



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:51 PM UTC

PDB ID : 4EMZ / pdb_00004emz
Title : HIV-1 Nef in complex with MHC-I cytoplasmic domain and Mu1 adaptin subunit of AP1 adaptor (second domain)
Authors : Jia, X.; Xiong, Y.
Deposited on : 2012-04-12
Resolution : 2.90 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

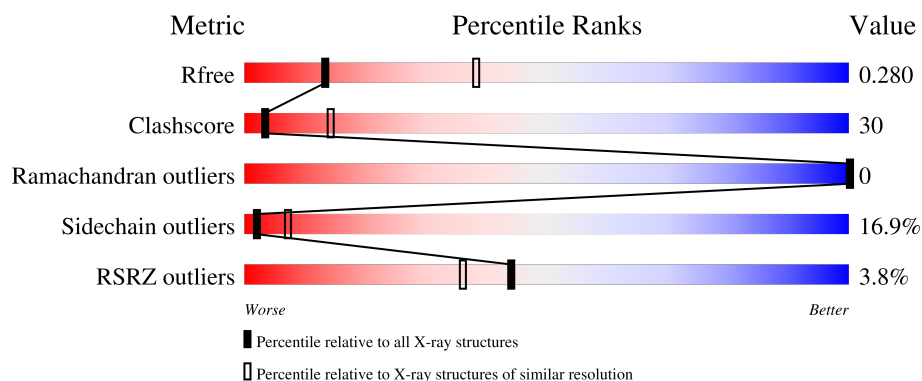
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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 $\leq 5\%$. 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	B	206	3% 33% 28% 5% 33%
1	C	206	6% 38% 24% 7% 31%
2	D	28	43% 18% 7% 32%
2	E	28	25% 25% 11% 39%
3	A	266	3% 48% 37% 9% ...

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Mol	Chain	Length	Quality of chain
3	M	266	2% 47% 37% 11%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6789 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 Protein Nef.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	C	142	Total	C	N	O	S	Se	0	0	0
			1193	775	210	204	2	2			
1	B	138	Total	C	N	O	S	Se	0	0	0
			1163	756	205	199	1	2			

- Molecule 2 is a protein called MHC-I.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	19	Total	C	N	O	0	0	0
			127	71	25	31			
2	E	17	Total	C	N	O	0	0	0
			113	64	23	26			

- Molecule 3 is a protein called AP-1 complex subunit mu-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	A	255	Total	C	N	O	S	Se	0	1	0
			2088	1341	367	374	1	5			
3	M	255	Total	C	N	O	S	Se	0	1	0
			2087	1341	367	373	1	5			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	2	Total	O	0	0
			2	2		
4	D	1	Total	O	0	0
			1	1		
4	B	2	Total	O	0	0
			2	2		
4	A	8	Total	O	0	0
			8	8		

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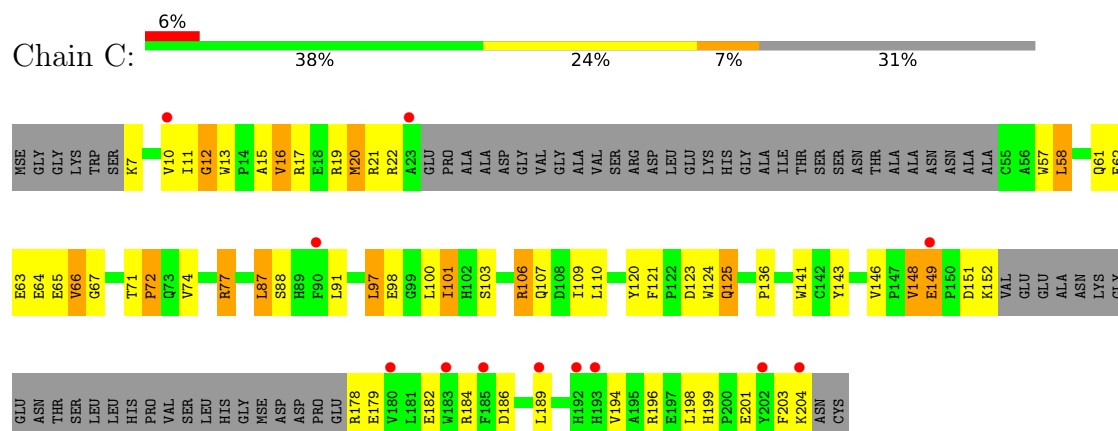
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	5	Total	O	0	0
			5	5		

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.

