Full wwPDB X-ray Structure Validation Report ⓘ

Aug 14, 2023 – 12:45 PM EDT

PDB ID	:	5W2M
Title	:	APOBEC3F Catalytic Domain Complex with a Single-Stranded DNA
Authors	:	Fang, Y.; Xiao, X.; Li, S.-X.; Wolfe, A.; Chen, X.S.
Deposited on	:	2017-06-06
Resolution	:	3.70 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 ⓘ 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 ⓘ) were used in the production of this report:

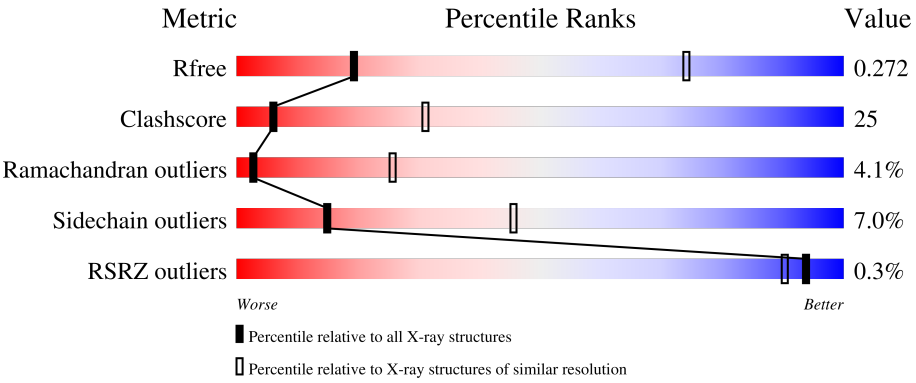
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.70 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	184	54% 39% 7%
1	B	184	% 53% 40% 7%
1	C	184	% 52% 40% 8%
1	D	184	51% 42% 8%
1	J	184	% 54% 39% 7%

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Mol	Chain	Length	Quality of chain
1	K	184	54% 39% 7%
1	L	184	51% 42% 8%
1	M	184	% 50% 42% 8%
2	E	10	10% 80% 10%
2	N	10	10% 80% 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12926 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 dC->dU-editing enzyme APOBEC-3F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	184	Total	C	N	O	S	0	0	0
			1565	1017	255	282	11			
1	B	184	Total	C	N	O	S	0	0	0
			1565	1017	255	282	11			
1	C	184	Total	C	N	O	S	0	0	0
			1565	1017	255	282	11			
1	D	184	Total	C	N	O	S	0	0	0
			1565	1017	255	282	11			
1	J	184	Total	C	N	O	S	0	0	0
			1565	1017	255	282	11			
1	K	184	Total	C	N	O	S	0	0	0
			1565	1017	255	282	11			
1	L	184	Total	C	N	O	S	0	0	0
			1565	1017	255	282	11			
1	M	184	Total	C	N	O	S	0	0	0
			1565	1017	255	282	11			

- Molecule 2 is a DNA chain called DNA (5'-D(P*TP*TP*TP*TP*TP*TP*TP*TP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	10	Total	C	N	O	P	0	0	0
			201	100	20	71	10			
2	N	10	Total	C	N	O	P	0	0	0
			201	100	20	71	10			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		

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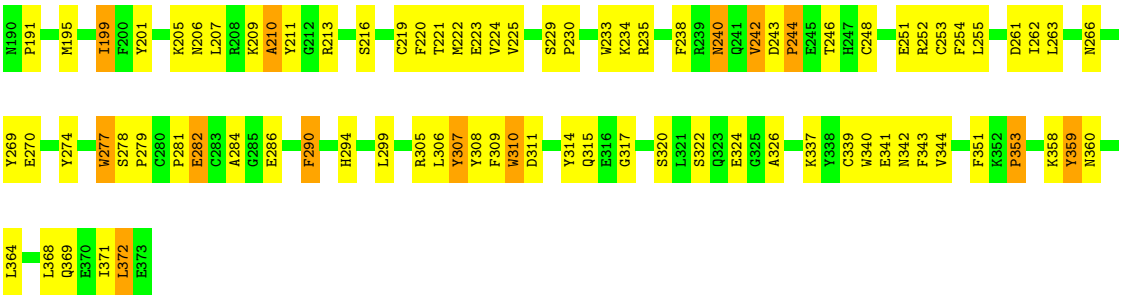
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	J	1	Total Zn 1 1	0	0
3	K	1	Total Zn 1 1	0	0

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.

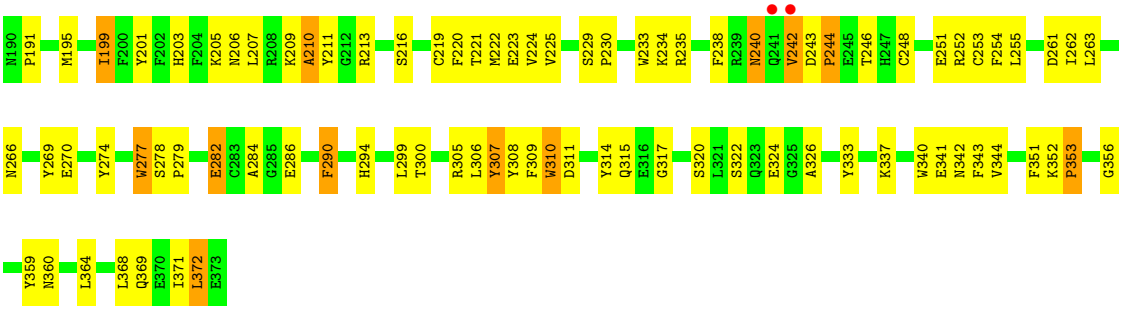
• Molecule 1: DNA dC->dU-editing enzyme APOBEC-3F

Chain A:



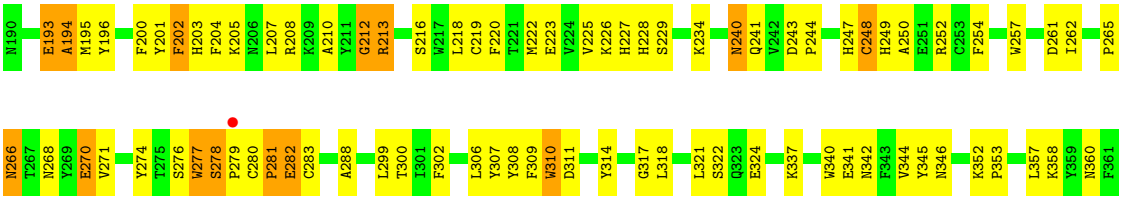
• Molecule 1: DNA dC->dU-editing enzyme APOBEC-3F

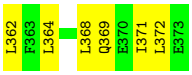
Chain B:



• Molecule 1: DNA dC->dU-editing enzyme APOBEC-3F

Chain C:



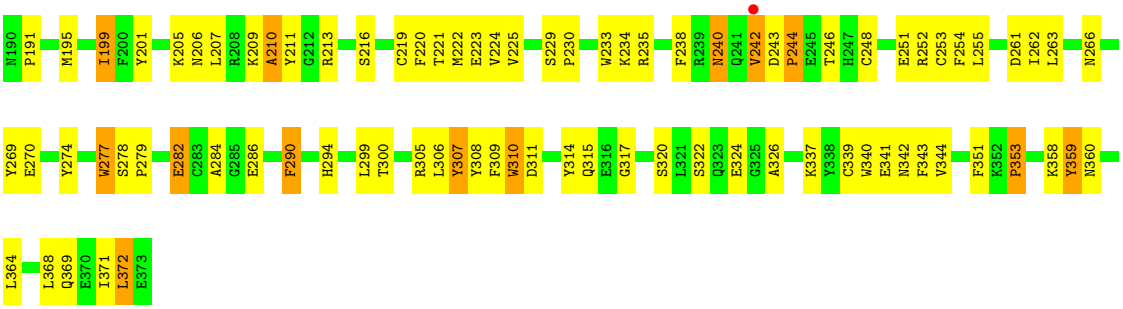


• Molecule 1: DNA dC->dU-editing enzyme APOBEC-3F

Chain D:

• Molecule 1: DNA dC->dU-editing enzyme APOBEC-3F

Chain J:

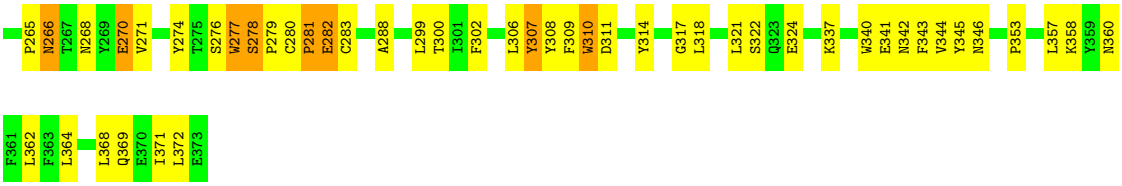


• Molecule 1: DNA dC->dU-editing enzyme APOBEC-3F

Chain K:

