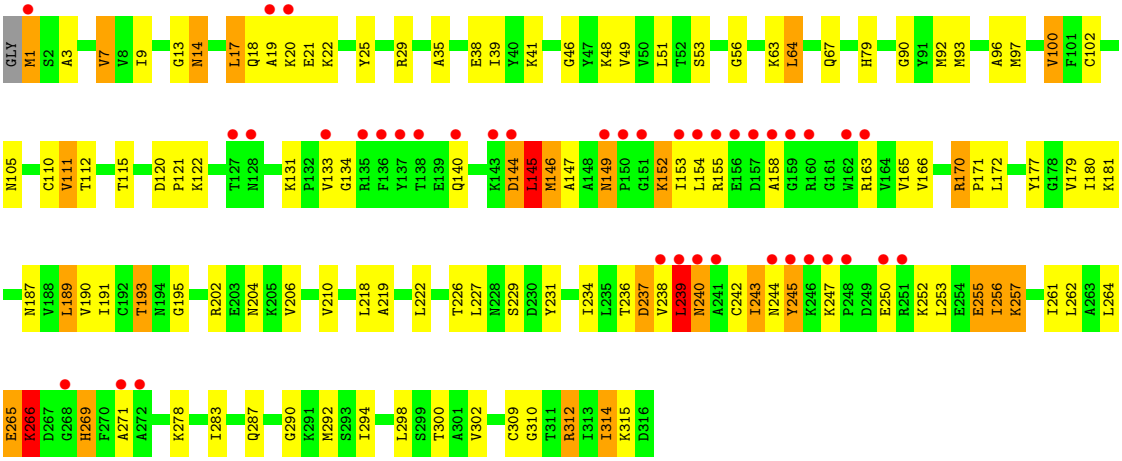
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	90	Total O 90 90	0	0
3	B	65	Total O 65 65	0	0
3	C	70	Total O 70 70	0	0
3	D	50	Total O 50 50	0	0

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.

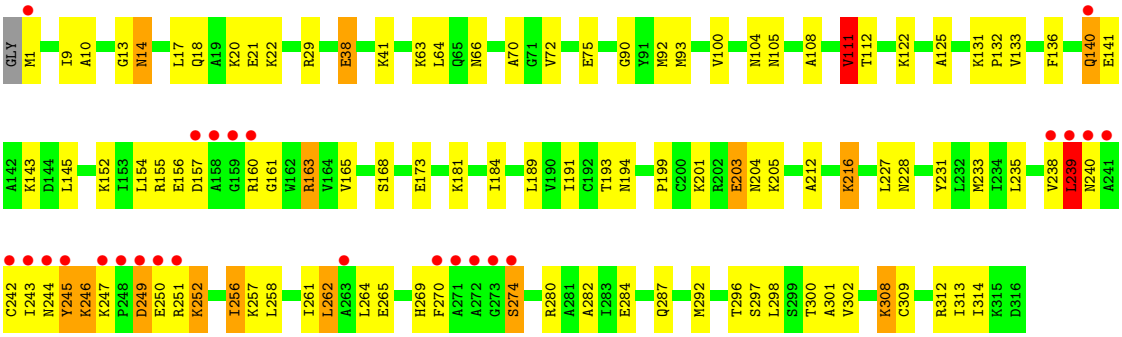
- Molecule 1: Carbamate kinase

Chain A:



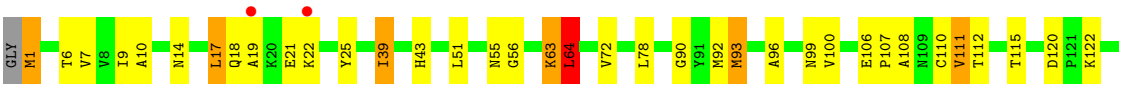
- Molecule 1: Carbamate kinase

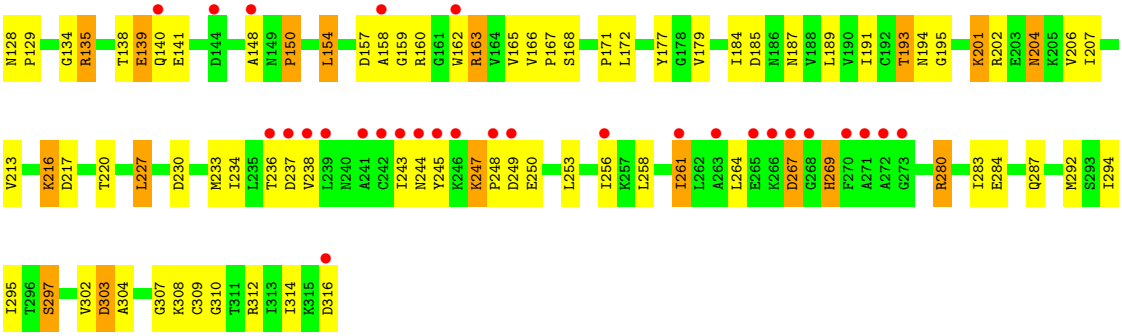
Chain B:



- Molecule 1: Carbamate kinase

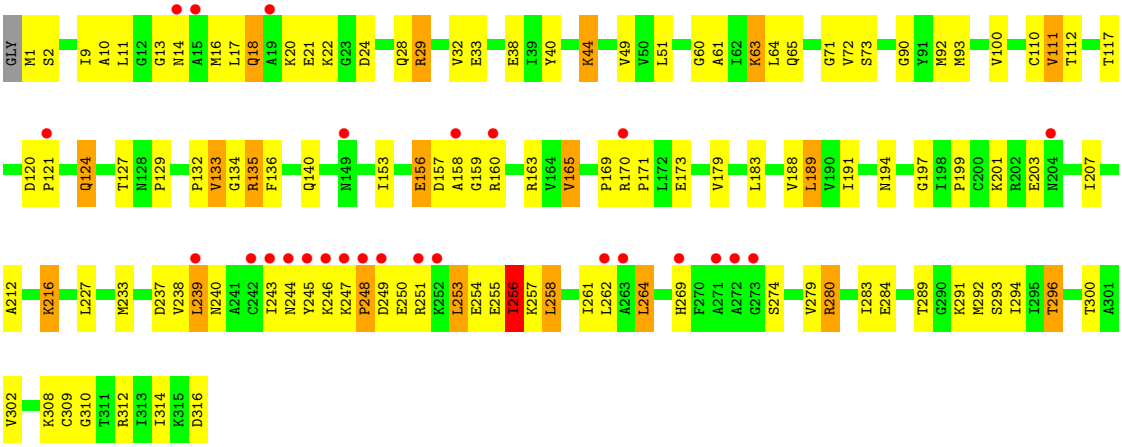
Chain C:





- Molecule 1: Carbamate kinase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	69.92Å 92.74Å 101.84Å 90.00° 106.22° 90.00°	Depositor
Resolution (Å)	46.10 – 2.40 46.13 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (46.10-2.40) 97.9 (46.13-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.62 (at 2.39Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.218 , 0.280 0.215 , 0.276	Depositor DCC
R_{free} test set	2009 reflections (4.13%)	wwPDB-VP
Wilson B-factor (Å^2)	29.4	Xtriage
Anisotropy	0.657	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 60.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9791	wwPDB-VP
Average B, all atoms (Å^2)	44.0	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 51.90 % 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 5.2508e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: 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	0/2398	0.68	2/3240 (0.1%)
1	B	0.58	0/2398	0.71	1/3240 (0.0%)
1	C	0.63	0/2398	0.71	2/3240 (0.1%)
1	D	0.59	0/2398	0.69	0/3240
All	All	0.60	0/9592	0.70	5/12960 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	111	VAL	CB-CA-C	-5.50	100.96	111.40
1	C	111	VAL	CB-CA-C	-5.36	101.22	111.40
1	B	111	VAL	CB-CA-C	-5.33	101.26	111.40
1	C	64	LEU	CA-CB-CG	5.10	127.03	115.30
1	A	51	LEU	CB-CG-CD1	-5.05	102.41	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	266	LYS	Peptide
1	B	108	ALA	Peptide
1	C	108	ALA	Peptide

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	2366	0	2430	97	0
1	B	2366	0	2430	79	0
1	C	2366	0	2430	112	0
1	D	2366	0	2430	87	0
2	A	13	0	5	3	0
2	B	13	0	5	2	0
2	C	13	0	5	0	0
2	D	13	0	5	1	0
3	A	90	0	0	6	0
3	B	65	0	0	6	0
3	C	70	0	0	2	0
3	D	50	0	0	0	0
All	All	9791	0	9740	356	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 18.