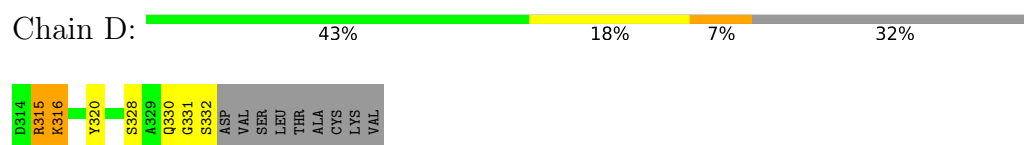
• Molecule 1: Protein Nef



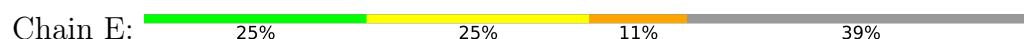
• Molecule 1: Protein Nef



• Molecule 2: MHC-I

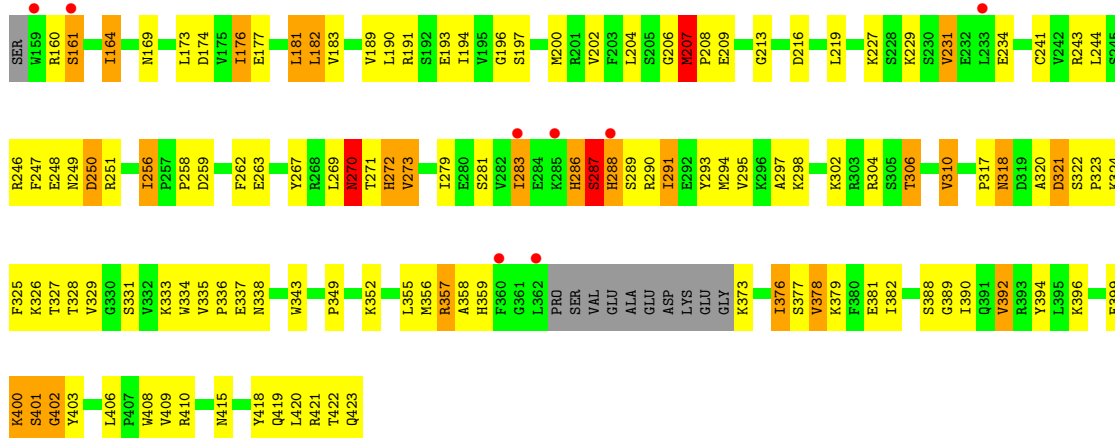


• Molecule 2: MHC-I

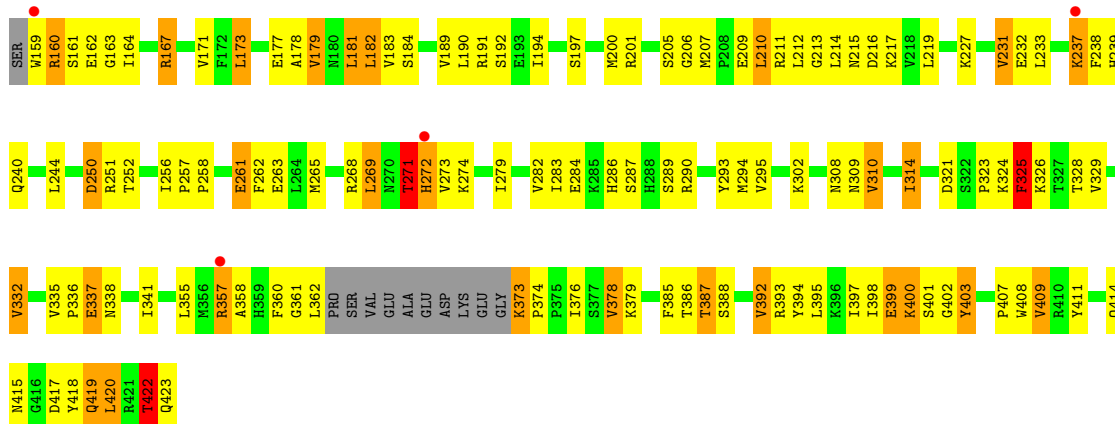




• Molecule 3: AP-1 complex subunit mu-1



• Molecule 3: AP-1 complex subunit mu-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.32Å 112.47Å 114.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 30.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (30.00-2.90) 99.3 (30.00-2.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.6.0116	Depositor
R, R_{free}	0.223 , 0.278 0.225 , 0.280	Depositor DCC
R_{free} test set	1317 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	77.2	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 84.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.015 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6789	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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](#)

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	B	1.01	0/1202	1.24	8/1629 (0.5%)
1	C	1.05	1/1232 (0.1%)	1.25	15/1669 (0.9%)
2	D	1.15	0/127	1.22	1/167 (0.6%)
2	E	1.02	0/113	1.17	0/148
3	A	0.97	0/2135	1.22	12/2871 (0.4%)
3	M	0.97	1/2134 (0.0%)	1.17	9/2871 (0.3%)
All	All	0.99	2/6943 (0.0%)	1.21	45/9355 (0.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	422	THR	CA-C	5.72	1.57	1.52
1	C	74	VAL	N-CA	-5.50	1.41	1.46

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	67	GLY	N-CA-C	8.04	120.24	112.04
3	A	402	GLY	N-CA-C	-7.80	103.31	112.83
1	C	199	HIS	CA-C-N	-7.70	112.27	119.82
1	C	199	HIS	C-N-CA	-7.70	112.27	119.82
1	B	65	GLU	N-CA-C	-7.61	96.53	109.24
2	D	316	LYS	CB-CA-C	-7.44	107.98	116.54
3	A	419	GLN	N-CA-C	7.03	121.14	108.69
1	C	148	VAL	N-CA-C	6.99	117.01	108.06
1	C	66	VAL	CB-CA-C	-6.79	102.25	111.63
3	A	207	MSE	CA-C-N	6.63	126.39	119.76
3	A	207	MSE	C-N-CA	6.63	126.39	119.76
1	C	72	PRO	CA-C-N	-6.58	112.34	122.60
1	C	72	PRO	C-N-CA	-6.58	112.34	122.60
1	C	72	PRO	N-CA-C	6.47	122.72	113.47
1	B	72	PRO	CA-C-N	-6.28	112.27	122.26
1	B	72	PRO	C-N-CA	-6.28	112.27	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	13	TRP	CA-C-N	-6.23	112.49	118.97
1	B	13	TRP	C-N-CA	-6.23	112.49	118.97
3	A	202	VAL	CB-CA-C	-6.15	102.56	110.98
3	M	325	PHE	N-CA-C	6.14	118.41	109.07
1	B	99	GLY	N-CA-C	-6.14	107.62	115.42
3	A	193	GLU	N-CA-C	5.91	117.93	110.24
3	A	288	HIS	N-CA-C	-5.83	101.42	110.10
1	C	74	VAL	CB-CA-C	-5.75	105.60	110.94
1	C	149	GLU	CA-C-N	-5.74	112.97	119.28
1	C	149	GLU	C-N-CA	-5.74	112.97	119.28
3	M	419	GLN	N-CA-C	5.73	118.84	108.69
3	A	273	VAL	CB-CA-C	-5.59	102.13	111.29
3	A	273	VAL	N-CA-C	5.55	120.89	109.34
3	A	216	ASP	N-CA-C	5.44	118.45	110.30
1	C	16	VAL	CB-CA-C	-5.35	105.07	112.24
1	C	12	GLY	CA-C-N	5.32	126.74	120.09
1	C	12	GLY	C-N-CA	5.32	126.74	120.09
1	B	80	THR	CB-CA-C	5.31	119.50	109.37
3	A	270	ASN	N-CA-C	5.29	117.13	111.36
3	M	402	GLY	N-CA-C	-5.24	100.76	113.18
3	M	417	ASP	N-CA-C	5.23	117.93	107.62
1	C	149	GLU	N-CA-C	5.21	121.33	109.81
3	M	397	ILE	N-CA-C	5.20	115.33	107.75
3	M	179	VAL	CB-CA-C	-5.19	105.62	111.23
3	M	265	MSE	N-CA-C	5.16	116.13	108.60
1	C	179	GLU	N-CA-C	5.13	117.15	110.43
3	M	271	THR	CB-CA-C	-5.05	99.68	109.68
3	M	409	VAL	N-CA-C	5.03	114.99	108.35
3	A	287	SER	N-CA-C	-5.02	103.91	110.53

