Full wwPDB X-ray Structure Validation Report (i)

Sep 10, 2023 – 12:56 PM EDT

PDB ID	:	4JZ8
Title	:	Carbamate kinase from Giardia lamblia bound to citric acid
Authors	:	Lim, K.; Herzberg, O.
Deposited on	:	2013-04-02
Resolution	:	2.10 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:

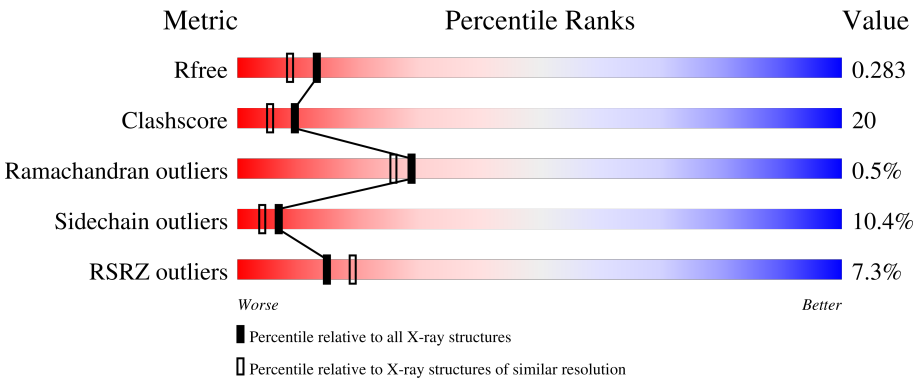
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	9% 65% 29% 5%
1	B	317	7% 57% 36% 6% •
1	C	317	9% 62% 30% 5% •
1	D	317	4% 68% 25% 5% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10081 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.

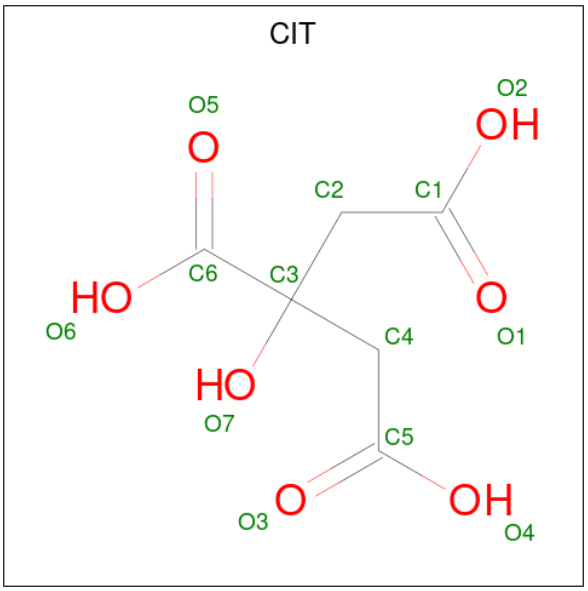
- Molecule 1 is a protein called Carbamate kinase.

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	311	2321	1453	401	448	19	0	0	0
1	C	311	2321	1453	401	448	19	0	0	0
1	D	311	2321	1453	401	448	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.

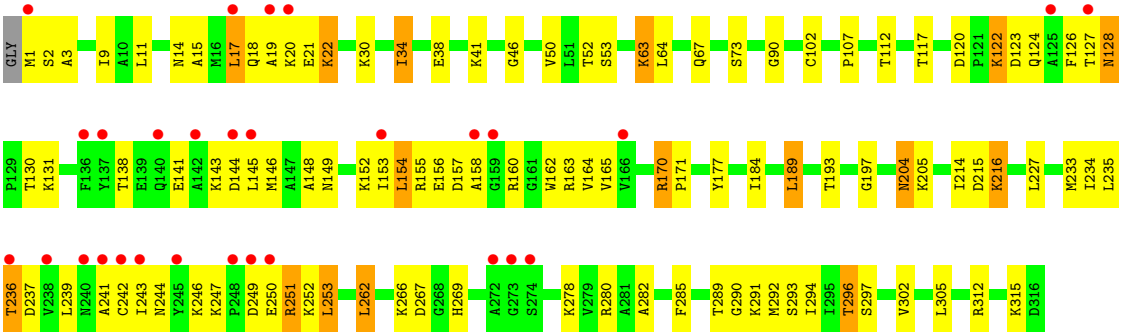
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	183	Total O 183 183	0	0
3	B	156	Total O 156 156	0	0
3	C	178	Total O 178 178	0	0
3	D	183	Total O 183 183	0	0

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.

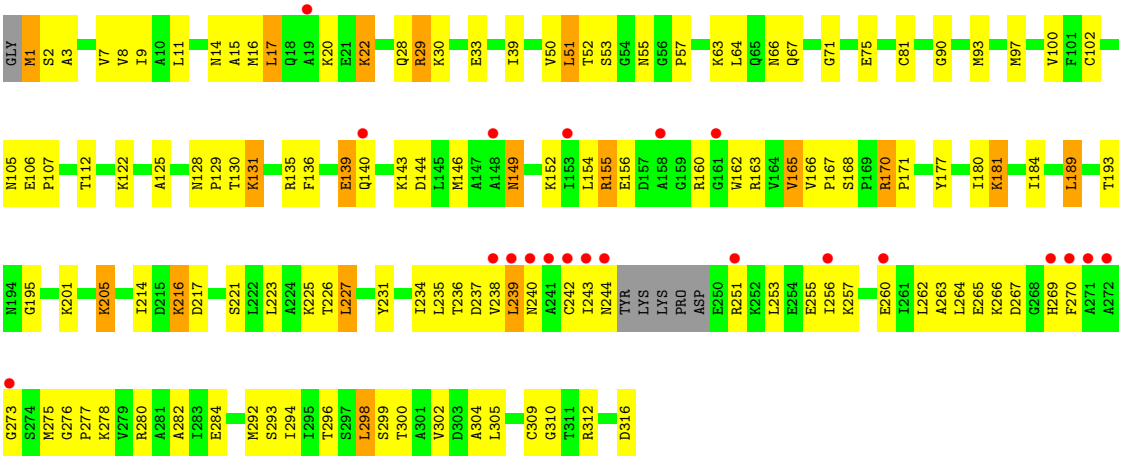
• Molecule 1: Carbamate kinase

Chain A:



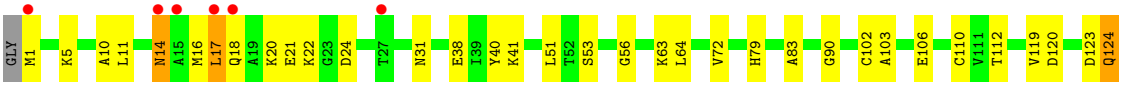
• Molecule 1: Carbamate kinase

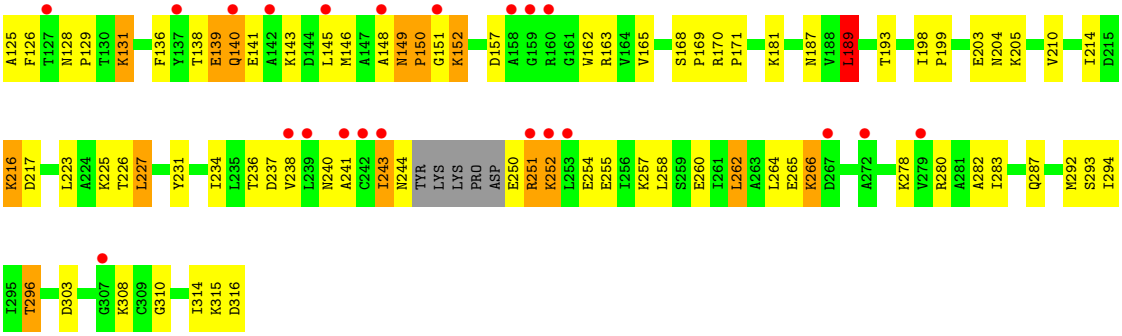
Chain B:



• Molecule 1: Carbamate kinase

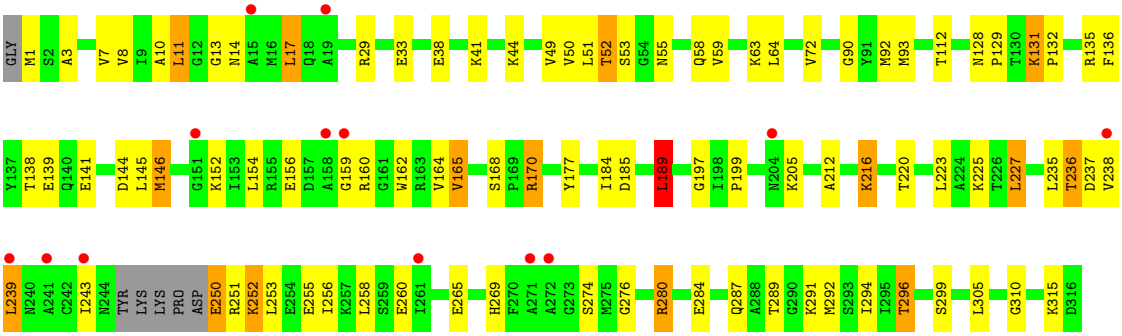
Chain C:





- 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	69.93Å 86.40Å 101.96Å 90.00° 106.53° 90.00°	Depositor
Resolution (Å)	46.30 – 2.10 46.25 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (46.30-2.10) 94.5 (46.25-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 2.10Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.218 , 0.286 0.216 , 0.283	Depositor DCC
R_{free} test set	2670 reflections (3.97%)	wwPDB-VP
Wilson B-factor (Å^2)	22.2	Xtriage
Anisotropy	0.665	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 75.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10081	wwPDB-VP
Average B, all atoms (Å^2)	31.0	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 32.81 % 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 8.8533e-04. 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	0.71	1/3240 (0.0%)
1	B	0.57	0/2350	0.69	2/3174 (0.1%)
1	C	0.58	0/2350	0.72	1/3174 (0.0%)
1	D	0.61	0/2350	0.73	1/3174 (0.0%)
All	All	0.59	0/9448	0.71	5/12762 (0.0%)

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	B	189	LEU	CA-CB-CG	6.84	131.02	115.30
1	A	189	LEU	CA-CB-CG	6.47	130.18	115.30
1	D	189	LEU	CA-CB-CG	5.47	127.88	115.30
1	C	189	LEU	CA-CB-CG	5.27	127.43	115.30
1	B	298	LEU	CA-CB-CG	5.08	126.99	115.30

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	2366	0	2430	84	0
1	B	2321	0	2383	122	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2321	0	2383	102	0
1	D	2321	0	2383	67	0
2	A	13	0	5	1	0
2	B	13	0	5	1	0
2	C	13	0	5	1	0
2	D	13	0	5	1	0
3	A	183	0	0	9	0
3	B	156	0	0	19	0
3	C	178	0	0	17	0
3	D	183	0	0	10	0
All	All	10081	0	9599	371	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 20.