All (356) 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:D:29:ARG:HA	1:D:92:MET:HE2	1.50	0.93
1:C:1:MET:N	1:C:187:ASN:HB3	1.85	0.91
1:B:140:GLN:NE2	1:C:22:LYS:HB3	1.86	0.90
1:C:129:PRO:HB2	1:C:165:VAL:HG12	1.52	0.90
1:C:233:MET:HG2	1:C:294:ILE:HB	1.54	0.89
1:C:243:ILE:HD12	1:C:269:HIS:CD2	2.11	0.85
1:C:236:THR:O	1:C:297:SER:HA	1.79	0.83
1:C:64:LEU:CD1	1:D:73:SER:HB2	2.10	0.82
1:C:292:MET:CE	1:C:312:ARG:HG2	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:ARG:O	1:C:163:ARG:HG3	1.81	0.79
1:B:29:ARG:HA	1:B:92:MET:HE2	1.64	0.79
1:B:90:GLY:HA3	1:B:112:THR:HG21	1.64	0.79
1:D:20:LYS:HE3	1:D:160:ARG:HB3	1.63	0.79
1:C:292:MET:HE2	1:C:294:ILE:HD11	1.65	0.78
1:D:29:ARG:CA	1:D:92:MET:HE2	2.14	0.78
1:C:292:MET:HE1	1:C:312:ARG:HG2	1.64	0.78
1:C:138:THR:HG22	1:C:140:GLN:H	1.48	0.78
1:A:266:LYS:HB2	1:A:266:LYS:NZ	1.99	0.77
1:A:243:ILE:HG13	1:A:269:HIS:CD2	2.19	0.77
1:C:292:MET:HE3	1:C:294:ILE:HG12	1.66	0.77
1:A:265:GLU:HG3	1:A:266:LYS:HD3	1.67	0.77
1:A:255:GLU:HG3	1:A:314:ILE:HD13	1.66	0.76
1:C:243:ILE:HG23	1:C:269:HIS:CD2	2.21	0.75
1:B:136:PHE:CD2	1:B:161:GLY:HA3	2.23	0.74
1:D:296:THR:HG23	1:D:310:GLY:HA3	1.70	0.73
1:B:160:ARG:HA	3:B:1008:HOH:O	1.89	0.73
1:B:280:ARG:O	1:B:284:GLU:HG3	1.89	0.73
1:D:129:PRO:HB2	1:D:165:VAL:HG13	1.71	0.73
1:A:244:ASN:HB3	1:A:247:LYS:HD3	1.71	0.73
1:A:266:LYS:HB2	1:A:266:LYS:HZ2	1.54	0.73
1:D:280:ARG:O	1:D:284:GLU:HG3	1.89	0.72
1:A:239:LEU:HG	1:A:240:ASN:HB2	1.71	0.72
1:D:10:ALA:HB1	1:D:216:LYS:HE2	1.72	0.72
1:D:90:GLY:HA3	1:D:112:THR:HG21	1.71	0.71
1:A:257:LYS:NZ	3:A:522:HOH:O	2.24	0.71
1:A:22:LYS:NZ	1:D:140:GLN:HB2	2.06	0.70
1:A:144:ASP:O	1:A:147:ALA:N	2.23	0.70
1:C:1:MET:H1	1:C:187:ASN:HB3	1.53	0.70
1:B:140:GLN:NE2	1:C:22:LYS:CB	2.55	0.70
1:C:93:MET:HB3	1:C:191:ILE:HD13	1.74	0.70
1:B:245:TYR:HD2	1:B:246:LYS:N	1.90	0.69
1:B:242:CYS:SG	1:B:252:LYS:HB3	2.31	0.69
1:A:14:ASN:HA	1:A:17:LEU:O	1.92	0.69
1:C:106:GLU:HG3	1:C:107:PRO:HD2	1.74	0.69
1:D:63:LYS:O	1:D:63:LYS:HD3	1.92	0.69
1:D:243:ILE:HB	1:D:269:HIS:ND1	2.08	0.69
1:C:1:MET:H2	1:C:187:ASN:HB3	1.59	0.68
1:D:170:ARG:HG2	1:D:171:PRO:HD2	1.75	0.68
1:C:25:TYR:CE1	1:C:92:MET:HE3	2.29	0.67
1:C:138:THR:HB	1:C:141:GLU:HG3	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ALA:HA	1:A:298:LEU:HD21	1.77	0.67
1:C:18:GLN:HA	1:C:18:GLN:OE1	1.93	0.67
1:A:149:ASN:N	1:A:149:ASN:OD1	2.28	0.66
1:A:90:GLY:HA3	1:A:112:THR:HG21	1.78	0.66
1:B:245:TYR:HD2	1:B:246:LYS:H	1.43	0.66
1:C:138:THR:HG22	1:C:140:GLN:N	2.11	0.66
1:D:296:THR:CG2	1:D:310:GLY:HA3	2.24	0.65
1:C:139:GLU:HB3	1:C:162:TRP:NE1	2.12	0.65
1:D:308:LYS:O	1:D:309:CYS:HB3	1.95	0.65
1:A:13:GLY:N	2:A:401:CIT:H41	2.12	0.65
1:B:258:LEU:HD21	1:B:287:GLN:HG2	1.78	0.65
1:C:303:ASP:N	1:C:303:ASP:OD2	2.28	0.65
1:B:296:THR:HG22	1:B:300:THR:OG1	1.98	0.64
1:C:64:LEU:CD2	1:C:135:ARG:HG2	2.27	0.64
1:A:181:LYS:NZ	3:A:563:HOH:O	2.30	0.64
1:B:244:ASN:HB3	1:B:247:LYS:HD3	1.78	0.64
1:C:64:LEU:HD12	1:D:73:SER:HB2	1.80	0.64
1:C:25:TYR:CD1	1:C:92:MET:HE3	2.33	0.63
1:B:136:PHE:HD2	1:B:161:GLY:HA3	1.62	0.63
1:A:25:TYR:CE1	1:A:92:MET:HE3	2.33	0.63
1:B:238:VAL:HG12	1:B:240:ASN:O	1.98	0.63
1:A:238:VAL:O	1:A:240:ASN:N	2.31	0.62
1:B:231:TYR:HE2	1:B:292:MET:HE1	1.64	0.62
1:B:282:ALA:HB1	1:B:313:ILE:HD12	1.81	0.62
1:B:309:CYS:O	1:B:312:ARG:NE	2.32	0.61
2:B:401:CIT:O3	2:B:401:CIT:H22	2.00	0.61
1:D:136:PHE:CE2	1:D:163:ARG:HD3	2.35	0.61
1:B:14:ASN:ND2	3:B:1030:HOH:O	2.33	0.61
1:C:1:MET:H2	1:C:187:ASN:CB	2.12	0.61
1:A:231:TYR:HE2	1:A:292:MET:HE1	1.64	0.61
1:D:254:GLU:O	1:D:256:ILE:HG22	2.01	0.61
1:A:22:LYS:HZ1	1:D:140:GLN:HB2	1.65	0.60
1:A:7:VAL:HG22	1:A:9:ILE:HG13	1.82	0.60
1:A:292:MET:HE3	1:A:294:ILE:HD11	1.83	0.60
1:D:261:ILE:HA	1:D:264:LEU:HB2	1.82	0.60
1:A:122:LYS:HG2	3:A:544:HOH:O	2.01	0.60
1:B:235:LEU:HD13	1:B:298:LEU:HA	1.84	0.60
1:C:294:ILE:HG21	1:C:304:ALA:HB1	1.84	0.60
1:C:158:ALA:C	1:C:160:ARG:H	2.06	0.59