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	B	1163	0	1120	75	0
1	C	1193	0	1153	67	0
2	D	127	0	110	6	0
2	E	113	0	101	24	0
3	A	2088	0	2117	130	0
3	M	2087	0	2119	118	0
4	A	8	0	0	1	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	1	0	0	0	0
4	M	5	0	0	0	0
All	All	6789	0	6720	405	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 30.

All (405) 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)
3:A:283:ILE:HG22	3:A:293:TYR:CD1	1.79	1.17
1:B:79:MSE:HE2	1:B:83:ALA:HB3	1.28	1.11
1:C:20:MSE:HA	1:C:109:ILE:HD11	1.31	1.09
3:M:286:HIS:CD2	3:M:290:ARG:CZ	2.38	1.07
3:M:286:HIS:HD2	3:M:290:ARG:NH1	1.54	1.03
2:E:315:ARG:HH11	2:E:315:ARG:HG3	1.21	0.98
3:A:160:ARG:NH1	3:A:161:SER:O	1.97	0.97
1:C:13:TRP:CZ3	1:C:20:MSE:CE	2.48	0.97
1:B:79:MSE:CE	1:B:83:ALA:HB3	1.94	0.97
2:E:316:LYS:CG	2:E:317:GLY:H	1.77	0.95
3:A:283:ILE:CG2	3:A:293:TYR:CD1	2.50	0.94
3:A:286:HIS:CD2	3:A:287:SER:N	2.34	0.94
3:M:159:TRP:CG	3:M:160:ARG:H	1.86	0.94
2:E:316:LYS:HG2	2:E:317:GLY:H	1.30	0.93
1:C:13:TRP:HZ3	1:C:20:MSE:CE	1.83	0.92
1:C:184:ARG:HH11	1:C:184:ARG:HB2	1.34	0.92
3:A:400:LYS:HD2	3:A:400:LYS:N	1.85	0.91
3:M:286:HIS:CD2	3:M:290:ARG:NH1	2.37	0.91
2:E:315:ARG:HG3	2:E:315:ARG:NH1	1.77	0.90
3:A:286:HIS:HD2	3:A:287:SER:N	1.68	0.88
3:A:164:ILE:HD11	3:A:206:GLY:O	1.75	0.86
3:A:399:GLU:HB3	3:A:403:TYR:CD2	2.10	0.86
3:A:283:ILE:HG21	3:A:293:TYR:CE1	2.11	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:314:ILE:HG12	3:M:341:ILE:HG23	1.58	0.85
3:M:159:TRP:CG	3:M:160:ARG:N	2.43	0.85
1:C:20:MSE:HA	1:C:109:ILE:CD1	2.06	0.84
2:E:316:LYS:CG	2:E:317:GLY:N	2.40	0.84
3:A:335:VAL:HG12	3:A:337:GLU:O	1.77	0.84
3:M:160:ARG:NH1	3:M:206:GLY:O	2.10	0.83
1:C:77:ARG:HH11	1:C:77:ARG:HG2	1.43	0.83
1:C:184:ARG:HB2	1:C:184:ARG:NH1	1.92	0.83
1:C:13:TRP:CH2	1:C:20:MSE:HE3	2.14	0.83
3:M:231:VAL:HG12	3:M:233:LEU:HD22	1.59	0.83
3:A:177:GLU:OE1	3:A:388:SER:OG	1.96	0.83
1:C:13:TRP:HZ3	1:C:20:MSE:HE1	1.43	0.82
1:B:101:ILE:HD11	1:B:180:VAL:CG1	2.09	0.82
3:A:328:THR:HG23	3:A:329:VAL:HG23	1.62	0.82
3:M:237:LYS:HD2	3:M:238:PHE:H	1.45	0.81
1:B:79:MSE:CE	1:B:83:ALA:CB	2.58	0.81
1:B:192:HIS:NE2	1:B:197:GLU:OE2	2.14	0.81
1:C:20:MSE:CA	1:C:109:ILE:HD11	2.11	0.81
1:C:194:VAL:HG12	1:C:198:LEU:CD1	2.10	0.81
3:A:283:ILE:CG2	3:A:293:TYR:CE1	2.66	0.80
3:A:272:HIS:ND1	3:A:272:HIS:C	2.39	0.79
1:B:79:MSE:HE2	1:B:83:ALA:CB	2.08	0.79
3:A:160:ARG:CZ	3:A:161:SER:O	2.31	0.79
3:M:177:GLU:OE1	3:M:388:SER:OG	2.02	0.78
1:B:59:GLU:OE1	1:B:60:ALA:N	2.17	0.78
3:M:378:VAL:HG13	3:M:418:TYR:CD2	2.19	0.78
3:M:184:SER:HB2	3:M:190:LEU:HD11	1.65	0.77
3:M:173:LEU:HD12	3:M:408:TRP:O	1.84	0.77
1:C:146:VAL:HG22	1:C:184:ARG:NH1	1.99	0.77
3:M:159:TRP:CD1	3:M:160:ARG:H	2.02	0.77
1:C:100:LEU:HD12	1:C:101:ILE:H	1.49	0.75
3:A:286:HIS:CD2	3:A:287:SER:H	2.01	0.75
3:A:321:ASP:C	3:A:321:ASP:OD2	2.29	0.75
1:B:133:VAL:CG2	1:B:135:TYR:CZ	2.71	0.74
3:M:268:ARG:O	3:M:269:LEU:HD12	1.87	0.74
1:B:178:ARG:HG2	1:B:179:GLU:N	2.03	0.74
