Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:19 AM GMT

PDB ID	:	3E6U
Title	:	Crystal structure of Human LanCL1
Authors	:	Zhang, W.; Zhu, G.; Li, X.; Rao, Z.; Zhang, C.
Deposited on	:	2008-08-16
Resolution	:	2.60 Å(reported)

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

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

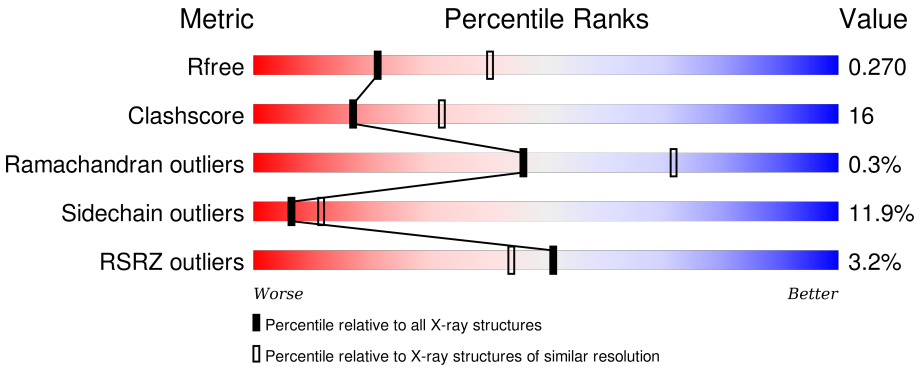
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	411	3% 73% 21% 5%
1	B	411	3% 64% 30%
1	C	411	3% 68% 27% 5%
1	D	411	3% 67% 27%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13228 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 LanC-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	S	0	0	0
			3283	2123	551	586	23			
1	C	409	Total	C	N	O	S	0	0	0
			3283	2123	551	586	23			
1	B	401	Total	C	N	O	S	0	0	0
			3213	2081	535	575	22			
1	D	399	Total	C	N	O	S	0	0	0
			3193	2067	533	571	22			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	HIS	-	EXPRESSION TAG	UNP O43813
A	-10	HIS	-	EXPRESSION TAG	UNP O43813
A	-9	HIS	-	EXPRESSION TAG	UNP O43813
A	-8	HIS	-	EXPRESSION TAG	UNP O43813
A	-7	HIS	-	EXPRESSION TAG	UNP O43813
A	-6	HIS	-	EXPRESSION TAG	UNP O43813
A	-5	SER	-	EXPRESSION TAG	UNP O43813
A	-4	MET	-	EXPRESSION TAG	UNP O43813
A	-3	ASP	-	EXPRESSION TAG	UNP O43813
A	-2	ILE	-	EXPRESSION TAG	UNP O43813
A	-1	GLU	-	EXPRESSION TAG	UNP O43813
A	0	PHE	-	EXPRESSION TAG	UNP O43813
C	-11	HIS	-	EXPRESSION TAG	UNP O43813
C	-10	HIS	-	EXPRESSION TAG	UNP O43813
C	-9	HIS	-	EXPRESSION TAG	UNP O43813
C	-8	HIS	-	EXPRESSION TAG	UNP O43813
C	-7	HIS	-	EXPRESSION TAG	UNP O43813
C	-6	HIS	-	EXPRESSION TAG	UNP O43813
C	-5	SER	-	EXPRESSION TAG	UNP O43813
C	-4	MET	-	EXPRESSION TAG	UNP O43813
C	-3	ASP	-	EXPRESSION TAG	UNP O43813

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	ILE	-	EXPRESSION TAG	UNP O43813
C	-1	GLU	-	EXPRESSION TAG	UNP O43813
C	0	PHE	-	EXPRESSION TAG	UNP O43813
B	-11	HIS	-	EXPRESSION TAG	UNP O43813
B	-10	HIS	-	EXPRESSION TAG	UNP O43813
B	-9	HIS	-	EXPRESSION TAG	UNP O43813
B	-8	HIS	-	EXPRESSION TAG	UNP O43813
B	-7	HIS	-	EXPRESSION TAG	UNP O43813
B	-6	HIS	-	EXPRESSION TAG	UNP O43813
B	-5	SER	-	EXPRESSION TAG	UNP O43813
B	-4	MET	-	EXPRESSION TAG	UNP O43813
B	-3	ASP	-	EXPRESSION TAG	UNP O43813
B	-2	ILE	-	EXPRESSION TAG	UNP O43813
B	-1	GLU	-	EXPRESSION TAG	UNP O43813
B	0	PHE	-	EXPRESSION TAG	UNP O43813
D	-11	HIS	-	EXPRESSION TAG	UNP O43813
D	-10	HIS	-	EXPRESSION TAG	UNP O43813
D	-9	HIS	-	EXPRESSION TAG	UNP O43813
D	-8	HIS	-	EXPRESSION TAG	UNP O43813
D	-7	HIS	-	EXPRESSION TAG	UNP O43813
D	-6	HIS	-	EXPRESSION TAG	UNP O43813
D	-5	SER	-	EXPRESSION TAG	UNP O43813
D	-4	MET	-	EXPRESSION TAG	UNP O43813
D	-3	ASP	-	EXPRESSION TAG	UNP O43813
D	-2	ILE	-	EXPRESSION TAG	UNP O43813
D	-1	GLU	-	EXPRESSION TAG	UNP O43813
D	0	PHE	-	EXPRESSION TAG	UNP O43813

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0

- Molecule 3 is water.

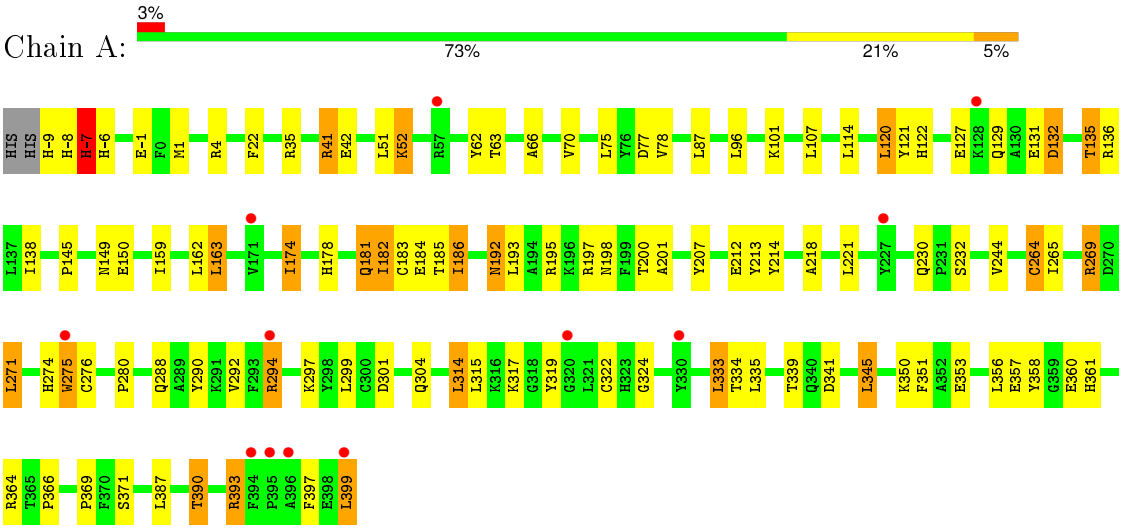
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	78	Total O 78 78	0	0
3	C	62	Total O 62 62	0	0
3	B	67	Total O 67 67	0	0
3	D	45	Total O 45 45	0	0

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.

