Full wwPDB X-ray Structure Validation Report

Feb 27, 2016 – 11:19 AM GMT

PDB ID	:	5CUY
Title	:	Crystal structure of Trypanosoma brucei Vacuolar Soluble Pyrophosphatases in apo form
Authors	:	Yang, Y.Y.; Ko, T.P.; Liu, W.D.; Zheng, Y.Y.; Chen, C.C.; Guo, R.T.
Deposited on	:	2015-07-25
Resolution	:	2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

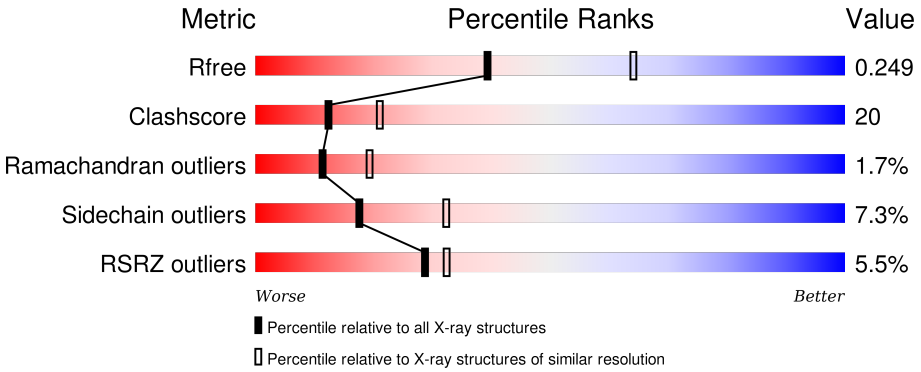
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	414	4% 60% 29% 5% 5%
1	B	414	6% 62% 27% 5% 6%
1	C	414	5% 63% 27% • 5%
1	D	414	6% 66% 25% • • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CIT	B	901	-	-	-	X
2	CIT	C	901	-	-	-	X
3	MG	A	902	-	-	-	X
3	MG	C	902	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13374 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.

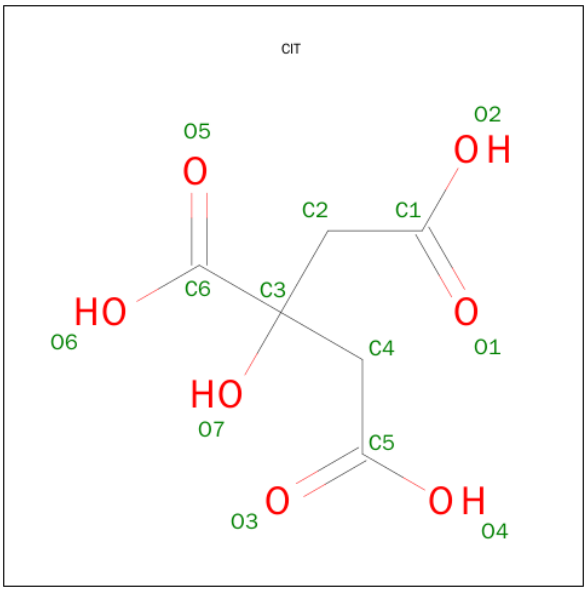
- Molecule 1 is a protein called Acidocalcisomal pyrophosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	0
			3157	2014	537	583	23			
1	B	388	Total	C	N	O	S	0	0	0
			3124	1990	534	577	23			
1	C	392	Total	C	N	O	S	0	0	0
			3161	2016	541	581	23			
1	D	396	Total	C	N	O	S	0	0	0
			3190	2033	546	588	23			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	406	ARG	LEU	engineered mutation	UNP Q384W3
B	406	ARG	LEU	engineered mutation	UNP Q384W3
C	406	ARG	LEU	engineered mutation	UNP Q384W3
D	406	ARG	LEU	engineered mutation	UNP Q384W3

- 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 MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	164	Total O 164 164	0	0

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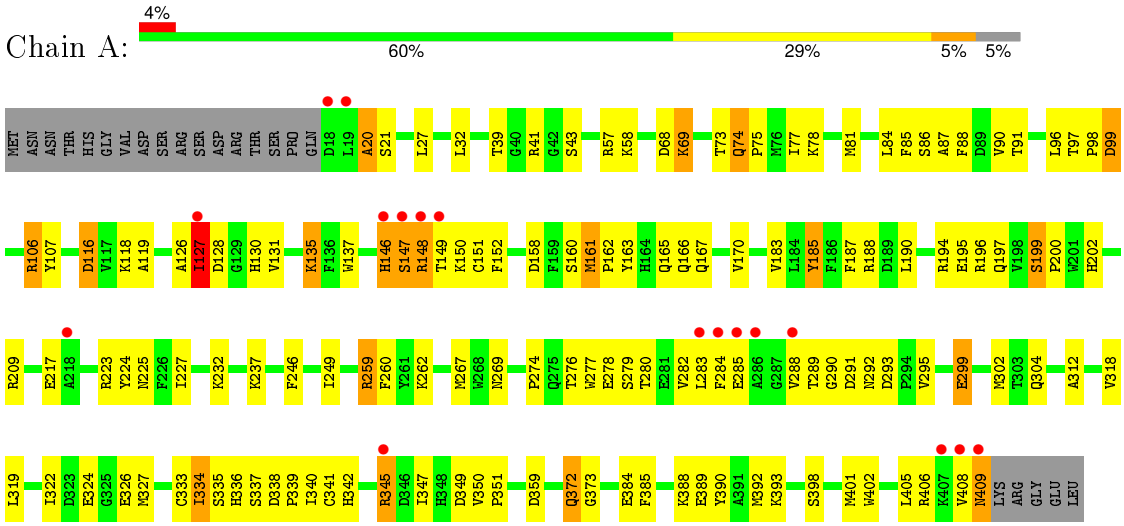
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	183	Total O 183 183	0	0
4	C	171	Total O 171 171	0	0
4	D	168	Total O 168 168	0	0

3 Residue-property plots (i)

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

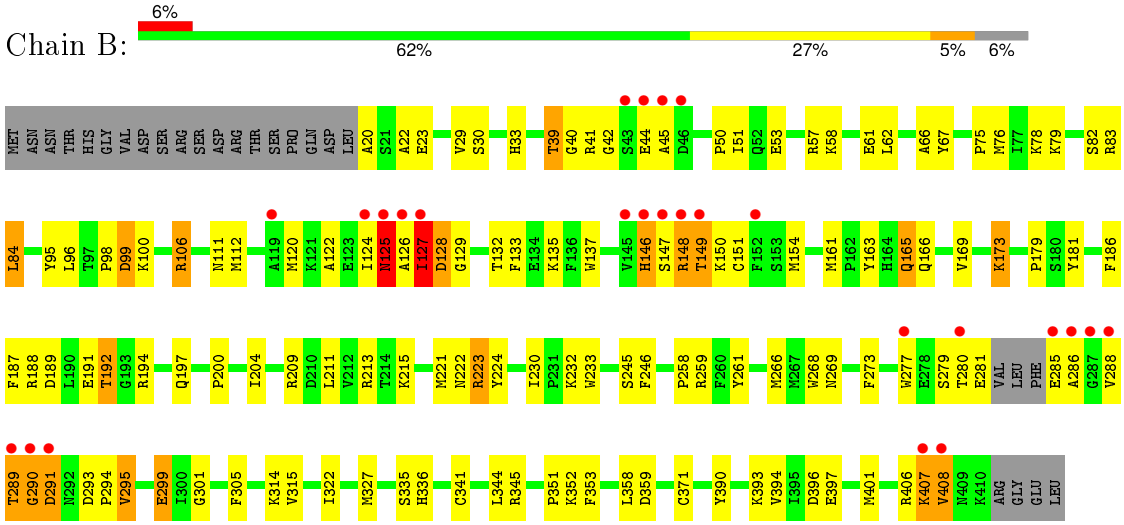
- Molecule 1: Acidocalcisomal pyrophosphatase

Chain A:



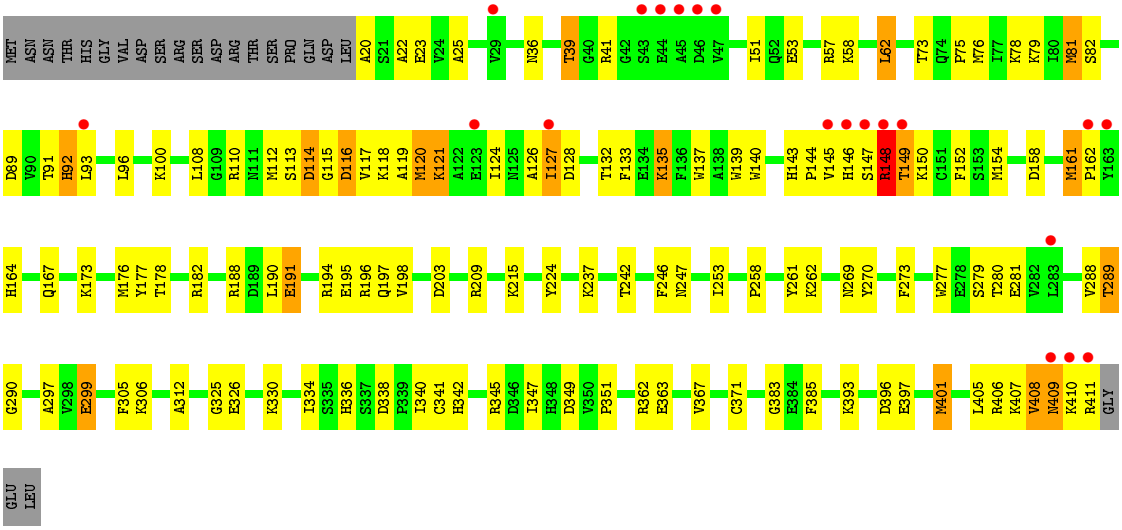
- Molecule 1: Acidocalcisomal pyrophosphatase

Chain B:

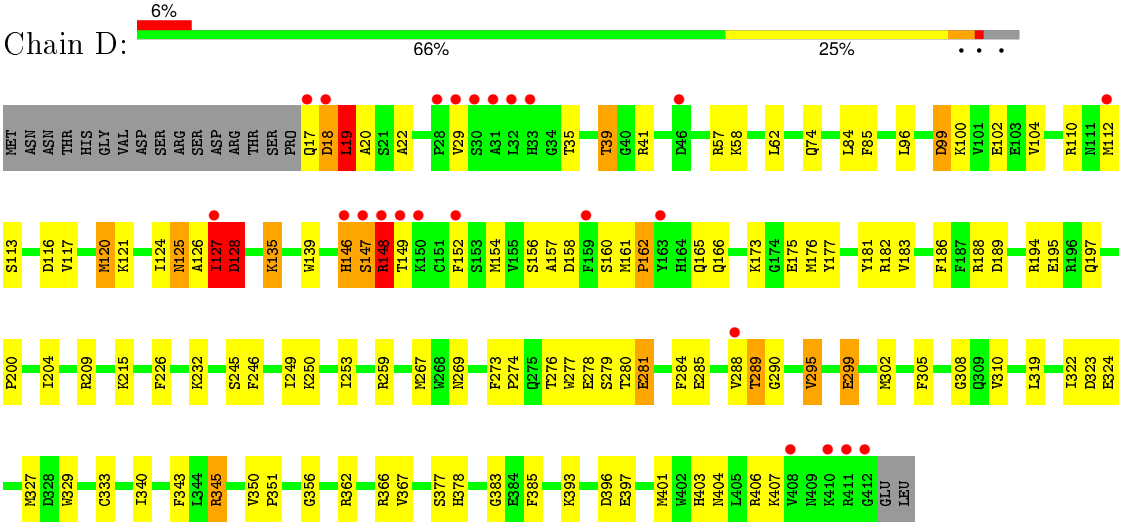


- Molecule 1: Acidocalcisomal pyrophosphatase

Chain C:



- Molecule 1: Acidocalcisomal pyrophosphatase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	199.92Å 70.14Å 141.76Å 90.00° 106.38° 90.00°	Depositor
Resolution (Å)	25.00 – 2.50 24.92 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.2 (25.00-2.50) 93.8 (24.92-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.16 (at 2.50Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.194 , 0.252 0.194 , 0.249	Depositor DCC
R_{free} test set	3114 reflections (5.05%)	DCC
Wilson B-factor (Å^2)	39.2	Xtriage
Anisotropy	0.866	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 47.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 61789 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13374	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.71	0/3245	0.85	0/4395
1	B	0.78	1/3210 (0.0%)	0.86	1/4344 (0.0%)
1	C	0.72	0/3249	0.83	0/4398
1	D	0.77	0/3278	0.85	1/4437 (0.0%)
All	All	0.74	1/12982 (0.0%)	0.85	2/17574 (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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	371	CYS	CB-SG	5.10	1.91	1.82