1:C:292:MET:HE3	1:C:312:ARG:HG2	1.84	0.59
1:D:110:CYS:HB2	1:D:189:LEU:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:ILE:HG13	1:B:257:LYS:N	2.18	0.59
1:A:310:GLY:O	1:A:312:ARG:HD3	2.02	0.59
1:C:216:LYS:HE2	1:C:217:ASP:OD1	2.02	0.59
1:A:238:VAL:C	1:A:240:ASN:H	2.05	0.59
1:C:307:GLY:O	1:C:312:ARG:NH1	2.36	0.59
1:C:204:ASN:O	1:C:204:ASN:ND2	2.29	0.58
1:C:179:VAL:HG11	1:D:111:VAL:HG21	1.86	0.58
1:B:13:GLY:N	2:B:401:CIT:O3	2.37	0.57
1:C:129:PRO:HB2	1:C:165:VAL:CG1	2.32	0.57
1:C:112:THR:HA	1:C:191:ILE:O	2.05	0.57
1:C:179:VAL:HG11	1:D:111:VAL:CG2	2.34	0.57
1:A:13:GLY:H	2:A:401:CIT:H41	1.67	0.57
1:B:243:ILE:HG21	1:B:269:HIS:ND1	2.19	0.57
1:D:135:ARG:HG2	1:D:136:PHE:N	2.20	0.57
1:A:261:ILE:HA	1:A:264:LEU:HD12	1.87	0.57
1:C:90:GLY:HA3	1:C:112:THR:HG21	1.86	0.57
1:B:247:LYS:HE2	1:B:249:ASP:OD2	2.05	0.56
1:C:202:ARG:HA	1:C:206:VAL:O	2.04	0.56
1:C:244:ASN:O	1:C:250:GLU:HB2	2.06	0.56
1:C:292:MET:CE	1:C:294:ILE:HG12	2.35	0.56
1:A:19:ALA:C	1:A:20:LYS:HD2	2.26	0.56
1:A:134:GLY:O	1:A:163:ARG:NH1	2.33	0.56
1:A:1:MET:N	3:A:560:HOH:O	2.39	0.55
1:B:201:LYS:HE3	1:B:203:GLU:HG3	1.87	0.55
1:C:138:THR:CG2	1:C:140:GLN:H	2.19	0.55
1:A:56:GLY:HA2	1:A:133:VAL:HG22	1.87	0.55
1:A:144:ASP:O	1:A:146:MET:N	2.39	0.55
1:D:132:PRO:HB2	1:D:163:ARG:HE	1.72	0.55
1:A:96:ALA:O	1:A:100:VAL:HG23	2.06	0.55
1:C:78:LEU:HD22	1:C:166:VAL:HG11	1.89	0.55
1:C:148:ALA:O	1:C:150:PRO:HD3	2.07	0.54
1:A:64:LEU:HD13	1:B:72:VAL:HG12	1.90	0.54
1:A:25:TYR:CD1	1:A:92:MET:HE3	2.41	0.54
1:A:56:GLY:N	2:A:401:CIT:O6	2.39	0.54
1:D:257:LYS:HG2	1:D:316:ASP:OD2	2.07	0.54
1:D:121:PRO:HG3	1:D:201:LYS:HB2	1.90	0.54
1:A:179:VAL:HG11	1:B:111:VAL:CG2	2.38	0.54
1:B:296:THR:HG22	1:B:297:SER:H	1.72	0.53
1:C:247:LYS:HG3	1:C:248:PRO:N	2.22	0.53
1:B:38:GLU:OE2	1:B:41:LYS:HD2	2.07	0.53
1:D:13:GLY:N	2:D:401:CIT:O4	2.25	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:SD	1:A:3:ALA:HB3	2.49	0.53
1:A:244:ASN:HB3	1:A:247:LYS:CD	2.37	0.53
1:A:231:TYR:CE2	1:A:292:MET:HE1	2.42	0.53
1:A:236:THR:OG1	1:A:237:ASP:N	2.38	0.53
1:D:24:ASP:OD2	1:D:24:ASP:N	2.42	0.53
1:C:1:MET:H2	1:C:187:ASN:CG	2.12	0.53
1:C:10:ALA:HB2	1:C:220:THR:HG21	1.90	0.53
1:B:10:ALA:HB1	1:B:216:LYS:HE2	1.90	0.52
1:B:181:LYS:O	1:B:184:ILE:HG12	2.09	0.52
1:B:274:SER:HA	3:B:1041:HOH:O	2.10	0.52
1:C:202:ARG:HG3	1:C:207:ILE:HG12	1.90	0.52
1:D:156:GLU:OE2	1:D:157:ASP:N	2.43	0.52
1:C:64:LEU:HD11	1:D:72:VAL:HG12	1.90	0.52
1:B:133:VAL:O	1:B:163:ARG:HG2	2.10	0.52
1:A:146:MET:CE	1:A:153:ILE:HG12	2.39	0.52
1:C:111:VAL:HG11	1:D:179:VAL:HG11	1.92	0.52
1:C:184:ILE:HG13	1:C:185:ASP:N	2.25	0.52
1:D:132:PRO:HB2	1:D:163:ARG:HH21	1.75	0.52
1:A:292:MET:CE	1:A:294:ILE:HD11	2.39	0.51
1:B:125:ALA:HB1	1:B:168:SER:H	1.75	0.51
1:A:187:ASN:HB3	3:A:560:HOH:O	2.09	0.51
1:B:104:ASN:HD22	1:B:104:ASN:N	2.08	0.51
1:C:308:LYS:O	1:C:309:CYS:HB3	2.10	0.51
1:D:16:MET:HG2	1:D:32:VAL:CG2	2.39	0.51
1:A:256:ILE:CG2	1:A:257:LYS:O	2.59	0.51
1:C:292:MET:HE2	1:C:294:ILE:CD1	2.39	0.51
1:C:243:ILE:HD12	1:C:269:HIS:CG	2.45	0.51
1:C:96:ALA:O	1:C:100:VAL:HG23	2.11	0.51
1:D:61:ALA:O	1:D:65:GLN:HG3	2.10	0.51
1:B:18:GLN:HB2	1:B:21:GLU:CD	2.31	0.51
1:A:38:GLU:OE2	1:A:41:LYS:HD2	2.11	0.51
1:A:48:LYS:HE2	1:A:187:ASN:OD1	2.11	0.51
1:C:115:THR:HG21	1:C:193:THR:HG23	1.93	0.51
1:A:262:LEU:HD23	1:A:262:LEU:O	2.10	0.50
1:A:234:ILE:HG21	1:A:278:LYS:HG2	1.92	0.50
1:B:243:ILE:CG2	1:B:269:HIS:ND1	2.75	0.50
1:D:250:GLU:O	1:D:251:ARG:HG2	2.11	0.50
1:C:247:LYS:HD3	1:C:249:ASP:OD1	2.10	0.50
1:D:49:VAL:HB	1:D:189:LEU:HD22	1.93	0.50
1:D:309:CYS:O	1:D:312:ARG:NE	2.25	0.50
1:B:231:TYR:CE2	1:B:292:MET:HE1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:ARG:N	1:D:92:MET:HE2	2.26	0.50
1:D:240:ASN:ND2	1:D:253:LEU:O	2.45	0.50
1:A:219:ALA:O	1:A:222:LEU:HB3	2.11	0.50
1:C:201:LYS:O	1:C:207:ILE:HA	2.12	0.50
1:B:66:ASN:HB3	1:B:75:GLU:HG3	1.94	0.50
1:C:243:ILE:O	1:C:250:GLU:HA	2.11	0.50
1:C:256:ILE:HD13	1:C:261:ILE:HG12	1.93	0.50