All (371) 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:63:LYS:HE3	3:D:584:HOH:O	1.54	1.05
1:C:214:ILE:HD12	3:C:542:HOH:O	1.61	1.00
1:D:236:THR:HG23	1:D:238:VAL:H	1.27	0.99
1:B:296:THR:HG22	1:B:310:GLY:HA3	1.49	0.95
1:C:138:THR:OG1	1:C:140:GLN:HG3	1.70	0.91
1:A:236:THR:OG1	1:A:237:ASP:N	2.06	0.89
1:B:144:ASP:HB2	3:B:577:HOH:O	1.71	0.89
1:B:231:TYR:HE2	1:B:292:MET:HE2	1.41	0.85
1:C:181:LYS:HD2	3:C:582:HOH:O	1.76	0.85
1:D:52:THR:HG21	1:D:220:THR:OG1	1.77	0.84
1:C:11:LEU:HD11	1:C:51:LEU:HD22	1.60	0.83
1:C:11:LEU:CD1	1:C:51:LEU:HD22	2.11	0.81
1:B:296:THR:CG2	1:B:310:GLY:HA3	2.11	0.80
1:D:1:MET:SD	1:D:3:ALA:HB3	2.23	0.79
1:C:240:ASN:ND2	1:C:254:GLU:OE2	2.16	0.78
1:C:292:MET:CE	1:C:294:ILE:HD11	2.13	0.78
1:B:170:ARG:NH1	1:B:284:GLU:OE2	2.16	0.78
1:C:292:MET:HE3	1:C:294:ILE:HD11	1.66	0.76
1:A:124:GLN:OE1	1:A:128:ASN:ND2	2.19	0.76
1:A:170:ARG:HG3	1:A:171:PRO:HD2	1.68	0.76
1:B:277:PRO:HA	1:B:280:ARG:HB3	1.66	0.76
1:A:145:LEU:HD21	1:A:152:LYS:HE2	1.68	0.75
1:B:231:TYR:CE2	1:B:292:MET:HE2	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:LYS:HB2	1:D:168:SER:HB2	1.68	0.74
1:C:11:LEU:O	1:C:216:LYS:HE2	1.87	0.74
1:C:204:ASN:ND2	3:C:556:HOH:O	2.20	0.73
1:D:92:MET:HB2	3:D:595:HOH:O	1.88	0.73
1:A:138:THR:OG1	1:A:141:GLU:HG3	1.89	0.73
1:C:265:GLU:OE2	1:C:280:ARG:NH1	2.22	0.73
1:B:296:THR:HG22	1:B:310:GLY:CA	2.19	0.72
1:B:90:GLY:HA3	1:B:112:THR:HG21	1.71	0.72
1:C:124:GLN:NE2	3:C:653:HOH:O	2.23	0.72
1:D:10:ALA:HA	1:D:52:THR:HG22	1.70	0.72
1:A:122:LYS:HB3	1:A:122:LYS:NZ	2.03	0.72
1:B:136:PHE:CE2	1:B:160:ARG:HB2	2.25	0.72
1:B:130:THR:HG22	3:B:558:HOH:O	1.90	0.71
1:A:145:LEU:HA	1:A:148:ALA:HB3	1.73	0.70
1:A:296:THR:HG22	1:A:297:SER:H	1.57	0.69
1:C:225:LYS:HD2	3:C:576:HOH:O	1.91	0.69
1:B:29:ARG:HH22	1:B:30:LYS:HE3	1.58	0.69
1:B:63:LYS:HE3	1:B:81:CYS:SG	2.33	0.69
1:C:187:ASN:ND2	3:C:591:HOH:O	2.26	0.68
1:B:225:LYS:NZ	3:B:576:HOH:O	2.19	0.68
1:C:148:ALA:O	1:C:150:PRO:HD3	1.92	0.68
1:B:1:MET:SD	1:B:3:ALA:HB3	2.33	0.68
1:B:11:LEU:HD13	1:B:51:LEU:HD22	1.74	0.68
1:D:14:ASN:HA	1:D:17:LEU:O	1.95	0.67
1:B:292:MET:CE	1:B:294:ILE:HD11	2.24	0.67
1:C:10:ALA:HB1	1:C:216:LYS:HD3	1.75	0.66
1:B:243:ILE:HG12	1:B:269:HIS:ND1	2.10	0.66
1:A:107:PRO:HA	3:A:1068:HOH:O	1.96	0.66
1:B:270:PHE:HB3	1:B:276:GLY:HA2	1.78	0.65
1:D:11:LEU:O	1:D:216:LYS:HE3	1.96	0.65
2:C:401:CIT:H21	3:C:648:HOH:O	1.97	0.65
1:B:242:CYS:SG	1:B:243:ILE:N	2.70	0.64
1:C:148:ALA:C	1:C:150:PRO:HD3	2.17	0.64
1:C:138:THR:CB	1:C:140:GLN:HG3	2.26	0.64
1:A:292:MET:HE2	1:A:294:ILE:HD11	1.80	0.64
2:A:401:CIT:C1	3:A:1030:HOH:O	2.46	0.63
1:C:149:ASN:O	1:C:151:GLY:N	2.32	0.63
1:A:236:THR:HG1	1:A:237:ASP:H	1.44	0.62
1:C:125:ALA:HB1	1:C:168:SER:H	1.63	0.62
1:C:79:HIS:HB3	1:C:210:VAL:O	1.98	0.62
1:B:29:ARG:NH2	1:B:30:LYS:HE3	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:LYS:HB2	1:C:168:SER:HB2	1.82	0.62
1:A:149:ASN:HD22	1:A:152:LYS:HD3	1.65	0.62
1:B:131:LYS:HB2	1:B:168:SER:HB2	1.82	0.62
1:C:199:PRO:HG3	1:C:214:ILE:HG12	1.81	0.62
1:D:265:GLU:OE1	1:D:280:ARG:HD2	1.99	0.61
1:A:53:SER:O	1:A:216:LYS:HG3	1.99	0.61
1:A:124:GLN:O	1:A:128:ASN:ND2	2.34	0.61
1:C:234:ILE:HG21	1:C:278:LYS:HG2	1.82	0.61
1:B:280:ARG:HB2	3:B:563:HOH:O	1.99	0.61
1:A:243:ILE:HD12	1:A:251:ARG:NH1	2.16	0.61
1:A:14:ASN:HA	1:A:17:LEU:O	2.00	0.60
1:A:154:LEU:HD23	1:A:162:TRP:HB3	1.83	0.60
1:A:30:LYS:O	1:A:34:ILE:HD12	2.02	0.60
1:B:239:LEU:HD11	1:B:300:THR:HG21	1.83	0.60
1:C:146:MET:HG3	1:C:152:LYS:O	2.02	0.60
1:D:135:ARG:NE	3:D:657:HOH:O	2.34	0.60
1:A:1:MET:N	3:A:1144:HOH:O	2.35	0.59
1:A:247:LYS:HE2	1:A:249:ASP:HB2	1.83	0.59
1:A:292:MET:CE	1:A:294:ILE:HD11	2.33	0.59
1:C:243:ILE:O	1:C:250:GLU:HA	2.02	0.59
1:D:289:THR:HB	1:D:291:LYS:HG3	1.85	0.58
1:C:204:ASN:O	1:C:205:LYS:HB2	2.02	0.58
1:B:236:THR:OG1	1:B:237:ASP:N	2.34	0.58
1:B:296:THR:HG21	1:B:304:ALA:HB2	1.85	0.58
1:A:170:ARG:HG3	1:A:171:PRO:CD	2.34	0.58
3:B:585:HOH:O	1:C:72:VAL:HG12	2.03	0.57
1:D:236:THR:HG23	1:D:237:ASP:N	2.19	0.57
1:B:105:ASN:ND2	3:B:566:HOH:O	2.37	0.57
1:A:1:MET:HB2	3:A:1138:HOH:O	2.03	0.57