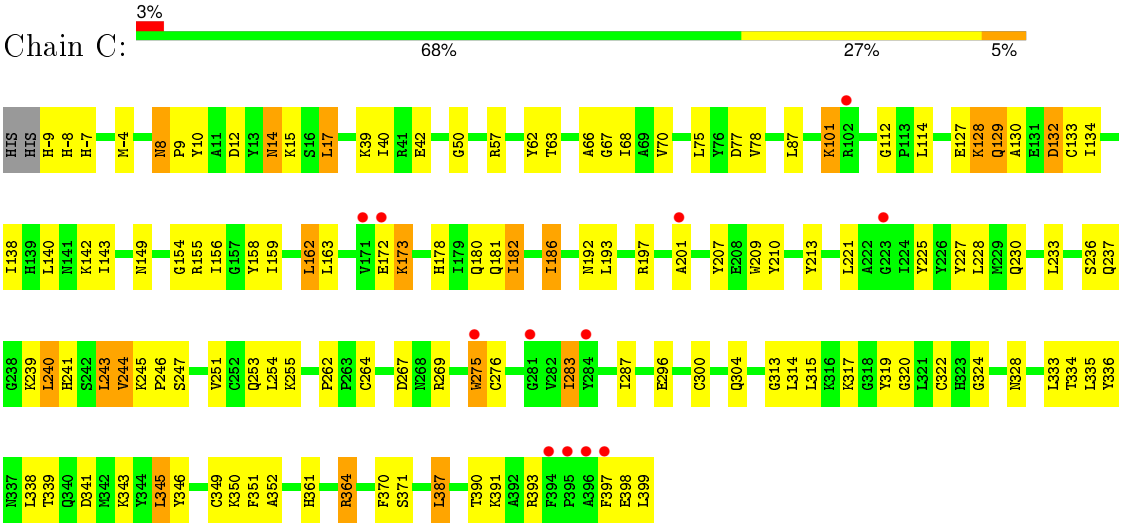
- Molecule 1: LanC-like protein 1

Chain A:



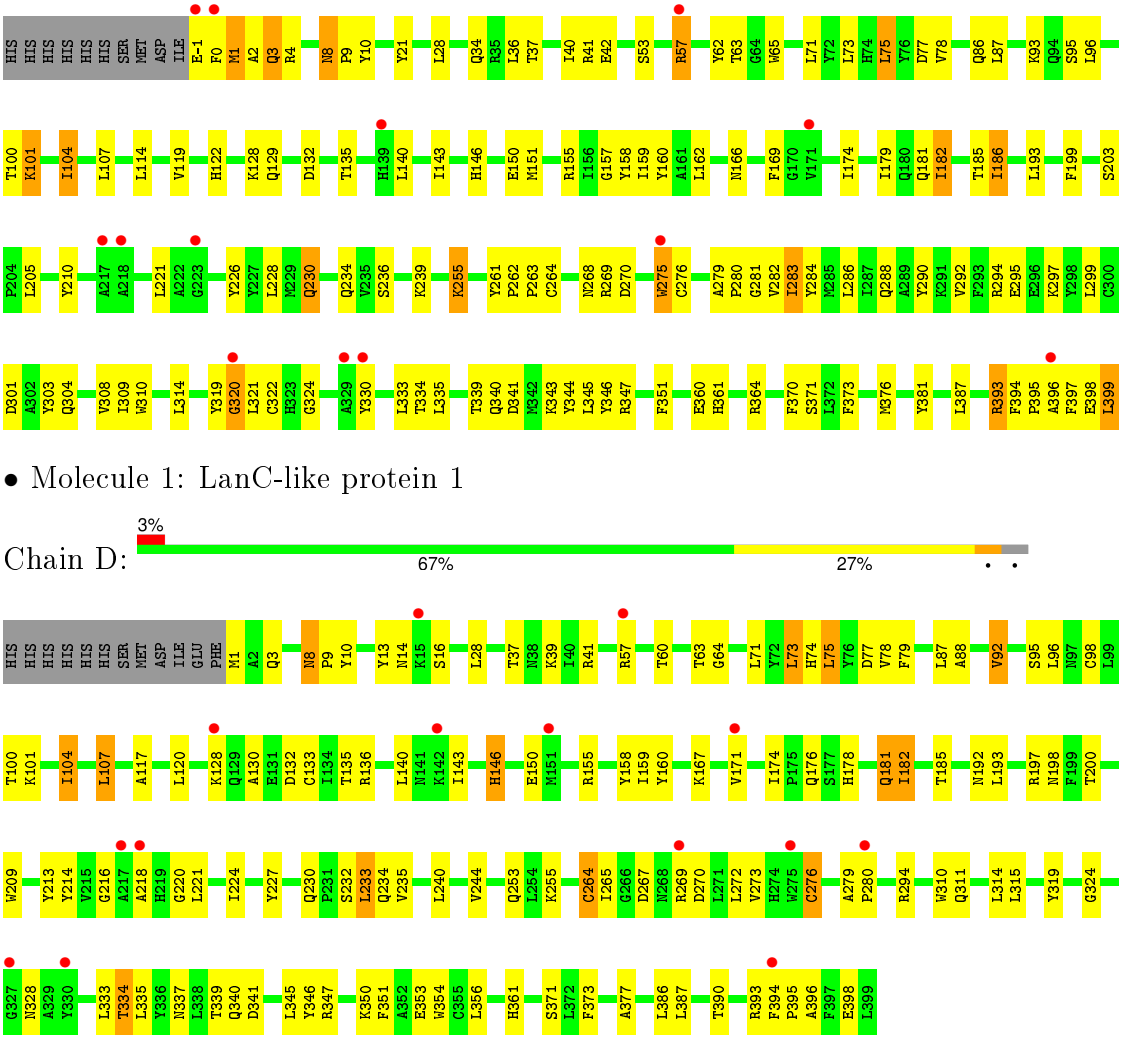
- Molecule 1: LanC-like protein 1

Chain C:



- Molecule 1: LanC-like protein 1

Chain B:



- Molecule 1: LanC-like protein 1

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	194.28Å 194.28Å 211.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	32.58 – 2.60 32.57 – 2.60	Depositor EDS
% Data completeness (in resolution range)	92.2 (32.58-2.60) 92.2 (32.57-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	8.60 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.4.0077	Depositor
R, R_{free}	0.246 , 0.275 0.242 , 0.270	Depositor DCC
R_{free} test set	5266 reflections (4.20%)	DCC
Wilson B-factor (Å^2)	67.7	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 60.7	EDS
Estimated twinning fraction	0.004 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Outliers	1 of 130560 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13228	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% 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: 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	0.46	0/3379	0.68	0/4582
1	B	0.50	0/3305	0.66	1/4482 (0.0%)
1	C	0.45	0/3379	0.64	0/4582
1	D	0.46	0/3284	0.64	0/4454
All	All	0.47	0/13347	0.65	1/18100 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	283	ILE	CB-CA-C	5.11	121.82	111.60

There are no chirality outliers.

There are no planarity outliers.