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	19	LEU	N-CA-C	-5.36	96.53	111.00
1	B	290	GLY	N-CA-C	5.11	125.89	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	185	TYR	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3157	0	3038	131	0
1	B	3124	0	3006	150	0
1	C	3161	0	3049	133	0
1	D	3190	0	3075	125	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	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	164	0	0	3	0
4	B	183	0	0	11	0
4	C	171	0	0	4	0
4	D	168	0	0	8	0
All	All	13374	0	12188	488	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 (488) 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:C:279:SER:H	1:C:401:MET:HE2	1.07	1.14
1:B:289:THR:HG22	1:B:290:GLY:H	1.12	1.06
1:D:378:HIS:HB3	4:D:1115:HOH:O	1.55	1.03
1:A:127:ILE:H	1:A:127:ILE:HD13	1.23	1.01
1:B:288:VAL:HG12	1:B:289:THR:H	1.28	0.99
1:A:340:ILE:HD13	1:D:302:MET:HE3	1.43	0.98
1:A:152:PHE:CZ	1:B:277:TRP:HH2	1.80	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:SER:O	1:D:162:PRO:HD3	1.64	0.97
1:A:276:THR:HB	1:A:398:SER:OG	1.67	0.94
1:B:289:THR:HG22	1:B:290:GLY:N	1.84	0.91
1:D:39:THR:HG22	1:D:41:ARG:H	1.35	0.90
1:A:151:CYS:HA	1:B:288:VAL:HG11	1.55	0.89
1:C:154:MET:HE3	1:D:406:ARG:HH11	1.36	0.87
1:B:39:THR:HG22	1:B:41:ARG:H	1.35	0.87
1:C:279:SER:H	1:C:401:MET:CE	1.85	0.86
1:C:279:SER:N	1:C:401:MET:HE2	1.88	0.86
1:C:289:THR:HG23	1:C:326:GLU:HG2	1.57	0.86
1:B:147:SER:O	1:B:149:THR:N	2.09	0.85
1:D:148:ARG:HG3	1:D:148:ARG:O	1.77	0.84
1:C:148:ARG:CZ	1:C:150:LYS:HE3	2.08	0.83
1:B:39:THR:HG21	1:B:45:ALA:HB2	1.61	0.83
1:B:132:THR:HG23	1:B:135:LYS:H	1.45	0.81
1:A:152:PHE:HE2	1:B:289:THR:HB	1.47	0.80
1:A:20:ALA:HA	1:C:351:PRO:HB2	1.61	0.80
1:B:322:ILE:HG12	1:B:327:MET:CE	2.12	0.80
1:B:148:ARG:HH11	1:B:150:LYS:HE3	1.47	0.80
1:C:154:MET:CE	1:D:406:ARG:HD2	2.12	0.79
1:A:161:MET:CE	1:A:161:MET:HA	2.13	0.79
1:B:166:GLN:HE21	1:B:187:PHE:HB3	1.48	0.79
1:A:146:HIS:O	1:A:148:ARG:HD2	1.82	0.79
1:C:39:THR:HG22	1:C:41:ARG:H	1.46	0.78
1:A:165:GLN:HG2	1:A:190:LEU:HD12	1.63	0.78
1:D:279:SER:H	1:D:401:MET:CE	1.97	0.77
1:C:132:THR:HG23	1:C:135:LYS:H	1.50	0.77
1:D:403:HIS:O	1:D:407:LYS:HD3	1.85	0.77
1:B:122:ALA:O	1:B:125:ASN:HB2	1.85	0.77
1:D:125:ASN:O	1:D:125:ASN:ND2	2.19	0.76
1:A:183:VAL:HB	1:A:249:ILE:HB	1.66	0.76
1:A:147:SER:O	1:A:148:ARG:HG2	1.85	0.76
1:B:147:SER:C	1:B:149:THR:H	1.89	0.76
1:B:209:ARG:HG2	1:B:221:MET:HE1	1.68	0.76
1:A:73:THR:O	1:A:77:ILE:HG12	1.86	0.76
1:C:154:MET:CE	1:D:406:ARG:HH11	2.00	0.75
1:D:39:THR:CG2	1:D:41:ARG:H	1.98	0.75
1:B:322:ILE:HG12	1:B:327:MET:HE1	1.68	0.75
1:C:132:THR:HG22	1:C:135:LYS:HB2	1.69	0.74
1:B:146:HIS:HD2	1:B:148:ARG:HH12	1.33	0.74
1:C:406:ARG:HD2	1:D:154:MET:HE3	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:THR:O	1:C:92:HIS:HB2	1.88	0.74
1:A:127:ILE:N	1:A:127:ILE:HD13	2.01	0.74
1:C:53:GLU:HG3	1:C:76:MET:HG2	1.70	0.73
1:C:209:ARG:HD3	1:D:165:GLN:OE1	1.88	0.73
1:B:281:GLU:HG2	4:B:1048:HOH:O	1.88	0.73
1:D:279:SER:H	1:D:401:MET:HE1	1.52	0.73
1:C:393:LYS:O	1:C:397:GLU:HG3	1.89	0.72
1:C:120:MET:HG3	1:C:139:TRP:CZ2	2.25	0.72
1:D:22:ALA:HB3	4:D:1006:HOH:O	1.91	0.71
1:A:27:LEU:HB2	1:A:32:LEU:HD21	1.73	0.71
1:C:143:HIS:N	1:C:144:PRO:HD3	2.04	0.71
1:D:125:ASN:ND2	1:D:135:LYS:HE3	2.05	0.71
1:B:132:THR:HG21	4:B:1150:HOH:O	1.89	0.71
1:D:186:PHE:CD2	1:D:197:GLN:HA	2.27	0.70
1:B:286:ALA:HA	1:B:408:VAL:HG13	1.72	0.70
1:D:57:ARG:O	1:D:58:LYS:HB2	1.92	0.70
1:D:393:LYS:HE3	1:D:397:GLU:OE2	1.91	0.70
1:C:148:ARG:HD3	1:C:150:LYS:HG3	1.72	0.69
1:B:53:GLU:HG3	1:B:76:MET:CG	2.23	0.69
1:B:148:ARG:HH11	1:B:150:LYS:CE	2.04	0.69
1:A:340:ILE:HG21	1:D:302:MET:HE1	1.75	0.68
1:C:39:THR:CG2	1:C:41:ARG:H	2.06	0.68
1:B:146:HIS:HD2	1:B:148:ARG:NH1	1.91	0.68
1:C:91:THR:OG1	1:C:93:LEU:HG	1.94	0.67
1:B:41:ARG:HB3	1:B:44:GLU:OE1	1.93	0.67
1:A:152:PHE:CE1	1:B:277:TRP:HH2	2.12	0.67
1:A:146:HIS:N	1:A:146:HIS:ND1	2.43	0.67
4:A:1069:HOH:O	1:C:20:ALA:HB1	1.94	0.66
1:D:117:VAL:O	1:D:121:LYS:HG3	1.94	0.66
1:B:53:GLU:OE2	1:B:79:LYS:HE2	1.95	0.66
1:D:125:ASN:HD21	1:D:135:LYS:HE3	1.61	0.66
1:B:289:THR:CG2	1:B:290:GLY:N	2.57	0.66
1:D:273:PHE:HD2	1:D:295:VAL:CG2	2.09	0.66
1:C:53:GLU:HG3	1:C:76:MET:CG	2.25	0.66
1:C:147:SER:C	1:C:149:THR:H	1.98	0.66
1:B:51:ILE:HB	1:B:79:LYS:HE3	1.78	0.66
1:B:166:GLN:NE2	1:B:187:PHE:HB3	2.11	0.65
1:D:278:GLU:OE1	1:D:329:TRP:CD1	2.49	0.65
1:C:114:ASP:OD1	1:C:115:GLY:N	2.30	0.65
1:D:120:MET:HB2	1:D:139:TRP:CZ2	2.31	0.65
1:A:151:CYS:HA	1:B:288:VAL:CG1	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:ASN:OD1	1:B:149:THR:HG22	1.96	0.65
1:D:215:LYS:HE2	2:D:901:CIT:O6	1.95	0.65
1:C:39:THR:HG23	1:C:41:ARG:HG2	1.77	0.65
1:C:89:ASP:OD2	1:C:92:HIS:HA	1.97	0.65
1:B:288:VAL:HG12	1:B:289:THR:N	2.07	0.65
1:A:126:ALA:HB2	1:A:131:VAL:HG22	1.79	0.64
1:A:127:ILE:H	1:A:127:ILE:CD1	1.93	0.64
1:A:152:PHE:CZ	1:B:277:TRP:CH2	2.73	0.64
1:B:293:ASP:HB3	1:B:294:PRO:HD2	1.80	0.64
1:D:273:PHE:HD2	1:D:295:VAL:HG22	1.63	0.63
1:B:148:ARG:NH1	1:B:150:LYS:HE3	2.13	0.63
1:B:232:LYS:HD3	1:B:233:TRP:CE2	2.33	0.63
1:A:340:ILE:HG21	1:D:302:MET:CE	2.29	0.63
1:C:78:LYS:HD2	1:C:137:TRP:NE1	2.14	0.63
1:C:100:LYS:HE2	1:C:100:LYS:HA	1.79	0.63
1:A:90:VAL:HG23	1:A:91:THR:HG23	1.81	0.63
1:B:148:ARG:HD2	1:B:150:LYS:HE3	1.79	0.63
1:C:407:LYS:O	1:C:409:ASN:N	2.31	0.63
1:A:269:ASN:HB2	1:A:299:GLU:HG3	1.81	0.62
1:D:188:ARG:HG3	1:D:195:GLU:HG2	1.81	0.62
1:B:106:ARG:HH11	1:B:106:ARG:HG3	1.64	0.62
1:A:97:THR:HB	1:A:98:PRO:HD2	1.82	0.61
1:B:322:ILE:HG12	1:B:327:MET:HE3	1.81	0.61
1:B:120:MET:HG2	1:B:124:ILE:HG13	1.81	0.61
1:A:152:PHE:CE2	1:B:289:THR:HB	2.32	0.61
1:B:314:LYS:NZ	1:B:344:LEU:O	2.27	0.61
1:D:404:ASN:ND2	4:D:1003:HOH:O	2.32	0.61
1:A:304:GLN:NE2	1:D:356:GLY:HA3	2.15	0.61
1:A:147:SER:O	1:A:149:THR:N	2.33	0.61
1:D:147:SER:C	1:D:149:THR:H	2.04	0.61
1:A:277:TRP:CE2	1:A:405:LEU:HD22	2.36	0.61
1:C:188:ARG:HG3	1:C:195:GLU:HG2	1.81	0.61
1:B:82:SER:HB2	1:B:133:PHE:CE2	2.35	0.61
1:A:20:ALA:HA	1:C:351:PRO:CB	2.31	0.60
1:A:161:MET:HA	1:A:161:MET:HE2	1.83	0.60
1:B:83:ARG:HD3	4:B:1159:HOH:O	2.01	0.60
1:D:99:ASP:O	1:D:102:GLU:HG2	2.01	0.60
1:A:350:VAL:HB	1:A:351:PRO:HD3	1.83	0.60
1:B:192:THR:HG21	1:B:194:ARG:HH21	1.66	0.60
1:A:73:THR:OG1	1:A:75:PRO:HD2	2.02	0.60
1:A:152:PHE:CE1	1:B:277:TRP:CH2	2.90	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:GLU:O	1:A:292:ASN:HA	2.02	0.59
1:A:409:ASN:ND2	1:B:154:MET:HG3	2.16	0.59
1:A:161:MET:HE1	1:A:162:PRO:HD2	1.84	0.59
1:C:132:THR:CG2	1:C:135:LYS:HB2	2.31	0.59
1:A:135:LYS:HD2	1:A:135:LYS:N	2.18	0.59
1:B:78:LYS:HE3	1:B:137:TRP:CD1	2.37	0.59
1:D:232:LYS:H	1:D:269:ASN:ND2	2.00	0.58
1:D:39:THR:HG23	1:D:41:ARG:HG2	1.85	0.58
1:C:145:VAL:HG13	4:C:1004:HOH:O	2.04	0.58
1:B:351:PRO:HB2	1:D:20:ALA:HA	1.85	0.58
1:D:19:LEU:HD23	1:D:19:LEU:N	2.18	0.58
1:D:17:GLN:N	4:D:1005:HOH:O	2.35	0.58
1:B:224:TYR:CD1	1:B:315:VAL:HG23	2.38	0.58
1:B:269:ASN:HD21	1:B:305:PHE:H	1.50	0.58
1:C:289:THR:OG1	1:C:290:GLY:N	2.37	0.58
1:A:165:GLN:HE22	1:B:221:MET:CE	2.17	0.58
1:C:57:ARG:O	1:C:58:LYS:HB2	2.04	0.58
1:C:176:MET:HG2	1:C:177:TYR:CE2	2.38	0.58
1:C:363:GLU:O	1:C:367:VAL:HG22	2.03	0.58
1:A:78:LYS:HE3	1:A:137:TRP:CD1	2.38	0.58
1:D:280:THR:HG22	1:D:290:GLY:O	2.04	0.58
1:C:289:THR:HG23	1:C:326:GLU:CG	2.31	0.57
1:C:139:TRP:O	1:C:143:HIS:HD2	1.87	0.57
1:C:288:VAL:HA	1:C:325:GLY:O	2.04	0.57