1:B:292:MET:HE3	1:B:294:ILE:HD11	1.85	0.57
1:D:170:ARG:NE	3:D:602:HOH:O	2.37	0.57
1:B:8:VAL:HG22	1:B:50:VAL:HB	1.87	0.57
1:D:7:VAL:HG13	1:D:7:VAL:O	2.04	0.57
1:B:129:PRO:HB2	1:B:165:VAL:HG13	1.85	0.57
1:B:309:CYS:O	1:B:312:ARG:NE	2.38	0.57
1:C:225:LYS:NZ	3:C:574:HOH:O	2.25	0.57
1:C:292:MET:HE2	1:C:294:ILE:HD11	1.85	0.57
1:B:71:GLY:CA	1:D:145:LEU:HD13	2.35	0.57
1:B:216:LYS:NZ	1:B:217:ASP:OD1	2.28	0.56
1:B:312:ARG:NH1	3:B:578:HOH:O	2.22	0.56
1:B:239:LEU:O	1:B:239:LEU:HD23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:THR:HG22	1:B:53:SER:H	1.70	0.56
1:C:260:GLU:O	1:C:264:LEU:HG	2.04	0.56
1:B:292:MET:HE1	1:B:294:ILE:HD11	1.87	0.56
1:B:234:ILE:HG21	1:B:278:LYS:HG2	1.86	0.56
1:D:258:LEU:HD21	1:D:287:GLN:HG3	1.87	0.56
1:B:140:GLN:HA	1:B:143:LYS:HE3	1.86	0.56
1:C:16:MET:O	1:C:17:LEU:HD13	2.05	0.56
1:B:231:TYR:CE2	1:B:292:MET:CE	2.89	0.55
1:D:265:GLU:OE2	1:D:280:ARG:NH1	2.39	0.55
1:B:177:TYR:CE1	1:B:227:LEU:HD12	2.40	0.55
1:A:102:CYS:SG	1:B:205:LYS:HG2	2.47	0.55
1:B:136:PHE:CE2	1:B:163:ARG:HD2	2.42	0.55
1:C:149:ASN:O	1:C:152:LYS:HB3	2.07	0.55
1:A:241:ALA:O	1:A:253:LEU:HB2	2.07	0.55
1:B:235:LEU:HD13	1:B:298:LEU:HA	1.89	0.55
1:B:52:THR:HG22	1:B:53:SER:N	2.22	0.55
1:C:262:LEU:HD22	1:C:266:LYS:HE3	1.89	0.55
1:C:243:ILE:HD11	1:C:251:ARG:HB3	1.88	0.54
1:C:170:ARG:HG3	1:C:171:PRO:HD2	1.88	0.54
1:B:97:MET:HA	1:B:100:VAL:HG12	1.89	0.54
1:A:289:THR:HG21	3:A:1053:HOH:O	2.07	0.54
1:C:139:GLU:O	1:C:143:LYS:HG2	2.08	0.54
1:D:239:LEU:O	1:D:239:LEU:HD12	2.08	0.54
1:B:125:ALA:O	1:B:167:PRO:HB3	2.08	0.54
1:D:184:ILE:HG13	1:D:185:ASP:N	2.23	0.54
1:D:255:GLU:O	1:D:256:ILE:HD13	2.07	0.53
1:A:90:GLY:HA3	1:A:112:THR:HG21	1.91	0.53
1:A:152:LYS:HE3	1:A:164:VAL:HG22	1.91	0.53
1:C:315:LYS:NZ	3:C:560:HOH:O	2.39	0.53
1:C:138:THR:HG23	1:C:141:GLU:OE1	2.08	0.53
1:A:145:LEU:CD2	1:A:152:LYS:HE2	2.38	0.53
1:C:138:THR:OG1	1:C:141:GLU:OE1	2.27	0.53
1:B:251:ARG:NH2	1:B:260:GLU:OE1	2.41	0.53
1:D:13:GLY:N	2:D:401:CIT:O4	2.31	0.53
1:D:156:GLU:OE2	1:D:159:GLY:HA2	2.08	0.53
1:A:145:LEU:O	1:A:149:ASN:HB2	2.08	0.52
1:D:152:LYS:HE3	1:D:164:VAL:HG21	1.91	0.52
1:B:11:LEU:HD13	1:B:51:LEU:CD2	2.39	0.52
1:B:14:ASN:C	1:B:16:MET:H	2.12	0.52
1:C:14:ASN:OD1	1:C:237:ASP:HB3	2.09	0.52
3:A:1141:HOH:O	1:B:135:ARG:HD3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:ILE:HG23	1:A:269:HIS:CD2	2.44	0.52
1:B:152:LYS:HE3	3:B:571:HOH:O	2.09	0.52
1:D:90:GLY:HA3	1:D:112:THR:HG21	1.91	0.52
1:B:14:ASN:HA	1:B:17:LEU:O	2.08	0.52
1:B:71:GLY:N	1:D:145:LEU:HD13	2.25	0.52
1:C:18:GLN:N	1:C:21:GLU:OE2	2.23	0.52
1:A:52:THR:HG22	1:A:53:SER:H	1.75	0.52
1:A:247:LYS:CB	1:A:249:ASP:H	2.23	0.52
1:B:14:ASN:C	1:B:16:MET:N	2.64	0.52
1:A:50:VAL:HG21	1:A:184:ILE:HD11	1.91	0.51
1:A:52:THR:HG22	1:A:53:SER:N	2.25	0.51
1:B:66:ASN:HB3	1:B:75:GLU:HG3	1.92	0.51
1:B:1:MET:HB3	3:B:611:HOH:O	2.10	0.51
1:A:154:LEU:HG	1:A:163:ARG:C	2.31	0.51
1:C:139:GLU:HA	1:C:162:TRP:CD1	2.44	0.51
1:D:58:GLN:CD	1:D:58:GLN:H	2.14	0.51
1:B:16:MET:HE1	1:B:93:MET:HE3	1.92	0.51
1:C:231:TYR:CE2	1:C:292:MET:HE1	2.46	0.51
1:A:38:GLU:OE2	1:A:41:LYS:NZ	2.23	0.51
1:A:143:LYS:C	1:A:145:LEU:H	2.14	0.51
1:C:119:VAL:HG12	3:C:542:HOH:O	2.11	0.51
1:B:11:LEU:HD23	1:B:15:ALA:HB1	1.93	0.50
1:B:282:ALA:HB1	1:B:293:SER:OG	2.10	0.50
1:B:170:ARG:HH12	1:B:284:GLU:CD	2.15	0.50
1:C:103:ALA:HA	3:C:581:HOH:O	2.11	0.50
1:C:22:LYS:HE2	1:C:24:ASP:OD2	2.11	0.50
1:A:128:ASN:O	1:A:130:THR:HG23	2.11	0.50
1:D:136:PHE:CE2	1:D:160:ARG:HB2	2.46	0.50
1:A:145:LEU:HG	1:A:149:ASN:ND2	2.27	0.50
1:B:9:ILE:HB	1:B:51:LEU:HD23	1.94	0.50
1:B:231:TYR:HD2	1:B:292:MET:HE3	1.76	0.50
1:B:52:THR:HG23	1:B:193:THR:O	2.12	0.50
1:B:180:ILE:O	1:B:184:ILE:HG12	2.12	0.50
1:C:241:ALA:HA	3:C:642:HOH:O	2.11	0.50
1:D:280:ARG:O	1:D:284:GLU:HG3	2.12	0.50
1:B:273:GLY:C	1:B:275:MET:H	2.16	0.49
1:B:105:ASN:ND2	3:B:618:HOH:O	2.32	0.49
1:B:125:ALA:HA	3:B:556:HOH:O	2.11	0.49
1:B:154:LEU:HA	1:B:163:ARG:O	2.12	0.49
1:D:131:LYS:HD3	1:D:132:PRO:HD2	1.94	0.49
1:C:203:GLU:O	1:C:204:ASN:C	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:LYS:HB3	1:A:122:LYS:HZ1	1.76	0.49
