Full wwPDB X-ray Structure Validation Report (i)

Aug 21, 2023 – 10:43 AM EDT

PDB ID	:	2PVC
Title	:	DNMT3L recognizes unmethylated histone H3 lysine 4
Authors	:	Cheng, X.
Deposited on	:	2007-05-09
Resolution	:	3.69 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 (1)) were used in the production of this report:

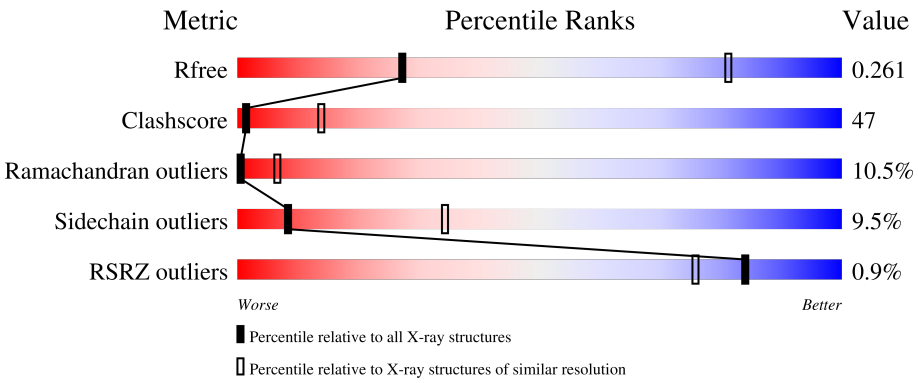
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 3.69 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	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)

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 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	386	34% 44% 11% • 10%
1	B	386	% 33% 45% 10% • 10%
1	C	386	% 34% 44% 11% • 10%
2	D	7	71% 29%
2	E	7	71% 29%

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Mol	Chain	Length	Quality of chain
2	F	7	71% 29%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8526 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 DNA (cytosine-5)-methyltransferase 3-like.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	347	2785	1780	477	507	21	0	0	0
1	A	347	2785	1780	477	507	21	0	0	0
1	C	347	2785	1780	477	507	21	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	278	GLY	ARG	conflict	UNP Q9UJW3
B	?	-	SER	deletion	UNP Q9UJW3
A	278	GLY	ARG	conflict	UNP Q9UJW3
A	?	-	SER	deletion	UNP Q9UJW3
C	278	GLY	ARG	conflict	UNP Q9UJW3
C	?	-	SER	deletion	UNP Q9UJW3

- Molecule 2 is a protein called Histone H3 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	D	7	54	31	12	11	0	0	0
2	E	7	54	31	12	11	0	0	0
2	F	7	54	31	12	11	0	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	B	3	3	3	0	0

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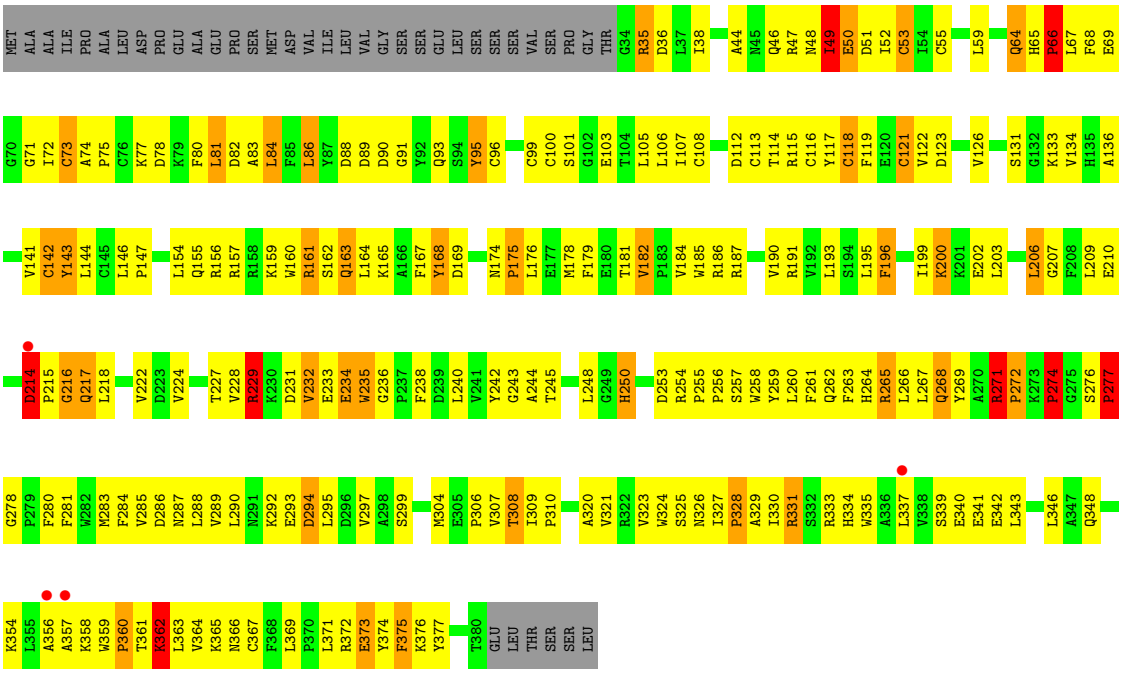
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	3	3	3	0	0
			Total	Zn		
3	C	3	3	3	0	0

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.

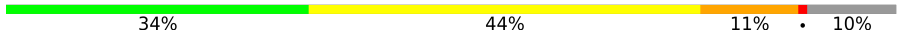
• Molecule 1: DNA (cytosine-5)-methyltransferase 3-like

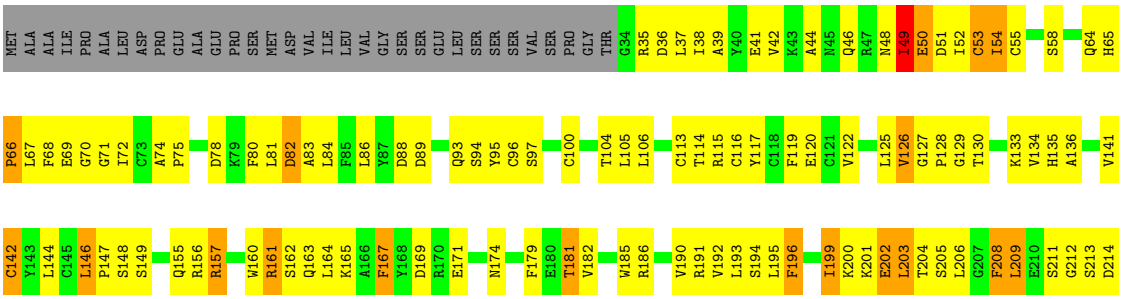
Chain B:

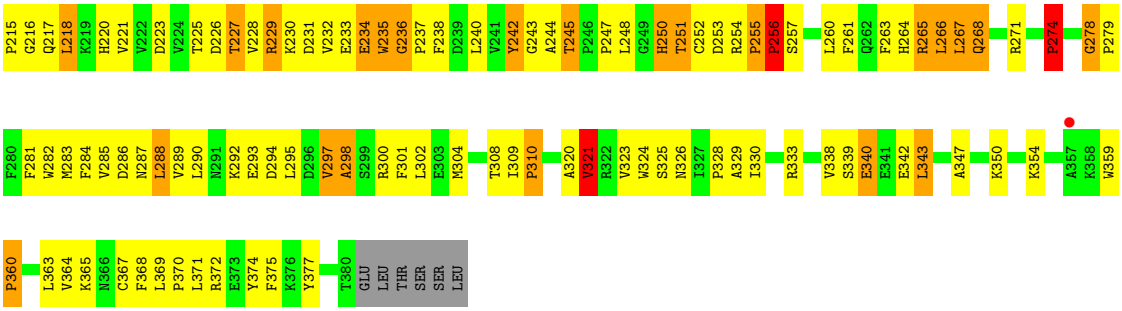


• Molecule 1: DNA (cytosine-5)-methyltransferase 3-like

Chain A:

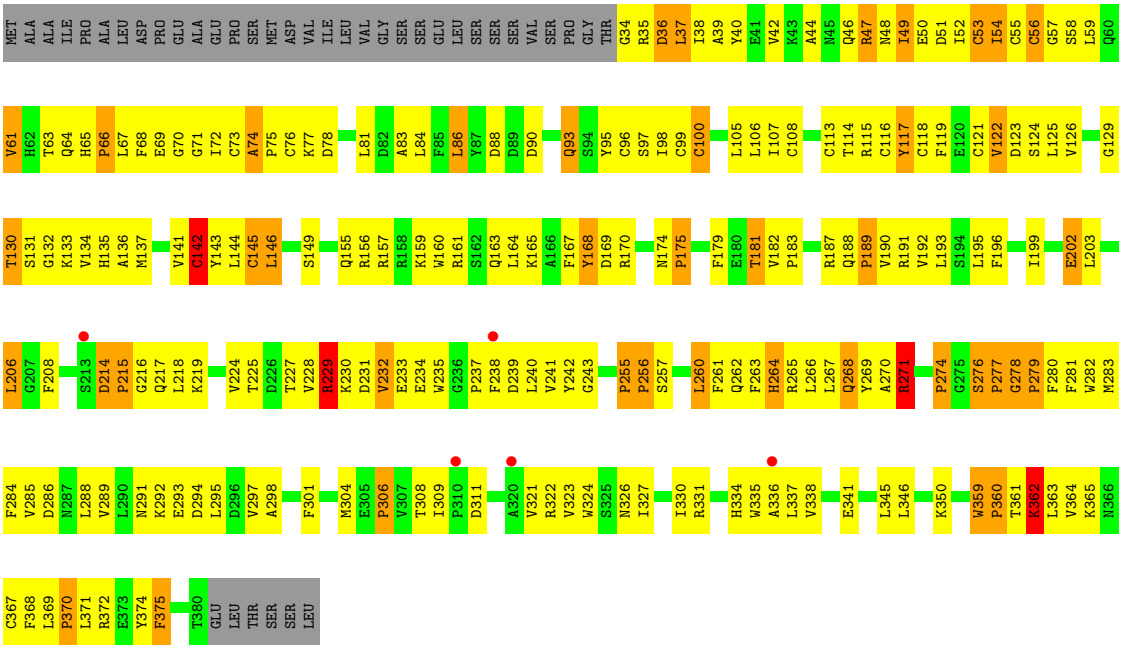






- Molecule 1: DNA (cytosine-5)-methyltransferase 3-like

Chain C:



- Molecule 2: Histone H3 peptide

Chain D:

- Molecule 2: Histone H3 peptide

Chain E:

- Molecule 2: Histone H3 peptide

Chain F:

A501
K504
A507

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	267.70Å 267.70Å 150.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.41 – 3.69 34.41 – 3.70	Depositor EDS
% Data completeness (in resolution range)	88.4 (34.41-3.69) 88.4 (34.41-3.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.98 (at 3.66Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.264 , 0.302 0.240 , 0.261	Depositor DCC
R_{free} test set	1513 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	142.1	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 112.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.55$, $< L^2 > = 0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8526	wwPDB-VP
Average B, all atoms (Å^2)	136.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% 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, 0.333 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: ZN

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	0.45	0/2863	0.69	0/3888
1	B	0.45	0/2863	0.73	0/3888
1	C	0.36	0/2863	0.60	0/3888
2	D	0.50	0/53	0.68	0/68
2	E	0.41	0/53	0.48	0/68
2	F	0.35	0/53	0.50	0/68
All	All	0.42	0/8748	0.67	0/11868

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	143	TYR	Sidechain

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	2785	0	2711	245	1
1	B	2785	0	2711	273	0
1	C	2785	0	2717	286	0
2	D	54	0	57	2	0
2	E	54	0	57	2	0
2	F	54	0	57	2	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
All	All	8526	0	8310	795	1

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 47.