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	3283	0	3197	101	0
1	B	3213	0	3140	119	0
1	C	3283	0	3197	116	0
1	D	3193	0	3125	87	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	78	0	0	27	0
3	B	67	0	0	20	0
3	C	62	0	0	16	0
3	D	45	0	0	10	0
All	All	13228	0	12659	418	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (418) 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:129:GLN:HG2	3:C:554:HOH:O	1.35	1.21
1:B:335:LEU:O	1:B:339:THR:HG22	1.44	1.17
1:D:176:GLN:CD	1:D:234:GLN:HE22	1.47	1.17
1:D:176:GLN:NE2	1:D:234:GLN:HE22	1.42	1.15
1:B:160:TYR:CE1	1:B:396:ALA:HA	1.85	1.10
1:A:197:ARG:HB3	3:A:563:HOH:O	1.52	1.08
1:C:304:GLN:HG2	3:C:537:HOH:O	1.54	1.07
1:B:398:GLU:O	1:B:399:LEU:OXT	1.72	1.07
1:C:-9:HIS:HB3	3:C:542:HOH:O	1.54	1.06
1:C:173:LYS:HA	1:C:173:LYS:HE2	1.40	1.04
1:C:128:LYS:HD2	1:C:128:LYS:O	1.58	1.03
1:C:172:GLU:HG3	1:C:172:GLU:O	1.60	1.02
1:B:160:TYR:HE1	1:B:396:ALA:HA	1.26	1.00
1:C:319:TYR:OH	1:C:361:HIS:HD2	1.43	1.00
1:B:0:PHE:HB2	1:B:3:GLN:OE1	1.61	0.98
1:B:284:TYR:CD1	3:B:512:HOH:O	2.22	0.93
1:A:335:LEU:O	1:A:339:THR:HG22	1.70	0.91
1:C:314:LEU:HD13	1:C:351:PHE:CZ	2.04	0.91
1:A:-8:HIS:N	1:A:-7:HIS:HB2	1.85	0.91
1:C:182:ILE:O	1:C:186:ILE:HG22	1.71	0.91
1:C:335:LEU:O	1:C:339:THR:HG22	1.71	0.90
1:D:176:GLN:CD	1:D:234:GLN:NE2	2.24	0.90
1:C:334:THR:HA	3:C:511:HOH:O	1.73	0.89
1:B:57:ARG:HD3	3:B:557:HOH:O	1.70	0.88
1:D:176:GLN:NE2	1:D:234:GLN:NE2	2.21	0.88
1:A:135:THR:HG23	3:A:520:HOH:O	1.73	0.87
1:B:304:GLN:HG2	3:B:514:HOH:O	1.73	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:TYR:HA	3:A:553:HOH:O	1.74	0.86
1:A:390:THR:HG22	3:A:513:HOH:O	1.75	0.86
1:A:-8:HIS:CA	1:A:-7:HIS:HB2	2.06	0.86
1:B:275:TRP:HH2	1:B:397:PHE:CD1	1.94	0.85
1:D:197:ARG:HB3	3:D:525:HOH:O	1.77	0.85
1:D:74:HIS:HD2	3:D:522:HOH:O	1.62	0.83
1:B:151:MET:CE	1:B:157:GLY:HA2	2.09	0.82
1:D:192:ASN:HB3	3:D:541:HOH:O	1.79	0.82
1:B:42:GLU:HG2	3:B:532:HOH:O	1.79	0.82
1:D:335:LEU:O	1:D:339:THR:HG22	1.78	0.81
1:B:151:MET:HE3	1:B:157:GLY:HA2	1.62	0.81
1:C:391:LYS:HE3	3:C:532:HOH:O	1.80	0.81
1:A:197:ARG:CB	3:A:563:HOH:O	2.20	0.80
1:B:275:TRP:HZ3	1:B:397:PHE:CD2	1.98	0.80
1:C:128:LYS:CD	1:C:128:LYS:O	2.30	0.79
1:A:62:TYR:HD2	1:A:63:THR:HG23	1.46	0.79
1:C:314:LEU:CD1	1:C:351:PHE:CZ	2.66	0.79
1:C:319:TYR:OH	1:C:361:HIS:CD2	2.32	0.78
1:A:4:ARG:HG2	3:A:540:HOH:O	1.84	0.77
1:A:41:ARG:CG	1:A:41:ARG:HH11	1.97	0.77
1:A:294:ARG:HH11	1:A:294:ARG:HG2	1.48	0.76
1:C:128:LYS:HD2	1:C:128:LYS:C	2.06	0.76
1:C:314:LEU:CD1	1:C:351:PHE:CE2	2.69	0.76
1:A:62:TYR:CD2	1:A:63:THR:HG23	2.20	0.75
1:C:255:LYS:HE3	3:C:537:HOH:O	1.87	0.75
1:D:319:TYR:OH	1:D:361:HIS:HD2	1.68	0.75
1:A:294:ARG:CG	1:A:294:ARG:HH11	2.00	0.74
1:A:197:ARG:CA	3:A:563:HOH:O	2.34	0.74
1:C:275:TRP:HZ3	1:C:397:PHE:CD2	2.06	0.74
1:A:63:THR:HA	1:A:371:SER:HB2	1.70	0.73
1:C:314:LEU:HD12	1:C:351:PHE:CE2	2.22	0.73
1:B:275:TRP:CH2	1:B:397:PHE:CD1	2.77	0.73
1:C:154:GLY:C	3:C:555:HOH:O	2.27	0.73
1:A:-8:HIS:H	1:A:-7:HIS:HB2	1.53	0.73
1:B:162:LEU:HD12	1:B:174:ILE:HD13	1.69	0.72
1:A:357:GLU:HB3	1:A:360:GLU:HG3	1.70	0.72
1:B:0:PHE:HB3	3:B:556:HOH:O	1.90	0.72
1:C:275:TRP:HZ3	1:C:397:PHE:CE2	2.08	0.72
1:B:284:TYR:CD1	1:B:397:PHE:HE2	2.08	0.72
1:C:101:LYS:HE2	3:C:515:HOH:O	1.89	0.72
1:A:214:TYR:CD1	3:A:553:HOH:O	2.43	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:LEU:HD13	1:C:351:PHE:CE1	2.25	0.71
1:A:275:TRP:CD1	1:A:276:CYS:N	2.58	0.71
1:A:198:ASN:N	3:A:563:HOH:O	2.22	0.70
1:B:104:ILE:HG12	1:B:158:TYR:HB2	1.73	0.70
1:C:275:TRP:CZ3	1:C:397:PHE:CD2	2.79	0.70
1:C:300:CYS:HB2	3:C:559:HOH:O	1.90	0.70
1:A:319:TYR:OH	1:A:361:HIS:HD2	1.73	0.70
1:A:317:LYS:HE3	1:C:-8:HIS:HE1	1.57	0.70
1:C:14:ASN:C	1:C:14:ASN:HD22	1.95	0.70
1:A:264:CYS:HB3	3:A:553:HOH:O	1.91	0.69
1:A:4:ARG:CG	3:A:540:HOH:O	2.39	0.69
1:D:178:HIS:O	1:D:182:ILE:HG22	1.92	0.69
1:B:360:GLU:HG2	3:B:560:HOH:O	1.93	0.69
1:A:1:MET:HB3	1:A:271:LEU:HA	1.75	0.68
1:B:159:ILE:HA	1:B:162:LEU:HD23	1.74	0.68
1:A:317:LYS:HE3	1:C:-8:HIS:CE1	2.29	0.68
1:C:398:GLU:O	1:C:399:LEU:HB2	1.91	0.68
1:A:230:GLN:HG2	1:A:399:LEU:HD13	1.76	0.68
1:C:172:GLU:O	1:C:172:GLU:CG	2.31	0.68
1:D:395:PRO:O	1:D:396:ALA:HB3	1.92	0.68
1:D:1:MET:N	3:D:533:HOH:O	2.26	0.68
1:C:66:ALA:O	1:C:70:VAL:HG23	1.93	0.67
1:B:398:GLU:O	1:B:399:LEU:C	2.32	0.67
1:D:233:LEU:O	1:D:234:GLN:C	2.32	0.66
1:C:14:ASN:ND2	1:C:17:LEU:H	1.93	0.66
1:A:178:HIS:O	1:A:182:ILE:HG22	1.96	0.65
1:B:275:TRP:CZ3	1:B:397:PHE:CG	2.85	0.65
1:A:288:GLN:O	1:A:292:VAL:HG23	1.96	0.65
1:C:-4:MET:HE1	1:D:197:ARG:HD3	1.79	0.65
1:C:149:ASN:HD22	1:C:207:TYR:HD1	1.44	0.65
1:C:8:ASN:C	1:C:8:ASN:HD22	2.00	0.65
1:D:310:TRP:CE3	1:D:347:ARG:HG2	2.32	0.65