1:A:244:ASN:HB3	1:A:247:LYS:HD3	1.93	0.49
1:B:231:TYR:CD2	1:B:292:MET:HE3	2.48	0.49
1:D:49:VAL:HB	1:D:189:LEU:HD22	1.94	0.49
1:B:139:GLU:HG2	1:B:162:TRP:NE1	2.28	0.49
1:A:19:ALA:C	1:A:21:GLU:N	2.65	0.49
1:C:22:LYS:HE2	1:C:24:ASP:HB3	1.95	0.49
1:C:124:GLN:CD	1:C:124:GLN:H	2.16	0.49
1:C:38:GLU:O	1:C:41:LYS:HB2	2.13	0.49
1:A:156:GLU:O	1:A:158:ALA:N	2.46	0.48
1:C:262:LEU:HD23	1:C:283:ILE:HD13	1.95	0.48
1:B:170:ARG:HG2	1:B:171:PRO:HD2	1.96	0.48
1:C:83:ALA:HA	1:C:198:ILE:HD11	1.95	0.48
1:D:29:ARG:O	1:D:33:GLU:HG3	2.13	0.48
1:B:135:ARG:HD2	3:B:586:HOH:O	2.14	0.48
1:B:11:LEU:O	1:B:216:LYS:HE3	2.13	0.48
1:A:290:GLY:CA	1:A:315:LYS:HD3	2.43	0.48
1:C:265:GLU:OE1	1:C:280:ARG:HD2	2.12	0.48
1:D:152:LYS:HE3	1:D:164:VAL:CG2	2.44	0.48
1:A:177:TYR:CE1	1:A:227:LEU:HD12	2.49	0.48
1:B:201:LYS:HE2	3:B:623:HOH:O	2.14	0.48
1:B:280:ARG:O	1:B:284:GLU:HG3	2.14	0.48
1:A:11:LEU:HD23	1:A:15:ALA:HB1	1.96	0.47
1:C:193:THR:HG22	1:C:193:THR:O	2.14	0.47
1:A:285:PHE:CE2	1:A:291:LYS:HB2	2.49	0.47
1:B:7:VAL:HG23	1:B:231:TYR:HB2	1.96	0.47
1:A:73:SER:HB2	1:B:64:LEU:HD12	1.96	0.47
1:B:17:LEU:HD13	1:B:28:GLN:HG2	1.96	0.47
1:B:256:ILE:HG22	1:B:257:LYS:O	2.14	0.47
1:C:243:ILE:O	1:C:244:ASN:HB2	2.13	0.47
1:D:53:SER:O	1:D:216:LYS:HG3	2.14	0.47
1:D:199:PRO:HG2	1:D:212:ALA:O	2.14	0.47
1:B:177:TYR:CD1	1:B:226:THR:HG22	2.49	0.47
1:A:52:THR:HG23	1:A:193:THR:O	2.15	0.47
1:B:263:ALA:O	1:B:266:LYS:HG2	2.14	0.47
1:D:296:THR:HG23	1:D:310:GLY:CA	2.44	0.47
1:A:120:ASP:O	1:A:126:PHE:HE2	1.98	0.47
1:C:11:LEU:HD11	1:C:51:LEU:CD2	2.41	0.47
1:D:11:LEU:HD22	1:D:51:LEU:HD22	1.97	0.47
1:B:57:PRO:HD3	2:B:401:CIT:O1	2.15	0.47
1:B:221:SER:O	1:B:225:LYS:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ARG:HB3	3:A:1105:HOH:O	2.15	0.46
1:C:5:LYS:HB2	1:C:5:LYS:HE3	1.62	0.46
1:A:267:ASP:HA	3:A:1182:HOH:O	2.15	0.46
1:B:154:LEU:HG	1:B:163:ARG:C	2.36	0.46
1:C:1:MET:HB2	3:C:590:HOH:O	2.15	0.46
1:B:257:LYS:HB3	1:B:316:ASP:OD1	2.16	0.46
1:C:146:MET:C	1:C:148:ALA:H	2.18	0.46
1:C:262:LEU:O	1:C:266:LYS:HD2	2.15	0.46
1:A:154:LEU:CD2	1:A:162:TRP:HB3	2.44	0.46
1:D:296:THR:HG23	1:D:310:GLY:HA3	1.98	0.46
1:A:22:LYS:HE2	1:A:22:LYS:HA	1.98	0.46
1:D:8:VAL:HG22	1:D:50:VAL:HB	1.97	0.46
1:D:250:GLU:OE2	1:D:252:LYS:NZ	2.39	0.46
1:A:18:GLN:HB3	1:A:19:ALA:H	1.31	0.46
1:C:129:PRO:HB2	1:C:165:VAL:HG13	1.97	0.46
1:B:263:ALA:HA	1:B:266:LYS:HD3	1.98	0.46
1:C:136:PHE:HE2	1:C:157:ASP:HB3	1.81	0.46
1:D:63:LYS:CE	3:D:584:HOH:O	2.35	0.46
1:D:93:MET:HG3	3:D:595:HOH:O	2.14	0.46
1:B:238:VAL:HG12	1:B:240:ASN:O	2.16	0.46
1:D:236:THR:CG2	1:D:238:VAL:H	2.13	0.46
1:A:9:ILE:HA	1:A:233:MET:O	2.16	0.45
1:C:102:CYS:SG	1:D:205:LYS:HB3	2.56	0.45
1:B:140:GLN:O	1:B:143:LYS:HG2	2.17	0.45
1:B:214:ILE:HG23	3:B:540:HOH:O	2.15	0.45
1:B:260:GLU:O	1:B:264:LEU:HG	2.16	0.45
1:A:214:ILE:HG22	1:A:215:ASP:O	2.17	0.45
1:C:11:LEU:HD13	1:C:51:LEU:HD22	1.97	0.45
1:A:243:ILE:HD11	1:A:253:LEU:HD11	1.98	0.45
1:B:146:MET:HG2	1:B:152:LYS:O	2.17	0.45
1:C:181:LYS:HE2	1:C:227:LEU:HD12	1.98	0.45
1:C:282:ALA:HB1	1:C:293:SER:OG	2.17	0.45
1:B:152:LYS:HE3	3:B:614:HOH:O	2.16	0.45
1:C:140:GLN:CD	3:C:644:HOH:O	2.56	0.45
1:D:138:THR:HG23	1:D:141:GLU:OE1	2.17	0.45
1:A:170:ARG:CG	1:A:171:PRO:HD2	2.42	0.44
1:C:56:GLY:HA3	3:C:553:HOH:O	2.17	0.44
1:C:145:LEU:O	1:C:145:LEU:HG	2.17	0.44
1:D:315:LYS:HG2	3:D:550:HOH:O	2.17	0.44
1:A:53:SER:C	1:A:216:LYS:HG3	2.37	0.44
1:B:128:ASN:HA	1:B:129:PRO:HD2	1.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:ARG:HH11	1:B:155:ARG:HG2	1.82	0.44
1:B:242:CYS:HA	1:B:251:ARG:O	2.17	0.44
1:C:90:GLY:HA3	1:C:112:THR:HG21	1.98	0.44
1:C:225:LYS:HG3	1:C:226:THR:N	2.33	0.44
1:C:237:ASP:OD1	1:C:237:ASP:N	2.49	0.44
1:D:146:MET:HE2	1:D:146:MET:HB2	1.91	0.44
1:C:140:GLN:NE2	3:C:644:HOH:O	2.51	0.44
1:C:257:LYS:HB2	1:C:260:GLU:HG3	2.00	0.44
1:C:110:CYS:HA	1:C:189:LEU:O	2.18	0.44
1:D:53:SER:C	1:D:216:LYS:HG3	2.38	0.44
1:A:1:MET:HE3	1:A:46:GLY:O	2.18	0.44
1:A:292:MET:HE3	1:A:294:ILE:CD1	2.48	0.44
1:B:231:TYR:CD2	1:B:292:MET:CE	3.01	0.44
1:D:129:PRO:HB2	1:D:165:VAL:HG13	1.99	0.44