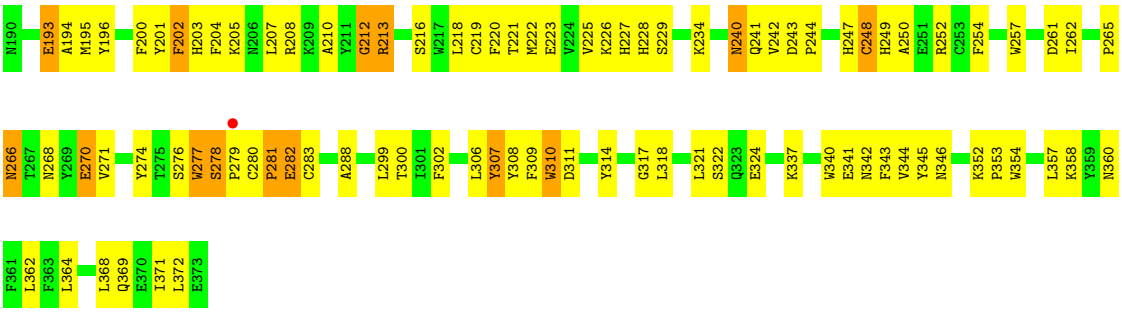
• Molecule 1: DNA dC->dU-editing enzyme APOBEC-3F

Chain L:



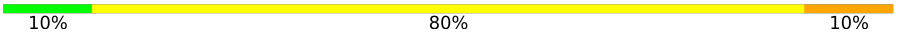
• Molecule 1: DNA dC->dU-editing enzyme APOBEC-3F

Chain M:



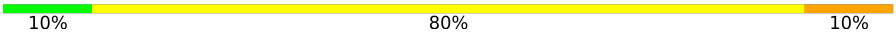
• Molecule 2: DNA (5'-D(P*TP*TP*TP*TP*TP*TP*TP*TP*TP*T)-3')

Chain E:



• Molecule 2: DNA (5'-D(P*TP*TP*TP*TP*TP*TP*TP*TP*TP*T)-3')

Chain N:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	68.19Å 108.49Å 108.55Å 79.60° 71.80° 71.75°	Depositor
Resolution (Å)	50.00 – 3.70 47.74 – 3.67	Depositor EDS
% Data completeness (in resolution range)	96.4 (50.00-3.70) 95.1 (47.74-3.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.35 (at 3.67Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.250 , 0.267 0.258 , 0.272	Depositor DCC
R_{free} test set	2866 reflections (9.84%)	wwPDB-VP
Wilson B-factor (Å^2)	87.7	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 33.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.327 for h,h-k,h-l 0.307 for -h,-l,-k 0.317 for -h,-h+l,-h+k	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	12926	wwPDB-VP
Average B, all atoms (Å^2)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.56% 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

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	0.37	0/1623	0.52	0/2204
1	B	0.36	0/1623	0.52	0/2204
1	C	0.38	0/1623	0.55	0/2204
1	D	0.38	0/1623	0.55	0/2204
1	J	0.36	0/1623	0.52	0/2204
1	K	0.37	0/1623	0.52	0/2204
1	L	0.38	0/1623	0.55	0/2204
1	M	0.38	0/1623	0.55	0/2204
2	E	0.72	1/220 (0.5%)	0.87	0/336
2	N	0.72	1/220 (0.5%)	0.86	0/336
All	All	0.39	2/13424 (0.0%)	0.55	0/18304

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	901	DT	OP3-P	-7.27	1.52	1.61
2	E	901	DT	OP3-P	-7.10	1.52	1.61

There are no bond angle outliers.

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	1565	0	1443	70	0
1	B	1565	0	1443	73	0
1	C	1565	0	1443	76	0
1	D	1565	0	1443	82	0
1	J	1565	0	1443	66	0
1	K	1565	0	1443	74	0
1	L	1565	0	1443	81	0
1	M	1565	0	1443	84	0
2	E	201	0	121	21	0
2	N	201	0	121	23	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
All	All	12926	0	11786	611	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 25.