1:C:258:LEU:HD21	1:C:287:GLN:HG3	1.94	0.50
1:D:258:LEU:O	1:D:262:LEU:HB2	2.11	0.50
1:A:177:TYR:CE1	1:A:226:THR:HG22	2.46	0.49
1:B:296:THR:CG2	1:B:300:THR:OG1	2.59	0.49
1:A:49:VAL:HB	1:A:189:LEU:HD13	1.93	0.49
1:C:168:SER:HA	1:C:213:VAL:O	2.12	0.49
1:A:18:GLN:HB2	1:A:21:GLU:OE2	2.12	0.49
1:A:145:LEU:HD12	1:A:149:ASN:HD21	1.77	0.49
1:B:239:LEU:HD12	1:B:240:ASN:N	2.28	0.49
1:D:191:ILE:HG22	1:D:194:ASN:HD21	1.77	0.49
1:B:136:PHE:CD2	1:B:163:ARG:HD3	2.47	0.49
1:B:233:MET:HE3	1:B:301:ALA:HB1	1.94	0.49
1:A:112:THR:HA	1:A:191:ILE:O	2.13	0.49
1:A:310:GLY:O	1:A:312:ARG:NH1	2.46	0.49
1:D:199:PRO:HG2	1:D:212:ALA:O	2.12	0.49
1:B:261:ILE:HA	1:B:264:LEU:HG	1.93	0.49
1:C:64:LEU:HD23	1:C:135:ARG:HA	1.94	0.49
1:B:140:GLN:HB2	1:C:22:LYS:HE3	1.95	0.48
1:D:289:THR:OG1	1:D:291:LYS:HG2	2.12	0.48
1:C:202:ARG:HG3	1:C:207:ILE:CG1	2.44	0.48
1:A:19:ALA:HB1	1:A:20:LYS:HD2	1.94	0.48
1:B:233:MET:CE	1:B:301:ALA:HB1	2.43	0.48
1:D:170:ARG:NH2	1:D:284:GLU:OE1	2.46	0.48
1:B:141:GLU:O	1:B:145:LEU:HB2	2.14	0.48
1:A:131:LYS:O	1:A:165:VAL:HA	2.14	0.48
1:C:64:LEU:HB2	1:C:134:GLY:HA2	1.95	0.48
1:D:63:LYS:HD3	1:D:63:LYS:C	2.34	0.48
1:B:29:ARG:CA	1:B:92:MET:HE2	2.37	0.47
1:D:244:ASN:HB3	1:D:247:LYS:HD3	1.96	0.47
1:B:308:LYS:O	1:B:309:CYS:HB3	2.14	0.47
1:D:134:GLY:O	1:D:163:ARG:NH1	2.47	0.47
1:D:245:TYR:CD1	1:D:246:LYS:HG3	2.49	0.47
1:A:22:LYS:HZ2	1:D:140:GLN:HB2	1.78	0.47
1:A:93:MET:HE2	1:A:191:ILE:HG23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ILE:HG23	1:A:190:VAL:HG11	1.97	0.47
1:D:158:ALA:C	1:D:160:ARG:H	2.17	0.47
1:A:238:VAL:HG12	1:A:240:ASN:O	2.15	0.47
1:C:25:TYR:CD1	1:C:92:MET:CE	2.97	0.47
1:D:29:ARG:O	1:D:33:GLU:HG3	2.14	0.47
1:D:18:GLN:HB2	1:D:21:GLU:OE2	2.13	0.47
1:A:145:LEU:HD12	1:A:149:ASN:ND2	2.30	0.47
1:D:40:TYR:CE2	1:D:44:LYS:HG3	2.50	0.47
1:B:244:ASN:O	1:B:250:GLU:HB2	2.14	0.47
1:D:158:ALA:O	1:D:160:ARG:N	2.48	0.47
1:A:152:LYS:O	1:A:153:ILE:HG13	2.15	0.47
1:C:17:LEU:HD12	1:C:17:LEU:HA	1.70	0.47
1:B:258:LEU:O	1:B:262:LEU:HB2	2.15	0.47
1:C:261:ILE:HG23	1:C:283:ILE:HD11	1.97	0.47
1:A:243:ILE:HG13	1:A:269:HIS:CG	2.51	0.46
1:C:64:LEU:HD23	1:C:135:ARG:HG2	1.95	0.46
1:B:201:LYS:HE3	1:B:203:GLU:CG	2.46	0.46
1:A:256:ILE:HG22	1:A:257:LYS:O	2.15	0.46
1:C:139:GLU:CD	1:C:139:GLU:H	2.14	0.46
1:D:248:PRO:C	1:D:250:GLU:H	2.18	0.46
1:A:238:VAL:C	1:A:240:ASN:N	2.69	0.46
1:B:112:THR:HA	1:B:191:ILE:O	2.15	0.46
1:A:309:CYS:O	1:A:312:ARG:NE	2.48	0.46
1:D:132:PRO:HB2	1:D:163:ARG:NE	2.31	0.46
1:A:29:ARG:NE	3:A:523:HOH:O	2.49	0.46
1:D:24:ASP:O	1:D:28:GLN:HG3	2.15	0.46
1:B:132:PRO:HB2	1:B:163:ARG:NH2	2.31	0.46
1:B:251:ARG:HH12	1:B:264:LEU:CD1	2.29	0.46
1:D:110:CYS:CB	1:D:189:LEU:HB3	2.46	0.45
1:B:63:LYS:HA	1:B:63:LYS:HD2	1.63	0.45
1:B:265:GLU:OE1	1:B:280:ARG:HD2	2.16	0.45
1:A:115:THR:HG21	1:A:193:THR:HG23	1.99	0.45
1:C:243:ILE:HG22	1:C:244:ASN:ND2	2.31	0.45
1:C:280:ARG:O	1:C:284:GLU:HG3	2.17	0.45
1:A:170:ARG:NH1	1:A:218:LEU:HD13	2.32	0.45
1:A:290:GLY:O	1:A:315:LYS:HB3	2.16	0.45
1:C:138:THR:HB	1:C:141:GLU:CG	2.45	0.45
1:C:292:MET:HE3	1:C:294:ILE:CG1	2.43	0.45
1:D:124:GLN:H	1:D:124:GLN:HG3	1.62	0.45
1:A:39:ILE:HB	1:A:97:MET:HE1	1.99	0.45
1:A:231:TYR:HD2	1:A:292:MET:HE2	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:LEU:HD23	1:C:172:LEU:N	2.32	0.45
1:C:243:ILE:CD1	1:C:269:HIS:HB3	2.47	0.45
1:D:132:PRO:HB2	1:D:163:ARG:NH2	2.31	0.45
1:A:146:MET:HA	1:A:149:ASN:O	2.16	0.45
1:A:283:ILE:O	1:A:287:GLN:HB2	2.17	0.45
1:B:296:THR:HG22	1:B:297:SER:N	2.32	0.45
1:C:154:LEU:HA	1:C:163:ARG:O	2.16	0.45
1:B:191:ILE:HG22	1:B:194:ASN:HD21	1.82	0.45
1:D:112:THR:HA	1:D:191:ILE:O	2.17	0.45
1:B:140:GLN:NE2	3:B:1059:HOH:O	2.50	0.44
1:A:1:MET:HE2	1:A:46:GLY:HA3	2.00	0.44
1:B:193:THR:O	1:B:193:THR:HG22	2.18	0.44
1:A:242:CYS:HB2	1:A:245:TYR:CD1	2.53	0.44
1:B:250:GLU:OE1	1:B:252:LYS:HE3	2.18	0.44
1:D:309:CYS:HA	1:D:312:ARG:HH21	1.80	0.44
1:B:245:TYR:CD1	1:B:250:GLU:OE1	2.70	0.44