3:A:291:ILE:O	3:A:359:HIS:HB2	1.86	0.74
3:A:321:ASP:OD2	3:A:322:SER:CB	2.35	0.74
3:M:268:ARG:O	3:M:269:LEU:CD1	2.35	0.74
1:C:63:GLU:HG3	3:A:333:LYS:HD2	1.70	0.73
3:A:250:ASP:OD1	3:A:250:ASP:C	2.29	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:378:VAL:HG13	3:A:418:TYR:CD2	2.23	0.73
3:A:183:VAL:HB	3:A:420:LEU:HD23	1.70	0.73
3:A:164:ILE:CD1	3:A:206:GLY:O	2.36	0.73
1:B:20:MSE:HG2	1:B:106:ARG:HG2	1.70	0.73
3:A:270:ASN:C	3:A:270:ASN:OD1	2.32	0.73
3:M:286:HIS:NE2	3:M:290:ARG:NH2	2.36	0.72
1:B:16:VAL:O	1:B:20:MSE:HB2	1.89	0.72
1:C:124:TRP:CZ3	1:C:125:GLN:HG3	2.25	0.72
1:C:203:PHE:O	1:C:204:LYS:HB2	1.90	0.71
1:C:194:VAL:HG12	1:C:198:LEU:HD11	1.72	0.71
1:B:133:VAL:HG23	1:B:135:TYR:CZ	2.25	0.71
1:B:103:SER:OG	1:B:106:ARG:HB2	1.90	0.70
3:A:194:ILE:HG13	3:A:271:THR:OG1	1.91	0.70
3:M:192:SER:HB3	3:M:271:THR:O	1.91	0.70
3:M:162:GLU:HG3	3:M:163:GLY:N	2.07	0.70
1:B:100:LEU:HD23	1:B:101:ILE:N	2.06	0.70
3:A:164:ILE:HD13	3:A:204:LEU:O	1.92	0.69
3:A:373:LYS:NZ	3:A:423:GLN:HA	2.07	0.69
3:A:249:ASN:O	3:A:250:ASP:CG	2.34	0.69
1:B:133:VAL:HG12	1:B:146:VAL:HG13	1.75	0.68
3:M:205:SER:O	3:M:403:TYR:OH	2.09	0.68
1:C:194:VAL:HG12	1:C:198:LEU:HD12	1.74	0.68
3:A:181:LEU:HD12	3:A:418:TYR:CZ	2.28	0.68
3:A:321:ASP:OD2	3:A:322:SER:HB3	1.94	0.67
1:C:146:VAL:CG2	1:C:184:ARG:NH1	2.57	0.67
1:B:105:ARG:O	1:B:109:ILE:HD12	1.95	0.67
2:E:327:ASP:C	2:E:327:ASP:OD1	2.35	0.67
3:M:373:LYS:HD3	3:M:374:PRO:HD2	1.75	0.67
1:C:100:LEU:HD11	1:C:106:ARG:CZ	2.25	0.67
1:B:185:PHE:C	1:B:185:PHE:CD2	2.73	0.67
3:M:420:LEU:HD13	3:M:420:LEU:N	2.09	0.67
3:M:378:VAL:HG13	3:M:418:TYR:HD2	1.59	0.66
2:E:315:ARG:HD3	2:E:316:LYS:HE2	1.76	0.66
2:D:315:ARG:HG3	2:D:316:LYS:HD3	1.77	0.66
3:A:337:GLU:O	3:A:338:ASN:HB2	1.96	0.66
3:M:212:LEU:HD21	3:M:214:LEU:HD21	1.78	0.66
1:C:106:ARG:O	1:C:109:ILE:HG12	1.95	0.66
3:M:310:VAL:HA	3:M:379:LYS:O	1.96	0.65
1:C:11:ILE:HG22	1:C:11:ILE:O	1.96	0.65
1:B:93:GLU:N	1:B:93:GLU:OE2	2.30	0.65
1:B:59:GLU:OE1	1:B:59:GLU:C	2.40	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:282:VAL:HG21	3:M:294:MSE:HE2	1.78	0.65
3:A:181:LEU:HD23	3:A:191:ARG:O	1.97	0.65
1:B:100:LEU:HD21	1:B:106:ARG:HH11	1.61	0.65
3:A:318:ASN:OD1	3:A:318:ASN:N	2.31	0.64
3:M:160:ARG:HG3	3:M:256:ILE:HG22	1.79	0.64
3:M:293:TYR:N	3:M:358:ALA:O	2.27	0.64
1:B:133:VAL:CG1	1:B:146:VAL:HG13	2.27	0.64
1:C:149:GLU:O	1:C:152:LYS:HG2	1.98	0.64
3:A:272:HIS:O	3:A:272:HIS:CG	2.50	0.64
1:C:15:ALA:O	1:C:19:ARG:HG3	1.98	0.63
1:B:124:TRP:CZ3	1:B:125:GLN:HG3	2.34	0.63
3:M:361:GLY:O	3:M:362:LEU:HD23	1.98	0.63
3:A:317:PRO:O	3:A:320:ALA:HB2	1.98	0.63
3:A:373:LYS:HE3	3:A:423:GLN:HG3	1.80	0.63
1:B:182:GLU:CD	1:B:184:ARG:HH11	2.06	0.63
2:E:315:ARG:NH1	2:E:315:ARG:CG	2.57	0.62
3:M:314:ILE:CG1	3:M:341:ILE:HG23	2.27	0.62
3:M:399:GLU:HB3	3:M:403:TYR:CD2	2.35	0.62
1:C:13:TRP:HH2	1:C:20:MSE:HE3	1.62	0.62
1:C:13:TRP:CZ3	1:C:20:MSE:HE3	2.29	0.62
3:A:373:LYS:HZ1	3:A:423:GLN:HA	1.63	0.62
3:M:162:GLU:HG3	3:M:163:GLY:H	1.65	0.62