All (611) 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:K:351:PHE:HB3	2:N:908:DT:H72	1.55	0.87
1:B:207:LEU:HB2	1:B:210:ALA:HB2	1.57	0.87
1:K:207:LEU:HB2	1:K:210:ALA:HB2	1.57	0.87
1:A:207:LEU:HB2	1:A:210:ALA:HB2	1.58	0.85
1:J:207:LEU:HB2	1:J:210:ALA:HB2	1.59	0.85
1:B:351:PHE:HB3	2:E:908:DT:H72	1.60	0.84
1:D:280:CYS:SG	1:D:281:PRO:HD2	2.19	0.82
1:M:280:CYS:SG	1:M:281:PRO:HD2	2.22	0.80
2:N:906:DT:H2"	2:N:907:DT:OP1	1.82	0.79
1:A:262:ILE:HG22	1:A:263:LEU:H	1.48	0.79
1:C:280:CYS:SG	1:C:281:PRO:HD2	2.24	0.78
2:E:906:DT:H2"	2:E:907:DT:OP1	1.82	0.78
1:L:280:CYS:SG	1:L:281:PRO:HD2	2.23	0.78
1:K:262:ILE:HG22	1:K:263:LEU:H	1.49	0.78
1:M:341:GLU:C	1:M:342:ASN:HD22	1.87	0.77
1:C:341:GLU:C	1:C:342:ASN:HD22	1.87	0.77
1:J:262:ILE:HG22	1:J:263:LEU:H	1.49	0.77
1:K:223:GLU:HB3	1:K:270:GLU:HB2	1.65	0.77
1:B:262:ILE:HG22	1:B:263:LEU:H	1.49	0.77
1:D:341:GLU:C	1:D:342:ASN:HD22	1.88	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:341:GLU:C	1:L:342:ASN:HD22	1.88	0.77
1:B:223:GLU:HB3	1:B:270:GLU:HB2	1.67	0.76
1:A:223:GLU:HB3	1:A:270:GLU:HB2	1.67	0.76
2:E:907:DT:OP1	2:E:907:DT:H4'	1.86	0.75
1:J:223:GLU:HB3	1:J:270:GLU:HB2	1.67	0.75
2:N:907:DT:OP1	2:N:907:DT:H4'	1.87	0.74
1:L:248:CYS:HB2	1:L:252:ARG:HB2	1.73	0.71
1:C:248:CYS:HB2	1:C:252:ARG:HB2	1.73	0.70
1:B:353:PRO:HG3	2:E:907:DT:H2'	1.74	0.70
1:D:248:CYS:HB2	1:D:252:ARG:HB2	1.74	0.69
1:M:248:CYS:HB2	1:M:252:ARG:HB2	1.75	0.69
1:K:353:PRO:HG3	2:N:907:DT:H2'	1.74	0.68
1:M:257:TRP:O	1:M:261:ASP:HB2	1.93	0.68
1:C:257:TRP:O	1:C:261:ASP:HB2	1.94	0.68
1:L:222:MET:CB	1:L:234:LYS:HB2	2.24	0.68
1:B:221:THR:HG23	1:B:343:PHE:HZ	1.59	0.68
1:C:222:MET:HG3	1:C:223:GLU:H	1.59	0.68
1:C:222:MET:CB	1:C:234:LYS:HB2	2.24	0.68
1:D:222:MET:CB	1:D:234:LYS:HB2	2.24	0.68
1:L:257:TRP:O	1:L:261:ASP:HB2	1.94	0.68
1:M:222:MET:CB	1:M:234:LYS:HB2	2.24	0.68
1:L:271:VAL:HG23	1:L:299:LEU:HD13	1.77	0.67
1:D:257:TRP:O	1:D:261:ASP:HB2	1.94	0.67
1:M:222:MET:HG3	1:M:223:GLU:H	1.60	0.67
1:D:222:MET:HB3	1:D:234:LYS:HB2	1.77	0.67
1:L:222:MET:HG3	1:L:223:GLU:H	1.59	0.67
1:J:307:TYR:HB3	1:J:314:TYR:CE2	2.29	0.67
1:L:222:MET:HB3	1:L:234:LYS:HB2	1.77	0.67
1:B:307:TYR:HB3	1:B:314:TYR:CE2	2.29	0.66
1:K:307:TYR:HB3	1:K:314:TYR:CE2	2.30	0.66
1:J:315:GLN:HG2	1:J:371:ILE:HD13	1.77	0.66
1:C:222:MET:HB3	1:C:234:LYS:HB2	1.76	0.66
1:A:307:TYR:HB3	1:A:314:TYR:CE2	2.31	0.66
1:J:221:THR:HG23	1:J:343:PHE:HZ	1.61	0.66
1:B:315:GLN:HG2	1:B:371:ILE:HD13	1.78	0.65
1:D:271:VAL:HG23	1:D:299:LEU:HD13	1.79	0.65
1:K:360:ASN:O	1:K:364:LEU:HD23	1.96	0.65
1:K:315:GLN:HG2	1:K:371:ILE:HD13	1.78	0.65
1:A:315:GLN:HG2	1:A:371:ILE:HD13	1.79	0.65
1:D:222:MET:HG3	1:D:223:GLU:H	1.61	0.65
1:B:360:ASN:O	1:B:364:LEU:HD23	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:271:VAL:HG23	1:M:299:LEU:HD13	1.79	0.65
1:A:360:ASN:O	1:A:364:LEU:HD23	1.97	0.65
1:M:222:MET:HB3	1:M:234:LYS:HB2	1.78	0.65
1:A:221:THR:HG23	1:A:343:PHE:HZ	1.61	0.64
1:C:271:VAL:HG23	1:C:299:LEU:HD13	1.79	0.64
1:J:195:MET:HB3	1:J:199:ILE:CG2	2.28	0.64
1:A:219:CYS:HB2	1:A:274:TYR:HB2	1.80	0.64
1:B:219:CYS:HB2	1:B:274:TYR:HB2	1.79	0.63
1:J:219:CYS:HB2	1:J:274:TYR:HB2	1.79	0.63
1:J:360:ASN:O	1:J:364:LEU:HD23	1.98	0.63
1:L:277:TRP:HA	1:L:277:TRP:CE3	2.34	0.63
1:B:195:MET:HB3	1:B:199:ILE:CG2	2.29	0.63
1:B:337:LYS:O	1:B:341:GLU:HG3	1.98	0.63
1:K:219:CYS:HB2	1:K:274:TYR:HB2	1.81	0.62
1:A:195:MET:HB3	1:A:199:ILE:CG2	2.29	0.62
1:K:221:THR:HG23	1:K:343:PHE:HZ	1.62	0.62
1:A:337:LYS:O	1:A:341:GLU:HG3	1.99	0.62
1:M:277:TRP:CE3	1:M:277:TRP:HA	2.35	0.62
1:A:320:SER:O	1:A:324:GLU:HG2	2.00	0.61
1:K:320:SER:O	1:K:324:GLU:HG2	2.00	0.61
1:D:277:TRP:HA	1:D:277:TRP:CE3	2.35	0.61
1:M:200:PHE:O	1:M:204:PHE:HB2	2.01	0.61
1:L:277:TRP:HA	1:L:277:TRP:HE3	1.65	0.61
1:D:342:ASN:HD22	1:D:342:ASN:N	1.98	0.61
1:M:277:TRP:HA	1:M:277:TRP:HE3	1.66	0.61
1:C:277:TRP:O	1:C:278:SER:O	2.19	0.61
1:K:337:LYS:O	1:K:341:GLU:HG3	2.00	0.61
1:B:320:SER:O	1:B:324:GLU:HG2	2.01	0.60
1:C:277:TRP:HA	1:C:277:TRP:CE3	2.35	0.60
1:J:320:SER:O	1:J:324:GLU:HG2	2.01	0.60
1:B:213:ARG:HG2	1:B:305:ARG:NH2	2.17	0.60
1:C:277:TRP:HA	1:C:277:TRP:HE3	1.67	0.60
1:J:337:LYS:O	1:J:341:GLU:HG3	2.00	0.60
1:K:195:MET:HB3	1:K:199:ILE:CG2	2.31	0.60
1:L:342:ASN:HD22	1:L:342:ASN:N	1.99	0.60
1:M:277:TRP:O	1:M:278:SER:O	2.20	0.60
1:K:213:ARG:HG2	1:K:305:ARG:NH2	2.16	0.60
1:K:201:TYR:O	1:K:205:LYS:HG3	2.02	0.59
1:M:309:PHE:O	1:M:371:ILE:HD11	2.02	0.59
1:C:309:PHE:O	1:C:371:ILE:HD11	2.02	0.59
1:J:205:LYS:HE2	1:J:207:LEU:HD11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:CYS:HB2	1:B:252:ARG:HB2	1.83	0.59
1:K:248:CYS:HB2	1:K:252:ARG:HB2	1.83	0.59
1:L:277:TRP:O	1:L:278:SER:O	2.20	0.59
1:D:277:TRP:HA	1:D:277:TRP:HE3	1.67	0.59
1:J:322:SER:OG	1:J:372:LEU:HD11	2.02	0.58
1:B:233:TRP:O	1:B:234:LYS:HG2	2.03	0.58
1:D:277:TRP:O	1:D:278:SER:O	2.21	0.58
1:J:248:CYS:HB2	1:J:252:ARG:HB2	1.83	0.58
1:A:213:ARG:HG2	1:A:305:ARG:NH2	2.18	0.58
1:B:222:MET:HB3	1:B:234:LYS:HB2	1.86	0.58
1:J:233:TRP:O	1:J:234:LYS:HG2	2.03	0.58
1:A:248:CYS:HB2	1:A:252:ARG:HB2	1.84	0.58
1:D:309:PHE:O	1:D:371:ILE:HD11	2.03	0.58
1:A:205:LYS:HE2	1:A:207:LEU:HD11	1.86	0.58
1:B:222:MET:CB	1:B:234:LYS:HB2	2.34	0.58
1:C:200:PHE:O	1:C:204:PHE:HB2	2.04	0.58
1:A:222:MET:CB	1:A:234:LYS:HB2	2.34	0.58
1:B:368:LEU:HD21	1:B:372:LEU:HD22	1.85	0.57
1:L:309:PHE:O	1:L:371:ILE:HD11	2.03	0.57
1:A:222:MET:HB3	1:A:234:LYS:HB2	1.86	0.57
1:K:205:LYS:HE2	1:K:207:LEU:HD11	1.86	0.57
1:D:202:PHE:HD2	1:D:202:PHE:O	1.87	0.57
1:J:222:MET:HB3	1:J:234:LYS:HB2	1.87	0.57
1:K:322:SER:OG	1:K:372:LEU:HD11	2.04	0.57
1:B:205:LYS:HE2	1:B:207:LEU:HD11	1.86	0.57
1:J:222:MET:CB	1:J:234:LYS:HB2	2.35	0.57
1:K:201:TYR:OH	1:K:351:PHE:O	2.18	0.57
1:A:233:TRP:O	1:A:234:LYS:HG2	2.04	0.57
1:A:322:SER:OG	1:A:372:LEU:HD11	2.04	0.57
1:C:243:ASP:HB2	1:C:244:PRO:HD2	1.87	0.57
1:K:222:MET:CB	1:K:234:LYS:HB2	2.35	0.57
1:C:342:ASN:HD22	1:C:342:ASN:N	1.98	0.57
1:K:222:MET:HB3	1:K:234:LYS:HB2	1.87	0.56
1:J:213:ARG:HG2	1:J:305:ARG:NH2	2.21	0.56
1:L:202:PHE:HD2	1:L:202:PHE:O	1.88	0.56
1:M:202:PHE:HD2	1:M:202:PHE:O	1.88	0.56
1:J:201:TYR:O	1:J:205:LYS:HG3	2.05	0.56
1:K:233:TRP:O	1:K:234:LYS:HG2	2.04	0.56
1:M:243:ASP:HB2	1:M:244:PRO:HD2	1.88	0.56
1:J:282:GLU:CD	1:J:282:GLU:H	2.09	0.56
1:M:342:ASN:HD22	1:M:342:ASN:N	1.99	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:SER:OG	1:B:372:LEU:HD11	2.05	0.56
1:B:282:GLU:H	1:B:282:GLU:CD	2.09	0.56
1:K:282:GLU:CD	1:K:282:GLU:H	2.08	0.56
1:K:368:LEU:HD21	1:K:372:LEU:HD22	1.87	0.56
1:A:282:GLU:CD	1:A:282:GLU:H	2.09	0.55
1:A:282:GLU:O	1:A:286:GLU:HB2	2.06	0.55
1:D:358:LYS:O	1:D:362:LEU:HG	2.06	0.55
1:J:368:LEU:HD21	1:J:372:LEU:HD22	1.87	0.55
1:A:368:LEU:HD21	1:A:372:LEU:HD22	1.87	0.55
1:D:243:ASP:HB2	1:D:244:PRO:HD2	1.88	0.55
1:M:358:LYS:O	1:M:362:LEU:HG	2.06	0.55
1:B:282:GLU:O	1:B:286:GLU:HB2	2.06	0.55
1:C:207:LEU:HB3	1:C:210:ALA:HB3	1.89	0.55
1:J:282:GLU:O	1:J:286:GLU:HB2	2.06	0.55
1:L:243:ASP:HB2	1:L:244:PRO:HD2	1.88	0.55
1:B:351:PHE:HB3	2:E:908:DT:C7	2.35	0.55
2:E:906:DT:H1'	2:E:907:DT:OP2	2.06	0.55
1:K:216:SER:HB3	1:K:277:TRP:HB2	1.88	0.55
1:M:201:TYR:O	1:M:205:LYS:HG3	2.07	0.55
1:M:207:LEU:HB3	1:M:210:ALA:HB3	1.89	0.55
1:B:201:TYR:O	1:B:205:LYS:HG3	2.07	0.55
1:M:344:VAL:O	1:M:346:ASN:N	2.40	0.55
1:A:290:PHE:HE2	1:A:294:HIS:ND1	2.05	0.55
1:C:344:VAL:O	1:C:346:ASN:N	2.40	0.55
2:E:910:DT:H3'	1:M:352:LYS:NZ	2.21	0.55
1:K:282:GLU:O	1:K:286:GLU:HB2	2.07	0.54
1:L:360:ASN:N	1:L:360:ASN:HD22	2.05	0.54
1:J:290:PHE:HE2	1:J:294:HIS:ND1	2.05	0.54
1:A:252:ARG:HH21	1:A:282:GLU:CG	2.19	0.54
1:J:224:VAL:HG22	1:J:269:TYR:CE1	2.42	0.54
2:N:906:DT:H1'	2:N:907:DT:OP2	2.06	0.54
1:B:224:VAL:HG22	1:B:269:TYR:CE1	2.43	0.54
1:B:224:VAL:HG22	1:B:269:TYR:HE1	1.73	0.54
1:B:252:ARG:HH21	1:B:282:GLU:CG	2.21	0.54
1:B:290:PHE:HE2	1:B:294:HIS:ND1	2.06	0.54
1:C:358:LYS:O	1:C:362:LEU:HG	2.08	0.54
1:D:358:LYS:HB2	2:E:901:DT:H1'	1.89	0.54
1:D:360:ASN:N	1:D:360:ASN:HD22	2.06	0.54
1:L:358:LYS:O	1:L:362:LEU:HG	2.08	0.54
1:M:360:ASN:HD22	1:M:360:ASN:N	2.05	0.54
1:K:299:LEU:O	1:K:326:ALA:HA	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:TYR:OH	1:A:351:PHE:O	2.20	0.54
1:M:322:SER:CB	1:M:372:LEU:HD11	2.38	0.54
1:C:360:ASN:N	1:C:360:ASN:HD22	2.06	0.53
1:D:240:ASN:HD22	1:D:240:ASN:N	2.06	0.53
1:J:224:VAL:HG22	1:J:269:TYR:HE1	1.73	0.53
1:D:207:LEU:HB3	1:D:210:ALA:HB3	1.89	0.53
1:D:368:LEU:HD23	1:D:368:LEU:C	2.29	0.53
1:J:277:TRP:HA	1:J:277:TRP:CE3	2.43	0.53
1:J:201:TYR:OH	1:J:351:PHE:O	2.18	0.53
1:B:277:TRP:HA	1:B:277:TRP:CE3	2.43	0.53
1:K:290:PHE:HE2	1:K:294:HIS:ND1	2.06	0.53
1:L:207:LEU:HB3	1:L:210:ALA:HB3	1.90	0.53
1:A:201:TYR:O	1:A:205:LYS:HG3	2.09	0.53
1:J:252:ARG:HH21	1:J:282:GLU:CG	2.22	0.53
1:A:224:VAL:HG22	1:A:269:TYR:CE1	2.43	0.53
1:D:344:VAL:O	1:D:346:ASN:N	2.42	0.53
1:L:344:VAL:O	1:L:346:ASN:N	2.41	0.53
1:A:277:TRP:CE3	1:A:277:TRP:HA	2.43	0.53
1:L:368:LEU:C	1:L:368:LEU:HD23	2.29	0.53
1:C:322:SER:CB	1:C:372:LEU:HD11	2.39	0.53
1:C:368:LEU:C	1:C:368:LEU:HD23	2.29	0.53
1:A:224:VAL:HG22	1:A:269:TYR:HE1	1.74	0.52