All (795) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:LYS:H	1:B:362:LYS:HD2	1.12	1.11
1:B:64:GLN:HB2	1:B:157:ARG:HH22	1.18	1.08
1:B:107:ILE:HG12	1:B:116:CYS:SG	1.99	1.02
1:A:242:TYR:HD2	1:A:243:GLY:N	1.57	1.02
1:C:69:GLU:HB3	1:C:155:GLN:HB3	1.41	1.00
1:C:214:ASP:HB2	1:C:215:PRO:HD3	1.45	0.96
1:A:268:GLN:H	1:A:268:GLN:HE21	1.14	0.95
1:A:260:LEU:HD21	1:A:302:LEU:HD11	1.49	0.95
1:B:185:TRP:HD1	1:B:186:ARG:HG2	1.32	0.95
1:C:286:ASP:HB3	1:C:322:ARG:HB2	1.46	0.94
1:C:192:VAL:HG22	1:C:240:LEU:HB3	1.49	0.94
1:C:67:LEU:HD12	1:C:67:LEU:H	1.34	0.91
1:B:325:SER:OG	1:B:327:ILE:HG13	1.70	0.91
1:A:74:ALA:HB3	1:A:75:PRO:HD3	1.53	0.90
1:B:245:THR:HG21	1:B:290:LEU:HD11	1.53	0.90
1:B:159:LYS:HA	1:B:159:LYS:HE2	1.51	0.90
1:C:159:LYS:HE2	1:C:159:LYS:HA	1.54	0.90
1:B:74:ALA:HB3	1:B:75:PRO:HD3	1.53	0.89
1:B:268:GLN:H	1:B:268:GLN:HE21	1.13	0.88
1:C:49:ILE:HD13	1:C:49:ILE:H	1.37	0.87
1:A:49:ILE:HD13	1:A:49:ILE:H	1.40	0.86
1:B:165:LYS:HG3	1:B:178:MET:HG3	1.57	0.86
1:C:74:ALA:HB3	1:C:75:PRO:HD3	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:362:LYS:H	1:C:362:LYS:HD2	1.41	0.86
1:A:214:ASP:HB2	1:A:215:PRO:HD3	1.56	0.85
1:C:268:GLN:H	1:C:268:GLN:HE21	1.22	0.85
1:B:67:LEU:HD12	1:B:67:LEU:H	1.42	0.84
1:B:69:GLU:HB3	1:B:155:GLN:HB3	1.59	0.84
1:B:49:ILE:HD13	1:B:49:ILE:H	1.42	0.84
1:A:242:TYR:CD2	1:A:243:GLY:N	2.46	0.83
1:A:67:LEU:HD12	1:A:67:LEU:H	1.43	0.83
1:B:35:ARG:O	1:B:38:ILE:HG22	1.78	0.83
1:A:129:GLY:HA2	1:C:123:ASP:OD2	1.80	0.82
1:B:64:GLN:HB2	1:B:157:ARG:NH2	1.93	0.81
1:B:285:VAL:HG22	1:B:323:VAL:HG22	1.62	0.81
1:B:185:TRP:CD1	1:B:186:ARG:HG2	2.14	0.81
1:B:66:PRO:HB2	1:B:67:LEU:HD12	1.63	0.81
1:A:202:GLU:CD	1:A:202:GLU:H	1.84	0.80
1:B:292:LYS:HG3	1:B:293:GLU:N	1.96	0.80
1:C:93:GLN:HG2	1:C:114:THR:O	1.82	0.80
1:C:35:ARG:HH22	1:C:99:CYS:HB3	1.46	0.79
1:B:362:LYS:HD2	1:B:362:LYS:N	1.96	0.79
1:C:96:CYS:HB3	1:C:100:CYS:H	1.47	0.79
1:B:65:HIS:ND1	1:B:72:ILE:HD11	1.98	0.79
1:A:144:LEU:HA	1:A:156:ARG:HD3	1.65	0.79
1:B:362:LYS:H	1:B:362:LYS:CD	1.95	0.78
1:B:81:LEU:HD11	1:B:167:PHE:HE2	1.49	0.78
1:C:240:LEU:HA	1:C:281:PHE:O	1.83	0.78
1:C:225:THR:N	1:C:262:GLN:HE22	1.82	0.78
1:B:292:LYS:HG3	1:B:293:GLU:H	1.47	0.77
1:B:65:HIS:HD2	1:B:68:PHE:H	1.32	0.77
1:B:182:VAL:HG23	1:B:374:TYR:HA	1.67	0.77
1:C:229:ARG:O	1:C:229:ARG:HG3	1.80	0.77
1:B:193:LEU:HB2	1:B:238:PHE:CE1	2.19	0.77
1:A:266:LEU:HD12	1:A:266:LEU:H	1.50	0.77
1:A:268:GLN:HE21	1:A:268:GLN:N	1.83	0.77
1:C:285:VAL:HG22	1:C:323:VAL:HG22	1.68	0.76
1:C:49:ILE:HG13	1:C:69:GLU:HG2	1.67	0.76
1:C:93:GLN:HG3	1:C:115:ARG:HA	1.66	0.76
1:A:228:VAL:O	1:A:231:ASP:HB2	1.86	0.76
1:C:35:ARG:NH2	1:C:121:CYS:SG	2.59	0.75
1:C:268:GLN:H	1:C:268:GLN:NE2	1.84	0.75
1:B:81:LEU:CD1	1:B:167:PHE:HE2	2.00	0.75
1:A:88:ASP:OD2	1:A:94:SER:HA	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:CYS:O	1:C:146:LEU:HD22	1.87	0.74
1:C:224:VAL:HG23	1:C:262:GLN:NE2	2.03	0.74
1:B:65:HIS:CD2	1:B:68:PHE:H	2.05	0.74
1:A:53:CYS:SG	1:A:55:CYS:HB2	2.27	0.74
1:A:67:LEU:HD23	1:A:144:LEU:HD11	1.68	0.74
1:C:96:CYS:H	1:C:100:CYS:HA	1.52	0.74
1:B:164:LEU:O	1:B:167:PHE:HB3	1.88	0.74
1:B:214:ASP:HB2	1:B:215:PRO:HD3	1.69	0.74
1:B:93:GLN:NE2	1:B:115:ARG:HG2	2.02	0.74
1:A:49:ILE:HD13	1:A:49:ILE:N	2.02	0.73
1:A:320:ALA:O	1:A:321:VAL:HG23	1.88	0.73
1:B:187:ARG:O	1:B:376:LYS:HB2	1.89	0.73
1:B:268:GLN:H	1:B:268:GLN:NE2	1.85	0.73
1:B:289:VAL:HG13	1:B:290:LEU:HD12	1.71	0.73
1:A:193:LEU:HB2	1:A:238:PHE:CZ	2.23	0.73
1:B:106:LEU:HD13	1:B:134:VAL:HG11	1.70	0.72
1:B:123:ASP:OD2	1:B:131:SER:HB3	1.89	0.72
1:A:285:VAL:HG22	1:A:323:VAL:HG22	1.69	0.72
1:B:268:GLN:HE21	1:B:268:GLN:N	1.86	0.72
1:A:191:ARG:NH1	1:A:237:PRO:HG2	2.04	0.72
1:C:72:ILE:HG22	1:C:73:CYS:N	2.05	0.71
1:B:202:GLU:OE1	1:B:361:THR:HG21	1.90	0.71
1:B:117:TYR:CE2	1:B:142:CYS:HB2	2.25	0.71
1:C:99:CYS:O	1:C:100:CYS:HB2	1.88	0.71
1:A:298:ALA:O	1:A:302:LEU:HD12	1.91	0.70
1:A:199:ILE:HG22	1:A:199:ILE:O	1.90	0.70
1:C:362:LYS:HD2	1:C:362:LYS:N	2.05	0.70
1:A:54:ILE:HG22	1:A:125:LEU:HD21	1.74	0.70
1:B:69:GLU:CB	1:B:155:GLN:HB3	2.21	0.70
1:B:274:PRO:HB3	1:A:274:PRO:HB3	1.73	0.70
1:A:67:LEU:HD12	1:A:67:LEU:N	2.06	0.70
1:C:195:LEU:HD12	1:C:263:PHE:HD1	1.54	0.70
1:A:54:ILE:CD1	1:A:70:GLY:HA3	2.21	0.70
1:C:130:THR:O	1:C:134:VAL:HG23	1.92	0.70
1:C:311:ASP:HB2	1:C:363:LEU:HD11	1.74	0.70
1:A:242:TYR:OH	1:A:359:TRP:CH2	2.45	0.69
1:C:35:ARG:HH22	1:C:99:CYS:CB	2.04	0.69
1:A:309:ILE:HD11	1:A:363:LEU:HB3	1.74	0.69
1:B:306:PRO:HG3	1:B:324:TRP:CZ2	2.28	0.69
1:A:190:VAL:HB	1:A:375:PHE:HD1	1.58	0.68
1:C:224:VAL:HG23	1:C:262:GLN:CD	2.13	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:LEU:N	1:B:86:LEU:CD2	2.56	0.68
1:C:191:ARG:HB2	1:C:239:ASP:OD1	1.93	0.68
1:B:190:VAL:HB	1:B:375:PHE:HD1	1.58	0.68
1:C:95:TYR:HB3	1:C:100:CYS:HA	1.75	0.68
1:A:245:THR:HG23	1:A:286:ASP:HA	1.76	0.68
1:A:289:VAL:HG13	1:A:290:LEU:HD12	1.76	0.68
1:C:228:VAL:HG12	1:C:229:ARG:N	2.09	0.68
1:C:113:CYS:HB2	1:C:145:CYS:SG	2.33	0.68
1:C:83:ALA:HA	1:C:86:LEU:CD2	2.24	0.68
1:B:66:PRO:O	1:B:157:ARG:HG3	1.94	0.67
1:B:260:LEU:C	1:B:260:LEU:HD13	2.15	0.67
1:C:69:GLU:CB	1:C:155:GLN:HB3	2.21	0.67
1:A:81:LEU:HD12	1:A:81:LEU:H	1.60	0.67
1:B:133:LYS:O	1:B:136:ALA:HB3	1.93	0.67
1:B:375:PHE:HD2	1:B:375:PHE:N	1.93	0.67
1:B:335:TRP:C	1:B:337:LEU:H	1.97	0.67
1:C:38:ILE:HG13	1:C:39:ALA:N	2.10	0.67
1:B:53:CYS:SG	1:B:55:CYS:HB2	2.35	0.66
1:C:55:CYS:HB3	1:C:76:CYS:SG	2.34	0.66
1:C:35:ARG:NH2	1:C:99:CYS:HB3	2.08	0.66
1:C:260:LEU:HD11	1:C:298:ALA:CA	2.25	0.66
1:B:199:ILE:CG2	1:B:203:LEU:HG	2.25	0.66
1:C:304:MET:HG3	1:C:324:TRP:HD1	1.60	0.66
1:A:66:PRO:O	1:A:157:ARG:HG3	1.95	0.66
1:B:375:PHE:N	1:B:375:PHE:CD2	2.62	0.66
1:A:35:ARG:O	1:A:38:ILE:HG12	1.94	0.66
1:A:260:LEU:HD13	1:A:260:LEU:C	2.16	0.66
1:A:147:PRO:HA	1:A:156:ARG:NH2	2.11	0.66
1:B:175:PRO:O	1:B:176:LEU:HD23	1.95	0.65
1:C:117:TYR:OH	1:C:142:CYS:SG	2.55	0.65
1:B:66:PRO:HG2	1:B:80:PHE:CE1	2.30	0.65
1:C:192:VAL:CG2	1:C:240:LEU:HB3	2.25	0.65
1:B:35:ARG:O	1:B:38:ILE:CG2	2.44	0.65
1:A:64:GLN:HB2	1:A:157:ARG:NH2	2.12	0.65
1:C:285:VAL:HG13	1:C:321:VAL:HG13	1.79	0.65
1:B:93:GLN:HE22	1:B:115:ARG:HG2	1.61	0.64
1:B:265:ARG:HD2	1:A:301:PHE:CD1	2.33	0.64
1:B:99:CYS:HB3	1:B:121:CYS:SG	2.36	0.64
1:B:199:ILE:HD11	1:B:242:TYR:CE2	2.32	0.64
1:A:244:ALA:HA	1:A:284:PHE:CE1	2.32	0.64
1:A:330:ILE:HD11	1:A:367:CYS:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:VAL:HG12	1:C:229:ARG:H	1.62	0.64
1:B:144:LEU:HD23	1:B:156:ARG:HD3	1.80	0.64
1:C:49:ILE:HD13	1:C:49:ILE:N	2.11	0.64
1:C:367:CYS:O	1:C:370:PRO:HD2	1.98	0.64
1:B:240:LEU:HD12	1:B:281:PHE:O	1.99	0.63
1:A:119:PHE:CE2	1:C:132:GLY:HA3	2.33	0.63
1:C:37:LEU:HD12	1:C:37:LEU:H	1.62	0.63
1:B:67:LEU:HD12	1:B:67:LEU:N	2.13	0.63
1:C:203:LEU:HD21	1:C:368:PHE:HD1	1.62	0.63
1:A:243:GLY:O	1:A:284:PHE:HD1	1.81	0.63