3:A:279:ILE:HB	3:A:420:LEU:CD1	2.30	0.61
3:A:378:VAL:HG13	3:A:418:TYR:HD2	1.63	0.61
3:M:286:HIS:CD2	3:M:290:ARG:NH2	2.68	0.61
2:E:325:GLY:O	3:A:396:LYS:HB3	2.01	0.61
3:A:279:ILE:HB	3:A:420:LEU:HD13	1.81	0.61
3:M:373:LYS:HD3	3:M:374:PRO:CD	2.31	0.61
3:M:314:ILE:HG12	3:M:341:ILE:CG2	2.29	0.60
1:C:65:GLU:O	3:M:302:LYS:HE3	2.01	0.60
3:M:286:HIS:HE2	3:M:290:ARG:NH2	1.96	0.60
2:E:316:LYS:HG3	2:E:317:GLY:N	2.17	0.59
1:C:101:ILE:N	1:C:101:ILE:HD12	2.17	0.59
1:C:20:MSE:O	1:C:106:ARG:HD2	2.03	0.59
1:C:77:ARG:HG2	1:C:77:ARG:NH1	2.13	0.59
2:E:315:ARG:HD3	2:E:316:LYS:CE	2.32	0.59
3:M:422:THR:O	3:M:423:GLN:C	2.46	0.58
1:B:16:VAL:O	1:B:20:MSE:CB	2.51	0.58
3:A:392:VAL:HG11	3:A:409:VAL:HG21	1.85	0.58
1:C:182:GLU:HG3	1:C:184:ARG:HH12	1.69	0.58
3:M:160:ARG:HB3	3:M:207:MSE:HE1	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:250:ASP:HB3	3:M:252:THR:OG1	2.03	0.58
1:C:12:GLY:O	1:C:16:VAL:HG23	2.04	0.58
1:B:101:ILE:HD11	1:B:180:VAL:HG12	1.84	0.58
3:M:184:SER:HB2	3:M:190:LEU:CD1	2.34	0.58
1:C:184:ARG:HH11	1:C:184:ARG:CB	2.11	0.58
1:B:79:MSE:HE1	1:B:83:ALA:HB1	1.86	0.57
3:A:279:ILE:HD13	3:A:297:ALA:HA	1.86	0.57
3:M:323:PRO:HB3	3:M:360:PHE:CE2	2.40	0.57
3:A:272:HIS:ND1	3:A:272:HIS:O	2.37	0.57
3:M:192:SER:CB	3:M:271:THR:O	2.53	0.57
3:M:314:ILE:HG22	3:M:376:ILE:HG12	1.87	0.57
1:B:149:GLU:HB2	1:B:150:PRO:HD3	1.87	0.56
1:C:67:GLY:HA3	3:M:385:PHE:CZ	2.39	0.56
3:A:326:LYS:HG2	3:A:327:THR:N	2.19	0.56
3:A:343:TRP:CZ2	3:A:356:MSE:HB2	2.40	0.56
3:A:288:HIS:O	3:A:289:SER:CB	2.54	0.56
3:A:243:ARG:HB2	3:A:246:ARG:HG3	1.88	0.56
1:C:149:GLU:HA	1:C:152:LYS:HE3	1.89	0.55
3:A:392:VAL:CG1	3:A:409:VAL:HG21	2.37	0.55
3:M:282:VAL:HG22	3:M:294:MSE:HB3	1.88	0.55
1:B:79:MSE:HE1	1:B:83:ALA:CB	2.36	0.55
1:B:133:VAL:HG21	1:B:135:TYR:CZ	2.41	0.55
3:M:244:LEU:H	3:M:244:LEU:HD12	1.70	0.55
1:C:103:SER:OG	1:C:106:ARG:HG3	2.07	0.55
3:A:378:VAL:CG1	3:A:418:TYR:HD2	2.20	0.55
1:B:9:SER:O	1:B:11:ILE:N	2.40	0.55
3:A:207:MSE:CE	4:A:503:HOH:O	2.55	0.55
2:E:328:SER:HB2	1:B:79:MSE:O	2.06	0.54
1:B:130:GLY:HA3	1:B:134:ARG:CZ	2.37	0.54
3:A:373:LYS:NZ	3:A:422:THR:O	2.40	0.54
3:M:217:LYS:HD3	3:M:232:GLU:HB2	1.88	0.54
3:M:337:GLU:OE1	3:M:337:GLU:N	2.29	0.54
1:B:101:ILE:HD12	1:B:181:LEU:O	2.07	0.54
3:A:337:GLU:O	3:A:338:ASN:CB	2.54	0.54
3:M:179:VAL:O	3:M:415:ASN:O	2.25	0.54
3:M:336:PRO:HD2	3:M:337:GLU:OE1	2.07	0.54
1:B:98:GLU:C	1:B:100:LEU:H	2.16	0.54
3:M:283:ILE:HD12	3:M:293:TYR:CE2	2.42	0.54
1:B:102:HIS:HE1	1:B:107:GLN:OE1	1.91	0.53
3:A:321:ASP:OD2	3:A:322:SER:HB2	2.07	0.53
3:M:250:ASP:O	3:M:251:ARG:HB2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:160:ARG:NH2	3:A:161:SER:O	2.40	0.53
1:B:179:GLU:HG3	1:B:181:LEU:HD21	1.90	0.53
3:A:378:VAL:CG1	3:A:418:TYR:CD2	2.91	0.53
3:M:159:TRP:CD2	3:M:160:ARG:N	2.76	0.53
2:E:327:ASP:HB2	3:A:394:TYR:CE2	2.43	0.53
1:B:136:PRO:HG3	1:B:143:TYR:O	2.08	0.53
1:C:20:MSE:CA	1:C:109:ILE:CD1	2.81	0.53
3:M:332:VAL:HG11	3:M:341:ILE:HD11	1.90	0.53