1:D:200:PHE:O	1:D:204:PHE:HB2	2.09	0.52
1:K:351:PHE:HB3	2:N:908:DT:C7	2.32	0.52
1:M:318:LEU:O	1:M:318:LEU:HD23	2.09	0.52
1:J:299:LEU:O	1:J:326:ALA:HA	2.09	0.52
1:B:201:TYR:OH	1:B:351:PHE:O	2.18	0.52
1:D:317:GLY:O	1:D:321:LEU:HB2	2.09	0.52
1:D:322:SER:CB	1:D:372:LEU:HD11	2.39	0.52
1:L:240:ASN:N	1:L:240:ASN:HD22	2.08	0.52
1:L:322:SER:CB	1:L:372:LEU:HD11	2.39	0.52
1:M:280:CYS:HB3	1:M:283:CYS:SG	2.50	0.52
1:B:299:LEU:O	1:B:326:ALA:HA	2.10	0.52
1:D:280:CYS:HB3	1:D:283:CYS:SG	2.50	0.52
1:K:277:TRP:CE3	1:K:277:TRP:HA	2.43	0.52
1:D:226:LYS:HB2	1:D:229:SER:HB3	1.92	0.52
1:M:207:LEU:HB3	1:M:210:ALA:CB	2.39	0.52
1:A:299:LEU:O	1:A:326:ALA:HA	2.10	0.52
1:J:255:LEU:HD22	1:J:290:PHE:CD1	2.45	0.52
1:L:248:CYS:CB	1:L:252:ARG:HB2	2.39	0.52
1:M:216:SER:HB3	1:M:277:TRP:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:317:GLY:O	1:C:321:LEU:HB2	2.09	0.52
1:D:201:TYR:O	1:D:205:LYS:HG3	2.08	0.52
1:M:368:LEU:C	1:M:368:LEU:HD23	2.30	0.52
1:J:195:MET:HB3	1:J:199:ILE:HG21	1.91	0.52
1:L:318:LEU:HD23	1:L:318:LEU:O	2.09	0.52
1:B:255:LEU:HD22	1:B:290:PHE:CD1	2.45	0.52
1:K:243:ASP:HB2	1:K:244:PRO:HD2	1.92	0.52
1:M:317:GLY:O	1:M:321:LEU:HB2	2.10	0.52
1:L:226:LYS:HB2	1:L:229:SER:HB3	1.92	0.51
1:M:225:VAL:HG23	1:M:268:ASN:HB2	1.92	0.51
1:C:225:VAL:HG23	1:C:268:ASN:HB2	1.92	0.51
1:K:224:VAL:HG22	1:K:269:TYR:CE1	2.45	0.51
1:L:271:VAL:HG23	1:L:299:LEU:CD1	2.40	0.51
1:A:243:ASP:HB2	1:A:244:PRO:HD2	1.93	0.51
1:B:310:TRP:CH2	1:D:270:GLU:HB2	2.45	0.51
1:L:207:LEU:HB3	1:L:210:ALA:CB	2.40	0.51
1:K:255:LEU:HD22	1:K:290:PHE:CD1	2.45	0.51
1:A:359:TYR:N	2:E:904:DT:OP2	2.37	0.51
1:C:318:LEU:O	1:C:318:LEU:HD23	2.11	0.51
1:D:207:LEU:HB3	1:D:210:ALA:CB	2.40	0.51
1:K:252:ARG:HH21	1:K:282:GLU:CG	2.23	0.51
1:L:222:MET:HB2	1:L:234:LYS:HB2	1.92	0.51
1:C:207:LEU:HB3	1:C:210:ALA:CB	2.40	0.51
1:C:240:ASN:N	1:C:240:ASN:HD22	2.08	0.51
1:K:224:VAL:HG22	1:K:269:TYR:HE1	1.76	0.51
1:L:317:GLY:O	1:L:321:LEU:HB2	2.11	0.51
1:C:202:PHE:HD2	1:C:202:PHE:O	1.94	0.51
1:M:226:LYS:HB2	1:M:229:SER:HB3	1.93	0.51
1:C:226:LYS:HB2	1:C:229:SER:HB3	1.93	0.51
1:D:248:CYS:CB	1:D:252:ARG:HB2	2.40	0.51
1:K:240:ASN:C	1:K:240:ASN:HD22	2.14	0.51
1:D:354:TRP:O	2:E:901:DT:H4'	2.10	0.50
1:M:222:MET:HB2	1:M:234:LYS:HB2	1.93	0.50
1:M:241:GLN:HB2	1:M:247:HIS:O	2.12	0.50
1:A:255:LEU:HD22	1:A:290:PHE:CD1	2.46	0.50
1:C:248:CYS:CB	1:C:252:ARG:HB2	2.40	0.50
1:D:216:SER:HB3	1:D:277:TRP:HB3	1.92	0.50
1:L:310:TRP:HD1	1:L:311:ASP:N	2.10	0.50
1:D:196:TYR:CD2	1:D:196:TYR:N	2.79	0.50
1:C:241:GLN:HB2	1:C:247:HIS:O	2.12	0.50
1:D:225:VAL:HG23	1:D:268:ASN:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:241:GLN:HB2	1:D:247:HIS:O	2.11	0.50
1:C:201:TYR:O	1:C:205:LYS:HG3	2.12	0.50
1:A:240:ASN:C	1:A:240:ASN:HD22	2.14	0.50
1:L:249:HIS:O	1:L:250:ALA:HB3	2.12	0.50
1:M:271:VAL:HG23	1:M:299:LEU:CD1	2.42	0.50
1:D:222:MET:HB2	1:D:234:LYS:HB2	1.93	0.50
1:D:271:VAL:HG23	1:D:299:LEU:CD1	2.41	0.50
1:L:193:GLU:O	1:L:194:ALA:HB2	2.11	0.50
1:A:191:PRO:HB3	1:A:238:PHE:CE1	2.47	0.50
1:A:242:VAL:HG12	1:A:242:VAL:O	2.11	0.50
1:C:193:GLU:O	1:C:194:ALA:HB2	2.12	0.50
1:L:309:PHE:HB2	1:L:371:ILE:HD11	1.94	0.50
1:L:201:TYR:O	1:L:205:LYS:HG3	2.11	0.49
1:C:222:MET:HB2	1:C:234:LYS:HB2	1.94	0.49
1:C:310:TRP:HD1	1:C:311:ASP:N	2.10	0.49
1:D:310:TRP:HD1	1:D:311:ASP:N	2.10	0.49
1:L:225:VAL:HG23	1:L:268:ASN:HB2	1.93	0.49
1:M:240:ASN:N	1:M:240:ASN:HD22	2.09	0.49
1:A:195:MET:HB3	1:A:199:ILE:HG21	1.94	0.49
1:C:219:CYS:HB2	1:C:274:TYR:HB2	1.94	0.49
1:J:243:ASP:HB2	1:J:244:PRO:HD2	1.93	0.49
1:C:249:HIS:O	1:C:250:ALA:HB3	2.13	0.49
1:D:309:PHE:HB2	1:D:371:ILE:HD11	1.94	0.49
1:J:340:TRP:HA	1:J:344:VAL:HG21	1.94	0.49
1:M:248:CYS:CB	1:M:252:ARG:HB2	2.41	0.49
1:D:352:LYS:NZ	2:N:910:DT:H3'	2.26	0.49
1:K:191:PRO:HB3	1:K:238:PHE:CE1	2.48	0.49
1:L:280:CYS:HB3	1:L:283:CYS:SG	2.53	0.49
1:B:243:ASP:HB2	1:B:244:PRO:HD2	1.93	0.49
1:C:271:VAL:HG23	1:C:299:LEU:CD1	2.43	0.49
1:D:219:CYS:HB2	1:D:274:TYR:HB2	1.94	0.49
1:K:216:SER:CB	1:K:277:TRP:HB2	2.43	0.49
1:L:200:PHE:O	1:L:204:PHE:HB2	2.13	0.49
1:C:216:SER:HB3	1:C:277:TRP:HB3	1.94	0.49
1:D:249:HIS:O	1:D:250:ALA:HB3	2.13	0.49
1:C:247:HIS:O	1:C:248:CYS:O	2.30	0.49
1:J:242:VAL:HG12	1:J:242:VAL:O	2.11	0.49
1:L:241:GLN:HB2	1:L:247:HIS:O	2.12	0.49
1:A:220:PHE:CD2	1:A:254:PHE:HE2	2.31	0.49
1:B:242:VAL:O	1:B:242:VAL:HG12	2.11	0.49
1:K:220:PHE:CD2	1:K:254:PHE:HE2	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:219:CYS:HB2	1:M:274:TYR:HB2	1.95	0.49
1:M:358:LYS:HB2	2:N:901:DT:H1'	1.95	0.49
1:A:340:TRP:HA	1:A:344:VAL:HG21	1.95	0.48
1:J:353:PRO:HD2	2:N:902:DT:H1'	1.94	0.48
1:K:240:ASN:C	1:K:240:ASN:ND2	2.67	0.48
1:C:240:ASN:ND2	1:C:240:ASN:O	2.46	0.48
1:K:195:MET:HB3	1:K:199:ILE:HG21	1.95	0.48
1:K:242:VAL:HG12	1:K:242:VAL:O	2.12	0.48
1:M:309:PHE:HB2	1:M:371:ILE:HD11	1.95	0.48
1:A:240:ASN:C	1:A:240:ASN:ND2	2.67	0.48
1:B:191:PRO:HB3	1:B:238:PHE:CE1	2.49	0.48
1:L:247:HIS:O	1:L:248:CYS:O	2.31	0.48
1:M:310:TRP:HD1	1:M:311:ASP:N	2.12	0.48
1:B:220:PHE:CD2	1:B:254:PHE:HE2	2.31	0.48
1:C:280:CYS:HB3	1:C:283:CYS:SG	2.53	0.48
1:M:247:HIS:O	1:M:248:CYS:O	2.31	0.48
1:B:195:MET:HB3	1:B:199:ILE:HG22	1.95	0.48
1:L:240:ASN:O	1:L:240:ASN:ND2	2.47	0.48
1:J:220:PHE:CD2	1:J:254:PHE:HE2	2.32	0.48
1:J:240:ASN:C	1:J:240:ASN:HD22	2.15	0.48
1:K:368:LEU:C	1:K:368:LEU:HD23	2.34	0.48
1:M:288:ALA:O	1:M:324:GLU:HG3	2.13	0.48
1:M:194:ALA:HB3	1:M:345:TYR:CZ	2.49	0.48
1:A:353:PRO:HD2	2:E:902:DT:H1'	1.94	0.48
1:B:240:ASN:HD22	1:B:240:ASN:C	2.16	0.48
1:D:288:ALA:O	1:D:324:GLU:HG3	2.14	0.48
1:D:318:LEU:HD23	1:D:318:LEU:O	2.13	0.48
1:J:251:GLU:OE1	1:J:279:PRO:HA	2.13	0.48
1:J:368:LEU:C	1:J:368:LEU:HD23	2.34	0.48
1:M:249:HIS:O	1:M:250:ALA:HB3	2.14	0.48
1:B:221:THR:HG23	1:B:343:PHE:CZ	2.45	0.47
1:B:340:TRP:HA	1:B:344:VAL:HG21	1.95	0.47
1:L:219:CYS:HB2	1:L:274:TYR:HB2	1.96	0.47
1:M:196:TYR:CD2	1:M:196:TYR:N	2.82	0.47
1:A:221:THR:HG23	1:A:343:PHE:CZ	2.46	0.47
1:C:309:PHE:HB2	1:C:371:ILE:HD11	1.95	0.47
1:J:340:TRP:HA	1:J:344:VAL:CG2	2.44	0.47
1:M:240:ASN:ND2	1:M:240:ASN:O	2.47	0.47
1:B:368:LEU:HD23	1:B:368:LEU:C	2.34	0.47
1:D:240:ASN:O	1:D:240:ASN:ND2	2.47	0.47
1:J:191:PRO:HB3	1:J:238:PHE:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:216:SER:HB3	1:J:277:TRP:HB2	1.97	0.47
1:J:240:ASN:C	1:J:240:ASN:ND2	2.68	0.47
1:B:240:ASN:C	1:B:240:ASN:ND2	2.68	0.47
1:B:307:TYR:HB3	1:B:314:TYR:HE2	1.78	0.47
1:D:247:HIS:O	1:D:248:CYS:O	2.32	0.47
1:L:216:SER:HB3	1:L:277:TRP:HB3	1.94	0.47
1:L:288:ALA:O	1:L:324:GLU:HG3	2.14	0.47
1:A:310:TRP:CH2	1:C:270:GLU:HB2	2.50	0.47
1:B:195:MET:HB3	1:B:199:ILE:HG21	1.97	0.47
1:L:306:LEU:HG	1:L:364:LEU:HD12	1.97	0.47
1:M:193:GLU:O	1:M:194:ALA:HB2	2.15	0.47
1:C:288:ALA:HB2	1:C:321:LEU:HA	1.96	0.47
1:D:193:GLU:O	1:D:194:ALA:HB2	2.14	0.47
1:D:282:GLU:CD	1:D:282:GLU:H	2.18	0.47
1:M:299:LEU:HD12	1:M:300:THR:H	1.79	0.47
2:N:907:DT:H2"	2:N:908:DT:H5"	1.96	0.47
1:A:368:LEU:C	1:A:368:LEU:HD23	2.35	0.47
1:B:340:TRP:HA	1:B:344:VAL:CG2	2.45	0.47
1:A:262:ILE:HG22	1:A:263:LEU:N	2.24	0.47
1:K:333:TYR:OH	2:N:908:DT:H71	2.14	0.47
1:M:280:CYS:HA	1:M:307:TYR:CD2	2.50	0.47
1:B:251:GLU:OE1	1:B:279:PRO:HA	2.15	0.46
1:C:288:ALA:O	1:C:324:GLU:HG3	2.15	0.46
1:D:288:ALA:HB2	1:D:321:LEU:HA	1.96	0.46
1:K:251:GLU:OE1	1:K:279:PRO:HA	2.15	0.46
1:C:280:CYS:HA	1:C:307:TYR:CD2	2.50	0.46
1:D:278:SER:OG	1:D:279:PRO:HD2	2.15	0.46
1:D:342:ASN:N	1:D:342:ASN:ND2	2.63	0.46
1:K:333:TYR:OH	2:N:908:DT:C7	2.63	0.46
1:M:282:GLU:CD	1:M:282:GLU:H	2.19	0.46
1:B:333:TYR:OH	2:E:908:DT:H71	2.16	0.46
1:J:206:ASN:HA	1:J:305:ARG:HG2	1.97	0.46
1:K:225:VAL:HG23	1:K:225:VAL:O	2.15	0.46
1:A:340:TRP:HA	1:A:344:VAL:CG2	2.46	0.46
1:C:337:LYS:O	1:C:341:GLU:HG3	2.15	0.46
1:C:353:PRO:HB2	2:E:909:DT:H2'	1.98	0.46
1:J:307:TYR:HB3	1:J:314:TYR:HE2	1.79	0.46
1:K:221:THR:HG23	1:K:343:PHE:CZ	2.47	0.46
1:A:251:GLU:OE1	1:A:279:PRO:HA	2.16	0.46
1:A:358:LYS:HB2	2:E:903:DT:O2	2.15	0.46
1:B:333:TYR:OH	2:E:908:DT:C7	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:GLY:C	1:C:213:ARG:HD2	2.35	0.46
1:B:216:SER:HB3	1:B:277:TRP:HB2	1.98	0.46
1:C:195:MET:SD	1:C:204:PHE:HE2	2.38	0.46
1:J:359:TYR:N	2:N:904:DT:OP2	2.38	0.46
1:K:310:TRP:CH2	1:M:270:GLU:HB2	2.51	0.46
1:L:342:ASN:N	1:L:342:ASN:ND2	2.63	0.46
1:J:262:ILE:HG22	1:J:263:LEU:N	2.25	0.46
1:K:209:LYS:O	1:K:211:TYR:N	2.49	0.46
1:C:342:ASN:N	1:C:342:ASN:ND2	2.63	0.46
1:M:306:LEU:HG	1:M:364:LEU:HD12	1.97	0.46
1:B:262:ILE:HG22	1:B:263:LEU:N	2.26	0.46
1:K:262:ILE:HG22	1:K:263:LEU:N	2.25	0.46
1:K:340:TRP:HA	1:K:344:VAL:CG2	2.46	0.46
1:J:221:THR:HG23	1:J:343:PHE:CZ	2.47	0.45
1:K:340:TRP:HA	1:K:344:VAL:HG21	1.98	0.45
1:M:288:ALA:HB2	1:M:321:LEU:HA	1.97	0.45
1:C:278:SER:OG	1:C:279:PRO:HD2	2.16	0.45
1:D:352:LYS:HZ2	2:N:910:DT:H3'	1.81	0.45
1:J:235:ARG:HG3	1:J:235:ARG:HH11	1.81	0.45
1:M:306:LEU:C	1:M:308:TYR:H	2.18	0.45
1:D:306:LEU:HG	1:D:364:LEU:HD12	1.99	0.45
2:E:903:DT:H2"	2:E:904:DT:OP1	2.16	0.45
1:L:288:ALA:HB2	1:L:321:LEU:HA	1.97	0.45
1:M:207:LEU:CB	1:M:210:ALA:HB3	2.45	0.45
1:M:342:ASN:N	1:M:342:ASN:ND2	2.63	0.45
1:B:209:LYS:O	1:B:211:TYR:N	2.50	0.45