1:C:224:VAL:HB	1:C:266:LEU:HD11	1.80	0.63
1:A:229:ARG:HG3	1:A:233:GLU:HG3	1.80	0.63
1:A:93:GLN:HE22	1:A:115:ARG:CZ	2.12	0.63
1:A:54:ILE:HD13	1:A:70:GLY:HA3	1.81	0.63
1:C:55:CYS:SG	1:C:99:CYS:HA	2.39	0.62
1:C:93:GLN:CG	1:C:115:ARG:HA	2.28	0.62
1:A:160:TRP:O	1:A:163:GLN:N	2.33	0.62
1:B:168:TYR:HD1	1:B:168:TYR:C	2.03	0.62
1:C:190:VAL:HG23	1:C:375:PHE:CD1	2.34	0.62
1:C:346:LEU:HD11	1:C:350:LYS:NZ	2.14	0.62
1:C:288:LEU:HD23	1:C:322:ARG:HE	1.63	0.62
1:A:196:PHE:N	1:A:196:PHE:CD2	2.65	0.62
1:C:369:LEU:O	1:C:372:ARG:N	2.30	0.62
1:B:168:TYR:C	1:B:168:TYR:CD1	2.74	0.61
1:B:184:VAL:HA	1:B:187:ARG:HE	1.65	0.61
1:C:192:VAL:HG13	1:C:240:LEU:O	2.00	0.61
1:A:66:PRO:HB2	1:A:67:LEU:HD12	1.82	0.61
1:A:230:LYS:O	1:A:234:GLU:HB2	2.00	0.61
1:A:295:LEU:HD23	1:A:295:LEU:C	2.21	0.61
1:C:327:ILE:HG23	1:C:371:LEU:HD21	1.83	0.61
1:B:83:ALA:HA	1:B:86:LEU:HD21	1.80	0.61
1:A:193:LEU:HD22	1:A:238:PHE:CE1	2.36	0.61
1:A:248:LEU:N	1:A:248:LEU:HD22	2.16	0.61
1:A:271:ARG:HG3	1:A:271:ARG:HH11	1.65	0.61
1:A:374:TYR:C	1:A:375:PHE:HD2	2.03	0.61
1:C:53:CYS:C	1:C:55:CYS:H	2.04	0.61
1:A:164:LEU:O	1:A:167:PHE:HB3	2.01	0.61
1:B:81:LEU:HD11	1:B:167:PHE:CE2	2.32	0.61
1:B:264:HIS:O	1:B:268:GLN:NE2	2.34	0.61
1:C:294:ASP:O	1:C:297:VAL:HB	2.00	0.61
1:B:190:VAL:HG23	1:B:375:PHE:CE1	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:LEU:HD11	1:B:320:ALA:HB3	1.82	0.61
1:B:343:LEU:HD22	1:B:343:LEU:H	1.65	0.60
1:A:185:TRP:CD1	1:A:186:ARG:HG2	2.35	0.60
1:B:181:THR:HA	1:B:374:TYR:CE2	2.36	0.60
1:B:276:SER:OG	1:B:277:PRO:HD2	2.00	0.60
1:A:268:GLN:H	1:A:268:GLN:NE2	1.91	0.60
1:A:67:LEU:H	1:A:67:LEU:CD1	2.14	0.60
1:A:242:TYR:HD2	1:A:242:TYR:C	2.04	0.60
1:C:190:VAL:HG23	1:C:375:PHE:HD1	1.65	0.60
1:C:142:CYS:SG	1:C:145:CYS:HB2	2.41	0.60
1:C:284:PHE:HD2	1:C:324:TRP:CE3	2.20	0.60
1:B:374:TYR:C	1:B:375:PHE:HD2	2.05	0.60
1:A:266:LEU:H	1:A:266:LEU:CD1	2.15	0.60
1:A:368:PHE:C	1:A:370:PRO:HD2	2.21	0.60
1:C:271:ARG:HG3	1:C:271:ARG:HH11	1.66	0.60
1:C:183:PRO:O	1:C:187:ARG:HG3	2.02	0.60
1:B:271:ARG:HG3	1:B:271:ARG:HH11	1.65	0.60
1:C:65:HIS:ND1	1:C:72:ILE:HD11	2.16	0.60
1:B:190:VAL:CB	1:B:375:PHE:HD1	2.15	0.60
1:B:48:ASN:O	1:B:50:GLU:N	2.34	0.60
1:B:335:TRP:C	1:B:337:LEU:N	2.55	0.60
1:C:53:CYS:HB3	1:C:58:SER:H	1.66	0.59
1:B:199:ILE:HD11	1:B:242:TYR:CZ	2.37	0.59
1:C:81:LEU:H	1:C:81:LEU:HD12	1.66	0.59
1:C:95:TYR:HB3	1:C:100:CYS:CA	2.32	0.59
1:C:268:GLN:NE2	1:C:268:GLN:N	2.49	0.59
1:A:297:VAL:O	1:A:300:ARG:N	2.23	0.59
1:A:201:LYS:O	1:A:204:THR:HB	2.02	0.59
1:A:268:GLN:N	1:A:268:GLN:NE2	2.49	0.59
1:B:122:VAL:O	1:B:126:VAL:HG23	2.02	0.59
1:B:274:PRO:HB3	1:A:274:PRO:CB	2.32	0.59
1:A:374:TYR:O	1:A:375:PHE:HD2	1.86	0.59
1:B:306:PRO:HG3	1:B:324:TRP:CE2	2.38	0.59
1:C:72:ILE:CG2	1:C:73:CYS:N	2.64	0.59
1:A:54:ILE:HG12	1:A:71:GLY:H	1.68	0.59
1:A:67:LEU:HD23	1:A:144:LEU:CD1	2.33	0.59
1:C:49:ILE:H	1:C:49:ILE:CD1	2.14	0.59
1:C:263:PHE:C	1:C:265:ARG:H	2.07	0.58
1:A:105:LEU:O	2:E:503:THR:HA	2.02	0.58
1:C:278:GLY:H	1:C:279:PRO:CD	2.16	0.58
1:B:115:ARG:HD3	1:B:144:LEU:HD12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:GLU:O	1:A:204:THR:N	2.36	0.58
1:C:96:CYS:SG	1:C:117:TYR:HA	2.44	0.58
1:A:119:PHE:CD2	1:C:132:GLY:HA3	2.39	0.58
1:B:144:LEU:HA	1:B:156:ARG:HD3	1.86	0.58
1:B:224:VAL:HG21	1:B:266:LEU:HD11	1.86	0.58
1:B:268:GLN:NE2	1:B:268:GLN:N	2.49	0.58
1:A:192:VAL:HG21	1:A:203:LEU:HD13	1.84	0.58
1:C:270:ALA:O	1:C:271:ARG:O	2.21	0.58
1:B:364:VAL:HA	1:B:367:CYS:SG	2.44	0.58
1:B:107:ILE:CG2	1:B:108:CYS:N	2.67	0.58
1:B:240:LEU:HA	1:B:281:PHE:O	2.04	0.58
1:B:248:LEU:N	1:B:248:LEU:HD22	2.19	0.58
1:B:287:ASN:ND2	1:B:360:PRO:HD2	2.19	0.58
1:B:281:PHE:HA	1:B:326:ASN:HD21	1.68	0.57
1:A:265:ARG:O	1:A:267:LEU:N	2.37	0.57
1:C:228:VAL:C	1:C:230:LYS:H	2.07	0.57
1:B:84:LEU:HD11	1:B:164:LEU:HD21	1.85	0.57
1:A:253:ASP:O	1:A:254:ARG:HG3	2.04	0.57
1:A:127:GLY:O	1:A:130:THR:HG23	2.04	0.57
1:A:374:TYR:C	1:A:375:PHE:CD2	2.78	0.57
1:C:306:PRO:HG3	1:C:324:TRP:CZ2	2.40	0.57
1:C:106:LEU:HD13	1:C:134:VAL:HG11	1.86	0.57
1:B:95:TYR:CD2	1:B:95:TYR:N	2.72	0.57
1:C:54:ILE:O	1:C:54:ILE:HG13	2.03	0.57
1:C:98:ILE:HD12	1:C:98:ILE:N	2.19	0.57
1:C:362:LYS:H	1:C:362:LYS:CD	2.14	0.57
1:C:69:GLU:N	1:C:155:GLN:O	2.34	0.57
1:C:84:LEU:N	1:C:86:LEU:HD23	2.19	0.57
1:C:335:TRP:C	1:C:337:LEU:H	2.08	0.57
1:B:146:LEU:HD23	1:B:146:LEU:H	1.69	0.57
1:A:193:LEU:HB2	1:A:238:PHE:CE2	2.40	0.57
1:C:182:VAL:HG23	1:C:374:TYR:HD2	1.70	0.57
1:C:243:GLY:O	1:C:284:PHE:HA	2.04	0.57
1:B:48:ASN:O	1:B:51:ASP:N	2.38	0.57
1:B:117:TYR:CZ	1:B:142:CYS:HB2	2.40	0.57
1:B:234:GLU:C	1:B:236:GLY:H	2.08	0.57
1:B:278:GLY:O	1:B:280:PHE:N	2.38	0.57
1:B:141:VAL:O	1:B:142:CYS:O	2.23	0.57
1:B:214:ASP:CB	1:B:215:PRO:HD3	2.34	0.57
1:B:107:ILE:HG22	1:B:108:CYS:N	2.20	0.56
1:C:375:PHE:N	1:C:375:PHE:CD2	2.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:ALA:C	1:B:358:LYS:H	2.07	0.56
1:A:199:ILE:HG22	1:A:203:LEU:HG	1.87	0.56
1:C:72:ILE:CG2	1:C:73:CYS:H	2.18	0.56
1:A:122:VAL:HG12	1:A:130:THR:OG1	2.06	0.56
1:C:321:VAL:HG12	1:C:323:VAL:HG23	1.86	0.56
1:B:160:TRP:O	1:B:163:GLN:N	2.38	0.56
1:B:309:ILE:HG13	1:B:363:LEU:HD12	1.87	0.56
1:C:66:PRO:HB2	1:C:67:LEU:HD12	1.88	0.56
1:B:95:TYR:N	1:B:95:TYR:HD2	2.04	0.56
1:A:339:SER:HB3	1:A:342:GLU:CG	2.36	0.56
1:C:86:LEU:N	1:C:86:LEU:HD22	2.21	0.56
1:C:260:LEU:HD11	1:C:298:ALA:HA	1.87	0.56
1:A:251:THR:HG22	1:A:252:CYS:H	1.70	0.56
1:A:260:LEU:HD21	1:A:302:LEU:CD1	2.31	0.56
1:A:339:SER:HB3	1:A:342:GLU:CD	2.26	0.56
1:C:96:CYS:N	1:C:100:CYS:HA	2.20	0.56
1:C:262:GLN:O	1:C:266:LEU:HD12	2.06	0.56
1:A:266:LEU:HD12	1:A:266:LEU:N	2.20	0.56
1:B:105:LEU:HD23	1:B:118:CYS:HA	1.88	0.55
1:B:106:LEU:HD13	1:B:134:VAL:CG1	2.37	0.55
1:C:214:ASP:HB2	1:C:215:PRO:CD	2.29	0.55
1:B:118:CYS:O	1:B:122:VAL:HG23	2.05	0.55
1:B:196:PHE:CD2	1:B:196:PHE:N	2.73	0.55
1:A:228:VAL:HG12	1:A:229:ARG:N	2.20	0.55
1:A:243:GLY:O	1:A:284:PHE:HA	2.06	0.55
1:A:297:VAL:HG12	1:A:298:ALA:N	2.21	0.55
1:C:54:ILE:HG21	1:C:70:GLY:HA3	1.89	0.55
1:C:68:PHE:CZ	1:C:144:LEU:HD21	2.41	0.55
1:C:117:TYR:CE2	1:C:142:CYS:HB2	2.41	0.55
1:B:99:CYS:SG	1:B:101:SER:HB2	2.46	0.55
1:A:339:SER:O	1:A:342:GLU:HB2	2.06	0.55
1:A:242:TYR:CD2	1:A:242:TYR:C	2.77	0.55
1:B:83:ALA:HA	1:B:86:LEU:CD2	2.37	0.55
1:B:107:ILE:HG22	1:B:108:CYS:O	2.06	0.55
1:B:142:CYS:O	1:B:146:LEU:HD22	2.07	0.55
1:B:182:VAL:CG2	1:B:374:TYR:HA	2.37	0.55
1:B:143:TYR:HA	1:B:146:LEU:CD2	2.37	0.55
1:A:50:GLU:OE2	1:A:69:GLU:HG3	2.06	0.55
1:C:263:PHE:C	1:C:265:ARG:N	2.61	0.55
1:C:369:LEU:HB2	1:C:370:PRO:HD3	1.88	0.55
1:C:335:TRP:O	1:C:338:VAL:HG23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:375:PHE:N	1:C:375:PHE:HD2	2.03	0.55
1:B:74:ALA:HB3	1:B:75:PRO:CD	2.31	0.54
1:A:289:VAL:CG1	1:A:290:LEU:HD12	2.37	0.54
1:C:374:TYR:C	1:C:375:PHE:HD2	2.10	0.54
1:B:286:ASP:OD2	1:B:289:VAL:HG12	2.07	0.54