1:B:178:ARG:CG	1:B:179:GLU:N	2.72	0.52
3:A:401:SER:O	3:A:403:TYR:CB	2.57	0.52
3:M:210:LEU:HG	3:M:257:PRO:HD3	1.91	0.52
1:B:182:GLU:CD	1:B:184:ARG:NH1	2.67	0.52
3:M:268:ARG:C	3:M:269:LEU:HD13	2.34	0.52
1:C:7:LYS:HA	1:C:10:VAL:HG23	1.91	0.52
1:B:133:VAL:HG12	1:B:146:VAL:HA	1.90	0.52
3:A:258:PRO:HG2	3:A:262:PHE:CD2	2.44	0.52
3:M:268:ARG:O	3:M:269:LEU:HD13	2.08	0.51
1:B:79:MSE:HG3	1:B:80:THR:N	2.25	0.51
1:B:182:GLU:OE1	1:B:184:ARG:NH1	2.37	0.51
3:A:244:LEU:O	3:A:247:PHE:N	2.44	0.51
3:M:239:HIS:ND1	3:M:240:GLN:N	2.58	0.51
3:A:244:LEU:O	3:A:248:GLU:OE2	2.28	0.51
3:A:246:ARG:O	3:A:249:ASN:O	2.29	0.51
3:A:401:SER:O	3:A:403:TYR:HB2	2.11	0.51
1:C:100:LEU:HD12	1:C:101:ILE:N	2.24	0.51
1:C:136:PRO:HG3	1:C:143:TYR:O	2.10	0.51
2:E:315:ARG:NE	2:E:316:LYS:HE3	2.26	0.51
3:A:160:ARG:O	3:A:207:MSE:SE	2.78	0.51
3:A:286:HIS:CD2	3:A:286:HIS:C	2.89	0.51
1:B:20:MSE:O	1:B:106:ARG:CG	2.59	0.51
3:A:219:LEU:C	3:A:219:LEU:HD23	2.36	0.51
3:A:381:GLU:HG2	3:A:382:ILE:N	2.26	0.51
1:C:13:TRP:CZ3	1:C:20:MSE:HE2	2.43	0.50
1:B:11:ILE:O	1:B:14:PRO:HD2	2.11	0.50
3:M:194:ILE:HD11	3:M:387:THR:HB	1.93	0.50
3:M:314:ILE:CG1	3:M:341:ILE:CG2	2.88	0.50
3:M:237:LYS:HD2	3:M:238:PHE:N	2.21	0.50
3:M:361:GLY:C	3:M:362:LEU:HG	2.37	0.50
3:M:378:VAL:CG1	3:M:418:TYR:CD2	2.91	0.50
3:M:378:VAL:CG2	3:M:379:LYS:N	2.75	0.50
1:B:130:GLY:CA	1:B:134:ARG:CZ	2.89	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:283:ILE:HG23	3:M:283:ILE:O	2.11	0.50
1:C:16:VAL:O	1:C:20:MSE:HB2	2.11	0.50
3:M:171:VAL:CG1	3:M:200:MSE:HE3	2.42	0.50
2:E:315:ARG:HH11	2:E:315:ARG:CG	2.02	0.50
3:M:209:GLU:OE1	3:M:256:ILE:HD11	2.12	0.50
3:A:206:GLY:O	3:A:207:MSE:HG2	2.12	0.49
3:A:287:SER:HB3	3:A:290:ARG:HB2	1.94	0.49
3:M:178:ALA:HA	3:M:414:GLN:O	2.12	0.49
1:B:102:HIS:CE1	1:B:107:GLN:OE1	2.65	0.49
3:A:379:LYS:HA	3:A:415:ASN:CG	2.37	0.49
3:M:282:VAL:CG2	3:M:294:MSE:HE2	2.41	0.49
1:C:201:GLU:CD	1:C:201:GLU:H	2.21	0.49
1:B:17:ARG:O	1:B:21:ARG:HG3	2.11	0.49
2:E:315:ARG:HE	2:E:316:LYS:HE3	1.77	0.49
1:B:133:VAL:HG23	1:B:135:TYR:CE2	2.47	0.49
3:A:189:VAL:C	3:A:190:LEU:HD23	2.38	0.49
2:D:331:GLY:O	2:D:332:SER:CB	2.61	0.49
3:A:287:SER:OG	3:A:288:HIS:O	2.29	0.49
3:M:239:HIS:HB2	3:M:263:GLU:O	2.13	0.49
3:A:208:PRO:O	3:A:256:ILE:HG23	2.13	0.49
1:C:7:LYS:HA	1:C:10:VAL:CG2	2.43	0.49
1:B:12:GLY:O	1:B:16:VAL:HG23	2.12	0.49
1:B:133:VAL:CG2	1:B:135:TYR:OH	2.60	0.49
3:A:182:LEU:HB3	3:A:190:LEU:HB2	1.94	0.48
3:A:288:HIS:O	3:A:289:SER:OG	2.29	0.48
3:A:325:PHE:HA	3:A:358:ALA:HA	1.95	0.48
3:M:182:LEU:HD13	3:M:190:LEU:HD22	1.94	0.48
3:M:233:LEU:HD23	3:M:233:LEU:H	1.78	0.48
3:M:268:ARG:C	3:M:269:LEU:CD1	2.86	0.48
2:E:316:LYS:HG2	2:E:317:GLY:N	2.08	0.48
3:A:286:HIS:HD2	3:A:287:SER:CA	2.26	0.48
1:B:9:SER:O	1:B:10:VAL:C	2.56	0.48
1:B:14:PRO:HA	1:B:17:ARG:NH1	2.29	0.48
3:M:419:GLN:C	3:M:420:LEU:HD13	2.38	0.48
1:C:146:VAL:HG22	1:C:184:ARG:HH12	1.79	0.48
3:A:286:HIS:CG	3:A:287:SER:H	2.32	0.48
3:A:401:SER:O	3:A:402:GLY:C	2.57	0.48
3:M:189:VAL:HB	3:M:272:HIS:CE1	2.49	0.48