1:D:288:VAL:HG21	1:D:322:ILE:HD13	1.84	0.57
1:B:148:ARG:HH11	1:B:150:LYS:NZ	2.02	0.57
1:C:91:THR:O	1:C:92:HIS:CB	2.53	0.57
1:C:147:SER:O	1:C:149:THR:N	2.37	0.57
1:A:98:PRO:HG2	1:A:99:ASP:OD1	2.04	0.57
1:C:81:MET:HE2	1:C:81:MET:HA	1.86	0.57
1:D:57:ARG:O	4:D:1001:HOH:O	2.17	0.57
1:D:278:GLU:OE1	1:D:329:TRP:HD1	1.87	0.57
1:B:336:HIS:HA	1:B:341:CYS:SG	2.45	0.57
1:B:232:LYS:H	1:B:269:ASN:ND2	2.02	0.57
1:D:146:HIS:HB2	4:D:1064:HOH:O	2.04	0.57
1:B:293:ASP:HB3	1:B:294:PRO:CD	2.34	0.56
1:A:390:TYR:HA	1:A:393:LYS:HD2	1.86	0.56
1:A:389:GLU:O	1:A:393:LYS:HG3	2.05	0.56
1:B:100:LYS:NZ	1:B:100:LYS:HB3	2.20	0.56
1:D:175:GLU:O	1:D:181:TYR:HB2	2.05	0.56
1:D:289:THR:HG23	1:D:290:GLY:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:THR:HA	1:C:247:ASN:HD22	1.70	0.56
1:D:128:ASP:OD1	1:D:128:ASP:N	2.39	0.56
1:C:118:LYS:HG3	1:C:119:ALA:N	2.21	0.56
1:B:53:GLU:HG3	1:B:76:MET:SD	2.45	0.56
1:B:273:PHE:HD2	1:B:295:VAL:HG22	1.71	0.56
1:B:53:GLU:CG	1:B:76:MET:HG2	2.36	0.55
1:B:299:GLU:HG2	1:B:305:PHE:CE2	2.42	0.55
1:B:22:ALA:HB3	4:B:1121:HOH:O	2.05	0.55
1:B:277:TRP:NE1	1:B:279:SER:HB3	2.22	0.55
1:B:146:HIS:CD2	1:B:148:ARG:HH12	2.18	0.55
1:B:215:LYS:HE2	2:B:901:CIT:O6	2.06	0.55
1:C:277:TRP:HH2	1:D:152:PHE:CE1	2.24	0.55
1:A:227:ILE:HD11	1:A:274:PRO:HB3	1.89	0.55
1:B:44:GLU:HG2	1:B:44:GLU:O	2.07	0.55
1:A:388:LYS:HD2	1:A:392:MET:CE	2.37	0.55
1:A:162:PRO:HG2	1:A:163:TYR:CD2	2.42	0.55
1:A:170:VAL:O	1:A:170:VAL:CG2	2.55	0.55
1:D:279:SER:H	1:D:401:MET:HE2	1.72	0.55
1:A:147:SER:C	1:A:149:THR:H	2.10	0.54
1:B:122:ALA:O	1:B:125:ASN:CB	2.55	0.54
1:B:53:GLU:HG3	1:B:76:MET:HG2	1.89	0.54
1:C:73:THR:HB	1:C:75:PRO:HD2	1.89	0.54
1:B:165:GLN:NE2	4:B:1005:HOH:O	2.40	0.54
1:B:277:TRP:NE1	1:B:279:SER:CB	2.71	0.54
1:A:170:VAL:O	1:A:170:VAL:HG23	2.06	0.54
1:A:166:GLN:HE21	1:A:187:PHE:HB3	1.72	0.54
1:A:188:ARG:NH1	1:A:195:GLU:OE2	2.41	0.54
1:C:280:THR:HA	1:C:289:THR:OG1	2.06	0.54
1:B:122:ALA:O	1:B:125:ASN:N	2.40	0.54
1:B:230:ILE:CD1	1:B:261:TYR:HE2	2.21	0.54
1:C:143:HIS:N	1:C:144:PRO:CD	2.71	0.54
1:A:304:GLN:HE22	1:D:356:GLY:HA3	1.73	0.54
1:B:192:THR:CG2	1:B:194:ARG:HH21	2.20	0.54
1:A:85:PHE:CE1	1:A:96:LEU:HD12	2.43	0.54
1:A:260:PHE:CD2	1:B:66:ALA:HA	2.42	0.54
1:B:352:LYS:NZ	1:D:345:ARG:HH12	2.05	0.54
1:A:279:SER:H	1:A:401:MET:CE	2.21	0.54
1:C:336:HIS:HA	1:C:341:CYS:SG	2.48	0.53
1:D:396:ASP:HB3	4:D:1119:HOH:O	2.06	0.53
1:A:373:GLY:HA2	1:C:57:ARG:NH2	2.23	0.53
1:C:408:VAL:HG12	1:C:408:VAL:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:SER:O	1:D:149:THR:N	2.41	0.53
1:C:126:ALA:O	1:C:128:ASP:N	2.41	0.53
1:C:148:ARG:HD3	1:C:150:LYS:CG	2.39	0.53
1:B:390:TYR:O	1:B:394:VAL:HG23	2.08	0.53
1:B:147:SER:C	1:B:149:THR:N	2.59	0.53
1:C:96:LEU:HB3	1:C:100:LYS:HB2	1.91	0.53
1:C:126:ALA:C	1:C:128:ASP:H	2.12	0.53
1:B:288:VAL:CG1	1:B:289:THR:H	2.12	0.53
1:C:167:GLN:HB2	1:C:190:LEU:HD21	1.91	0.53
1:A:185:TYR:CD1	1:A:200:PRO:HD3	2.43	0.53
1:A:289:THR:HG23	1:A:290:GLY:N	2.24	0.53
1:A:289:THR:HG22	1:A:326:GLU:HG2	1.90	0.52
1:A:267:MET:HG2	1:D:267:MET:HG2	1.92	0.52
1:C:215:LYS:HE2	2:C:901:CIT:O6	2.09	0.52
1:A:285:GLU:HB3	1:A:288:VAL:HG21	1.92	0.52
1:A:165:GLN:HE22	1:B:221:MET:HE1	1.72	0.52
1:D:127:ILE:HD11	1:D:135:LYS:NZ	2.25	0.52
1:A:166:GLN:NE2	1:A:187:PHE:HB3	2.25	0.52
1:C:280:THR:O	1:C:289:THR:OG1	2.20	0.52
1:D:166:GLN:NE2	1:D:189:ASP:HA	2.24	0.52
1:C:154:MET:CE	1:D:406:ARG:CD	2.87	0.52
1:A:336:HIS:HA	1:A:341:CYS:SG	2.50	0.52
1:C:148:ARG:NH2	4:C:1004:HOH:O	2.42	0.52
1:D:269:ASN:HD21	1:D:305:PHE:H	1.57	0.52
1:D:57:ARG:O	1:D:58:LYS:CB	2.55	0.52
1:B:258:PRO:HD3	4:B:1021:HOH:O	2.10	0.51
1:C:161:MET:O	1:C:161:MET:HG2	2.10	0.51
1:A:223:ARG:NH1	2:A:901:CIT:O5	2.42	0.51
1:A:57:ARG:O	1:A:58:LYS:HB2	2.10	0.51
1:A:262:LYS:HB2	1:A:372:GLN:NE2	2.25	0.51
1:B:197:GLN:HG2	1:B:246:PHE:CG	2.45	0.51
1:C:53:GLU:CG	1:C:76:MET:HG2	2.40	0.51
1:A:116:ASP:O	1:A:119:ALA:HB3	2.11	0.51
1:A:402:TRP:CZ2	1:A:406:ARG:HD2	2.45	0.51
1:B:269:ASN:ND2	1:B:305:PHE:H	2.09	0.51
1:B:197:GLN:HG2	1:B:246:PHE:CD1	2.46	0.51
1:C:113:SER:O	1:C:117:VAL:HG23	2.11	0.51
1:B:20:ALA:C	1:B:22:ALA:N	2.64	0.50
1:C:362:ARG:NH1	1:C:383:GLY:O	2.42	0.50
1:A:334:ILE:HG13	1:A:335:SER:N	2.25	0.50
1:C:277:TRP:HH2	1:D:152:PHE:CZ	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:MET:HE1	1:D:406:ARG:HD2	1.91	0.50
1:B:407:LYS:O	1:B:408:VAL:C	2.50	0.50
1:C:81:MET:CE	1:C:108:LEU:HD11	2.41	0.50
1:D:84:LEU:O	1:D:84:LEU:HD23	2.12	0.50
1:D:112:MET:HE3	1:D:139:TRP:HH2	1.76	0.50
1:D:188:ARG:NH1	1:D:195:GLU:OE2	2.44	0.50
1:A:232:LYS:HB3	1:A:304:GLN:HB2	1.94	0.50
1:A:285:GLU:HB3	1:A:288:VAL:CG2	2.43	0.49
1:D:249:ILE:CD1	1:D:308:GLY:HA2	2.42	0.49
1:C:176:MET:O	1:C:177:TYR:HB2	2.12	0.49
1:B:189:ASP:OD1	1:B:191:GLU:HB2	2.12	0.49
1:A:69:LYS:HG2	1:C:371:CYS:O	2.12	0.49
1:B:122:ALA:O	1:B:125:ASN:CA	2.60	0.49
1:A:27:LEU:HB2	1:A:32:LEU:CD2	2.42	0.49
1:B:223:ARG:NH1	2:B:901:CIT:O5	2.45	0.49
1:C:161:MET:SD	1:C:161:MET:N	2.86	0.49
1:D:29:VAL:O	1:D:29:VAL:HG12	2.12	0.49
1:D:323:ASP:OD1	1:D:324:GLU:HG3	2.12	0.49
1:C:164:HIS:ND1	1:C:191:GLU:HB2	2.27	0.49
1:B:23:GLU:O	1:D:362:ARG:NH2	2.44	0.49
1:D:160:SER:C	1:D:162:PRO:HD3	2.32	0.49
1:B:39:THR:CG2	1:B:41:ARG:H	2.16	0.49
1:C:147:SER:C	1:C:149:THR:N	2.66	0.49
1:D:279:SER:C	1:D:281:GLU:H	2.16	0.49
1:B:127:ILE:HA	4:B:1026:HOH:O	2.13	0.49
1:D:319:LEU:HB2	1:D:385:PHE:CE1	2.48	0.49
1:D:176:MET:O	1:D:177:TYR:HB2	2.12	0.49
1:B:232:LYS:O	1:B:233:TRP:HB2	2.13	0.49
1:C:128:ASP:OD1	1:C:128:ASP:N	2.45	0.49
1:B:95:TYR:CD1	1:B:95:TYR:C	2.85	0.49
1:C:299:GLU:HG2	1:C:305:PHE:HE2	1.78	0.48
1:B:192:THR:CG2	1:B:194:ARG:NH2	2.76	0.48
1:D:362:ARG:NH1	1:D:383:GLY:O	2.40	0.48
1:B:100:LYS:HZ2	1:B:100:LYS:HB3	1.77	0.48
1:C:203:ASP:OD1	1:D:156:SER:HB2	2.13	0.48
1:B:20:ALA:C	1:B:22:ALA:H	2.16	0.48
1:A:262:LYS:HG3	4:B:1017:HOH:O	2.14	0.48
1:C:277:TRP:CE2	1:C:405:LEU:HD22	2.48	0.48
1:A:57:ARG:NH1	1:A:68:ASP:OD1	2.47	0.48
1:C:253:ILE:HD13	1:C:258:PRO:HA	1.95	0.48
1:D:299:GLU:HA	1:D:333:CYS:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:HIS:CE1	1:A:402:TRP:HE1	2.31	0.48
1:B:266:MET:HG3	1:B:268:TRP:O	2.14	0.48
1:C:113:SER:O	1:C:115:GLY:N	2.47	0.48
1:C:410:LYS:HG3	1:C:411:ARG:N	2.29	0.48
1:B:200:PRO:HA	1:B:204:ILE:CD1	2.44	0.48
1:D:39:THR:CG2	1:D:41:ARG:N	2.74	0.48
1:A:39:THR:HG21	1:A:87:ALA:CB	2.44	0.48
1:A:278:GLU:O	1:A:292:ASN:CA	2.61	0.48
1:C:118:LYS:O	1:C:121:LYS:HG2	2.14	0.48
1:A:194:ARG:HH22	1:A:196:ARG:HD3	1.79	0.48
1:D:284:PHE:CD2	1:D:285:GLU:HG2	2.49	0.48
1:D:188:ARG:CG	1:D:195:GLU:HG2	2.44	0.47
1:A:128:ASP:OD2	1:A:130:HIS:HB2	2.14	0.47
1:D:284:PHE:CE2	1:D:327:MET:CE	2.96	0.47
1:C:120:MET:CE	1:C:124:ILE:HD12	2.44	0.47
1:D:110:ARG:O	1:D:110:ARG:HG2	2.15	0.47
1:B:277:TRP:HD1	1:B:401:MET:HG3	1.80	0.47
1:C:113:SER:OG	1:C:116:ASP:OD1	2.32	0.47
1:D:113:SER:O	1:D:116:ASP:N	2.47	0.47
1:C:117:VAL:O	1:C:120:MET:HB3	2.14	0.47
1:C:176:MET:HG2	1:C:177:TYR:CD2	2.50	0.47
1:C:196:ARG:NH2	1:D:157:ALA:O	2.48	0.47
1:D:200:PRO:HA	1:D:204:ILE:HG13	1.96	0.47
1:B:106:ARG:NH1	1:B:106:ARG:HG3	2.28	0.47
1:B:98:PRO:HD3	1:B:129:GLY:O	2.15	0.47
1:B:345:ARG:HE	1:B:345:ARG:HB2	1.61	0.47
1:A:342:HIS:HB2	4:A:1021:HOH:O	2.15	0.47
1:A:152:PHE:CZ	1:B:290:GLY:N	2.83	0.46
1:A:289:THR:CG2	1:A:326:GLU:HG2	2.45	0.46
1:A:150:LYS:HA	1:B:290:GLY:HA2	1.96	0.46
1:C:148:ARG:NH1	1:C:150:LYS:HE3	2.29	0.46