2:E:907:DT:H2"	2:E:908:DT:H5"	1.96	0.45
1:M:278:SER:OG	1:M:279:PRO:HD2	2.16	0.45
1:C:207:LEU:CB	1:C:210:ALA:HB3	2.46	0.45
1:C:265:PRO:O	1:C:266:ASN:OD1	2.35	0.45
1:C:306:LEU:HG	1:C:364:LEU:HD12	1.98	0.45
1:D:212:GLY:C	1:D:213:ARG:HD2	2.36	0.45
1:K:206:ASN:HA	1:K:305:ARG:HG2	1.98	0.45
1:K:310:TRP:CD1	1:K:310:TRP:C	2.90	0.45
1:M:212:GLY:C	1:M:213:ARG:HD2	2.36	0.45
1:B:206:ASN:HA	1:B:305:ARG:HG2	1.99	0.45
1:D:337:LYS:O	1:D:341:GLU:HG3	2.17	0.45
1:L:207:LEU:CB	1:L:210:ALA:HB3	2.46	0.45
1:L:337:LYS:O	1:L:341:GLU:HG3	2.17	0.45
1:B:225:VAL:HG23	1:B:225:VAL:O	2.16	0.45
1:C:306:LEU:C	1:C:308:TYR:H	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:243:ASP:HB2	1:D:244:PRO:CD	2.47	0.45
1:L:306:LEU:C	1:L:308:TYR:H	2.19	0.45
1:D:322:SER:HB3	1:D:372:LEU:HD11	1.99	0.45
1:L:278:SER:OG	1:L:279:PRO:HD2	2.16	0.45
1:C:243:ASP:HB2	1:C:244:PRO:CD	2.46	0.45
1:C:322:SER:HB3	1:C:372:LEU:HD11	1.99	0.45
1:D:299:LEU:HD12	1:D:300:THR:H	1.82	0.45
1:L:280:CYS:HA	1:L:307:TYR:CD2	2.51	0.45
1:L:353:PRO:HB2	2:N:909:DT:H2'	1.99	0.45
1:A:206:ASN:HA	1:A:305:ARG:HG2	1.98	0.44
1:L:322:SER:HB3	1:L:372:LEU:HD11	1.99	0.44
1:M:354:TRP:O	2:N:901:DT:H4'	2.17	0.44
1:B:310:TRP:CZ3	1:D:270:GLU:HG3	2.52	0.44
1:D:280:CYS:HA	1:D:307:TYR:CD2	2.51	0.44
1:L:243:ASP:HB2	1:L:244:PRO:CD	2.47	0.44
1:B:311:ASP:O	1:B:315:GLN:HG3	2.17	0.44
1:C:196:TYR:CD2	1:C:196:TYR:N	2.86	0.44
1:D:207:LEU:CB	1:D:210:ALA:HB3	2.46	0.44
1:L:299:LEU:HD12	1:L:300:THR:H	1.83	0.44
1:M:265:PRO:O	1:M:266:ASN:OD1	2.35	0.44
1:B:310:TRP:CD1	1:B:310:TRP:C	2.90	0.44
1:C:226:LYS:O	1:C:228:HIS:N	2.51	0.44
1:D:195:MET:SD	1:D:204:PHE:HE2	2.40	0.44
1:L:196:TYR:CD2	1:L:196:TYR:N	2.82	0.44
1:C:299:LEU:HD12	1:C:300:THR:H	1.82	0.44
1:J:209:LYS:O	1:J:211:TYR:N	2.51	0.44
1:J:225:VAL:HG23	1:J:225:VAL:O	2.17	0.44
1:K:243:ASP:HB2	1:K:244:PRO:CD	2.48	0.44
1:M:243:ASP:HB2	1:M:244:PRO:CD	2.46	0.44
1:A:225:VAL:O	1:A:225:VAL:HG23	2.17	0.44
1:L:306:LEU:O	1:L:308:TYR:N	2.41	0.44
1:C:282:GLU:CD	1:C:282:GLU:H	2.21	0.44
1:J:278:SER:HB3	1:J:307:TYR:H	1.83	0.44
1:M:322:SER:HB3	1:M:372:LEU:HD11	1.99	0.44
1:A:243:ASP:HB2	1:A:244:PRO:CD	2.48	0.44
1:L:265:PRO:O	1:L:266:ASN:OD1	2.35	0.44
1:A:310:TRP:CD1	1:A:310:TRP:C	2.92	0.44
1:B:352:LYS:HD2	2:E:908:DT:H2'	1.98	0.44
1:C:369:GLN:HA	1:C:369:GLN:NE2	2.33	0.44
1:D:306:LEU:C	1:D:308:TYR:H	2.20	0.44
1:L:274:TYR:CE1	1:L:302:PHE:HD2	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:TRP:CD1	1:A:351:PHE:HA	2.53	0.43
1:D:306:LEU:HD22	1:D:314:TYR:OH	2.18	0.43
1:J:310:TRP:CD1	1:J:310:TRP:C	2.91	0.43
1:K:307:TYR:HB3	1:K:314:TYR:HE2	1.79	0.43
1:J:310:TRP:CH2	1:L:270:GLU:HB2	2.53	0.43
1:A:209:LYS:O	1:A:211:TYR:N	2.52	0.43
1:D:194:ALA:HB3	1:D:345:TYR:CZ	2.53	0.43
1:L:220:PHE:CD2	1:L:254:PHE:HE2	2.36	0.43
1:L:282:GLU:H	1:L:282:GLU:CD	2.22	0.43
1:L:369:GLN:HA	1:L:369:GLN:NE2	2.33	0.43
1:M:226:LYS:O	1:M:228:HIS:N	2.52	0.43
1:D:360:ASN:O	1:D:364:LEU:HD23	2.18	0.43
1:M:220:PHE:CD2	1:M:254:PHE:HE2	2.36	0.43
1:B:278:SER:HB3	1:B:307:TYR:H	1.84	0.43
1:J:358:LYS:HB2	2:N:903:DT:O2	2.18	0.43
1:L:212:GLY:C	1:L:213:ARG:HD2	2.39	0.43
1:B:235:ARG:HG3	1:B:235:ARG:HH11	1.84	0.43
1:D:274:TYR:CE1	1:D:302:PHE:HD2	2.37	0.43
1:K:284:ALA:HB3	1:K:317:GLY:HA3	2.00	0.43
1:L:226:LYS:O	1:L:228:HIS:N	2.51	0.43
1:M:337:LYS:O	1:M:341:GLU:HG3	2.19	0.43
1:M:360:ASN:O	1:M:364:LEU:HD23	2.18	0.43
1:C:306:LEU:HD22	1:C:314:TYR:OH	2.19	0.43
1:C:352:LYS:HA	1:C:353:PRO:HD2	1.90	0.43
1:D:265:PRO:O	1:D:266:ASN:OD1	2.36	0.43
1:M:203:HIS:O	1:M:276:SER:HB2	2.19	0.43
1:M:274:TYR:CE1	1:M:302:PHE:HD2	2.37	0.43
1:D:369:GLN:HA	1:D:369:GLN:NE2	2.33	0.43
1:J:311:ASP:O	1:J:315:GLN:HG3	2.19	0.43
1:L:221:THR:HG23	1:L:343:PHE:HZ	1.84	0.43
1:A:195:MET:HB3	1:A:199:ILE:HG22	2.00	0.42
1:A:310:TRP:CZ3	1:C:270:GLU:HG3	2.54	0.42
1:A:311:ASP:O	1:A:315:GLN:HG3	2.19	0.42
1:C:203:HIS:O	1:C:276:SER:HB2	2.19	0.42
1:J:243:ASP:HB2	1:J:244:PRO:CD	2.48	0.42
1:L:306:LEU:HD22	1:L:314:TYR:OH	2.19	0.42
1:A:307:TYR:HB3	1:A:314:TYR:HE2	1.80	0.42
1:B:243:ASP:HB2	1:B:244:PRO:CD	2.48	0.42
1:C:213:ARG:HD2	1:C:213:ARG:N	2.34	0.42
1:D:213:ARG:HD2	1:D:213:ARG:N	2.34	0.42
1:L:357:LEU:HD23	1:L:357:LEU:C	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:SER:HB3	1:A:307:TYR:H	1.84	0.42
1:C:360:ASN:O	1:C:364:LEU:HD23	2.18	0.42
1:D:203:HIS:O	1:D:276:SER:HB2	2.18	0.42
1:L:195:MET:SD	1:L:204:PHE:HE2	2.42	0.42
1:M:213:ARG:HD2	1:M:213:ARG:N	2.34	0.42
1:D:281:PRO:HD3	1:D:307:TYR:CG	2.54	0.42
1:B:284:ALA:HB3	1:B:317:GLY:HA3	2.00	0.42
1:D:220:PHE:CD2	1:D:254:PHE:HE2	2.37	0.42
1:J:360:ASN:HD22	1:J:360:ASN:HA	1.61	0.42
1:L:242:VAL:HG12	1:L:242:VAL:O	2.20	0.42
1:M:195:MET:SD	1:M:204:PHE:HE2	2.43	0.42
1:M:281:PRO:HD3	1:M:307:TYR:CG	2.54	0.42
1:M:352:LYS:HA	1:M:353:PRO:HD2	1.90	0.42
1:M:360:ASN:O	1:M:364:LEU:HB2	2.20	0.42
1:B:199:ILE:CD1	1:B:203:HIS:HD2	2.33	0.42
1:D:306:LEU:O	1:D:308:TYR:N	2.42	0.42
1:M:218:LEU:HD23	1:M:218:LEU:C	2.40	0.42
1:M:369:GLN:HA	1:M:369:GLN:NE2	2.35	0.42
2:N:903:DT:H2"	2:N:904:DT:OP1	2.19	0.42
1:A:353:PRO:HD2	2:E:902:DT:C1'	2.49	0.42
1:C:274:TYR:CE1	1:C:302:PHE:HD2	2.37	0.42
1:D:226:LYS:O	1:D:228:HIS:N	2.52	0.42
1:K:278:SER:HB3	1:K:307:TYR:H	1.85	0.42
1:L:222:MET:SD	1:L:271:VAL:HG12	2.60	0.42
1:M:306:LEU:HD22	1:M:314:TYR:OH	2.20	0.42
1:B:340:TRP:CD1	1:B:351:PHE:HA	2.54	0.42
1:J:278:SER:HB2	1:J:306:LEU:HA	2.02	0.42
2:N:906:DT:O2	2:N:906:DT:O4'	2.38	0.42
1:K:310:TRP:CZ3	1:M:270:GLU:HG3	2.55	0.42
1:D:221:THR:HG23	1:D:343:PHE:HZ	1.85	0.42
1:J:299:LEU:HD12	1:J:300:THR:H	1.84	0.42
1:L:213:ARG:HD2	1:L:213:ARG:N	2.35	0.42
1:B:213:ARG:N	1:B:213:ARG:HD2	2.34	0.41
1:C:218:LEU:C	1:C:218:LEU:HD23	2.41	0.41
1:L:194:ALA:HB3	1:L:345:TYR:CZ	2.55	0.41
1:M:242:VAL:HG12	1:M:242:VAL:O	2.19	0.41
1:J:213:ARG:N	1:J:213:ARG:HD2	2.34	0.41
1:L:321:LEU:HD23	1:L:321:LEU:O	2.20	0.41
1:M:307:TYR:O	1:M:308:TYR:HB2	2.20	0.41
1:A:235:ARG:HG3	1:A:235:ARG:HH11	1.86	0.41
1:B:229:SER:HB3	1:B:230:PRO:CD	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:ALA:HB3	1:C:345:TYR:CZ	2.55	0.41
1:D:357:LEU:C	1:D:357:LEU:HD23	2.40	0.41
2:E:906:DT:O2	2:E:906:DT:O4'	2.37	0.41
1:K:356:GLY:O	1:K:360:ASN:HB2	2.21	0.41
1:L:281:PRO:HD3	1:L:307:TYR:CG	2.55	0.41
1:A:284:ALA:HB3	1:A:317:GLY:HA3	2.01	0.41
1:K:351:PHE:O	1:K:352:LYS:HB3	2.20	0.41
1:L:369:GLN:CA	1:L:369:GLN:HE21	2.33	0.41
1:A:252:ARG:HH21	1:A:282:GLU:HG2	1.85	0.41
1:D:321:LEU:O	1:D:321:LEU:HD23	2.20	0.41
1:K:356:GLY:CA	2:N:907:DT:OP2	2.69	0.41
1:L:203:HIS:O	1:L:276:SER:HB2	2.19	0.41
1:C:220:PHE:CD2	1:C:254:PHE:HE2	2.38	0.41
1:C:357:LEU:C	1:C:357:LEU:HD23	2.40	0.41
1:D:307:TYR:O	1:D:308:TYR:HB2	2.20	0.41
1:J:310:TRP:CZ3	1:L:270:GLU:HG3	2.55	0.41
1:M:357:LEU:C	1:M:357:LEU:HD23	2.40	0.41
1:B:299:LEU:HD12	1:B:300:THR:H	1.85	0.41
1:B:351:PHE:O	1:B:352:LYS:HB3	2.20	0.41
1:C:281:PRO:HD3	1:C:307:TYR:CG	2.55	0.41
1:D:280:CYS:SG	1:D:281:PRO:CD	3.00	0.41
1:J:235:ARG:HH21	1:J:342:ASN:HB3	1.86	0.41
1:K:281:PRO:HD3	1:K:314:TYR:CE2	2.56	0.41
1:L:225:VAL:HG12	1:L:231:VAL:HG22	2.03	0.41
1:A:277:TRP:HA	1:A:277:TRP:HE3	1.85	0.41
1:J:284:ALA:HB3	1:J:317:GLY:HA3	2.02	0.41
1:K:235:ARG:HH21	1:K:342:ASN:HB3	1.85	0.41
1:B:278:SER:HB2	1:B:306:LEU:HA	2.03	0.41
1:B:356:GLY:CA	2:E:907:DT:OP2	2.68	0.41
1:B:360:ASN:HD22	1:B:360:ASN:HA	1.62	0.41
1:C:360:ASN:O	1:C:364:LEU:HB2	2.21	0.41
1:K:213:ARG:HD2	1:K:213:ARG:N	2.35	0.41
1:K:311:ASP:O	1:K:315:GLN:HG3	2.21	0.41
1:K:340:TRP:CD1	1:K:351:PHE:HA	2.56	0.41
1:M:306:LEU:O	1:M:308:TYR:N	2.40	0.41
1:A:235:ARG:HH21	1:A:342:ASN:HB3	1.85	0.41
1:A:281:PRO:HD3	1:A:314:TYR:CE2	2.56	0.41
1:A:278:SER:HB2	1:A:306:LEU:HA	2.02	0.40
1:B:235:ARG:HH21	1:B:342:ASN:HB3	1.86	0.40
1:J:229:SER:HB3	1:J:230:PRO:CD	2.51	0.40
1:K:358:LYS:HB3	2:N:906:DT:O3'	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:360:ASN:O	1:L:364:LEU:HD23	2.20	0.40
1:M:221:THR:HG23	1:M:343:PHE:HZ	1.85	0.40
1:A:229:SER:HB3	1:A:230:PRO:CD	2.51	0.40
1:A:339:CYS:C	1:A:341:GLU:H	2.24	0.40
1:K:235:ARG:HG3	1:K:235:ARG:HH11	1.87	0.40
1:L:307:TYR:O	1:L:308:TYR:HB2	2.21	0.40
1:M:321:LEU:HD23	1:M:321:LEU:O	2.20	0.40
1:A:213:ARG:HD2	1:A:213:ARG:N	2.35	0.40
1:A:216:SER:HB3	1:A:277:TRP:HB2	2.03	0.40
1:D:242:VAL:O	1:D:242:VAL:HG12	2.21	0.40
1:J:339:CYS:C	1:J:341:GLU:H	2.24	0.40
1:K:277:TRP:HA	1:K:277:TRP:HE3	1.85	0.40
1:K:281:PRO:HG3	1:K:314:TYR:CE1	2.56	0.40
1:K:299:LEU:HD12	1:K:300:THR:H	1.86	0.40
1:K:352:LYS:HD2	2:N:908:DT:H2'	2.04	0.40
1:M:218:LEU:HD23	1:M:219:CYS:N	2.36	0.40
2:N:907:DT:O2	2:N:907:DT:O4'	2.39	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	182/184 (99%)	141 (78%)	33 (18%)	8 (4%)	2	24
1	B	182/184 (99%)	141 (78%)	33 (18%)	8 (4%)	2	24
1	C	182/184 (99%)	142 (78%)	33 (18%)	7 (4%)	3	27
1	D	182/184 (99%)	142 (78%)	33 (18%)	7 (4%)	3	27
1	J	182/184 (99%)	141 (78%)	33 (18%)	8 (4%)	2	24
1	K	182/184 (99%)	141 (78%)	33 (18%)	8 (4%)	2	24
1	L	182/184 (99%)	142 (78%)	33 (18%)	7 (4%)	3	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	M	182/184 (99%)	142 (78%)	33 (18%)	7 (4%)	3 27
All	All	1456/1472 (99%)	1132 (78%)	264 (18%)	60 (4%)	3 26