1:C:87:LEU:HD13	1:C:141:TRP:CZ3	2.49	0.47
3:A:181:LEU:HA	3:A:191:ARG:O	2.13	0.47
3:A:231:VAL:CG2	3:A:388:SER:HB2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:378:VAL:CG1	3:M:418:TYR:HD2	2.26	0.47
1:B:94:LYS:HA	1:B:94:LYS:HD3	1.44	0.47
3:A:298:LYS:HA	3:A:352:LYS:O	2.14	0.47
3:A:294:MSE:HA	3:A:357:ARG:HD3	1.95	0.47
3:A:271:THR:HG23	3:A:273:VAL:HG22	1.96	0.47
1:C:148:VAL:O	1:C:152:LYS:HE3	2.14	0.47
2:D:331:GLY:O	2:D:332:SER:HB3	2.14	0.47
3:A:241:CYS:HB2	3:A:256:ILE:O	2.14	0.47
3:A:243:ARG:CB	3:A:246:ARG:HG3	2.45	0.47
3:M:279:ILE:HB	3:M:420:LEU:HD23	1.96	0.47
1:B:127:TYR:HB3	1:B:134:ARG:HB3	1.97	0.47
3:A:334:TRP:O	3:A:336:PRO:HD3	2.15	0.47
3:M:314:ILE:HG22	3:M:376:ILE:CG1	2.44	0.47
3:M:337:GLU:H	3:M:337:GLU:CD	2.10	0.47
3:M:335:VAL:HG12	3:M:338:ASN:H	1.80	0.46
3:A:173:LEU:HD11	3:A:200:MSE:HE3	1.98	0.46
1:B:92:LYS:HD2	1:B:185:PHE:CD1	2.51	0.46
3:M:197:SER:HB2	3:M:263:GLU:OE1	2.16	0.46
3:M:392:VAL:CG1	3:M:409:VAL:HG21	2.46	0.46
3:M:160:ARG:HB3	3:M:207:MSE:CE	2.45	0.46
3:M:325:PHE:HB3	3:M:357:ARG:O	2.15	0.46
1:B:136:PRO:CG	1:B:143:TYR:O	2.63	0.46
3:A:306:THR:HG23	3:A:349:PRO:HA	1.98	0.46
3:M:420:LEU:N	3:M:420:LEU:CD1	2.79	0.46
1:C:58:LEU:O	3:A:324:LYS:HA	2.16	0.46
1:B:88:SER:HB3	1:B:142:CYS:HB2	1.96	0.46
3:A:169:ASN:HB3	3:A:204:LEU:HD23	1.98	0.46
1:C:11:ILE:O	1:C:11:ILE:CG2	2.64	0.45
3:M:273:VAL:O	3:M:274:LYS:C	2.58	0.45
3:A:322:SER:N	3:A:323:PRO:HD3	2.31	0.45
3:M:181:LEU:HD23	3:M:191:ARG:O	2.17	0.45
1:C:203:PHE:O	1:C:204:LYS:CB	2.64	0.45
2:E:318:GLY:O	3:A:410:ARG:NH1	2.44	0.45
1:B:121:PHE:HA	1:B:122:PRO:HD3	1.81	0.45
1:B:101:ILE:HD11	1:B:180:VAL:HG13	1.93	0.45
3:A:271:THR:O	3:A:271:THR:HG22	2.17	0.45
3:A:399:GLU:HB3	3:A:403:TYR:CE2	2.52	0.45
1:B:146:VAL:CG2	1:B:184:ARG:HB2	2.47	0.45
3:M:290:ARG:HA	3:M:361:GLY:HA2	1.99	0.45
1:B:71:THR:HG23	3:A:304[A]:ARG:HH12	1.82	0.45
3:M:201[A]:ARG:HG3	3:M:261:GLU:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:315:ARG:CD	2:E:316:LYS:HE2	2.45	0.44
1:B:79:MSE:CE	1:B:80:THR:H	2.29	0.44
2:E:322:GLN:NE2	3:A:406:LEU:HD22	2.32	0.44
2:E:320:TYR:HB3	3:A:408:TRP:HB3	2.00	0.44
1:B:10:VAL:HG23	1:B:11:ILE:N	2.33	0.44
1:C:7:LYS:O	1:C:10:VAL:HB	2.17	0.44
3:M:336:PRO:CD	3:M:337:GLU:OE1	2.66	0.44
1:C:196:ARG:HA	1:C:203:PHE:CD1	2.53	0.44
3:A:283:ILE:H	3:A:283:ILE:HG12	1.60	0.44
1:B:80:THR:HG22	1:B:83:ALA:H	1.83	0.44
3:A:288:HIS:N	3:A:288:HIS:CD2	2.86	0.44
3:A:325:PHE:CD2	3:A:325:PHE:C	2.96	0.44
2:E:325:GLY:O	3:A:396:LYS:CB	2.66	0.44
3:M:233:LEU:HD23	3:M:233:LEU:N	2.32	0.44
3:M:239:HIS:CG	3:M:240:GLN:N	2.86	0.44
3:M:269:LEU:HD12	3:M:269:LEU:HA	1.59	0.44
1:B:11:ILE:C	1:B:14:PRO:HD2	2.42	0.43
3:M:159:TRP:CE3	3:M:160:ARG:O	2.71	0.43
3:M:271:THR:O	3:M:271:THR:HG23	2.17	0.43
3:M:386:THR:CG2	3:M:411:TYR:HB3	2.47	0.43
3:A:164:ILE:H	3:A:164:ILE:HG13	1.62	0.43
3:M:258:PRO:HD2	3:M:262:PHE:CE2	2.53	0.43
3:A:287:SER:HB3	3:A:290:ARG:CB	2.49	0.43
3:M:332:VAL:CG1	3:M:341:ILE:HD11	2.48	0.43