1:D:147:SER:C	1:D:149:THR:N	2.68	0.46
1:A:57:ARG:O	1:A:58:LYS:CB	2.63	0.46
1:D:350:VAL:N	1:D:351:PRO:CD	2.78	0.46
1:C:120:MET:HG3	1:C:139:TRP:CE2	2.50	0.46
1:C:405:LEU:HG	1:D:154:MET:HE2	1.98	0.46
1:B:169:VAL:HB	1:B:186:PHE:HB2	1.97	0.46
1:B:39:THR:CG2	1:B:41:ARG:HB2	2.45	0.46
1:D:279:SER:N	1:D:401:MET:HE1	2.25	0.46
1:B:299:GLU:HG2	1:B:305:PHE:HE2	1.81	0.46
1:C:110:ARG:HD3	1:C:112:MET:CE	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:PHE:HE2	1:B:289:THR:CB	2.22	0.46
1:D:39:THR:CG2	1:D:41:ARG:HB2	2.46	0.46
1:A:384:GLU:HG3	1:C:25:ALA:HA	1.97	0.46
1:B:39:THR:HG21	1:B:45:ALA:CB	2.40	0.46
1:C:78:LYS:HB2	1:C:137:TRP:CZ2	2.50	0.46
1:B:209:ARG:NH2	4:B:1008:HOH:O	2.46	0.46
1:D:17:GLN:N	1:D:19:LEU:HD21	2.31	0.46
1:A:322:ILE:HD11	1:A:327:MET:CE	2.46	0.46
1:A:284:PHE:CD2	1:A:327:MET:HE3	2.51	0.46
1:C:20:ALA:C	1:C:22:ALA:H	2.19	0.45
1:C:409:ASN:O	1:C:411:ARG:O	2.34	0.45
1:B:57:ARG:O	1:B:58:LYS:HB2	2.17	0.45
1:C:242:THR:HA	1:C:247:ASN:ND2	2.30	0.45
1:C:126:ALA:C	1:C:128:ASP:N	2.68	0.45
1:C:198:VAL:HB	1:C:203:ASP:HB2	1.99	0.45
1:A:319:LEU:HB2	1:A:385:PHE:CE1	2.52	0.45
1:A:345:ARG:N	1:A:349:ASP:OD2	2.44	0.45
1:A:284:PHE:CE2	1:A:327:MET:HE3	2.52	0.45
1:C:182:ARG:HG2	1:C:182:ARG:HH11	1.82	0.45
1:A:146:HIS:CD2	1:A:148:ARG:NH1	2.85	0.45
1:B:215:LYS:CE	2:B:901:CIT:O6	2.65	0.45
1:D:127:ILE:HD11	1:D:135:LYS:HZ3	1.82	0.45
1:C:53:GLU:HB3	4:C:1127:HOH:O	2.15	0.45
1:D:215:LYS:CE	2:D:901:CIT:O6	2.64	0.45
1:C:393:LYS:HD2	1:C:397:GLU:OE2	2.17	0.45
1:D:269:ASN:ND2	1:D:305:PHE:H	2.13	0.45
1:A:41:ARG:HD2	1:A:88:PHE:CE1	2.52	0.45
1:C:82:SER:HB2	1:C:133:PHE:CE2	2.52	0.45
1:A:282:VAL:HB	1:A:401:MET:HE3	2.00	0.44
1:D:18:ASP:OD1	1:D:18:ASP:N	2.50	0.44
1:B:327:MET:HA	1:B:327:MET:CE	2.48	0.44
1:A:167:GLN:OE1	1:B:213:ARG:HD3	2.18	0.44
1:B:273:PHE:HD2	1:B:295:VAL:CG2	2.31	0.44
1:C:406:ARG:HD2	1:D:154:MET:CE	2.44	0.44
1:C:51:ILE:HD12	1:C:76:MET:HG2	1.99	0.44
1:C:197:GLN:HG2	1:C:246:PHE:CG	2.53	0.44
1:B:84:LEU:HD23	1:B:84:LEU:N	2.33	0.44
1:B:353:PHE:N	1:B:353:PHE:CD1	2.86	0.44
1:C:53:GLU:H	1:C:53:GLU:CD	2.21	0.44
1:B:99:ASP:OD1	1:B:99:ASP:N	2.45	0.44
1:B:222:ASN:OD1	1:B:224:TYR:HE1	2.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:GLU:OE2	1:B:188:ARG:NH2	2.49	0.44
1:A:340:ILE:HD13	1:D:302:MET:CE	2.31	0.44
1:A:126:ALA:C	1:A:128:ASP:H	2.21	0.44
1:D:232:LYS:H	1:D:269:ASN:HD22	1.64	0.43
1:A:280:THR:HG23	1:A:292:ASN:HB2	2.00	0.43
1:A:279:SER:H	1:A:401:MET:HE1	1.82	0.43
1:D:124:ILE:O	1:D:125:ASN:CG	2.56	0.43
1:D:85:PHE:CE1	1:D:96:LEU:HD12	2.52	0.43
1:B:393:LYS:HE3	1:B:393:LYS:HB2	1.67	0.43
1:D:182:ARG:HH11	1:D:182:ARG:HG2	1.83	0.43
1:A:408:VAL:CG1	1:A:409:ASN:N	2.81	0.43
1:D:350:VAL:HB	1:D:351:PRO:HD3	2.00	0.43
1:D:245:SER:O	1:D:246:PHE:HB2	2.17	0.43
1:B:211:LEU:HA	1:B:211:LEU:HD12	1.87	0.43
1:A:147:SER:C	1:A:149:THR:N	2.71	0.43
1:D:120:MET:CE	1:D:124:ILE:HD12	2.48	0.43
1:B:75:PRO:O	1:B:79:LYS:HD3	2.18	0.43
1:A:278:GLU:O	1:A:292:ASN:N	2.49	0.43
1:B:20:ALA:HB3	4:B:1072:HOH:O	2.18	0.43
1:D:343:PHE:N	1:D:343:PHE:CD1	2.87	0.43
1:C:81:MET:HE1	1:C:108:LEU:HD11	2.00	0.43
1:C:173:LYS:HE2	1:C:173:LYS:HB2	1.77	0.43
1:B:277:TRP:HE1	1:B:279:SER:HB3	1.84	0.43
1:B:406:ARG:HA	1:B:406:ARG:HD2	1.89	0.43
1:A:126:ALA:HB1	1:A:130:HIS:O	2.18	0.43
1:B:299:GLU:OE2	1:B:301:GLY:N	2.45	0.43
1:C:269:ASN:HB2	1:C:299:GLU:HG3	2.01	0.43
1:A:194:ARG:NH2	1:A:196:ARG:HD3	2.33	0.43
1:A:163:TYR:CD1	1:B:161:MET:HG2	2.54	0.43
1:A:165:GLN:CG	1:A:190:LEU:HD12	2.43	0.43
1:C:393:LYS:HD2	1:C:397:GLU:CD	2.39	0.43
1:D:186:PHE:CD2	1:D:197:GLN:CA	3.00	0.43
1:A:190:LEU:HA	1:A:190:LEU:HD23	1.88	0.42
1:D:120:MET:HB2	1:D:139:TRP:CE2	2.54	0.42
1:C:237:LYS:HE2	1:C:261:TYR:CE1	2.54	0.42
1:C:338:ASP:OD2	1:C:340:ILE:HG12	2.19	0.42
1:A:276:THR:OG1	1:A:295:VAL:HG12	2.19	0.42
1:D:121:LYS:HB3	1:D:121:LYS:NZ	2.34	0.42
1:C:121:LYS:H	1:C:121:LYS:HG2	1.64	0.42
1:B:40:GLY:C	1:B:42:GLY:H	2.22	0.42
1:D:74:GLN:NE2	4:D:1013:HOH:O	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:TYR:OH	1:C:330:LYS:NZ	2.51	0.42
1:B:112:MET:CE	1:B:112:MET:HA	2.49	0.42
1:B:291:ASP:OD1	1:B:291:ASP:O	2.37	0.42
1:B:126:ALA:C	1:B:128:ASP:H	2.23	0.42
1:A:237:LYS:HD3	1:A:259:ARG:HB3	2.00	0.42
1:A:322:ILE:HD11	1:A:327:MET:HE1	2.01	0.42
1:B:83:ARG:CD	4:B:1159:HOH:O	2.64	0.42
1:C:363:GLU:HA	1:C:363:GLU:OE1	2.19	0.42
1:C:36:ASN:O	1:C:62:LEU:HD22	2.20	0.42
1:C:81:MET:CA	1:C:81:MET:HE2	2.49	0.42
1:A:225:ASN:O	1:A:274:PRO:HD2	2.20	0.42
1:B:163:TYR:CE2	1:B:211:LEU:HD22	2.54	0.42
1:A:107:TYR:CZ	1:B:179:PRO:HB2	2.55	0.42
1:A:302:MET:CE	1:D:340:ILE:HG21	2.50	0.42
1:B:50:PRO:HA	1:B:61:GLU:OE1	2.20	0.42
1:D:120:MET:HG3	1:D:121:LYS:N	2.34	0.42
1:D:127:ILE:N	1:D:127:ILE:HD12	2.34	0.42
1:C:20:ALA:C	1:C:22:ALA:N	2.73	0.42
1:D:126:ALA:C	1:D:128:ASP:H	2.23	0.42
1:D:183:VAL:HB	1:D:249:ILE:HB	2.02	0.42
1:B:277:TRP:NE1	1:B:279:SER:HB2	2.35	0.41
1:C:277:TRP:CD1	1:C:405:LEU:HD22	2.55	0.41
1:B:173:LYS:O	1:B:181:TYR:HA	2.20	0.41
1:B:62:LEU:HA	1:B:62:LEU:HD12	1.85	0.41
1:B:111:ASN:HD22	1:B:111:ASN:HA	1.61	0.41
1:D:280:THR:HA	1:D:289:THR:HG23	2.01	0.41
1:D:100:LYS:O	1:D:104:VAL:HG23	2.20	0.41
1:B:279:SER:O	1:B:401:MET:CE	2.69	0.41
1:D:39:THR:HG21	1:D:41:ARG:HB2	2.02	0.41
1:B:125:ASN:C	1:B:125:ASN:HD22	2.23	0.41
1:D:188:ARG:HG3	1:D:195:GLU:CG	2.50	0.41
1:C:345:ARG:HB2	1:C:349:ASP:OD2	2.20	0.41
1:C:124:ILE:HG23	1:C:135:LYS:CG	2.51	0.41
1:A:74:GLN:HB3	1:A:75:PRO:HD3	2.02	0.41
1:C:127:ILE:HG22	1:C:127:ILE:O	2.20	0.41
1:A:318:VAL:HG22	1:A:319:LEU:N	2.36	0.41
1:C:273:PHE:CE2	1:C:297:ALA:HB2	2.55	0.41
1:C:280:THR:CA	1:C:289:THR:OG1	2.69	0.41
1:A:359:ASP:CG	1:C:23:GLU:HG2	2.41	0.41
1:D:366:ARG:HA	1:D:377:SER:HB2	2.02	0.41
1:D:274:PRO:O	1:D:276:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:ASP:HA	1:A:339:PRO:HD3	1.94	0.41
1:D:17:GLN:C	1:D:19:LEU:H	2.24	0.41
1:C:342:HIS:CG	1:C:342:HIS:O	2.73	0.41
1:C:152:PHE:CZ	1:D:277:TRP:HH2	2.39	0.41
1:B:285:GLU:HB2	1:B:286:ALA:H	1.67	0.41
1:B:53:GLU:CG	1:B:76:MET:CG	2.95	0.41
1:A:90:VAL:HG23	1:A:91:THR:N	2.36	0.41
1:C:58:LYS:HE2	1:C:58:LYS:HB2	1.94	0.41
1:A:199:SER:O	1:A:200:PRO:C	2.58	0.41
1:A:161:MET:HA	1:A:161:MET:HE1	1.98	0.41
1:C:110:ARG:NE	1:C:140:TRP:CZ3	2.88	0.41
1:A:277:TRP:CD2	1:A:405:LEU:HD22	2.56	0.40
1:D:289:THR:HG23	1:D:290:GLY:O	2.21	0.40
1:D:284:PHE:CD2	1:D:327:MET:HE3	2.55	0.40
1:A:347:ILE:HG12	1:A:385:PHE:HB3	2.02	0.40
1:A:197:GLN:HE21	1:A:246:PHE:HB3	1.86	0.40
1:D:120:MET:CB	1:D:139:TRP:CZ2	3.03	0.40
1:B:120:MET:HG2	1:B:124:ILE:CG1	2.49	0.40
1:A:324:GLU:O	1:A:326:GLU:HG3	2.21	0.40
1:B:358:LEU:O	1:B:359:ASP:C	2.60	0.40
1:B:67:TYR:CE2	1:D:367:VAL:HG11	2.56	0.40
1:C:347:ILE:HG12	1:C:385:PHE:HB3	2.03	0.40
1:A:299:GLU:HA	1:A:333:CYS:O	2.22	0.40
1:C:79:LYS:HE3	4:C:1073:HOH:O	2.21	0.40
1:B:39:THR:HG22	1:B:41:ARG:N	2.17	0.40
1:B:146:HIS:O	1:B:148:ARG:HG2	2.22	0.40
1:D:226:PHE:O	1:D:310:VAL:HA	2.21	0.40
1:A:106:ARG:HD3	4:A:1120:HOH:O	2.21	0.40
1:C:224:TYR:O	1:C:312:ALA:HA	2.22	0.40
1:A:224:TYR:O	1:A:312:ALA:HA	2.22	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	390/414 (94%)	361 (93%)	24 (6%)	5 (1%)	15 26
1	B	384/414 (93%)	351 (91%)	27 (7%)	6 (2%)	12 21
1	C	390/414 (94%)	358 (92%)	22 (6%)	10 (3%)	7 10
1	D	394/414 (95%)	365 (93%)	23 (6%)	6 (2%)	13 22
All	All	1558/1656 (94%)	1435 (92%)	96 (6%)	27 (2%)	11 19