1:C:173:LYS:CA	1:C:173:LYS:HE2	2.18	0.64
1:C:339:THR:HG23	1:C:341:ASP:H	1.62	0.64
1:B:230:GLN:HA	1:B:230:GLN:OE1	1.97	0.64
1:D:8:ASN:ND2	1:D:10:TYR:H	1.95	0.64
1:B:275:TRP:CH2	1:B:397:PHE:CG	2.85	0.64
1:D:160:TYR:CE1	1:D:396:ALA:HA	2.31	0.64
1:A:181:GLN:O	1:A:185:THR:HG23	1.98	0.64
1:A:132:ASP:C	1:A:132:ASP:OD1	2.36	0.64
1:B:8:ASN:C	1:B:8:ASN:HD22	1.99	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:THR:HA	3:B:510:HOH:O	1.98	0.64
1:B:275:TRP:CZ3	1:B:397:PHE:CD2	2.84	0.64
1:D:14:ASN:ND2	1:D:16:SER:HB3	2.13	0.64
1:B:339:THR:O	1:B:340:GLN:HB2	1.98	0.63
1:B:393:ARG:HG3	1:B:398:GLU:HB3	1.80	0.63
1:B:398:GLU:O	1:B:399:LEU:HG	1.97	0.63
1:D:8:ASN:HD22	1:D:10:TYR:H	1.44	0.63
1:A:357:GLU:O	1:A:360:GLU:HG2	1.98	0.63
1:D:339:THR:O	1:D:340:GLN:HB2	1.98	0.62
1:C:251:VAL:HA	1:C:254:LEU:HD12	1.80	0.62
1:C:-4:MET:HA	1:C:-4:MET:HE3	1.80	0.62
1:A:290:TYR:CD1	1:A:299:LEU:HB2	2.36	0.61
1:B:160:TYR:CE1	1:B:396:ALA:CA	2.75	0.61
1:B:284:TYR:CD1	1:B:397:PHE:CE2	2.89	0.61
1:D:101:LYS:O	1:D:143:ILE:HD12	2.00	0.61
1:C:275:TRP:HH2	1:C:397:PHE:CD1	2.18	0.60
1:A:393:ARG:HD2	3:A:532:HOH:O	1.99	0.60
1:B:319:TYR:OH	1:B:361:HIS:HD2	1.83	0.60
1:C:128:LYS:CD	1:C:128:LYS:C	2.70	0.60
1:D:319:TYR:OH	1:D:361:HIS:CD2	2.54	0.60
1:D:181:GLN:O	1:D:185:THR:HG23	2.01	0.60
1:A:41:ARG:HG3	1:A:41:ARG:HH11	1.67	0.60
1:B:395:PRO:O	1:B:396:ALA:HB3	2.01	0.60
1:B:41:ARG:HD3	3:B:524:HOH:O	2.01	0.60
1:A:77:ASP:HB3	3:A:574:HOH:O	2.00	0.60
1:D:14:ASN:HD21	1:D:16:SER:HB3	1.67	0.60
1:B:279:ALA:O	1:B:283:ILE:HG22	2.02	0.59
1:B:166:ASN:O	1:B:169:PHE:O	2.21	0.59
1:B:86:GLN:HG3	3:B:571:HOH:O	2.02	0.59
1:C:230:GLN:HG2	1:C:399:LEU:HD13	1.82	0.59
1:C:364:ARG:HG2	3:C:539:HOH:O	2.02	0.59
1:D:92:VAL:HG11	1:D:117:ALA:HA	1.84	0.59
1:B:0:PHE:O	1:B:1:MET:C	2.38	0.59
1:A:264:CYS:CB	3:A:553:HOH:O	2.51	0.59
1:A:159:ILE:HG22	1:A:163:LEU:HD22	1.85	0.59
1:B:339:THR:HG23	1:B:341:ASP:H	1.68	0.58
1:C:155:ARG:N	3:C:555:HOH:O	2.35	0.58
1:C:178:HIS:O	1:C:182:ILE:HG12	2.02	0.58
1:C:-4:MET:HA	1:C:-4:MET:CE	2.33	0.58
1:D:310:TRP:CZ3	1:D:347:ARG:HG2	2.39	0.58
1:B:65:TRP:HB2	1:B:95:SER:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ARG:NH1	1:A:294:ARG:HG2	2.16	0.58
1:D:213:TYR:HB2	1:D:265:ILE:CG1	2.33	0.58
1:C:156:ILE:O	1:C:159:ILE:HB	2.04	0.58
1:B:155:ARG:HB3	1:B:182:ILE:HD11	1.84	0.58
1:A:218:ALA:HB2	1:A:276:CYS:HA	1.86	0.58
1:A:317:LYS:CE	1:C:-8:HIS:HE1	2.15	0.58
1:C:158:TYR:O	1:C:162:LEU:HD22	2.04	0.57
1:C:275:TRP:CZ3	1:C:397:PHE:CE2	2.92	0.57
1:A:107:LEU:HD13	3:A:562:HOH:O	2.04	0.57
1:D:235:VAL:HG12	1:D:235:VAL:O	2.03	0.57
1:C:275:TRP:CD1	1:C:276:CYS:N	2.73	0.57
1:B:151:MET:HE1	1:B:157:GLY:HA2	1.86	0.57
1:C:197:ARG:HD3	1:B:210:TYR:CE1	2.40	0.57
1:A:145:PRO:HD2	3:A:576:HOH:O	2.04	0.57
1:B:8:ASN:ND2	1:B:10:TYR:H	2.02	0.56
1:A:301:ASP:O	1:A:304:GLN:HB3	2.05	0.56
1:B:0:PHE:O	1:B:2:ALA:N	2.39	0.56
1:A:35:ARG:NH2	1:A:356:LEU:HD12	2.20	0.56
1:A:275:TRP:CD1	1:A:322:CYS:HA	2.41	0.56
1:D:213:TYR:HB2	1:D:265:ILE:HG12	1.87	0.56
1:A:63:THR:HA	1:A:371:SER:CB	2.35	0.56
1:B:186:ILE:HD12	1:B:228:LEU:HD21	1.88	0.56
1:C:63:THR:HA	1:C:371:SER:HB2	1.86	0.56
1:B:179:ILE:O	1:B:182:ILE:HG22	2.06	0.56
1:C:186:ILE:CD1	1:C:228:LEU:HD21	2.36	0.55
1:B:1:MET:O	1:B:2:ALA:C	2.41	0.55
1:B:122:HIS:CG	1:B:169:PHE:CE1	2.94	0.55
1:B:284:TYR:CE1	3:B:512:HOH:O	2.55	0.55
1:C:186:ILE:C	1:C:186:ILE:HD13	2.27	0.55
1:A:195:ARG:HD3	3:A:523:HOH:O	2.06	0.55
1:C:275:TRP:CH2	1:C:397:PHE:CG	2.94	0.55
1:A:62:TYR:HD2	1:A:63:THR:CG2	2.20	0.54
1:B:286:LEU:HD22	1:B:301:ASP:CB	2.38	0.54
1:C:364:ARG:NH2	3:C:503:HOH:O	2.38	0.54
1:B:286:LEU:HD22	1:B:301:ASP:HB2	1.89	0.54
1:C:156:ILE:HA	1:C:159:ILE:HG13	1.90	0.54
1:A:66:ALA:O	1:A:70:VAL:HG23	2.08	0.54
1:D:74:HIS:CD2	3:D:522:HOH:O	2.47	0.53
1:C:275:TRP:HH2	1:C:397:PHE:CG	2.26	0.53
1:B:104:ILE:O	1:B:104:ILE:HG12	2.09	0.53
1:A:192:ASN:N	1:A:192:ASN:HD22	2.05	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:TYR:OH	1:A:361:HIS:CD2	2.59	0.53
1:A:200:THR:HG22	3:A:507:HOH:O	2.09	0.53
1:A:275:TRP:CG	1:A:276:CYS:N	2.76	0.53
1:D:214:TYR:O	1:D:220:GLY:HA3	2.09	0.53
1:C:129:GLN:HA	1:C:132:ASP:HB2	1.90	0.53
1:A:178:HIS:O	1:A:182:ILE:CG2	2.57	0.52
1:B:295:GLU:OE2	1:B:297:LYS:HE2	2.09	0.52
1:B:262:PRO:HG2	3:B:550:HOH:O	2.08	0.52
1:B:399:LEU:OXT	1:B:399:LEU:HG	2.08	0.52
1:C:296:GLU:HG3	3:C:559:HOH:O	2.09	0.52
1:B:53:SER:HB3	3:B:553:HOH:O	2.08	0.52
1:B:186:ILE:CD1	1:B:228:LEU:HD21	2.40	0.52
1:B:288:GLN:NE2	1:B:292:VAL:HG23	2.24	0.52
1:B:0:PHE:H	1:B:3:GLN:NE2	2.07	0.52
1:A:4:ARG:CZ	3:A:540:HOH:O	2.57	0.52
1:B:8:ASN:HD22	1:B:9:PRO:N	2.07	0.52
1:A:4:ARG:CD	3:A:540:HOH:O	2.57	0.52
1:D:155:ARG:HB3	1:D:182:ILE:HD11	1.92	0.52