1:C:341:GLU:O	1:C:345:LEU:HG	2.08	0.54
1:B:67:LEU:HD23	1:B:144:LEU:HD11	1.88	0.54
1:C:192:VAL:O	1:C:218:LEU:HD12	2.08	0.54
1:B:320:ALA:O	1:B:321:VAL:HG23	2.08	0.54
1:B:165:LYS:NZ	1:B:178:MET:O	2.34	0.54
1:B:187:ARG:NH1	1:B:372:ARG:O	2.41	0.54
1:A:194:SER:HA	1:A:242:TYR:O	2.07	0.54
1:C:53:CYS:HB3	1:C:58:SER:N	2.23	0.54
1:C:291:ASN:O	1:C:293:GLU:N	2.41	0.54
1:C:361:THR:O	1:C:363:LEU:N	2.41	0.54
1:C:268:GLN:HE21	1:C:268:GLN:N	1.98	0.54
1:B:48:ASN:HB3	1:B:51:ASP:OD2	2.08	0.53
1:B:49:ILE:C	1:B:51:ASP:H	2.12	0.53
1:C:86:LEU:CD2	1:C:86:LEU:N	2.70	0.53
1:C:264:HIS:ND1	1:C:301:PHE:HB3	2.23	0.53
1:C:304:MET:HB2	1:C:331:ARG:NH2	2.23	0.53
1:A:363:LEU:H	1:A:363:LEU:CD2	2.20	0.53
1:C:81:LEU:HA	1:C:84:LEU:CG	2.39	0.53
1:A:80:PHE:HD2	1:A:100:CYS:SG	2.31	0.53
1:C:72:ILE:HG22	1:C:73:CYS:H	1.73	0.53
1:B:86:LEU:N	1:B:86:LEU:HD23	2.22	0.53
1:B:286:ASP:CG	1:B:290:LEU:HD13	2.28	0.53
1:C:263:PHE:O	1:C:265:ARG:N	2.42	0.53
1:B:266:LEU:O	1:B:269:TYR:HB2	2.09	0.53
1:A:192:VAL:O	1:A:218:LEU:HA	2.09	0.53
1:B:141:VAL:O	1:B:141:VAL:HG23	2.09	0.53
1:C:206:LEU:HD23	1:C:365:LYS:HG2	1.91	0.53
1:C:278:GLY:O	1:C:280:PHE:N	2.42	0.53
1:B:67:LEU:H	1:B:67:LEU:CD1	2.16	0.53
1:A:182:VAL:HG23	1:A:374:TYR:HD2	1.73	0.53
1:A:199:ILE:HG13	1:A:242:TYR:CD1	2.43	0.53
1:C:67:LEU:H	1:C:67:LEU:CD1	2.12	0.53
1:C:164:LEU:O	1:C:167:PHE:HB3	2.08	0.53
1:A:375:PHE:CD2	1:A:375:PHE:N	2.76	0.52
1:C:330:ILE:HG23	1:C:331:ARG:HD2	1.90	0.52
1:B:66:PRO:HG3	1:B:167:PHE:CD1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:GLU:O	1:B:236:GLY:N	2.42	0.52
1:A:294:ASP:O	1:A:297:VAL:HB	2.09	0.52
1:B:64:GLN:HA	1:B:71:GLY:HA2	1.91	0.52
1:C:74:ALA:HB3	1:C:75:PRO:CD	2.34	0.52
1:B:73:CYS:SG	1:B:75:PRO:HD2	2.49	0.52
1:B:81:LEU:O	1:B:83:ALA:N	2.43	0.52
1:A:202:GLU:HG2	1:A:203:LEU:H	1.74	0.52
1:A:257:SER:O	1:A:260:LEU:HB3	2.10	0.52
1:C:38:ILE:HD11	1:C:125:LEU:HD23	1.92	0.52
1:C:260:LEU:HD11	1:C:298:ALA:HB2	1.91	0.52
1:A:288:LEU:HD11	1:A:320:ALA:HB3	1.91	0.52
2:E:502:ARG:HG2	2:E:503:THR:H	1.74	0.52
1:B:65:HIS:HD2	1:B:68:PHE:N	2.06	0.52
2:D:506:THR:HG22	2:D:507:ALA:N	2.25	0.52
1:A:52:ILE:HG13	1:A:52:ILE:O	2.10	0.52
1:B:48:ASN:O	1:B:49:ILE:C	2.47	0.52
1:A:217:GLN:OE1	1:A:217:GLN:HA	2.10	0.52
1:A:245:THR:CG2	1:A:286:ASP:HA	2.40	0.52
1:C:227:THR:O	1:C:265:ARG:NH2	2.42	0.52
1:B:160:TRP:O	1:B:162:SER:N	2.43	0.52
1:C:59:LEU:HD12	1:C:59:LEU:N	2.25	0.52
1:B:195:LEU:HD13	1:B:266:LEU:HD13	1.91	0.52
1:A:363:LEU:CD2	1:A:363:LEU:N	2.73	0.52
1:C:35:ARG:O	1:C:124:SER:HB2	2.09	0.52
1:C:306:PRO:HG3	1:C:324:TRP:HE1	1.75	0.52
1:C:293:GLU:O	1:C:297:VAL:HG23	2.10	0.52
1:A:202:GLU:CD	1:A:202:GLU:N	2.59	0.51
1:B:86:LEU:HD23	1:B:86:LEU:H	1.75	0.51
1:B:333:ARG:HH12	1:B:366:ASN:HB2	1.74	0.51
1:B:160:TRP:O	1:B:161:ARG:C	2.49	0.51
1:B:199:ILE:O	1:B:200:LYS:C	2.49	0.51
1:B:248:LEU:HD22	1:B:248:LEU:H	1.74	0.51
1:C:38:ILE:O	1:C:42:VAL:HG23	2.09	0.51
1:C:309:ILE:O	1:C:309:ILE:HG13	2.11	0.51
1:A:136:ALA:HB2	1:C:135:HIS:CE1	2.46	0.51
1:C:284:PHE:HD2	1:C:324:TRP:HE3	1.58	0.51
1:A:38:ILE:HG22	1:A:52:ILE:HD12	1.92	0.51
1:B:248:LEU:H	1:B:248:LEU:CD2	2.24	0.51
1:C:68:PHE:HA	1:C:155:GLN:O	2.10	0.51
1:A:53:CYS:HA	1:A:71:GLY:O	2.10	0.51
1:C:65:HIS:HB3	1:C:70:GLY:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:TYR:CD2	1:C:117:TYR:N	2.79	0.51
1:B:191:ARG:HA	1:B:217:GLN:HB3	1.93	0.51
1:A:160:TRP:O	1:A:162:SER:N	2.44	0.51
1:C:369:LEU:O	1:C:371:LEU:N	2.43	0.51
1:A:368:PHE:O	1:A:370:PRO:HD2	2.10	0.51
1:C:361:THR:HB	1:C:362:LYS:HD2	1.93	0.51
1:C:367:CYS:C	1:C:369:LEU:H	2.14	0.51
1:B:77:LYS:HE3	1:B:78:ASP:OD2	2.11	0.51
1:B:207:GLY:HA3	1:B:377:TYR:CE1	2.46	0.51
1:A:93:GLN:NE2	1:A:115:ARG:CZ	2.74	0.50
1:A:211:SER:O	1:A:213:SER:N	2.44	0.50
1:A:298:ALA:O	1:A:302:LEU:CD1	2.59	0.50
1:B:156:ARG:HG2	1:B:156:ARG:HH11	1.76	0.50
1:C:323:VAL:HG12	1:C:324:TRP:N	2.24	0.50
1:B:83:ALA:HB1	1:B:86:LEU:HG	1.93	0.50
1:A:48:ASN:O	1:A:49:ILE:C	2.50	0.50
1:C:95:TYR:N	1:C:95:TYR:CD2	2.80	0.50
1:C:113:CYS:CB	1:C:145:CYS:SG	2.99	0.50
1:B:199:ILE:HG21	1:B:203:LEU:HG	1.91	0.50
1:A:95:TYR:HB3	1:A:100:CYS:O	2.10	0.50
1:A:106:LEU:HD13	1:A:134:VAL:HG11	1.93	0.50
1:C:202:GLU:OE1	1:C:361:THR:HG21	2.11	0.50
1:A:38:ILE:O	1:A:42:VAL:HG23	2.11	0.50
1:A:255:PRO:O	1:A:256:PRO:C	2.50	0.50
1:B:65:HIS:O	1:B:157:ARG:NH2	2.43	0.50
1:B:176:LEU:HD13	1:B:331:ARG:CZ	2.42	0.50
1:A:142:CYS:O	1:A:146:LEU:HD22	2.12	0.50
1:A:340:GLU:CD	1:A:340:GLU:H	2.15	0.50
1:A:83:ALA:HA	1:A:86:LEU:CD2	2.42	0.50
1:A:244:ALA:HA	1:A:284:PHE:CD1	2.47	0.49
1:C:159:LYS:HE2	1:C:159:LYS:CA	2.35	0.49
1:B:361:THR:O	1:B:363:LEU:N	2.45	0.49
1:C:346:LEU:HD11	1:C:350:LYS:HZ2	1.77	0.49
1:A:147:PRO:HA	1:A:156:ARG:HH21	1.74	0.49
1:A:220:HIS:CD2	1:A:221:VAL:N	2.80	0.49
1:C:95:TYR:N	1:C:95:TYR:HD2	2.09	0.49
1:B:308:THR:HG22	1:B:334:HIS:HE1	1.77	0.49
1:C:224:VAL:C	1:C:262:GLN:HE22	2.16	0.49
1:B:67:LEU:HD23	1:B:144:LEU:CD1	2.43	0.49
1:B:343:LEU:HD22	1:B:343:LEU:N	2.27	0.49
1:B:346:LEU:HD12	1:B:346:LEU:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:TYR:N	1:A:95:TYR:CD2	2.80	0.49
1:A:223:ASP:OD1	1:A:225:THR:HG22	2.12	0.49
1:C:129:GLY:O	1:C:133:LYS:HG3	2.13	0.49
1:C:228:VAL:O	1:C:230:LYS:N	2.44	0.49
1:B:216:GLY:O	1:B:218:LEU:N	2.42	0.49
1:A:44:ALA:O	1:A:46:GLN:HG3	2.13	0.49
1:B:66:PRO:HG2	1:B:80:PHE:HE1	1.74	0.49
1:B:167:PHE:O	1:B:168:TYR:C	2.51	0.49
1:B:287:ASN:C	1:B:288:LEU:HG	2.32	0.49
1:A:372:ARG:HG2	1:A:372:ARG:HH11	1.77	0.49
1:B:244:ALA:HA	1:B:284:PHE:CE1	2.48	0.49
1:C:68:PHE:CE2	1:C:144:LEU:HD21	2.48	0.49
1:C:278:GLY:N	1:C:279:PRO:CD	2.76	0.49
1:C:295:LEU:C	1:C:297:VAL:H	2.15	0.49
1:B:176:LEU:HD13	1:B:331:ARG:NH1	2.28	0.48
1:B:190:VAL:HG23	1:B:375:PHE:HE1	1.76	0.48
1:B:340:GLU:CD	1:B:340:GLU:H	2.16	0.48
1:A:220:HIS:HD2	1:A:221:VAL:N	2.11	0.48
1:A:228:VAL:HG12	1:A:229:ARG:H	1.78	0.48
1:A:286:ASP:OD2	1:A:287:ASN:N	2.46	0.48
1:C:361:THR:C	1:C:363:LEU:H	2.15	0.48
1:C:195:LEU:HD12	1:C:263:PHE:CD1	2.43	0.48
1:B:274:PRO:CB	1:A:274:PRO:HB3	2.40	0.48
1:C:83:ALA:HA	1:C:86:LEU:HD23	1.93	0.48
1:C:126:VAL:HG21	1:C:143:TYR:OH	2.13	0.48
1:C:81:LEU:H	1:C:81:LEU:CD1	2.26	0.48
1:C:181:THR:HA	1:C:374:TYR:CE2	2.49	0.48
1:C:188:GLN:HB3	1:C:189:PRO:HD2	1.95	0.48
1:A:128:PRO:HG2	1:C:36:ASP:HB3	1.95	0.48
1:A:199:ILE:O	1:A:203:LEU:HB2	2.13	0.48
1:A:214:ASP:HB2	1:A:215:PRO:CD	2.37	0.48
1:C:63:THR:HG23	1:C:64:GLN:N	2.28	0.48
1:A:165:LYS:HE3	1:A:169:ASP:OD2	2.13	0.48
1:C:203:LEU:HD22	1:C:208:PHE:HD1	1.78	0.48
1:B:59:LEU:N	1:B:59:LEU:HD12	2.28	0.48
1:B:304:MET:HG3	1:B:304:MET:O	2.13	0.48
1:A:113:CYS:SG	1:A:115:ARG:HG3	2.53	0.48
1:C:264:HIS:CE1	1:C:301:PHE:HB3	2.49	0.48
1:A:65:HIS:CD2	1:A:68:PHE:H	2.32	0.48
1:C:53:CYS:SG	1:C:76:CYS:SG	3.12	0.48
1:B:44:ALA:C	1:B:46:GLN:H	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:CYS:HB2	1:B:118:CYS:HB2	1.96	0.48