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	ARG
1	B	148	ARG
1	C	92	HIS
1	C	148	ARG
1	C	149	THR
1	C	408	VAL
1	D	128	ASP
1	A	20	ALA
1	B	125	ASN
1	B	289	THR
1	B	408	VAL
1	C	114	ASP
1	C	127	ILE
1	C	158	ASP
1	C	281	GLU
1	D	127	ILE
1	D	147	SER
1	D	148	ARG
1	A	21	SER
1	B	149	THR
1	C	409	ASN
1	D	158	ASP
1	A	127	ILE
1	A	147	SER
1	D	161	MET
1	B	127	ILE
1	C	162	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	341/361 (94%)	313 (92%)	28 (8%)	14	27
1	B	337/361 (93%)	310 (92%)	27 (8%)	15	28
1	C	341/361 (94%)	321 (94%)	20 (6%)	24	44
1	D	344/361 (95%)	319 (93%)	25 (7%)	17	32
All	All	1363/1444 (94%)	1263 (93%)	100 (7%)	17	32

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	SER
1	A	69	LYS
1	A	74	GLN
1	A	81	MET
1	A	84	LEU
1	A	86	SER
1	A	99	ASP
1	A	106	ARG
1	A	116	ASP
1	A	118	LYS
1	A	127	ILE
1	A	135	LYS
1	A	146	HIS
1	A	158	ASP
1	A	160	SER
1	A	161	MET
1	A	199	SER
1	A	209	ARG
1	A	259	ARG
1	A	283	LEU
1	A	291	ASP
1	A	293	ASP
1	A	299	GLU
1	A	334	ILE