1:D:8:ASN:HD22	1:D:8:ASN:C	2.13	0.52
1:A:52:LYS:HE2	3:A:536:HOH:O	2.08	0.52
1:D:339:THR:HG23	1:D:341:ASP:H	1.75	0.52
1:D:240:LEU:HA	1:D:244:VAL:CG1	2.40	0.52
1:D:107:LEU:HD12	3:D:510:HOH:O	2.10	0.52
1:A:339:THR:HG23	1:A:341:ASP:H	1.73	0.51
1:D:13:TYR:HB2	1:D:346:TYR:CD1	2.45	0.51
1:B:279:ALA:N	1:B:280:PRO:CD	2.72	0.51
1:D:100:THR:HG23	3:D:543:HOH:O	2.10	0.51
1:C:314:LEU:CD1	1:C:351:PHE:CE1	2.91	0.51
1:D:264:CYS:SG	1:D:267:ASP:OD2	2.54	0.51
1:D:104:ILE:HG12	1:D:158:TYR:HB2	1.93	0.51
1:B:282:VAL:C	3:B:525:HOH:O	2.49	0.51
1:D:63:THR:HA	1:D:371:SER:HB2	1.94	0.50
1:A:366:PRO:HG2	1:A:369:PRO:HA	1.93	0.50
1:D:395:PRO:O	1:D:396:ALA:CB	2.58	0.50
1:B:319:TYR:OH	1:B:361:HIS:CD2	2.64	0.50
1:C:8:ASN:HD22	1:C:9:PRO:N	2.09	0.50
1:D:140:LEU:O	1:D:143:ILE:HG12	2.12	0.50
1:C:313:GLY:O	1:C:328:ASN:ND2	2.28	0.50
1:C:320:GLY:N	1:C:324:GLY:HA3	2.26	0.50
1:B:304:GLN:O	1:B:308:VAL:HG23	2.10	0.50
1:B:314:LEU:CD1	1:B:351:PHE:CZ	2.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:TYR:CZ	1:C:247:SER:HB3	2.47	0.50
1:B:236:SER:OG	1:B:239:LYS:HD2	2.11	0.50
1:B:284:TYR:N	3:B:525:HOH:O	2.45	0.50
1:C:230:GLN:HB3	1:C:233:LEU:HD13	1.94	0.50
1:C:50:GLY:HA3	1:C:370:PHE:CE1	2.47	0.50
1:B:280:PRO:HG3	1:B:309:ILE:HG12	1.94	0.49
1:C:130:ALA:O	1:C:133:CYS:HB2	2.12	0.49
1:B:107:LEU:HD21	1:B:373:PHE:CE2	2.47	0.49
1:B:230:GLN:HG3	1:B:399:LEU:HD11	1.94	0.49
1:C:275:TRP:CD1	1:C:322:CYS:HA	2.47	0.49
1:D:218:ALA:HB2	1:D:276:CYS:HA	1.94	0.49
1:A:-8:HIS:N	1:A:-7:HIS:CB	2.66	0.49
1:A:41:ARG:CG	1:A:41:ARG:NH1	2.68	0.49
1:C:62:TYR:CD2	1:C:63:THR:HG23	2.46	0.49
1:C:236:SER:OG	1:C:239:LYS:HG3	2.13	0.49
1:C:173:LYS:CA	1:C:173:LYS:CE	2.86	0.49
1:A:41:ARG:HG2	1:A:41:ARG:HH11	1.74	0.49
1:B:158:TYR:CE1	1:B:162:LEU:HD21	2.48	0.49
1:B:37:THR:O	1:B:41:ARG:HG3	2.12	0.49
1:D:220:GLY:O	1:D:224:ILE:HG13	2.13	0.49
1:B:262:PRO:CG	3:B:550:HOH:O	2.61	0.49
1:A:35:ARG:HH22	1:A:356:LEU:HD12	1.77	0.49
1:D:78:VAL:HG23	1:D:79:PHE:CD1	2.47	0.49
1:B:283:ILE:HA	1:B:286:LEU:HD12	1.95	0.49
1:B:62:TYR:HD2	1:B:63:THR:HG23	1.77	0.49
1:A:275:TRP:HH2	1:A:397:PHE:CD1	2.30	0.48
1:C:243:LEU:O	1:C:246:PRO:HD2	2.13	0.48
1:C:134:ILE:HD12	1:C:173:LYS:HG2	1.96	0.48
1:A:62:TYR:CD2	1:A:63:THR:CG2	2.93	0.48
1:C:343:LYS:O	1:C:346:TYR:HB3	2.13	0.48
1:A:41:ARG:NH1	3:A:526:HOH:O	2.47	0.48
1:B:146:HIS:CD2	3:B:522:HOH:O	2.67	0.48
1:A:213:TYR:CB	1:A:265:ILE:HD12	2.43	0.48
1:A:182:ILE:O	1:A:186:ILE:HG22	2.14	0.48
1:B:71:LEU:HG	1:B:75:LEU:HD22	1.95	0.47
1:C:186:ILE:HD12	1:C:228:LEU:HD21	1.94	0.47
1:C:159:ILE:HA	1:C:162:LEU:HD23	1.96	0.47
1:A:121:TYR:CD1	1:A:129:GLN:HB3	2.50	0.47
1:C:67:GLY:O	1:C:70:VAL:HB	2.14	0.47
1:B:226:TYR:CE2	1:B:284:TYR:HB3	2.50	0.47
1:D:132:ASP:O	1:D:136:ARG:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:LYS:HD2	1:C:39:LYS:HA	1.68	0.47
1:A:197:ARG:HA	3:A:563:HOH:O	2.10	0.47
1:A:212:GLU:HB2	1:A:214:TYR:CE2	2.50	0.47
1:D:394:PHE:CD2	1:D:395:PRO:HD2	2.49	0.47
1:A:183:CYS:HA	1:A:186:ILE:HG23	1.96	0.47
1:B:255:LYS:HB2	1:B:261:TYR:CE2	2.49	0.47
1:B:158:TYR:O	1:B:162:LEU:HD22	2.14	0.47
1:B:8:ASN:HD22	1:B:10:TYR:H	1.62	0.47
1:B:275:TRP:CD1	1:B:322:CYS:HA	2.50	0.47
1:C:14:ASN:ND2	1:C:14:ASN:C	2.65	0.47
1:D:240:LEU:HA	1:D:244:VAL:HG12	1.97	0.47
1:B:62:TYR:CD2	1:B:63:THR:HG23	2.49	0.47
1:C:336:TYR:CD1	1:C:345:LEU:HB2	2.51	0.47
1:C:237:GLN:O	1:C:241:HIS:HD2	1.98	0.47
1:C:336:TYR:HA	1:C:339:THR:CG2	2.45	0.46
1:A:159:ILE:HG22	1:A:163:LEU:CD2	2.45	0.46
1:A:274:HIS:O	1:A:280:PRO:HD2	2.15	0.46
1:A:138:ILE:HD11	1:A:174:ILE:HG13	1.96	0.46
1:B:283:ILE:HG23	3:B:512:HOH:O	2.15	0.46
1:C:12:ASP:HB2	3:C:548:HOH:O	2.15	0.46
1:D:279:ALA:N	1:D:280:PRO:CD	2.78	0.46
1:D:28:LEU:HD11	1:D:386:LEU:O	2.14	0.46
1:A:186:ILE:O	1:A:186:ILE:HG13	2.12	0.46
1:D:334:THR:HG23	1:D:398:GLU:OE1	2.14	0.46
1:B:321:LEU:O	1:B:394:PHE:HZ	1.98	0.46
1:D:71:LEU:HD22	1:D:377:ALA:HB1	1.96	0.46
1:C:262:PRO:HB2	1:C:267:ASP:HB2	1.97	0.46
1:A:314:LEU:HD13	1:A:351:PHE:CZ	2.51	0.46
1:C:264:CYS:HB2	1:C:267:ASP:OD1	2.16	0.46
1:D:1:MET:HB2	1:D:270:ASP:O	2.16	0.46
1:A:297:LYS:HE2	3:A:567:HOH:O	2.16	0.46
1:C:315:LEU:C	1:C:317:LYS:N	2.69	0.46
1:B:310:TRP:CE3	1:B:347:ARG:HG2	2.51	0.46
1:D:233:LEU:O	1:D:235:VAL:HG23	2.16	0.45
1:B:36:LEU:O	1:B:40:ILE:HG13	2.16	0.45
1:C:350:LYS:HA	1:C:350:LYS:HD3	1.71	0.45
1:C:240:LEU:HA	1:C:244:VAL:HG13	1.98	0.45
1:B:122:HIS:CD2	1:B:169:PHE:CE1	3.04	0.45
1:D:182:ILE:C	1:D:182:ILE:HD13	2.37	0.45
1:B:288:GLN:HE21	1:B:292:VAL:HG23	1.82	0.45
1:B:322:CYS:HB2	1:B:373:PHE:HD1	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:213:TYR:HB2	1:D:265:ILE:HG13	1.98	0.45
1:C:314:LEU:CD1	1:C:351:PHE:CD2	2.99	0.45
1:C:156:ILE:N	3:C:555:HOH:O	2.50	0.45