1:B:232:VAL:HA	1:B:235:TRP:CE3	2.49	0.48
1:A:240:LEU:HA	1:A:281:PHE:O	2.14	0.48
1:C:81:LEU:HD12	1:C:81:LEU:N	2.27	0.48
1:C:141:VAL:O	1:C:142:CYS:O	2.32	0.48
1:B:80:PHE:O	1:B:84:LEU:HD23	2.14	0.47
1:B:174:ASN:N	1:B:175:PRO:HD3	2.28	0.47
1:A:192:VAL:HG12	1:A:193:LEU:N	2.28	0.47
1:A:297:VAL:O	1:A:300:ARG:HB2	2.14	0.47
1:C:95:TYR:HB3	1:C:100:CYS:C	2.33	0.47
1:A:235:TRP:O	1:A:236:GLY:O	2.32	0.47
1:C:149:SER:HB3	1:C:155:GLN:OE1	2.14	0.47
1:C:179:PHE:CD1	1:C:278:GLY:O	2.68	0.47
1:C:181:THR:HA	1:C:374:TYR:HE2	1.79	0.47
1:B:295:LEU:C	1:B:295:LEU:HD23	2.35	0.47
1:C:169:ASP:HA	1:C:175:PRO:HG3	1.95	0.47
1:C:190:VAL:HG22	1:C:192:VAL:HG23	1.95	0.47
1:C:193:LEU:HD13	1:C:238:PHE:HE1	1.78	0.47
1:C:216:GLY:C	1:C:218:LEU:H	2.17	0.47
1:B:229:ARG:O	1:B:233:GLU:HG3	2.14	0.47
1:B:366:ASN:HB3	1:B:369:LEU:HD12	1.97	0.47
1:A:292:LYS:O	1:A:293:GLU:C	2.51	0.47
1:A:363:LEU:N	1:A:363:LEU:HD22	2.29	0.47
1:C:66:PRO:O	1:C:157:ARG:HG3	2.15	0.47
1:B:227:THR:O	1:B:265:ARG:NH2	2.47	0.47
1:A:244:ALA:CB	1:A:285:VAL:HB	2.43	0.47
1:A:80:PHE:HA	1:A:100:CYS:SG	2.55	0.47
1:A:83:ALA:HA	1:A:86:LEU:HD23	1.95	0.47
1:A:116:CYS:O	1:A:117:TYR:CG	2.68	0.47
1:A:330:ILE:HD12	1:A:330:ILE:HA	1.81	0.47
1:C:63:THR:OG1	1:C:170:ARG:NH2	2.48	0.47
1:C:285:VAL:HG13	1:C:321:VAL:CG1	2.44	0.47
1:B:86:LEU:N	1:B:86:LEU:HD22	2.30	0.47
1:A:114:THR:HG21	1:A:372:ARG:HG2	1.96	0.47
1:C:240:LEU:HD13	1:C:281:PHE:HB2	1.97	0.47
1:C:289:VAL:O	1:C:289:VAL:HG22	2.15	0.47
1:B:243:GLY:O	1:B:284:PHE:HA	2.15	0.47
1:A:49:ILE:H	1:A:49:ILE:CD1	2.18	0.47
1:A:200:LYS:O	1:A:201:LYS:C	2.52	0.47
1:A:372:ARG:HD3	1:A:377:TYR:HB2	1.97	0.47
1:B:310:PRO:HD2	1:B:335:TRP:CD1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:GLU:CD	1:B:361:THR:HG21	2.35	0.46
1:B:271:ARG:HD3	1:B:272:PRO:HD2	1.97	0.46
1:A:65:HIS:ND1	1:A:72:ILE:HD11	2.30	0.46
1:B:276:SER:O	1:B:277:PRO:C	2.54	0.46
1:B:364:VAL:O	1:B:365:LYS:C	2.54	0.46
1:C:49:ILE:CG1	1:C:69:GLU:HG2	2.42	0.46
1:C:241:VAL:O	1:C:283:MET:N	2.43	0.46
1:B:83:ALA:CB	1:B:86:LEU:HG	2.45	0.46
1:A:160:TRP:O	1:A:161:ARG:C	2.52	0.46
1:C:192:VAL:HG12	1:C:193:LEU:N	2.30	0.46
1:C:260:LEU:HD11	1:C:298:ALA:CB	2.44	0.46
1:C:295:LEU:C	1:C:297:VAL:N	2.68	0.46
1:B:117:TYR:CE1	1:B:143:TYR:HD1	2.33	0.46
1:A:147:PRO:O	1:A:149:SER:N	2.48	0.46
1:C:96:CYS:HB3	1:C:99:CYS:SG	2.55	0.46
1:C:160:TRP:O	1:C:161:ARG:C	2.54	0.46
1:B:113:CYS:SG	1:B:115:ARG:HG3	2.56	0.46
1:C:88:ASP:HB2	1:C:90:ASP:OD2	2.14	0.46
1:C:161:ARG:HG2	1:C:161:ARG:HH11	1.80	0.46
1:B:134:VAL:C	1:B:136:ALA:N	2.65	0.46
1:B:343:LEU:H	1:B:343:LEU:CD2	2.26	0.46
1:B:364:VAL:O	1:B:367:CYS:N	2.43	0.46
1:A:81:LEU:HD21	1:A:171:GLU:CB	2.46	0.46
1:A:104:THR:HG23	1:A:119:PHE:HD1	1.80	0.46
1:C:97:SER:C	1:C:98:ILE:HD12	2.36	0.46
1:C:225:THR:CA	1:C:262:GLN:HE22	2.27	0.46
1:C:232:VAL:HG11	1:C:269:TYR:O	2.15	0.46
1:B:48:ASN:ND2	1:B:50:GLU:HG3	2.30	0.46
1:B:293:GLU:O	1:B:295:LEU:N	2.49	0.46
1:A:48:ASN:O	1:A:51:ASP:N	2.44	0.46
1:C:193:LEU:HB2	1:C:238:PHE:CD1	2.51	0.46
1:A:50:GLU:OE2	1:A:70:GLY:N	2.49	0.46
1:A:261:PHE:O	1:A:264:HIS:HB3	2.15	0.46
1:A:283:MET:CB	1:A:325:SER:HB2	2.46	0.46
1:C:214:ASP:CB	1:C:215:PRO:HD3	2.30	0.46
1:C:261:PHE:C	1:C:263:PHE:N	2.68	0.46
1:C:306:PRO:HG3	1:C:324:TRP:NE1	2.30	0.46
1:C:364:VAL:O	1:C:367:CYS:N	2.42	0.46
1:A:78:ASP:O	1:A:82:ASP:HB2	2.16	0.46
1:A:320:ALA:CB	1:A:343:LEU:HD11	2.46	0.46
1:B:214:ASP:C	1:B:216:GLY:H	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:VAL:O	1:A:126:VAL:HG23	2.16	0.46
1:C:86:LEU:CD2	1:C:86:LEU:H	2.28	0.46
1:C:228:VAL:C	1:C:230:LYS:N	2.69	0.46
1:B:72:ILE:HG22	1:B:73:CYS:O	2.16	0.45
1:B:190:VAL:HG23	1:B:375:PHE:CD1	2.51	0.45
1:B:330:ILE:HA	1:B:330:ILE:HD12	1.80	0.45
1:A:141:VAL:HG23	1:A:141:VAL:O	2.16	0.45
1:C:69:GLU:OE2	1:C:155:GLN:HG2	2.16	0.45
1:C:142:CYS:SG	1:C:143:TYR:N	2.88	0.45
1:B:293:GLU:C	1:B:295:LEU:H	2.19	0.45
1:A:49:ILE:O	1:A:51:ASP:N	2.50	0.45
1:A:141:VAL:O	1:A:142:CYS:O	2.33	0.45
1:C:52:ILE:O	1:C:54:ILE:N	2.50	0.45
1:C:144:LEU:HA	1:C:156:ARG:HD3	1.98	0.45
1:C:163:GLN:O	1:C:167:PHE:HB2	2.17	0.45
1:B:53:CYS:O	1:B:55:CYS:N	2.49	0.45
1:B:88:ASP:OD1	2:D:506:THR:HG21	2.15	0.45
1:B:295:LEU:C	1:B:297:VAL:N	2.66	0.45
1:B:299:SER:OG	1:B:306:PRO:HD3	2.16	0.45
1:A:50:GLU:OE1	1:A:157:ARG:NH2	2.48	0.45
1:A:292:LYS:HG3	1:A:293:GLU:N	2.32	0.45
1:A:321:VAL:O	1:A:321:VAL:HG12	2.16	0.45
1:B:49:ILE:C	1:B:51:ASP:N	2.70	0.45
1:B:49:ILE:O	1:B:51:ASP:N	2.49	0.45
1:B:117:TYR:CE2	1:B:142:CYS:CB	2.98	0.45
1:B:154:LEU:HD12	1:B:154:LEU:HA	1.86	0.45
1:B:199:ILE:HG22	1:B:203:LEU:HG	1.97	0.45
1:A:226:ASP:O	1:A:227:THR:C	2.54	0.45
1:C:206:LEU:HD13	1:C:206:LEU:O	2.16	0.45
1:B:168:TYR:HD1	1:B:168:TYR:O	1.99	0.45
1:B:290:LEU:HD12	1:B:290:LEU:N	2.32	0.45
1:A:35:ARG:NH1	1:A:120:GLU:OE2	2.49	0.45
1:C:40:TYR:O	1:C:44:ALA:HB3	2.16	0.45
1:C:228:VAL:CG1	1:C:229:ARG:N	2.77	0.45
1:C:284:PHE:CD2	1:C:324:TRP:CE3	3.03	0.45
1:B:68:PHE:CD2	1:B:154:LEU:HG	2.51	0.45
1:B:112:ASP:OD1	1:B:184:VAL:HG21	2.16	0.45
1:B:143:TYR:HA	1:B:146:LEU:HD22	1.98	0.45
1:B:354:LYS:HD2	1:B:354:LYS:N	2.30	0.45
1:A:48:ASN:O	1:A:50:GLU:N	2.50	0.45
1:A:83:ALA:C	1:A:86:LEU:HD23	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:GLU:C	1:A:342:GLU:H	2.20	0.45
1:A:248:LEU:N	1:A:248:LEU:CD2	2.80	0.45
1:C:53:CYS:C	1:C:55:CYS:N	2.70	0.45
1:C:53:CYS:SG	1:C:55:CYS:HB3	2.56	0.45
1:B:47:ARG:HG3	1:B:47:ARG:HH11	1.82	0.45
1:A:260:LEU:C	1:A:260:LEU:CD1	2.85	0.45
1:C:261:PHE:O	1:C:263:PHE:N	2.50	0.45
1:A:174:ASN:CG	1:A:174:ASN:O	2.55	0.45
1:C:74:ALA:CB	1:C:75:PRO:HD3	2.37	0.45
1:C:117:TYR:OH	1:C:142:CYS:HB2	2.17	0.45
1:A:96:CYS:SG	1:A:117:TYR:HA	2.57	0.45
1:A:136:ALA:HB2	1:C:135:HIS:HE1	1.80	0.45
1:C:113:CYS:SG	1:C:115:ARG:HG3	2.57	0.45
1:C:219:LYS:HD2	1:C:219:LYS:HA	1.75	0.45
1:C:309:ILE:HD12	1:C:363:LEU:O	2.17	0.45
1:B:202:GLU:HG3	1:B:361:THR:HG23	1.98	0.44
1:A:49:ILE:C	1:A:51:ASP:H	2.21	0.44
1:A:67:LEU:HD21	1:A:115:ARG:NH2	2.32	0.44
1:A:104:THR:O	1:A:105:LEU:HD23	2.17	0.44
1:A:84:LEU:N	1:A:86:LEU:HD23	2.32	0.44
1:A:192:VAL:HB	1:A:218:LEU:HB2	2.00	0.44
1:C:137:MET:O	2:F:501:ALA:N	2.51	0.44
1:A:240:LEU:HD12	1:A:281:PHE:O	2.17	0.44
1:C:135:HIS:O	1:C:135:HIS:CD2	2.70	0.44
1:B:80:PHE:HA	1:B:100:CYS:SG	2.57	0.44
1:B:134:VAL:C	1:B:136:ALA:H	2.20	0.44
1:B:217:GLN:OE1	1:B:217:GLN:HA	2.17	0.44
1:A:104:THR:CG2	1:A:119:PHE:HD1	2.31	0.44
1:A:245:THR:HG23	1:A:285:VAL:O	2.17	0.44
1:A:363:LEU:H	1:A:363:LEU:HD23	1.82	0.44
1:B:242:TYR:CG	1:B:243:GLY:N	2.85	0.44
1:B:307:VAL:HG11	1:B:330:ILE:O	2.18	0.44
1:A:93:GLN:HE22	1:A:115:ARG:NH2	2.16	0.44
1:A:260:LEU:HD23	1:A:284:PHE:CE2	2.53	0.44
1:A:261:PHE:HE2	1:A:301:PHE:CZ	2.35	0.44
1:C:61:VAL:HA	1:C:72:ILE:O	2.17	0.44
1:C:192:VAL:CG1	1:C:193:LEU:N	2.81	0.44
1:B:96:CYS:HB2	1:B:118:CYS:CB	2.48	0.44
1:A:204:THR:HG22	1:A:205:SER:N	2.31	0.44
1:A:340:GLU:C	1:A:342:GLU:N	2.70	0.44