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Mol	Chain	Res	Type
1	A	337	SER
1	A	345	ARG
1	A	372	GLN
1	A	409	ASN
1	B	29	VAL
1	B	30	SER
1	B	33	HIS
1	B	39	THR
1	B	84	LEU
1	B	96	LEU
1	B	99	ASP
1	B	106	ARG
1	B	125	ASN
1	B	127	ILE
1	B	128	ASP
1	B	146	HIS
1	B	151	CYS
1	B	165	GLN
1	B	173	LYS
1	B	192	THR
1	B	223	ARG
1	B	245	SER
1	B	259	ARG
1	B	280	THR
1	B	291	ASP
1	B	295	VAL
1	B	299	GLU
1	B	335	SER
1	B	396	ASP
1	B	397	GLU
1	B	407	LYS
1	C	39	THR
1	C	62	LEU
1	C	81	MET
1	C	116	ASP
1	C	120	MET
1	C	121	LYS
1	C	135	LYS
1	C	146	HIS
1	C	148	ARG
1	C	161	MET
1	C	178	THR

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Mol	Chain	Res	Type
1	C	191	GLU
1	C	194	ARG
1	C	262	LYS
1	C	289	THR
1	C	299	GLU
1	C	306	LYS
1	C	334	ILE
1	C	396	ASP
1	C	401	MET
1	D	18	ASP
1	D	19	LEU
1	D	35	THR
1	D	39	THR
1	D	62	LEU
1	D	99	ASP
1	D	120	MET
1	D	125	ASN
1	D	127	ILE
1	D	128	ASP
1	D	135	LYS
1	D	146	HIS
1	D	148	ARG
1	D	162	PRO
1	D	173	LYS
1	D	194	ARG
1	D	209	ARG
1	D	250	LYS
1	D	253	ILE
1	D	259	ARG
1	D	281	GLU
1	D	289	THR
1	D	295	VAL
1	D	299	GLU
1	D	345	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	GLN
1	A	130	HIS
1	A	165	GLN
1	A	166	GLN