1:C:387:LEU:HA	1:C:387:LEU:HD12	1.85	0.45
1:B:203:SER:OG	1:B:205:LEU:O	2.29	0.44
1:B:63:THR:HA	1:B:371:SER:HB2	1.99	0.44
1:B:330:TYR:HB2	1:B:394:PHE:HD1	1.81	0.44
1:A:357:GLU:O	1:A:360:GLU:CG	2.64	0.44
1:C:197:ARG:HD2	1:C:213:TYR:OH	2.18	0.44
1:C:140:LEU:O	1:C:143:ILE:HG12	2.18	0.44
1:B:303:TYR:HD2	1:B:344:TYR:HH	1.62	0.44
1:C:283:ILE:HD13	1:C:287:ILE:HG12	1.99	0.44
1:B:-1:GLU:O	1:B:4:ARG:NH1	2.42	0.44
1:A:297:LYS:CE	3:A:567:HOH:O	2.65	0.44
1:D:96:LEU:HA	1:D:96:LEU:HD23	1.56	0.43
1:B:1:MET:HE2	1:B:270:ASP:OD2	2.18	0.43
1:D:253:GLN:HG2	1:D:253:GLN:O	2.19	0.43
1:D:351:PHE:O	1:D:354:TRP:HB3	2.17	0.43
1:B:320:GLY:O	1:B:324:GLY:HA3	2.18	0.43
1:D:88:ALA:O	1:D:92:VAL:HG23	2.17	0.43
1:D:214:TYR:HA	1:D:264:CYS:HB3	1.99	0.43
1:D:240:LEU:HD12	1:D:244:VAL:HG11	2.00	0.43
1:A:-1:GLU:OE1	1:A:269:ARG:NH2	2.40	0.43
1:A:201:ALA:HB3	3:A:527:HOH:O	2.19	0.43
1:A:120:LEU:O	1:A:120:LEU:HG	2.18	0.43
1:C:127:GLU:OE1	1:C:127:GLU:HA	2.18	0.43
1:B:1:MET:O	1:B:3:GLN:N	2.52	0.43
1:A:149:ASN:HD22	1:A:207:TYR:HD1	1.65	0.43
1:C:155:ARG:O	1:C:159:ILE:HG12	2.19	0.43
1:D:14:ASN:HD22	1:D:16:SER:H	1.66	0.43
1:B:122:HIS:CD2	1:B:169:PHE:HE1	2.37	0.43
1:D:315:LEU:HD11	1:D:328:ASN:HD21	1.84	0.43
1:A:350:LYS:O	1:A:353:GLU:HB3	2.19	0.43
1:C:251:VAL:O	1:C:254:LEU:HB2	2.19	0.43
1:A:4:ARG:NH1	3:A:540:HOH:O	2.51	0.42
1:A:41:ARG:NH1	1:A:41:ARG:HG3	2.33	0.42
1:C:296:GLU:HA	1:C:296:GLU:OE1	2.19	0.42
1:A:315:LEU:HD12	1:A:324:GLY:HA2	2.01	0.42
1:B:100:THR:C	1:B:101:LYS:HG2	2.39	0.42
1:A:-8:HIS:CB	1:A:-7:HIS:HB2	2.49	0.42
1:A:314:LEU:CD1	1:A:351:PHE:CZ	3.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:LYS:HE3	1:C:101:LYS:HB2	1.86	0.42
1:B:281:GLY:O	3:B:525:HOH:O	2.22	0.42
1:D:95:SER:O	1:D:98:CYS:HB2	2.20	0.42
1:C:201:ALA:HB3	3:C:563:HOH:O	2.18	0.42
1:C:244:VAL:O	1:C:245:LYS:C	2.58	0.42
1:D:350:LYS:O	1:D:353:GLU:HB3	2.18	0.42
1:D:60:THR:O	1:D:64:GLY:N	2.47	0.42
1:D:73:LEU:HD23	3:D:526:HOH:O	2.18	0.42
1:C:227:TYR:O	1:C:233:LEU:HD22	2.19	0.42
1:C:8:ASN:ND2	1:C:10:TYR:H	2.18	0.42
1:A:-7:HIS:HB3	1:A:-6:HIS:H	1.39	0.42
1:A:357:GLU:O	1:A:358:TYR:C	2.57	0.42
1:C:50:GLY:HA3	1:C:370:PHE:CZ	2.54	0.42
1:B:343:LYS:O	1:B:346:TYR:HB3	2.20	0.42
1:D:209:TRP:HE3	1:D:214:TYR:CE2	2.38	0.42
1:D:227:TYR:O	1:D:233:LEU:HD22	2.19	0.42
1:D:107:LEU:HD21	1:D:373:PHE:CZ	2.55	0.42
1:C:149:ASN:HA	1:C:155:ARG:H	1.86	0.41
1:B:330:TYR:CB	1:B:394:PHE:HD1	2.33	0.41
1:A:51:LEU:HD23	1:A:51:LEU:HA	1.87	0.41
1:D:39:LYS:HG2	1:D:356:LEU:HD22	2.03	0.41
1:A:213:TYR:HB3	1:A:265:ILE:HD12	2.01	0.41
1:B:21:TYR:O	1:B:28:LEU:HA	2.21	0.41
1:D:130:ALA:O	1:D:133:CYS:HB2	2.20	0.41
1:D:146:HIS:CD2	3:D:512:HOH:O	2.72	0.41
1:B:275:TRP:HZ3	1:B:397:PHE:CE2	2.38	0.41
1:C:335:LEU:C	1:C:339:THR:HG22	2.39	0.41
1:B:314:LEU:HD13	1:B:351:PHE:CZ	2.55	0.41
1:A:127:GLU:O	1:A:131:GLU:HB2	2.21	0.41
1:C:209:TRP:O	1:C:210:TYR:C	2.57	0.41
1:B:381:TYR:CZ	1:B:395:PRO:HB3	2.56	0.41
1:B:395:PRO:O	1:B:396:ALA:CB	2.66	0.41
1:B:262:PRO:CD	3:B:550:HOH:O	2.68	0.41
1:C:349:CYS:O	1:C:352:ALA:HB3	2.20	0.41
1:B:140:LEU:O	1:B:143:ILE:HG12	2.21	0.41
1:D:8:ASN:HD22	1:D:9:PRO:N	2.19	0.41
1:D:265:ILE:HG12	1:D:265:ILE:H	1.66	0.41
1:B:262:PRO:HA	1:B:263:PRO:HD3	1.86	0.41
1:B:290:TYR:CZ	1:B:299:LEU:HD22	2.56	0.41
1:C:68:ILE:H	1:C:68:ILE:HG12	1.70	0.41
1:D:75:LEU:HA	1:D:75:LEU:HD12	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:ILE:HG23	1:C:178:HIS:NE2	2.35	0.41
1:C:62:TYR:HD2	1:C:63:THR:HG23	1.86	0.41
1:B:96:LEU:HA	1:B:96:LEU:HD23	1.88	0.41
1:B:370:PHE:HA	1:B:376:MET:H	1.86	0.41
1:D:255:LYS:HB2	1:D:255:LYS:HE3	1.89	0.41
1:D:1:MET:HE3	1:D:273:VAL:HG22	2.02	0.41
1:C:315:LEU:C	1:C:317:LYS:H	2.24	0.41
1:D:37:THR:O	1:D:41:ARG:HG3	2.21	0.41
1:D:234:GLN:H	1:D:234:GLN:CD	2.23	0.40
1:D:337:ASN:HD21	1:D:390:THR:HA	1.86	0.40
1:A:96:LEU:HA	1:A:96:LEU:HD23	1.84	0.40
1:A:333:LEU:HA	1:A:333:LEU:HD12	1.94	0.40
1:B:93:LYS:HD3	3:B:517:HOH:O	2.21	0.40
1:D:198:ASN:N	3:D:525:HOH:O	2.34	0.40
1:B:186:ILE:C	1:B:186:ILE:HD13	2.42	0.40
1:A:122:HIS:HD2	1:A:127:GLU:OE1	2.04	0.40
1:A:22:PHE:CD1	1:A:345:LEU:HD13	2.57	0.40
1:B:288:GLN:HE21	1:B:292:VAL:CG2	2.35	0.40
1:D:315:LEU:HD12	1:D:324:GLY:HA2	2.02	0.40
1:D:233:LEU:O	1:D:235:VAL:N	2.54	0.40
1:D:159:ILE:HD11	1:D:182:ILE:HD12	2.04	0.40
1:C:39:LYS:O	1:C:40:ILE:C	2.59	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	407/411 (99%)	369 (91%)	37 (9%)	1 (0%)	52 77
1	B	399/411 (97%)	359 (90%)	38 (10%)	2 (0%)	34 60
1	C	407/411 (99%)	368 (90%)	38 (9%)	1 (0%)	52 77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	397/411 (97%)	359 (90%)	37 (9%)	1 (0%)	46 72
All	All	1610/1644 (98%)	1455 (90%)	150 (9%)	5 (0%)	46 72