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	210	ALA
1	A	353	PRO
1	B	210	ALA
1	B	353	PRO
1	C	208	ARG
1	C	227	HIS
1	C	248	CYS
1	C	278	SER
1	D	208	ARG
1	D	227	HIS
1	D	248	CYS
1	D	278	SER
1	J	210	ALA
1	J	353	PRO
1	K	210	ALA
1	K	353	PRO
1	L	208	ARG
1	L	227	HIS
1	L	248	CYS
1	L	278	SER
1	M	208	ARG
1	M	227	HIS
1	M	248	CYS
1	M	278	SER
1	A	246	THR
1	B	246	THR
1	C	262	ILE
1	D	262	ILE
1	J	246	THR
1	K	246	THR
1	L	262	ILE
1	M	262	ILE
1	A	372	LEU
1	B	372	LEU
1	C	212	GLY
1	D	212	GLY

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Mol	Chain	Res	Type
1	J	372	LEU
1	K	372	LEU
1	L	212	GLY
1	M	212	GLY
1	A	242	VAL
1	A	266	ASN
1	A	308	TYR
1	B	266	ASN
1	J	266	ASN
1	J	308	TYR
1	K	266	ASN
1	K	308	TYR
1	M	307	TYR
1	B	242	VAL
1	B	308	TYR
1	C	194	ALA
1	D	307	TYR
1	J	242	VAL
1	K	242	VAL
1	L	307	TYR
1	A	244	PRO
1	B	244	PRO
1	J	244	PRO
1	K	244	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	169/169 (100%)	157 (93%)	12 (7%)	14	45
1	B	169/169 (100%)	157 (93%)	12 (7%)	14	45
1	C	169/169 (100%)	158 (94%)	11 (6%)	17	48
1	D	169/169 (100%)	157 (93%)	12 (7%)	14	45
1	J	169/169 (100%)	157 (93%)	12 (7%)	14	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	K	169/169 (100%)	157 (93%)	12 (7%)	14 45
1	L	169/169 (100%)	157 (93%)	12 (7%)	14 45
1	M	169/169 (100%)	158 (94%)	11 (6%)	17 48
All	All	1352/1352 (100%)	1258 (93%)	94 (7%)	15 45