1:B:251:ARG:NH2	3:B:1015:HOH:O	2.35	0.44
1:D:60:GLY:CA	1:D:133:VAL:HG13	2.48	0.44
1:D:239:LEU:HG	1:D:240:ASN:OD1	2.17	0.44
1:B:140:GLN:HE22	1:C:22:LYS:HB3	1.79	0.44
1:C:18:GLN:O	1:C:19:ALA:C	2.56	0.44
1:C:158:ALA:O	1:C:160:ARG:N	2.51	0.44
1:D:296:THR:HB	1:D:300:THR:OG1	2.16	0.44
1:B:145:LEU:HD13	1:D:71:GLY:CA	2.48	0.43
1:C:6:THR:N	1:C:230:ASP:OD2	2.34	0.43
1:C:171:PRO:C	1:C:172:LEU:HD23	2.39	0.43
1:A:140:GLN:O	1:A:144:ASP:HB2	2.18	0.43
1:C:1:MET:HE1	1:C:43:HIS:O	2.19	0.43
1:C:18:GLN:HB2	1:C:21:GLU:OE2	2.18	0.43
1:C:55:ASN:CG	1:C:195:GLY:HA3	2.38	0.43
1:B:70:ALA:O	3:B:1009:HOH:O	2.21	0.43
1:D:13:GLY:O	1:D:17:LEU:N	2.44	0.43
1:A:171:PRO:HB2	1:A:222:LEU:HD22	1.99	0.43
1:D:201:LYS:O	1:D:207:ILE:HA	2.18	0.43
1:D:255:GLU:HB2	1:D:312:ARG:NH1	2.33	0.43
1:A:244:ASN:HB2	1:A:250:GLU:HA	2.00	0.43
1:D:9:ILE:HA	1:D:233:MET:O	2.18	0.43
1:A:53:SER:O	1:A:195:GLY:N	2.52	0.43
1:C:14:ASN:HA	1:C:17:LEU:O	2.18	0.43
1:D:247:LYS:HE2	1:D:247:LYS:HB3	1.69	0.43
1:D:279:VAL:O	1:D:283:ILE:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:TYR:CD2	1:A:292:MET:HE2	2.53	0.42
1:C:111:VAL:CG1	1:D:179:VAL:HG11	2.49	0.42
1:A:79:HIS:HB3	1:A:210:VAL:O	2.19	0.42
1:C:1:MET:SD	1:C:43:HIS:CD2	3.12	0.42
1:C:120:ASP:OD1	1:C:122:LYS:HG2	2.19	0.42
1:A:243:ILE:HD11	1:A:269:HIS:HB3	2.01	0.42
1:C:158:ALA:C	1:C:160:ARG:N	2.73	0.42
1:C:177:TYR:HE1	1:C:227:LEU:HD12	1.85	0.42
1:C:250:GLU:O	1:C:250:GLU:HG2	2.18	0.42
1:C:292:MET:CE	1:C:294:ILE:CG1	2.98	0.42
1:C:166:VAL:HA	1:C:167:PRO:HD3	1.87	0.42
1:D:29:ARG:HD2	1:D:33:GLU:OE2	2.19	0.42
1:A:102:CYS:SG	1:B:205:LYS:HB3	2.60	0.42
1:B:9:ILE:HA	1:B:233:MET:O	2.19	0.42
1:C:310:GLY:O	1:C:312:ARG:NH2	2.50	0.42
1:C:294:ILE:CG2	1:C:304:ALA:HB1	2.49	0.42
1:A:18:GLN:O	1:A:19:ALA:C	2.58	0.42
1:A:93:MET:O	1:A:97:MET:HB2	2.20	0.42
1:D:170:ARG:NH2	1:D:284:GLU:OE2	2.46	0.42
1:B:154:LEU:HA	1:B:163:ARG:O	2.20	0.41
1:C:128:ASN:O	1:C:128:ASN:CG	2.57	0.41
1:C:234:ILE:HD12	1:C:295:ILE:HG12	2.02	0.41
1:D:169:PRO:HD3	1:D:212:ALA:HB1	2.01	0.41
1:C:194:ASN:ND2	3:C:505:HOH:O	2.50	0.41
1:B:131:LYS:HA	1:B:132:PRO:HD3	1.78	0.41
1:B:204:ASN:O	1:B:205:LYS:HB2	2.20	0.41
1:C:10:ALA:HB1	1:C:216:LYS:HE3	2.02	0.41
1:C:39:ILE:HD12	1:C:39:ILE:HA	1.89	0.41
1:D:120:ASP:HA	1:D:121:PRO:HD3	1.95	0.41
1:A:202:ARG:HA	1:A:206:VAL:O	2.21	0.41
1:A:256:ILE:HG21	1:A:261:ILE:HB	2.02	0.41
1:D:117:THR:OG1	1:D:197:GLY:HA3	2.21	0.41
1:C:51:LEU:HA	1:C:51:LEU:HD23	1.91	0.41
1:D:11:LEU:O	1:D:216:LYS:HE3	2.20	0.41
1:D:292:MET:CE	1:D:294:ILE:HD11	2.51	0.41
1:C:138:THR:CG2	1:C:140:GLN:HB3	2.51	0.41
1:D:183:LEU:HB3	1:D:188:VAL:HB	2.03	0.41
1:D:300:THR:HB	1:D:309:CYS:SG	2.60	0.41
1:A:179:VAL:HG11	1:B:111:VAL:HG21	2.03	0.41
1:A:242:CYS:SG	1:A:252:LYS:HG2	2.61	0.41
1:C:7:VAL:HG22	1:C:9:ILE:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:201:LYS:HE3	1:D:203:GLU:HG3	2.03	0.41
1:D:292:MET:HE2	1:D:294:ILE:HD11	2.03	0.41
1:A:154:LEU:O	1:A:155:ARG:HG2	2.21	0.41
1:A:300:THR:HB	1:A:309:CYS:SG	2.61	0.41
1:B:199:PRO:HG2	1:B:212:ALA:O	2.21	0.41
1:A:120:ASP:HA	1:A:121:PRO:HD3	1.83	0.40
1:B:136:PHE:CE2	1:B:163:ARG:HD3	2.57	0.40
1:B:264:LEU:N	1:B:264:LEU:HD23	2.37	0.40
1:C:177:TYR:CE1	1:C:227:LEU:HD12	2.57	0.40
1:D:248:PRO:O	1:D:250:GLU:N	2.51	0.40
1:A:63:LYS:O	1:A:67:GLN:HG3	2.21	0.40
1:D:296:THR:CG2	1:D:310:GLY:CA	2.98	0.40
1:A:179:VAL:HG11	1:B:111:VAL:HG22	2.02	0.40
1:B:245:TYR:CG	1:B:250:GLU:OE1	2.74	0.40
1:B:156:GLU:OE2	1:B:157:ASP:N	2.54	0.40
1:C:63:LYS:HA	1:C:63:LYS:HD3	1.57	0.40
1:C:99:ASN:O	3:C:559:HOH:O	2.22	0.40
1:C:227:LEU:HD12	1:C:227:LEU:HA	1.92	0.40
1:C:264:LEU:HA	1:C:267:ASP:HB2	2.02	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	314/317 (99%)	294 (94%)	15 (5%)	5 (2%)	9 13
1	B	314/317 (99%)	294 (94%)	19 (6%)	1 (0%)	41 55
1	C	314/317 (99%)	288 (92%)	23 (7%)	3 (1%)	15 23
1	D	314/317 (99%)	284 (90%)	25 (8%)	5 (2%)	9 13
All	All	1256/1268 (99%)	1160 (92%)	82 (6%)	14 (1%)	14 20