1:A:282:ALA:HB1	1:A:293:SER:OG	2.18	0.43
1:C:53:SER:C	1:C:216:LYS:HG3	2.37	0.43
1:D:10:ALA:HB1	1:D:216:LYS:HE2	2.00	0.43
1:B:125:ALA:HB1	1:B:168:SER:H	1.83	0.43
1:C:149:ASN:C	1:C:151:GLY:H	2.22	0.43
1:D:1:MET:SD	1:D:3:ALA:N	2.90	0.43
1:A:243:ILE:HG22	1:A:244:ASN:ND2	2.34	0.43
1:C:223:LEU:HD11	1:C:227:LEU:HD22	1.99	0.43
1:C:236:THR:HG23	1:C:238:VAL:H	1.81	0.43
1:A:63:LYS:O	1:A:67:GLN:HG3	2.19	0.43
1:A:233:MET:HG2	1:A:235:LEU:HD21	1.99	0.43
1:C:296:THR:HG23	1:C:310:GLY:CA	2.49	0.43
1:A:243:ILE:HD12	1:A:251:ARG:HH11	1.82	0.43
1:A:262:LEU:HD22	1:A:266:LYS:HD3	2.01	0.43
1:B:155:ARG:HG2	1:B:155:ARG:NH1	2.34	0.43
1:B:181:LYS:HE2	1:B:181:LYS:HB3	1.55	0.43
1:C:22:LYS:HG3	1:C:24:ASP:OD2	2.19	0.43
1:C:123:ASP:O	1:C:126:PHE:HD2	2.02	0.43
1:B:16:MET:HE1	1:B:93:MET:CE	2.48	0.43
1:B:39:ILE:HB	1:B:97:MET:HE1	1.99	0.43
1:C:216:LYS:HD2	1:C:217:ASP:N	2.34	0.43
1:C:231:TYR:HE2	1:C:292:MET:HE1	1.82	0.43
1:C:119:VAL:HG11	1:C:169:PRO:HG2	2.00	0.43
1:D:146:MET:HG3	3:D:603:HOH:O	2.18	0.43
1:D:197:GLY:C	3:D:510:HOH:O	2.56	0.43
1:D:223:LEU:HG	1:D:227:LEU:HD22	1.99	0.43
1:C:258:LEU:HD11	1:C:283:ILE:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:GLU:HG2	3:B:626:HOH:O	2.19	0.42
1:B:266:LYS:HG3	1:B:267:ASP:OD2	2.19	0.42
1:D:243:ILE:HG22	1:D:269:HIS:HB3	2.01	0.42
1:A:1:MET:SD	1:A:3:ALA:HB3	2.58	0.42
1:B:253:LEU:HD23	1:B:256:ILE:HD12	2.01	0.42
1:B:277:PRO:HA	1:B:280:ARG:CB	2.43	0.42
1:D:139:GLU:HG3	1:D:162:TRP:NE1	2.35	0.42
1:A:146:MET:SD	1:A:153:ILE:HA	2.60	0.42
1:B:243:ILE:HG21	1:B:269:HIS:ND1	2.34	0.42
1:C:128:ASN:ND2	3:C:587:HOH:O	2.48	0.42
1:D:260:GLU:HG2	3:D:668:HOH:O	2.18	0.42
1:A:11:LEU:HD23	1:A:15:ALA:CB	2.49	0.42
1:B:106:GLU:HG3	1:B:107:PRO:HD2	2.02	0.42
1:C:119:VAL:HG11	1:C:214:ILE:HD11	2.01	0.42
1:C:296:THR:HG23	1:C:310:GLY:HA3	2.01	0.42
1:A:117:THR:OG1	1:A:197:GLY:HA3	2.20	0.42
1:A:205:LYS:HB3	1:B:102:CYS:SG	2.60	0.42
1:C:181:LYS:HA	1:C:181:LYS:HD3	1.82	0.42
1:C:243:ILE:O	1:C:244:ASN:CB	2.68	0.42
1:A:292:MET:HE3	1:A:312:ARG:HG2	2.02	0.42
1:A:204:ASN:O	1:A:205:LYS:HB2	2.20	0.42
1:C:303:ASP:HB3	1:C:308:LYS:HB2	2.01	0.42
1:D:7:VAL:CG1	1:D:49:VAL:HG22	2.49	0.42
1:B:255:GLU:CG	3:B:626:HOH:O	2.68	0.41
1:C:283:ILE:O	1:C:287:GLN:HB2	2.20	0.41
1:D:156:GLU:OE2	1:D:159:GLY:CA	2.68	0.41
1:A:247:LYS:HB2	1:A:249:ASP:H	1.85	0.41
1:A:22:LYS:HD3	3:A:1131:HOH:O	2.20	0.41
1:B:33:GLU:HG2	3:B:644:HOH:O	2.20	0.41
1:B:149:ASN:HB2	1:B:152:LYS:HG3	2.03	0.41
1:A:143:LYS:O	1:A:145:LEU:N	2.53	0.41
1:A:154:LEU:HD23	1:A:163:ARG:N	2.36	0.41
1:B:253:LEU:HD12	1:B:253:LEU:N	2.35	0.41
1:B:17:LEU:HD12	1:B:17:LEU:HA	1.87	0.41
1:C:252:LYS:H	1:C:252:LYS:HG2	1.61	0.41
1:D:292:MET:CE	1:D:294:ILE:HD11	2.51	0.41
1:B:129:PRO:HA	1:B:167:PRO:HA	2.03	0.41
1:B:243:ILE:CG2	1:B:244:ASN:N	2.84	0.41
1:C:138:THR:HB	1:C:140:GLN:HG3	2.01	0.41
1:D:236:THR:HG23	1:D:238:VAL:N	2.12	0.41
1:A:177:TYR:CD1	1:A:227:LEU:HD12	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:LYS:HD2	3:B:586:HOH:O	2.21	0.41
1:C:40:TYR:OH	1:C:106:GLU:OE2	2.30	0.41
1:D:55:ASN:O	1:D:59:VAL:HG12	2.21	0.41
1:D:235:LEU:HD23	1:D:235:LEU:HA	1.82	0.41
1:B:1:MET:HB2	1:B:2:SER:H	1.64	0.41
1:B:55:ASN:CG	1:B:195:GLY:HA3	2.41	0.41
1:B:177:TYR:CD1	1:B:227:LEU:HD12	2.55	0.41
1:C:17:LEU:HD12	1:C:17:LEU:HA	1.89	0.41
1:D:1:MET:SD	1:D:3:ALA:CB	3.04	0.41
1:A:242:CYS:SG	1:A:252:LYS:HD3	2.61	0.40
1:B:131:LYS:HB3	1:B:166:VAL:HG22	2.02	0.40
1:D:154:LEU:HG	1:D:164:VAL:HA	2.03	0.40
1:A:294:ILE:HG22	1:A:296:THR:OG1	2.21	0.40
1:C:157:ASP:OD1	1:C:163:ARG:NH2	2.49	0.40
1:D:38:GLU:HA	1:D:41:LYS:HD2	2.03	0.40
1:B:223:LEU:O	1:B:227:LEU:HD13	2.22	0.40
1:A:234:ILE:HG21	1:A:278:LYS:HG2	2.03	0.40
1:C:21:GLU:OE2	1:C:31:ASN:ND2	2.54	0.40
1:C:262:LEU:CD2	1:C:266:LYS:HE3	2.52	0.40
1:D:128:ASN:HA	1:D:129:PRO:HD2	1.99	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%)	292 (93%)	18 (6%)	4 (1%)	12 7
1	B	307/317 (97%)	294 (96%)	13 (4%)	0	100 100
1	C	307/317 (97%)	290 (94%)	16 (5%)	1 (0%)	41 41
1	D	307/317 (97%)	295 (96%)	11 (4%)	1 (0%)	41 41
All	All	1235/1268 (97%)	1171 (95%)	58 (5%)	6 (0%)	29 26