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	199	ILE
1	A	240	ASN
1	A	253	CYS
1	A	261	ASP
1	A	277	TRP
1	A	282	GLU
1	A	290	PHE
1	A	307	TYR
1	A	309	PHE
1	A	310	TRP
1	A	359	TYR
1	A	369	GLN
1	B	199	ILE
1	B	240	ASN
1	B	253	CYS
1	B	261	ASP
1	B	277	TRP
1	B	282	GLU
1	B	290	PHE
1	B	307	TYR
1	B	309	PHE
1	B	310	TRP
1	B	359	TYR
1	B	369	GLN
1	C	193	GLU
1	C	202	PHE
1	C	213	ARG
1	C	240	ASN
1	C	266	ASN
1	C	270	GLU
1	C	277	TRP
1	C	281	PRO
1	C	282	GLU

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Mol	Chain	Res	Type
1	C	310	TRP
1	C	340	TRP
1	D	193	GLU
1	D	197	PRO
1	D	202	PHE
1	D	213	ARG
1	D	240	ASN
1	D	266	ASN
1	D	270	GLU
1	D	277	TRP
1	D	281	PRO
1	D	282	GLU
1	D	310	TRP
1	D	340	TRP
1	J	199	ILE
1	J	240	ASN
1	J	253	CYS
1	J	261	ASP
1	J	277	TRP
1	J	282	GLU
1	J	290	PHE
1	J	307	TYR
1	J	309	PHE
1	J	310	TRP
1	J	359	TYR
1	J	369	GLN
1	K	199	ILE
1	K	240	ASN
1	K	253	CYS
1	K	261	ASP
1	K	277	TRP
1	K	282	GLU
1	K	290	PHE
1	K	307	TYR
1	K	309	PHE
1	K	310	TRP
1	K	359	TYR
1	K	369	GLN
1	L	193	GLU
1	L	197	PRO
1	L	202	PHE
1	L	213	ARG