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	-7	HIS
1	B	1	MET
1	C	112	GLY
1	D	216	GLY
1	B	320	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	341/343 (99%)	300 (88%)	41 (12%)	6 11
1	B	333/343 (97%)	293 (88%)	40 (12%)	6 11
1	C	341/343 (99%)	300 (88%)	41 (12%)	6 11
1	D	331/343 (96%)	293 (88%)	38 (12%)	7 12
All	All	1346/1372 (98%)	1186 (88%)	160 (12%)	6 11

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-9	HIS
1	A	-7	HIS
1	A	41	ARG
1	A	42	GLU
1	A	52	LYS
1	A	75	LEU
1	A	78	VAL
1	A	87	LEU
1	A	101	LYS

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Mol	Chain	Res	Type
1	A	114	LEU
1	A	120	LEU
1	A	132	ASP
1	A	135	THR
1	A	136	ARG
1	A	150	GLU
1	A	162	LEU
1	A	163	LEU
1	A	174	ILE
1	A	181	GLN
1	A	182	ILE
1	A	184	GLU
1	A	186	ILE
1	A	192	ASN
1	A	193	LEU
1	A	221	LEU
1	A	232	SER
1	A	244	VAL
1	A	264	CYS
1	A	269	ARG
1	A	271	LEU
1	A	275	TRP
1	A	294	ARG
1	A	314	LEU
1	A	333	LEU
1	A	334	THR
1	A	345	LEU
1	A	364	ARG
1	A	387	LEU
1	A	390	THR
1	A	393	ARG
1	A	399	LEU
1	C	-7	HIS
1	C	8	ASN
1	C	14	ASN
1	C	15	LYS
1	C	17	LEU
1	C	42	GLU
1	C	57	ARG
1	C	75	LEU
1	C	77	ASP
1	C	78	VAL