1:B:164:LEU:C	1:B:164:LEU:HD23	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:SER:HB3	1:B:342:GLU:HG3	2.00	0.44
1:C:133:LYS:O	1:C:136:ALA:HB3	2.18	0.44
1:A:286:ASP:OD2	1:A:289:VAL:HG12	2.18	0.44
1:C:50:GLU:HA	1:C:71:GLY:N	2.33	0.44
1:C:77:LYS:O	1:C:81:LEU:HD13	2.17	0.44
1:C:81:LEU:HA	1:C:84:LEU:HG	1.99	0.44
1:C:93:GLN:O	2:F:504:LYS:NZ	2.50	0.44
1:C:323:VAL:CG1	1:C:324:TRP:N	2.81	0.44
1:B:47:ARG:HG3	1:B:47:ARG:NH1	2.33	0.44
1:A:83:ALA:CA	1:A:86:LEU:HD23	2.48	0.44
1:C:105:LEU:HB3	1:C:116:CYS:HB3	2.00	0.44
1:C:113:CYS:SG	1:C:114:THR:N	2.91	0.44
1:C:134:VAL:C	1:C:136:ALA:H	2.22	0.44
1:C:283:MET:SD	1:C:368:PHE:HE2	2.40	0.44
1:C:38:ILE:CG1	1:C:39:ALA:N	2.81	0.43
1:C:237:PRO:O	1:C:238:PHE:HD2	2.00	0.43
1:B:248:LEU:N	1:B:248:LEU:CD2	2.81	0.43
1:B:309:ILE:HG13	1:B:309:ILE:O	2.18	0.43
1:A:244:ALA:HB1	1:A:285:VAL:HB	2.00	0.43
1:A:260:LEU:HD13	1:A:261:PHE:N	2.33	0.43
1:A:65:HIS:HD2	1:A:68:PHE:H	1.66	0.43
1:A:359:TRP:HA	1:A:360:PRO:HD3	1.79	0.43
1:C:71:GLY:O	1:C:72:ILE:HG13	2.19	0.43
1:C:227:THR:HG23	1:C:231:ASP:CB	2.48	0.43
1:B:343:LEU:HA	1:B:346:LEU:HB3	2.01	0.43
1:A:228:VAL:O	1:A:229:ARG:C	2.56	0.43
1:A:271:ARG:HG3	1:A:271:ARG:NH1	2.33	0.43
1:C:81:LEU:HA	1:C:84:LEU:HD11	2.00	0.43
1:B:77:LYS:CE	1:B:78:ASP:OD2	2.67	0.43
1:B:107:ILE:HG12	1:B:116:CYS:HG	1.77	0.43
1:B:161:ARG:HH11	1:B:161:ARG:HG2	1.84	0.43
1:B:187:ARG:HH12	1:B:373:GLU:HA	1.84	0.43
1:A:38:ILE:HA	1:A:41:GLU:HB2	2.01	0.43
1:C:284:PHE:CD2	1:C:324:TRP:HE3	2.37	0.43
1:A:338:VAL:HG12	1:A:343:LEU:CD2	2.49	0.43
1:C:132:GLY:O	1:C:135:HIS:N	2.52	0.43
1:B:90:ASP:OD2	1:B:91:GLY:N	2.52	0.43
1:A:310:PRO:HG3	1:A:338:VAL:HG21	2.00	0.43
1:A:368:PHE:C	1:A:370:PRO:CD	2.87	0.43
1:C:160:TRP:O	1:C:163:GLN:N	2.52	0.43
1:B:71:GLY:O	1:B:72:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:LEU:HD13	1:A:343:LEU:HA	1.78	0.43
1:C:276:SER:OG	1:C:277:PRO:HD2	2.19	0.43
1:B:214:ASP:C	1:B:216:GLY:N	2.73	0.42
1:B:234:GLU:C	1:B:236:GLY:N	2.72	0.42
1:C:56:CYS:O	1:C:56:CYS:SG	2.77	0.42
1:C:108:CYS:SG	1:C:145:CYS:SG	3.15	0.42
1:C:144:LEU:HD22	1:C:156:ARG:HG3	2.01	0.42
1:C:228:VAL:CG1	1:C:229:ARG:H	2.28	0.42
1:C:271:ARG:HG3	1:C:271:ARG:NH1	2.32	0.42
1:B:255:PRO:HA	1:B:256:PRO:HD3	1.95	0.42
1:A:53:CYS:HA	1:A:71:GLY:C	2.40	0.42
1:C:359:TRP:HA	1:C:360:PRO:HD3	1.83	0.42
1:B:228:VAL:O	1:B:231:ASP:N	2.49	0.42
1:A:165:LYS:HG2	1:A:169:ASP:OD2	2.19	0.42
1:C:288:LEU:HD23	1:C:322:ARG:NE	2.33	0.42
1:A:133:LYS:O	1:A:136:ALA:N	2.51	0.42
1:A:208:PHE:CD1	1:A:208:PHE:N	2.87	0.42
1:C:174:ASN:O	1:C:175:PRO:O	2.38	0.42
1:C:203:LEU:HD21	1:C:368:PHE:CD1	2.50	0.42
1:B:323:VAL:CG1	1:B:324:TRP:N	2.82	0.42
1:B:325:SER:OG	1:B:326:ASN:N	2.52	0.42
1:B:343:LEU:O	1:B:346:LEU:N	2.52	0.42
1:A:251:THR:HG22	1:A:252:CYS:N	2.33	0.42
1:C:327:ILE:HG23	1:C:371:LEU:CD2	2.49	0.42
1:B:206:LEU:HD21	1:B:365:LYS:HG2	2.01	0.42
1:B:333:ARG:HH12	1:B:366:ASN:CB	2.32	0.42
1:A:338:VAL:HG12	1:A:343:LEU:HD22	2.01	0.42
1:C:196:PHE:N	1:C:196:PHE:CD2	2.86	0.42
1:B:193:LEU:HB2	1:B:238:PHE:CZ	2.54	0.42
1:B:243:GLY:O	1:B:284:PHE:HD1	2.02	0.42
1:C:37:LEU:O	1:C:40:TYR:HB3	2.19	0.42
1:B:164:LEU:O	1:B:165:LYS:C	2.58	0.42
1:B:287:ASN:HD21	1:B:360:PRO:HD2	1.83	0.42
1:A:245:THR:HG22	1:A:284:PHE:CZ	2.55	0.42
1:A:323:VAL:CG1	1:A:324:TRP:N	2.83	0.42
1:A:364:VAL:O	1:A:367:CYS:N	2.31	0.42
1:C:81:LEU:HA	1:C:84:LEU:HD21	2.02	0.42
1:C:156:ARG:HH11	1:C:156:ARG:HG2	1.84	0.42
1:B:258:TRP:O	1:B:261:PHE:N	2.53	0.42
1:B:271:ARG:HG3	1:B:271:ARG:NH1	2.33	0.42
1:A:37:LEU:H	1:A:37:LEU:CD1	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:ALA:O	1:A:350:LYS:HB2	2.20	0.42
1:C:121:CYS:O	1:C:122:VAL:C	2.57	0.42
1:C:188:GLN:HB3	1:C:189:PRO:CD	2.50	0.42
1:B:228:VAL:O	1:B:229:ARG:C	2.58	0.42
1:C:241:VAL:HB	1:C:282:TRP:CB	2.50	0.42
1:C:260:LEU:O	1:C:263:PHE:HB3	2.20	0.42
1:C:264:HIS:CD2	1:C:264:HIS:O	2.73	0.42
1:C:267:LEU:HB3	1:C:268:GLN:NE2	2.35	0.42
1:C:306:PRO:HG3	1:C:324:TRP:HZ2	1.81	0.42
1:B:216:GLY:C	1:B:218:LEU:H	2.21	0.41
1:C:192:VAL:HB	1:C:218:LEU:HD13	2.02	0.41
1:B:88:ASP:O	1:B:91:GLY:N	2.42	0.41
1:B:123:ASP:OD2	1:B:131:SER:CB	2.62	0.41
1:B:280:PHE:O	1:B:326:ASN:ND2	2.49	0.41
1:A:209:LEU:HD12	1:A:209:LEU:HA	1.79	0.41
1:C:36:ASP:O	1:C:38:ILE:N	2.53	0.41
1:C:53:CYS:O	1:C:57:GLY:N	2.48	0.41
1:C:199:ILE:HG13	1:C:242:TYR:CD2	2.55	0.41
1:B:267:LEU:C	1:B:267:LEU:HD13	2.41	0.41
1:B:335:TRP:O	1:B:337:LEU:N	2.53	0.41
1:A:199:ILE:CG2	1:A:203:LEU:HG	2.51	0.41
1:A:208:PHE:CE2	1:A:371:LEU:HB2	2.56	0.41
1:A:290:LEU:HD12	1:A:290:LEU:N	2.35	0.41
1:B:69:GLU:OE2	1:B:155:GLN:HG2	2.21	0.41
1:B:262:GLN:O	1:B:263:PHE:C	2.58	0.41
1:C:34:GLY:C	1:C:36:ASP:H	2.24	0.41
1:C:165:LYS:O	1:C:168:TYR:N	2.53	0.41
1:B:215:PRO:O	1:B:216:GLY:C	2.59	0.41
1:B:254:ARG:O	1:B:255:PRO:C	2.59	0.41
1:A:161:ARG:HG2	1:A:181:THR:HG1	1.84	0.41
1:A:190:VAL:HG23	1:A:375:PHE:CE1	2.55	0.41
1:C:46:GLN:O	1:C:47:ARG:O	2.39	0.41
1:C:260:LEU:CD1	1:C:298:ALA:HB2	2.51	0.41
1:B:371:LEU:C	1:B:373:GLU:N	2.74	0.41
1:A:81:LEU:H	1:A:81:LEU:CD1	2.32	0.41
1:A:104:THR:C	1:A:105:LEU:HG	2.41	0.41
1:C:107:ILE:CG2	1:C:108:CYS:N	2.82	0.41
1:B:285:VAL:HG13	1:B:321:VAL:HG13	2.03	0.41
1:B:356:ALA:C	1:B:358:LYS:N	2.74	0.41
1:A:179:PHE:CD1	1:A:279:PRO:HA	2.55	0.41
1:A:282:TRP:NE1	1:A:326:ASN:HB3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:HIS:NE2	1:B:253:ASP:HA	2.35	0.41
1:B:356:ALA:O	1:B:358:LYS:N	2.54	0.41
1:A:38:ILE:O	1:A:39:ALA:C	2.59	0.41
1:A:84:LEU:HD23	1:A:84:LEU:HA	1.88	0.41
1:A:199:ILE:HG22	1:A:203:LEU:CG	2.48	0.41
1:A:368:PHE:O	1:A:371:LEU:HG	2.21	0.41
1:C:255:PRO:HA	1:C:256:PRO:HD3	1.86	0.41
1:A:97:SER:HB2	1:A:117:TYR:CE1	2.56	0.41
1:A:260:LEU:O	1:A:263:PHE:HB3	2.20	0.41
1:C:193:LEU:HD13	1:C:238:PHE:CE1	2.56	0.41
1:C:281:PHE:HA	1:C:326:ASN:HD21	1.86	0.41
1:B:262:GLN:HE22	1:B:265:ARG:NH1	2.19	0.40
1:A:80:PHE:HD1	1:A:167:PHE:CE2	2.39	0.40
1:A:135:HIS:CD2	1:A:135:HIS:O	2.74	0.40
1:C:48:ASN:HB3	1:C:51:ASP:OD2	2.21	0.40
1:B:84:LEU:HD22	1:B:84:LEU:HA	1.73	0.40
1:B:179:PHE:CE1	1:B:278:GLY:O	2.74	0.40
1:B:341:GLU:H	1:B:341:GLU:HG2	1.53	0.40
1:B:361:THR:O	1:B:362:LYS:C	2.60	0.40
1:A:244:ALA:HB1	1:A:285:VAL:O	2.21	0.40
1:C:48:ASN:ND2	1:C:50:GLU:HG2	2.36	0.40
1:C:369:LEU:O	1:C:370:PRO:C	2.59	0.40
1:A:232:VAL:HA	1:A:235:TRP:CE3	2.55	0.40
1:A:278:GLY:HA2	1:A:279:PRO:HD3	1.87	0.40
1:C:48:ASN:O	1:C:51:ASP:N	2.51	0.40
1:C:130:THR:O	1:C:131:SER:C	2.60	0.40
1:B:196:PHE:CE1	1:B:259:TYR:HD2	2.40	0.40
1:C:99:CYS:O	1:C:100:CYS:CB	2.59	0.40
1:C:117:TYR:CZ	1:C:142:CYS:HB2	2.57	0.40
1:C:261:PHE:O	1:C:262:GLN:C	2.59	0.40
1:B:258:TRP:O	1:B:261:PHE:HB2	2.22	0.40
1:B:265:ARG:HD2	1:A:301:PHE:CE1	2.56	0.40
1:B:283:MET:HG2	1:B:284:PHE:N	2.36	0.40
1:C:308:THR:HG22	1:C:334:HIS:HE1	1.86	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:GLU:OE2	1:A:342:GLU:OE2[7_555]	2.11	0.09