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	239	LEU
1	A	271	ALA
1	B	239	LEU
1	D	249	ASP
1	A	145	LEU
1	A	158	ALA
1	A	255	GLU
1	D	18	GLN
1	D	159	GLY
1	C	159	GLY
1	C	56	GLY
1	D	248	PRO
1	D	256	ILE
1	C	150	PRO

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	257/257 (100%)	221 (86%)	36 (14%)	3 4
1	B	257/257 (100%)	221 (86%)	36 (14%)	3 4
1	C	257/257 (100%)	224 (87%)	33 (13%)	4 5
1	D	257/257 (100%)	220 (86%)	37 (14%)	3 3
All	All	1028/1028 (100%)	886 (86%)	142 (14%)	3 4

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	7	VAL
1	A	14	ASN
1	A	17	LEU
1	A	64	LEU
1	A	100	VAL

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Mol	Chain	Res	Type
1	A	105	ASN
1	A	110	CYS
1	A	111	VAL
1	A	144	ASP
1	A	145	LEU
1	A	146	MET
1	A	149	ASN
1	A	152	LYS
1	A	166	VAL
1	A	170	ARG
1	A	172	LEU
1	A	189	LEU
1	A	193	THR
1	A	204	ASN
1	A	227	LEU
1	A	229	SER
1	A	237	ASP
1	A	239	LEU
1	A	240	ASN
1	A	243	ILE
1	A	245	TYR
1	A	253	LEU
1	A	256	ILE
1	A	257	LYS
1	A	265	GLU
1	A	266	LYS
1	A	269	HIS
1	A	302	VAL
1	A	312	ARG
1	A	314	ILE
1	B	1	MET
1	B	14	ASN
1	B	17	LEU
1	B	20	LYS
1	B	22	LYS
1	B	38	GLU
1	B	64	LEU
1	B	93	MET
1	B	100	VAL
1	B	105	ASN
1	B	111	VAL
1	B	122	LYS

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Mol	Chain	Res	Type
1	B	140	GLN
1	B	143	LYS
1	B	152	LYS
1	B	155	ARG
1	B	163	ARG
1	B	165	VAL
1	B	173	GLU
1	B	189	LEU
1	B	203	GLU
1	B	216	LYS
1	B	227	LEU
1	B	228	ASN
1	B	239	LEU
1	B	245	TYR
1	B	246	LYS
1	B	249	ASP
1	B	252	LYS
1	B	256	ILE
1	B	262	LEU
1	B	270	PHE
1	B	274	SER
1	B	302	VAL
1	B	308	LYS
1	B	314	ILE
1	C	1	MET
1	C	17	LEU
1	C	39	ILE
1	C	63	LYS
1	C	64	LEU
1	C	72	VAL
1	C	93	MET
1	C	110	CYS
1	C	135	ARG
1	C	139	GLU
1	C	154	LEU
1	C	157	ASP
1	C	163	ARG
1	C	189	LEU
1	C	193	THR
1	C	201	LYS
1	C	204	ASN
1	C	216	LYS

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Mol	Chain	Res	Type
1	C	227	LEU
1	C	237	ASP
1	C	238	VAL
1	C	245	TYR
1	C	247	LYS
1	C	253	LEU
1	C	261	ILE
1	C	267	ASP
1	C	269	HIS
1	C	280	ARG
1	C	297	SER
1	C	302	VAL
1	C	303	ASP
1	C	314	ILE
1	C	316	ASP
1	D	1	MET
1	D	2	SER
1	D	14	ASN
1	D	22	LYS
1	D	29	ARG
1	D	38	GLU
1	D	44	LYS
1	D	51	LEU
1	D	63	LYS
1	D	64	LEU
1	D	93	MET
1	D	100	VAL
1	D	111	VAL
1	D	124	GLN
1	D	127	THR
1	D	133	VAL
1	D	135	ARG
1	D	153	ILE
1	D	156	GLU
1	D	165	VAL
1	D	173	GLU
1	D	189	LEU
1	D	216	LYS
1	D	227	LEU
1	D	237	ASP
1	D	238	VAL
1	D	239	LEU

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Mol	Chain	Res	Type
1	D	253	LEU
1	D	256	ILE
1	D	258	LEU
1	D	264	LEU
1	D	274	SER
1	D	280	ARG
1	D	293	SER
1	D	296	THR
1	D	302	VAL
1	D	314	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	95	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	D	401	-	12,12,12	1.17	0	17,17,17	2.18	7 (41%)
2	CIT	A	401	-	12,12,12	1.00	0	17,17,17	2.14	7 (41%)
2	CIT	C	401	-	12,12,12	1.01	0	17,17,17	1.88	4 (23%)
2	CIT	B	401	-	12,12,12	1.08	0	17,17,17	1.80	3 (17%)

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	D	401	-	-	7/16/16/16	-
2	CIT	A	401	-	-	5/16/16/16	-
2	CIT	C	401	-	-	9/16/16/16	-
2	CIT	B	401	-	-	6/16/16/16	-

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	CIT	O6-C6-C3	5.09	121.90	113.05
2	D	401	CIT	O6-C6-C3	5.06	121.83	113.05
2	B	401	CIT	O6-C6-C3	4.72	121.25	113.05
2	C	401	CIT	C3-C4-C5	-4.22	103.60	113.81
2	C	401	CIT	O6-C6-C3	3.81	119.66	113.05
2	A	401	CIT	O2-C1-C2	3.30	124.95	114.35
2	D	401	CIT	O5-C6-C3	-3.16	117.78	122.25
2	D	401	CIT	O2-C1-C2	2.97	123.88	114.35
2	A	401	CIT	C3-C2-C1	2.54	119.97	113.81
2	C	401	CIT	O2-C1-C2	2.44	122.19	114.35
2	D	401	CIT	C2-C3-C6	-2.43	104.89	110.11
2	D	401	CIT	O4-C5-C4	2.32	121.81	114.35
2	B	401	CIT	O4-C5-C4	2.28	121.68	114.35
2	B	401	CIT	O5-C6-C3	-2.25	119.07	122.25
2	A	401	CIT	O7-C3-C2	2.24	114.64	109.40
2	D	401	CIT	O4-C5-O3	-2.19	117.83	123.30
2	A	401	CIT	O2-C1-O1	-2.19	117.83	123.30
2	A	401	CIT	C3-C4-C5	-2.11	108.71	113.81
2	A	401	CIT	O5-C6-C3	-2.09	119.29	122.25
2	D	401	CIT	C3-C2-C1	2.09	118.88	113.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	CIT	O4-C5-C4	2.05	120.92	114.35