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Mol	Chain	Res	Type
1	C	87	LEU
1	C	101	LYS
1	C	114	LEU
1	C	128	LYS
1	C	129	GLN
1	C	132	ASP
1	C	142	LYS
1	C	162	LEU
1	C	163	LEU
1	C	173	LYS
1	C	180	GLN
1	C	181	GLN
1	C	182	ILE
1	C	186	ILE
1	C	192	ASN
1	C	193	LEU
1	C	221	LEU
1	C	240	LEU
1	C	243	LEU
1	C	244	VAL
1	C	253	GLN
1	C	269	ARG
1	C	275	TRP
1	C	283	ILE
1	C	333	LEU
1	C	338	LEU
1	C	345	LEU
1	C	364	ARG
1	C	387	LEU
1	C	390	THR
1	C	393	ARG
1	B	3	GLN
1	B	8	ASN
1	B	34	GLN
1	B	57	ARG
1	B	73	LEU
1	B	75	LEU
1	B	77	ASP
1	B	78	VAL
1	B	87	LEU
1	B	101	LYS
1	B	104	ILE

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Mol	Chain	Res	Type
1	B	114	LEU
1	B	119	VAL
1	B	128	LYS
1	B	129	GLN
1	B	132	ASP
1	B	135	THR
1	B	150	GLU
1	B	181	GLN
1	B	182	ILE
1	B	185	THR
1	B	186	ILE
1	B	193	LEU
1	B	199	PHE
1	B	221	LEU
1	B	230	GLN
1	B	234	GLN
1	B	255	LYS
1	B	264	CYS
1	B	268	ASN
1	B	269	ARG
1	B	275	TRP
1	B	276	CYS
1	B	294	ARG
1	B	333	LEU
1	B	345	LEU
1	B	364	ARG
1	B	387	LEU
1	B	393	ARG
1	B	399	LEU
1	D	3	GLN
1	D	8	ASN
1	D	57	ARG
1	D	73	LEU
1	D	75	LEU
1	D	77	ASP
1	D	87	LEU
1	D	92	VAL
1	D	104	ILE
1	D	107	LEU
1	D	120	LEU
1	D	128	LYS
1	D	135	THR

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Mol	Chain	Res	Type
1	D	146	HIS
1	D	150	GLU
1	D	167	LYS
1	D	171	VAL
1	D	174	ILE
1	D	181	GLN
1	D	182	ILE
1	D	193	LEU
1	D	200	THR
1	D	221	LEU
1	D	230	GLN
1	D	232	SER
1	D	233	LEU
1	D	264	CYS
1	D	269	ARG
1	D	272	LEU
1	D	276	CYS
1	D	294	ARG
1	D	311	GLN
1	D	314	LEU
1	D	333	LEU
1	D	334	THR
1	D	345	LEU
1	D	387	LEU
1	D	393	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-8	HIS
1	A	34	GLN
1	A	89	HIS
1	A	122	HIS
1	A	129	GLN
1	A	192	ASN
1	A	268	ASN
1	A	274	HIS
1	A	277	HIS
1	A	337	ASN
1	A	361	HIS
1	C	-8	HIS
1	C	-6	HIS

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Mol	Chain	Res	Type
1	C	8	ASN
1	C	14	ASN
1	C	38	ASN
1	C	86	GLN
1	C	97	ASN
1	C	192	ASN
1	C	237	GLN
1	C	241	HIS
1	C	274	HIS
1	C	311	GLN
1	C	337	ASN
1	C	361	HIS
1	B	3	GLN
1	B	8	ASN
1	B	34	GLN
1	B	89	HIS
1	B	97	ASN
1	B	122	HIS
1	B	176	GLN
1	B	181	GLN
1	B	192	ASN
1	B	274	HIS
1	B	288	GLN
1	B	311	GLN
1	B	361	HIS
1	D	3	GLN
1	D	8	ASN
1	D	14	ASN
1	D	89	HIS
1	D	176	GLN
1	D	192	ASN
1	D	234	GLN
1	D	274	HIS
1	D	311	GLN
1	D	337	ASN
1	D	361	HIS

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 4 ligands modelled in this entry, 4 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

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	409/411 (99%)	0.07	12 (2%)	55	48	54, 70, 94, 98	0
1	B	401/411 (97%)	0.15	13 (3%)	51	44	18, 72, 96, 102	0
1	C	409/411 (99%)	0.07	12 (2%)	55	48	56, 72, 96, 100	0
1	D	399/411 (97%)	0.24	14 (3%)	48	40	37, 74, 99, 107	0
All	All	1618/1644 (98%)	0.13	51 (3%)	51	44	18, 72, 96, 107	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	171	VAL	4.2
1	B	0	PHE	4.2
1	D	128	LYS	3.9
1	A	171	VAL	3.6
1	D	171	VAL	3.6
1	B	-1	GLU	3.4
1	B	396	ALA	3.3
1	A	399	LEU	3.2
1	D	275	TRP	3.0
1	C	201	ALA	3.0
1	A	396	ALA	2.9
1	B	275	TRP	2.8
1	A	394	PHE	2.8
1	B	171	VAL	2.7
1	C	394	PHE	2.7
1	B	57	ARG	2.6
1	D	280	PRO	2.6
1	B	139	HIS	2.6
1	C	396	ALA	2.6
1	D	218	ALA	2.5
1	D	269	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	294	ARG	2.5
1	D	217	ALA	2.5
1	A	395	PRO	2.5
1	B	329	ALA	2.4
1	D	151	MET	2.4
1	B	218	ALA	2.3
1	C	395	PRO	2.3
1	B	330	TYR	2.3
1	C	102	ARG	2.3
1	D	394	PHE	2.3
1	A	275	TRP	2.3
1	A	330	TYR	2.3
1	A	57	ARG	2.2
1	C	284	TYR	2.2
1	C	397	PHE	2.2
1	A	320	GLY	2.2
1	A	227	TYR	2.2
1	C	281	GLY	2.1
1	B	223	GLY	2.1
1	B	217	ALA	2.1
1	D	142	LYS	2.1
1	C	275	TRP	2.1
1	D	15	LYS	2.1
1	D	327	GLY	2.1
1	A	128	LYS	2.1
1	D	57	ARG	2.1
1	D	330	TYR	2.1
1	C	223	GLY	2.1
1	B	320	GLY	2.0
1	C	172	GLU	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

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
2	ZN	C	502	1/1	0.97	0.18	-1.01	66,66,66,66	0
2	ZN	A	501	1/1	0.97	0.18	-1.20	64,64,64,64	0
2	ZN	D	504	1/1	0.96	0.16	-	67,67,67,67	0
2	ZN	B	503	1/1	0.98	0.17	-	65,65,65,65	0

6.5 Other polymers

There are no such residues in this entry.