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	345/386 (89%)	237 (69%)	68 (20%)	40 (12%)	0 5
1	B	345/386 (89%)	240 (70%)	72 (21%)	33 (10%)	0 8
1	C	345/386 (89%)	233 (68%)	75 (22%)	37 (11%)	0 6
2	D	5/7 (71%)	4 (80%)	1 (20%)	0	100 100
2	E	5/7 (71%)	5 (100%)	0	0	100 100
2	F	5/7 (71%)	4 (80%)	1 (20%)	0	100 100
All	All	1050/1179 (89%)	723 (69%)	217 (21%)	110 (10%)	0 6

All (110) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	49	ILE
1	B	142	CYS
1	B	200	LYS
1	B	235	TRP
1	B	277	PRO
1	A	142	CYS
1	A	203	LEU
1	A	250	HIS
1	A	265	ARG
1	A	321	VAL
1	C	47	ARG
1	C	142	CYS
1	C	175	PRO
1	C	256	PRO
1	C	271	ARG
1	C	274	PRO
1	C	277	PRO
1	C	362	LYS
1	B	66	PRO
1	B	82	ASP

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Mol	Chain	Res	Type
1	B	103	GLU
1	B	161	ARG
1	B	216	GLY
1	B	217	GLN
1	B	265	ARG
1	B	274	PRO
1	B	329	ALA
1	B	362	LYS
1	A	49	ILE
1	A	53	CYS
1	A	58	SER
1	A	66	PRO
1	A	89	ASP
1	A	148	SER
1	A	161	ARG
1	A	202	GLU
1	A	212	GLY
1	A	227	THR
1	A	235	TRP
1	A	247	PRO
1	A	256	PRO
1	A	266	LEU
1	A	278	GLY
1	A	333	ARG
1	C	37	LEU
1	C	53	CYS
1	C	66	PRO
1	C	100	CYS
1	C	189	PRO
1	C	229	ARG
1	C	255	PRO
1	C	292	LYS
1	B	50	GLU
1	B	53	CYS
1	B	89	ASP
1	B	169	ASP
1	B	214	ASP
1	B	257	SER
1	B	294	ASP
1	B	357	ALA
1	A	50	GLU
1	A	167	PHE