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	CIT	C2-C3-C4-C5
2	A	401	CIT	O7-C3-C4-C5
2	A	401	CIT	C6-C3-C4-C5
2	B	401	CIT	C2-C3-C4-C5
2	B	401	CIT	O7-C3-C4-C5
2	B	401	CIT	C6-C3-C4-C5
2	C	401	CIT	C1-C2-C3-O7
2	C	401	CIT	C1-C2-C3-C4
2	C	401	CIT	C1-C2-C3-C6
2	D	401	CIT	C1-C2-C3-O7
2	B	401	CIT	C1-C2-C3-O7
2	B	401	CIT	C1-C2-C3-C6
2	D	401	CIT	C1-C2-C3-C6
2	D	401	CIT	C1-C2-C3-C4
2	B	401	CIT	C1-C2-C3-C4
2	C	401	CIT	O7-C3-C6-O5
2	C	401	CIT	C2-C3-C6-O5
2	C	401	CIT	C2-C3-C6-O6
2	C	401	CIT	C4-C3-C6-O5
2	C	401	CIT	C4-C3-C6-O6
2	D	401	CIT	C4-C3-C6-O5
2	A	401	CIT	O2-C1-C2-C3
2	C	401	CIT	O7-C3-C6-O6
2	D	401	CIT	C4-C3-C6-O6
2	A	401	CIT	O1-C1-C2-C3
2	D	401	CIT	O1-C1-C2-C3
2	D	401	CIT	O2-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 6 short contacts:

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

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	316/317 (99%)	0.69	40 (12%)	3	3	18, 39, 93, 110	0
1	B	316/317 (99%)	0.27	25 (7%)	12	11	17, 36, 80, 97	0
1	C	316/317 (99%)	0.44	31 (9%)	7	7	18, 38, 80, 96	0
1	D	316/317 (99%)	0.27	26 (8%)	11	10	17, 36, 82, 108	0
All	All	1264/1268 (99%)	0.42	122 (9%)	7	7	17, 37, 84, 110	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	271	ALA	7.1
1	A	150	PRO	6.9
1	D	248	PRO	6.7
1	C	316	ASP	6.5
1	B	239	LEU	6.1
1	A	151	GLY	5.8
1	D	15	ALA	5.6
1	B	271	ALA	5.6
1	B	243	ILE	5.5
1	A	153	ILE	5.5
1	A	162	TRP	5.4
1	A	140	GLN	5.2
1	A	160	ARG	5.1
1	D	242	CYS	5.0
1	A	136	PHE	4.9
1	B	245	TYR	4.9
1	D	245	TYR	4.9
1	C	272	ALA	4.9
1	A	159	GLY	4.8
1	C	245	TYR	4.7
1	B	244	ASN	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	158	ALA	4.6
1	A	149	ASN	4.3
1	A	158	ALA	4.3
1	C	243	ILE	4.2
1	D	246	LYS	4.2
1	D	249	ASP	4.1
1	B	248	PRO	4.1
1	D	263	ALA	4.1
1	B	1	MET	4.1
1	D	243	ILE	4.0
1	A	245	TYR	4.0
1	C	19	ALA	4.0
1	A	157	ASP	3.9
1	D	269	HIS	3.9
1	C	248	PRO	3.8
1	D	251	ARG	3.8
1	A	138	THR	3.8
1	A	272	ALA	3.8
1	B	249	ASP	3.8
1	C	246	LYS	3.8
1	D	158	ALA	3.7
1	A	246	LYS	3.7
1	B	242	CYS	3.7
1	A	137	TYR	3.7
1	B	247	LYS	3.7
1	D	19	ALA	3.7
1	C	242	CYS	3.6
1	B	251	ARG	3.5
1	B	273	GLY	3.5
1	A	19	ALA	3.5
1	C	239	LEU	3.4
1	A	241	ALA	3.4
1	C	148	ALA	3.4
1	A	156	GLU	3.3
1	B	159	GLY	3.3
1	D	273	GLY	3.3
1	D	252	LYS	3.2
1	C	256	ILE	3.1
1	B	238	VAL	3.1
1	A	133	VAL	3.0
1	A	155	ARG	3.0
1	C	270	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	244	ASN	3.0
1	A	244	ASN	3.0
1	D	244	ASN	3.0
1	A	20	LYS	3.0
1	C	144	ASP	3.0
1	C	249	ASP	3.0
1	D	262	LEU	3.0
1	A	135	ARG	2.9
1	C	140	GLN	2.9
1	A	268	GLY	2.9
1	A	238	VAL	2.8
1	A	248	PRO	2.8
1	B	240	ASN	2.8
1	C	238	VAL	2.8
1	D	204	ASN	2.7
1	B	272	ALA	2.7
1	C	271	ALA	2.7
1	A	163	ARG	2.7
1	D	271	ALA	2.7
1	C	273	GLY	2.7
1	B	241	ALA	2.7
1	C	263	ALA	2.6
1	A	154	LEU	2.6
1	A	143	LYS	2.5
1	A	127	THR	2.5
1	D	272	ALA	2.5
1	D	160	ARG	2.5
1	C	241	ALA	2.5
1	D	121	PRO	2.4
1	B	140	GLN	2.4
1	A	128	ASN	2.4
1	C	236	THR	2.4
1	A	251	ARG	2.4
1	A	239	LEU	2.3
1	C	268	GLY	2.3
1	C	237	ASP	2.3
1	C	266	LYS	2.3
1	A	144	ASP	2.3
1	C	261	ILE	2.3
1	D	247	LYS	2.3
1	A	250	GLU	2.3
1	A	240	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	149	ASN	2.2
1	A	1	MET	2.2
1	B	270	PHE	2.2
1	B	250	GLU	2.2
1	C	267	ASP	2.2
1	B	160	ARG	2.2
1	B	274	SER	2.2
1	D	14	ASN	2.1
1	C	158	ALA	2.1
1	B	263	ALA	2.1
1	D	239	LEU	2.1
1	A	247	LYS	2.0
1	C	22	LYS	2.0
1	B	157	ASP	2.0
1	C	265	GLU	2.0
1	C	162	TRP	2.0
1	D	170	ARG	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 monosaccharides 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(Å^2)	Q<0.9
2	CIT	B	401	13/13	0.86	0.19	38,45,54,60	0
2	CIT	D	401	13/13	0.88	0.17	35,46,51,52	0
2	CIT	A	401	13/13	0.90	0.18	38,48,58,59	0
2	CIT	C	401	13/13	0.93	0.17	36,42,50,52	0

6.5 Other polymers (i)

There are no such residues in this entry.