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	ASP
1	A	157	ASP
1	C	150	PRO
1	A	250	GLU
1	A	123	ASP
1	D	276	GLY

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%)	229 (89%)	28 (11%)	6 3
1	B	252/257 (98%)	226 (90%)	26 (10%)	7 4
1	C	252/257 (98%)	228 (90%)	24 (10%)	8 5
1	D	252/257 (98%)	225 (89%)	27 (11%)	6 3
All	All	1013/1028 (98%)	908 (90%)	105 (10%)	7 4

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	17	LEU
1	A	20	LYS
1	A	22	LYS
1	A	34	ILE
1	A	63	LYS
1	A	64	LEU
1	A	122	LYS
1	A	127	THR
1	A	128	ASN
1	A	131	LYS
1	A	154	LEU
1	A	155	ARG
1	A	165	VAL

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Mol	Chain	Res	Type
1	A	170	ARG
1	A	189	LEU
1	A	204	ASN
1	A	216	LYS
1	A	236	THR
1	A	239	LEU
1	A	246	LYS
1	A	251	ARG
1	A	253	LEU
1	A	262	LEU
1	A	280	ARG
1	A	296	THR
1	A	302	VAL
1	A	305	LEU
1	B	1	MET
1	B	17	LEU
1	B	20	LYS
1	B	22	LYS
1	B	29	ARG
1	B	51	LEU
1	B	67	GLN
1	B	122	LYS
1	B	131	LYS
1	B	139	GLU
1	B	149	ASN
1	B	155	ARG
1	B	156	GLU
1	B	165	VAL
1	B	170	ARG
1	B	181	LYS
1	B	189	LEU
1	B	205	LYS
1	B	216	LYS
1	B	227	LEU
1	B	239	LEU
1	B	262	LEU
1	B	265	GLU
1	B	299	SER
1	B	302	VAL
1	B	305	LEU
1	C	14	ASN
1	C	17	LEU

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Mol	Chain	Res	Type
1	C	20	LYS
1	C	63	LYS
1	C	64	LEU
1	C	120	ASP
1	C	124	GLN
1	C	131	LYS
1	C	139	GLU
1	C	140	GLN
1	C	149	ASN
1	C	152	LYS
1	C	189	LEU
1	C	216	LYS
1	C	227	LEU
1	C	243	ILE
1	C	251	ARG
1	C	252	LYS
1	C	255	GLU
1	C	262	LEU
1	C	266	LYS
1	C	296	THR
1	C	314	ILE
1	C	316	ASP
1	D	11	LEU
1	D	17	LEU
1	D	44	LYS
1	D	52	THR
1	D	64	LEU
1	D	72	VAL
1	D	131	LYS
1	D	144	ASP
1	D	146	MET
1	D	165	VAL
1	D	170	ARG
1	D	177	TYR
1	D	189	LEU
1	D	216	LYS
1	D	225	LYS
1	D	227	LEU
1	D	236	THR
1	D	239	LEU
1	D	250	GLU
1	D	251	ARG