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Mol	Chain	Res	Type
1	L	240	ASN
1	L	266	ASN
1	L	270	GLU
1	L	277	TRP
1	L	281	PRO
1	L	282	GLU
1	L	310	TRP
1	L	340	TRP
1	M	193	GLU
1	M	202	PHE
1	M	213	ARG
1	M	240	ASN
1	M	266	ASN
1	M	270	GLU
1	M	277	TRP
1	M	281	PRO
1	M	282	GLU
1	M	310	TRP
1	M	340	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	HIS
1	A	227	HIS
1	A	240	ASN
1	A	247	HIS
1	A	249	HIS
1	A	315	GLN
1	A	342	ASN
1	A	360	ASN
1	B	198	HIS
1	B	227	HIS
1	B	240	ASN
1	B	247	HIS
1	B	315	GLN
1	B	342	ASN
1	B	360	ASN
1	C	228	HIS
1	C	240	ASN
1	C	247	HIS
1	C	249	HIS

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Mol	Chain	Res	Type
1	C	266	ASN
1	C	294	HIS
1	C	315	GLN
1	C	342	ASN
1	C	360	ASN
1	C	369	GLN
1	D	240	ASN
1	D	247	HIS
1	D	249	HIS
1	D	266	ASN
1	D	294	HIS
1	D	315	GLN
1	D	342	ASN
1	D	360	ASN
1	D	369	GLN
1	J	227	HIS
1	J	240	ASN
1	J	247	HIS
1	J	315	GLN
1	J	342	ASN
1	J	360	ASN
1	K	227	HIS
1	K	240	ASN
1	K	247	HIS
1	K	315	GLN
1	K	342	ASN
1	K	360	ASN
1	L	228	HIS
1	L	240	ASN
1	L	247	HIS
1	L	249	HIS
1	L	266	ASN
1	L	294	HIS
1	L	315	GLN
1	L	342	ASN
1	L	360	ASN
1	L	369	GLN
1	M	240	ASN
1	M	247	HIS
1	M	249	HIS
1	M	266	ASN
1	M	294	HIS

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Mol	Chain	Res	Type
1	M	315	GLN
1	M	342	ASN
1	M	360	ASN
1	M	369	GLN

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 monosaccharides 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	184/184 (100%)	-0.27	0 100 100	80, 103, 141, 157	0
1	B	184/184 (100%)	-0.28	2 (1%) 80 71	79, 104, 142, 157	0
1	C	184/184 (100%)	-0.21	1 (0%) 91 85	81, 105, 139, 155	0
1	D	184/184 (100%)	-0.16	0 100 100	77, 105, 140, 154	0
1	J	184/184 (100%)	-0.25	1 (0%) 91 85	80, 103, 143, 157	0
1	K	184/184 (100%)	-0.35	0 100 100	78, 104, 143, 157	0
1	L	184/184 (100%)	-0.23	0 100 100	79, 105, 139, 154	0
1	M	184/184 (100%)	-0.20	1 (0%) 91 85	79, 105, 139, 155	0
2	E	10/10 (100%)	-0.34	0 100 100	82, 100, 156, 177	0
2	N	10/10 (100%)	-0.37	0 100 100	83, 102, 156, 177	0
All	All	1492/1492 (100%)	-0.25	5 (0%) 94 90	77, 105, 143, 177	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	242	VAL	4.1
1	C	279	PRO	3.8
1	B	241	GLN	2.5
1	B	242	VAL	2.4
1	M	279	PRO	2.4

6.2 Non-standard residues in protein, DNA, RNA chains

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, 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	B-factors(Å^2)	Q<0.9
3	ZN	B	801	1/1	0.69	0.08	221,221,221,221	0
3	ZN	K	801	1/1	0.69	0.14	221,221,221,221	0
3	ZN	A	801	1/1	0.72	0.12	225,225,225,225	0
3	ZN	J	801	1/1	0.77	0.10	225,225,225,225	0

6.5 Other polymers (i)

There are no such residues in this entry.