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Mol	Chain	Res	Type
1	A	171	HIS
1	A	197	GLN
1	A	304	GLN
1	A	409	ASN
1	B	125	ASN
1	B	146	HIS
1	B	166	GLN
1	B	197	GLN
1	B	269	ASN
1	B	409	ASN
1	C	92	HIS
1	C	130	HIS
1	C	143	HIS
1	C	166	GLN
1	C	247	ASN
1	C	404	ASN
1	D	125	ASN
1	D	143	HIS
1	D	166	GLN
1	D	269	ASN
1	D	304	GLN
1	D	404	ASN
1	D	409	ASN

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

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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	901	-	3,12,12	0.58	0	3,17,17	0.42	0
2	CIT	B	901	-	3,12,12	0.45	0	3,17,17	0.51	0
2	CIT	C	901	-	3,12,12	0.68	0	3,17,17	0.40	0
2	CIT	D	901	-	3,12,12	0.36	0	3,17,17	0.68	0

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	901	-	-	0/6/16/16	0/0/0/0
2	CIT	B	901	-	-	0/6/16/16	0/0/0/0
2	CIT	C	901	-	-	0/6/16/16	0/0/0/0
2	CIT	D	901	-	-	0/6/16/16	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	CIT	1	0
2	B	901	CIT	3	0
2	C	901	CIT	1	0
2	D	901	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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	392/414 (94%)	0.04	17 (4%)	39	44	25, 48, 86, 106	0
1	B	388/414 (93%)	-0.02	26 (6%)	21	23	27, 42, 86, 111	0
1	C	392/414 (94%)	0.00	20 (5%)	32	36	26, 47, 95, 119	0
1	D	396/414 (95%)	0.08	24 (6%)	25	27	26, 44, 87, 106	0
All	All	1568/1656 (94%)	0.03	87 (5%)	29	32	25, 45, 90, 119	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	149	THR	9.9
1	B	287	GLY	9.0
1	D	149	THR	8.2
1	A	147	SER	7.5
1	A	286	ALA	6.9
1	C	146	HIS	6.8
1	B	288	VAL	6.8
1	A	408	VAL	6.8
1	B	286	ALA	6.7
1	B	289	THR	5.9
1	B	148	ARG	5.8
1	B	45	ALA	5.6
1	D	147	SER	5.5
1	B	149	THR	5.2
1	B	285	GLU	5.1
1	B	152	PHE	5.0
1	B	44	GLU	5.0
1	D	127	ILE	5.0
1	B	46	ASP	4.9
1	C	148	ARG	4.9
1	C	149	THR	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	43	SER	4.7
1	D	32	LEU	4.6
1	C	46	ASP	4.6
1	D	412	GLY	4.6
1	D	146	HIS	4.5
1	B	145	VAL	4.4
1	D	17	GLN	4.4
1	D	148	ARG	4.4
1	B	124	ILE	4.3
1	B	147	SER	4.3
1	C	44	GLU	4.3
1	A	284	PHE	4.2
1	B	125	ASN	4.2
1	D	33	HIS	4.0
1	C	47	VAL	4.0
1	D	31	ALA	3.9
1	B	146	HIS	3.9
1	A	18	ASP	3.9
1	C	127	ILE	3.8
1	C	411	ARG	3.7
1	A	148	ARG	3.5
1	C	43	SER	3.4
1	A	218	ALA	3.3
1	D	410	LYS	3.3
1	A	146	HIS	3.2
1	C	147	SER	3.2
1	B	290	GLY	3.2
1	C	163	TYR	3.1
1	D	18	ASP	3.1
1	D	411	ARG	3.1
1	B	127	ILE	3.0
1	A	285	GLU	3.0
1	A	127	ILE	2.9
1	B	407	LYS	2.9
1	C	410	LYS	2.9
1	D	46	ASP	2.8
1	C	409	ASN	2.8
1	C	45	ALA	2.7
1	D	29	VAL	2.7
1	B	280	THR	2.6
1	D	150	LYS	2.6
1	D	30	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	162	PRO	2.6
1	A	288	VAL	2.6
1	A	283	LEU	2.5
1	B	119	ALA	2.5
1	A	345	ARG	2.4
1	D	28	PRO	2.4
1	B	277	TRP	2.4
1	A	407	LYS	2.4
1	B	126	ALA	2.4
1	D	288	VAL	2.4
1	C	93	LEU	2.3
1	C	123	GLU	2.3
1	D	163	TYR	2.2
1	D	159	PHE	2.2
1	A	19	LEU	2.2
1	C	283	LEU	2.2
1	A	409	ASN	2.2
1	B	291	ASP	2.1
1	B	408	VAL	2.1
1	C	29	VAL	2.1
1	D	408	VAL	2.1
1	D	112	MET	2.1
1	D	152	PHE	2.0
1	C	145	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	MG	C	902	1/1	0.88	0.27	7.29	49,49,49,49	0
2	CIT	C	901	13/13	0.82	0.25	5.19	108,108,110,111	0
2	CIT	B	901	13/13	0.89	0.24	4.18	87,90,93,93	0
3	MG	A	902	1/1	0.94	0.33	3.51	49,49,49,49	0
2	CIT	D	901	13/13	0.88	0.22	1.82	104,106,106,106	0
2	CIT	A	901	13/13	0.85	0.23	1.78	107,108,111,111	0
3	MG	B	902	1/1	0.90	0.12	-0.99	59,59,59,59	0
3	MG	D	902	1/1	0.83	0.27	-	49,49,49,49	0

6.5 Other polymers (i)

There are no such residues in this entry.