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Mol	Chain	Res	Type
1	A	236	GLY
1	A	274	PRO
1	A	298	ALA
1	A	310	PRO
1	A	329	ALA
1	A	365	LYS
1	C	78	ASP
1	C	118	CYS
1	C	181	THR
1	C	217	GLN
1	C	257	SER
1	C	264	HIS
1	C	306	PRO
1	B	64	GLN
1	A	157	ARG
1	A	216	GLY
1	A	255	PRO
1	C	74	ALA
1	C	93	GLN
1	C	336	ALA
1	B	210	GLU
1	B	250	HIS
1	B	360	PRO
1	A	229	ARG
1	A	297	VAL
1	A	304	MET
1	A	360	PRO
1	A	369	LEU
1	C	61	VAL
1	C	232	VAL
1	C	235	TRP
1	C	278	GLY
1	C	279	PRO
1	B	229	ARG
1	A	126	VAL
1	A	251	THR
1	C	214	ASP
1	C	233	GLU
1	C	360	PRO
1	B	175	PRO
1	B	271	ARG
1	A	199	ILE

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Mol	Chain	Res	Type
1	C	54	ILE
1	C	370	PRO
1	B	328	PRO
1	C	215	PRO
1	B	147	PRO
1	B	232	VAL

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	311/344 (90%)	283 (91%)	28 (9%)	9	37
1	B	311/344 (90%)	273 (88%)	38 (12%)	5	24
1	C	311/344 (90%)	287 (92%)	24 (8%)	13	43
2	D	5/5 (100%)	5 (100%)	0	100	100
2	E	5/5 (100%)	5 (100%)	0	100	100
2	F	5/5 (100%)	5 (100%)	0	100	100
All	All	948/1047 (90%)	858 (90%)	90 (10%)	8	34

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	35	ARG
1	B	36	ASP
1	B	49	ILE
1	B	52	ILE
1	B	66	PRO
1	B	73	CYS
1	B	81	LEU
1	B	84	LEU
1	B	86	LEU
1	B	95	TYR
1	B	114	THR
1	B	118	CYS

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Mol	Chain	Res	Type
1	B	119	PHE
1	B	121	CYS
1	B	163	GLN
1	B	168	TYR
1	B	182	VAL
1	B	196	PHE
1	B	206	LEU
1	B	209	LEU
1	B	214	ASP
1	B	222	VAL
1	B	229	ARG
1	B	234	GLU
1	B	268	GLN
1	B	271	ARG
1	B	272	PRO
1	B	274	PRO
1	B	277	PRO
1	B	294	ASP
1	B	308	THR
1	B	328	PRO
1	B	331	ARG
1	B	348	GLN
1	B	359	TRP
1	B	362	LYS
1	B	373	GLU
1	B	375	PHE
1	A	36	ASP
1	A	49	ILE
1	A	54	ILE
1	A	82	ASP
1	A	146	LEU
1	A	155	GLN
1	A	181	THR
1	A	195	LEU
1	A	196	PHE
1	A	206	LEU
1	A	208	PHE
1	A	209	LEU
1	A	218	LEU
1	A	234	GLU
1	A	242	TYR
1	A	245	THR

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Mol	Chain	Res	Type
1	A	250	HIS
1	A	256	PRO
1	A	267	LEU
1	A	268	GLN
1	A	274	PRO
1	A	288	LEU
1	A	308	THR
1	A	321	VAL
1	A	328	PRO
1	A	340	GLU
1	A	343	LEU
1	A	354	LYS
1	C	36	ASP
1	C	49	ILE
1	C	56	CYS
1	C	86	LEU
1	C	117	TYR
1	C	119	PHE
1	C	122	VAL
1	C	130	THR
1	C	142	CYS
1	C	145	CYS
1	C	146	LEU
1	C	168	TYR
1	C	202	GLU
1	C	206	LEU
1	C	229	ARG
1	C	234	GLU
1	C	260	LEU
1	C	268	GLN
1	C	271	ARG
1	C	274	PRO
1	C	276	SER
1	C	359	TRP
1	C	362	LYS
1	C	375	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	48	ASN
1	B	65	HIS

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Mol	Chain	Res	Type
1	B	93	GLN
1	B	220	HIS
1	B	262	GLN
1	B	268	GLN
1	B	287	ASN
1	B	334	HIS
2	D	505	GLN
1	A	48	ASN
1	A	93	GLN
1	A	135	HIS
1	A	268	GLN
1	A	334	HIS
1	C	48	ASN
1	C	135	HIS
1	C	262	GLN
1	C	268	GLN
1	C	334	HIS
1	C	349	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)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	347/386 (89%)	-0.56	1 (0%)	94	90	42, 113, 192, 202	0
1	B	347/386 (89%)	-0.56	4 (1%)	79	69	47, 98, 201, 202	0
1	C	347/386 (89%)	-0.08	5 (1%)	75	64	80, 189, 202, 202	0
2	D	7/7 (100%)	-0.11	0	100	100	129, 138, 195, 196	0
2	E	7/7 (100%)	0.40	0	100	100	190, 193, 201, 202	0
2	F	7/7 (100%)	0.26	0	100	100	157, 179, 199, 200	0
All	All	1062/1179 (90%)	-0.39	10 (0%)	84	76	42, 136, 202, 202	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	320	ALA	2.6
1	B	337	LEU	2.5
1	B	357	ALA	2.4
1	B	214	ASP	2.3
1	C	336	ALA	2.3
1	A	357	ALA	2.3
1	C	238	PHE	2.2
1	C	213	SER	2.1
1	C	310	PRO	2.1
1	B	356	ALA	2.1

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
3	ZN	C	607	1/1	0.94	0.07	164,164,164,164	1
3	ZN	C	608	1/1	0.98	0.24	69,69,69,69	1
3	ZN	B	604	1/1	0.98	0.08	61,61,61,61	1
3	ZN	A	603	1/1	0.99	0.19	115,115,115,115	0
3	ZN	C	609	1/1	0.99	0.09	129,129,129,129	0
3	ZN	A	601	1/1	0.99	0.09	111,111,111,111	1
3	ZN	A	602	1/1	1.00	0.25	58,58,58,58	1
3	ZN	B	606	1/1	1.00	0.18	71,71,71,71	0
3	ZN	B	605	1/1	1.00	0.22	14,14,14,14	1

6.5 Other polymers (i)

There are no such residues in this entry.