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Mol	Chain	Res	Type
1	D	252	LYS
1	D	253	LEU
1	D	274	SER
1	D	280	ARG
1	D	296	THR
1	D	299	SER
1	D	305	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	ASN
1	A	269	HIS
1	D	240	ASN

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	A	401	-	12,12,12	1.22	0	17,17,17	1.42	4 (23%)
2	CIT	C	401	-	12,12,12	1.10	0	17,17,17	1.85	6 (35%)
2	CIT	B	401	-	12,12,12	1.21	1 (8%)	17,17,17	1.59	4 (23%)
2	CIT	D	401	-	12,12,12	1.66	1 (8%)	17,17,17	1.66	5 (29%)

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	-	-	1/16/16/16	-
2	CIT	C	401	-	-	2/16/16/16	-
2	CIT	B	401	-	-	1/16/16/16	-
2	CIT	D	401	-	-	1/16/16/16	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	CIT	C3-C6	-4.07	1.49	1.53
2	B	401	CIT	C3-C6	-2.30	1.51	1.53

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	CIT	O6-C6-C3	3.56	119.23	113.05
2	D	401	CIT	O6-C6-C3	3.41	118.98	113.05
2	A	401	CIT	O2-C1-O1	-3.38	114.88	123.30
2	B	401	CIT	O6-C6-C3	2.88	118.05	113.05
2	D	401	CIT	C3-C4-C5	-2.71	107.25	113.81
2	C	401	CIT	C3-C4-C5	-2.55	107.64	113.81
2	C	401	CIT	O4-C5-C4	2.54	122.51	114.35
2	C	401	CIT	O2-C1-O1	-2.48	117.11	123.30
2	D	401	CIT	O2-C1-O1	-2.48	117.11	123.30
2	D	401	CIT	C4-C3-C6	-2.36	105.04	110.11
2	B	401	CIT	C3-C2-C1	-2.35	108.12	113.81
2	A	401	CIT	C3-C4-C5	-2.34	108.16	113.81
2	D	401	CIT	O5-C6-C3	-2.32	118.97	122.25
2	B	401	CIT	O2-C1-O1	-2.30	117.57	123.30
2	A	401	CIT	O2-C1-C2	2.28	121.66	114.35
2	B	401	CIT	C4-C3-C6	-2.26	105.24	110.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	CIT	C4-C3-C2	2.11	114.66	109.16
2	A	401	CIT	O6-C6-C3	2.07	116.64	113.05
2	C	401	CIT	O4-C5-O3	-2.01	118.28	123.30

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	CIT	1	0
2	C	401	CIT	1	0
2	B	401	CIT	1	0
2	D	401	CIT	1	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%)	0.49	29 (9%)	9	11	14, 27, 60, 76	0
1	B	311/317 (98%)	0.39	21 (6%)	17	21	14, 29, 58, 71	0
1	C	311/317 (98%)	0.52	28 (9%)	9	12	12, 28, 56, 67	0
1	D	311/317 (98%)	0.21	13 (4%)	36	42	13, 25, 47, 70	0
All	All	1249/1268 (98%)	0.41	91 (7%)	15	19	12, 27, 57, 76	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	243	ILE	8.4
1	C	239	LEU	7.0
1	A	245	TYR	6.9
1	A	248	PRO	6.8
1	B	240	ASN	6.1
1	C	158	ALA	6.0
1	B	19	ALA	5.9
1	D	158	ALA	5.7
1	B	238	VAL	5.2
1	A	158	ALA	5.1
1	C	18	GLN	4.8
1	D	15	ALA	4.8
1	D	272	ALA	4.7
1	A	241	ALA	4.6
1	D	243	ILE	4.6
1	C	242	CYS	4.5
1	A	127	THR	4.1
1	A	274	SER	4.1
1	C	140	GLN	4.0
1	C	137	TYR	4.0
1	C	127	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	159	GLY	3.8
1	C	14	ASN	3.8
1	B	270	PHE	3.8
1	D	239	LEU	3.7
1	A	140	GLN	3.7
1	B	158	ALA	3.6
1	C	1	MET	3.6
1	C	142	ALA	3.6
1	B	272	ALA	3.5
1	A	153	ILE	3.5
1	D	151	GLY	3.5
1	B	269	HIS	3.5
1	C	159	GLY	3.4
1	A	159	GLY	3.4
1	C	272	ALA	3.3
1	B	241	ALA	3.3
1	C	252	LYS	3.3
1	D	241	ALA	3.3
1	A	137	TYR	3.3
1	A	136	PHE	3.2
1	C	241	ALA	3.2
1	C	238	VAL	3.2
1	A	240	ASN	3.1
1	D	271	ALA	3.1
1	B	243	ILE	3.1
1	C	27	THR	3.1
1	B	256	ILE	3.1
1	D	19	ALA	3.0
1	C	145	LEU	3.0
1	A	19	ALA	3.0
1	A	250	GLU	2.9
1	C	251	ARG	2.9
1	A	144	ASP	2.8
1	A	272	ALA	2.8
1	C	17	LEU	2.8
1	C	148	ALA	2.8
1	D	204	ASN	2.7
1	A	242	CYS	2.7
1	D	238	VAL	2.6
1	A	145	LEU	2.6
1	A	166	VAL	2.5
1	C	151	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	273	GLY	2.5
1	B	140	GLN	2.5
1	B	148	ALA	2.4
1	A	17	LEU	2.4
1	C	15	ALA	2.4
1	C	253	LEU	2.4
1	A	249	ASP	2.4
1	A	125	ALA	2.3
1	A	236	THR	2.3
1	A	20	LYS	2.3
1	B	251	ARG	2.3
1	B	242	CYS	2.3
1	C	307	GLY	2.3
1	B	271	ALA	2.2
1	D	261	ILE	2.2
1	B	244	ASN	2.2
1	B	260	GLU	2.2
1	A	273	GLY	2.1
1	B	239	LEU	2.1
1	C	160	ARG	2.1
1	C	279	VAL	2.1
1	B	153	ILE	2.1
1	C	243	ILE	2.1
1	B	161	GLY	2.1
1	A	142	ALA	2.0
1	C	267	ASP	2.0
1	A	238	VAL	2.0
1	A	1	MET	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	A	401	13/13	0.86	0.18	21,32,37,48	0
2	CIT	B	401	13/13	0.86	0.14	33,37,47,50	0
2	CIT	D	401	13/13	0.88	0.17	25,32,39,39	0
2	CIT	C	401	13/13	0.89	0.20	24,31,39,40	0

6.5 Other polymers (i)

There are no such residues in this entry.