1:B:127:TYR:CD2	1:B:145:LEU:HD11	2.52	0.43
1:B:139:PHE:HB2	1:B:193:HIS:CE1	2.53	0.43
3:A:213:GLY:HA3	3:A:394:TYR:CE2	2.54	0.43
3:A:389:GLY:O	3:A:390:ILE:C	2.60	0.43
1:C:186:ASP:HB3	1:C:189:LEU:CD1	2.49	0.43
1:B:133:VAL:HG21	1:B:135:TYR:OH	2.18	0.43
1:C:21:ARG:O	1:C:22:ARG:C	2.61	0.43
1:C:194:VAL:O	1:C:198:LEU:HD12	2.19	0.43
3:A:258:PRO:HG2	3:A:262:PHE:CG	2.53	0.43
3:M:181:LEU:HD23	3:M:181:LEU:HA	1.87	0.43
3:M:183:VAL:HB	3:M:420:LEU:HD12	2.00	0.43
3:M:287:SER:C	3:M:289:SER:N	2.76	0.43
1:C:57:TRP:CD1	1:C:57:TRP:N	2.87	0.42
1:C:121:PHE:CE1	3:M:393:ARG:HA	2.54	0.42
2:D:320:TYR:HB3	3:M:408:TRP:HB3	2.01	0.42
2:E:316:LYS:HG3	2:E:317:GLY:H	1.68	0.42
3:M:159:TRP:CE2	3:M:160:ARG:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:TRP:CH2	1:C:125:GLN:HG3	2.53	0.42
1:B:197:GLU:O	1:B:200:PRO:HD3	2.19	0.42
3:A:379:LYS:HA	3:A:415:ASN:OD1	2.19	0.42
3:A:244:LEU:O	3:A:247:PHE:HB3	2.19	0.42
3:A:291:ILE:O	3:A:359:HIS:CB	2.61	0.42
3:M:181:LEU:HD12	3:M:418:TYR:CZ	2.54	0.42
3:M:361:GLY:O	3:M:362:LEU:CD2	2.67	0.42
1:B:98:GLU:HG3	1:B:99:GLY:N	2.34	0.42
3:A:270:ASN:OD1	3:A:270:ASN:O	2.36	0.42
3:M:308:ASN:O	3:M:309:ASN:C	2.61	0.42
3:A:183:VAL:CB	3:A:420:LEU:HD23	2.45	0.42
3:M:215:ASN:O	3:M:215:ASN:CG	2.63	0.42
1:B:11:ILE:O	1:B:11:ILE:CG1	2.67	0.42
3:M:167:ARG:O	3:M:167:ARG:HG3	2.18	0.42
3:M:392:VAL:HG11	3:M:409:VAL:HG21	2.01	0.42
1:C:194:VAL:CG1	1:C:198:LEU:HD11	2.44	0.42
2:E:315:ARG:CD	2:E:316:LYS:CE	2.98	0.42
1:C:13:TRP:CH2	1:C:20:MSE:CE	2.81	0.41
3:M:399:GLU:HG3	3:M:400:LYS:N	2.31	0.41
3:A:290:ARG:HD2	3:A:290:ARG:HA	1.81	0.41
1:C:196:ARG:HG3	1:C:203:PHE:CG	2.55	0.41
3:A:310:VAL:HA	3:A:379:LYS:O	2.20	0.41
3:M:211:ARG:O	3:M:395:LEU:HD12	2.20	0.41
3:A:376:ILE:HG22	3:A:377:SER:N	2.36	0.41
1:C:97:LEU:HD23	1:C:97:LEU:HA	1.84	0.41
1:B:13:TRP:O	1:B:14:PRO:C	2.60	0.41
3:A:302:LYS:HD2	3:A:304[B]:ARG:HH11	1.84	0.41
3:M:167:ARG:HG2	3:M:167:ARG:HH11	1.85	0.41
1:C:101:ILE:H	1:C:101:ILE:HD12	1.85	0.41
2:D:315:ARG:HG2	2:D:316:LYS:HB2	2.02	0.41
3:A:164:ILE:CD1	3:A:204:LEU:O	2.66	0.41
3:A:196:GLY:HA3	3:A:267:TYR:CZ	2.56	0.41
3:A:271:THR:CG2	3:A:273:VAL:HG22	2.51	0.41
3:A:357:ARG:HH11	3:A:357:ARG:CG	2.34	0.41
3:A:399:GLU:HG2	3:A:403:TYR:CD1	2.56	0.41
3:M:395:LEU:HD23	3:M:407:PRO:HB3	2.03	0.41
3:M:321:ASP:O	3:M:360:PHE:HB3	2.21	0.41
1:C:120:TYR:O	1:C:121:PHE:C	2.64	0.40
1:C:22:ARG:CZ	3:A:289:SER:HB3	2.51	0.40
2:D:315:ARG:O	2:D:316:LYS:C	2.64	0.40
1:B:77:ARG:HB2	1:B:78:PRO:CD	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:181:LEU:HD23	3:A:181:LEU:HA	1.80	0.40
3:A:288:HIS:CD2	3:A:288:HIS:H	2.39	0.40
3:A:343:TRP:CH2	3:A:356:MSE:HB2	2.57	0.40
1:B:77:ARG:HB2	1:B:78:PRO:HD2	2.03	0.40
3:A:250:ASP:O	3:A:251:ARG:HB2	2.21	0.40
3:M:213:GLY:HA3	3:M:394:TYR:CE1	2.56	0.40
1:B:148:VAL:CG1	1:B:182:GLU:CD	2.95	0.40
1:C:17:ARG:O	1:C:20:MSE:HB3	2.22	0.40
1:C:77:ARG:NH1	1:C:77:ARG:CG	2.75	0.40
3:A:174:ASP:HB3	3:A:176:ILE:HD11	2.02	0.40
3:A:251:ARG:HA	3:A:251:ARG:HD3	1.88	0.40
3:A:287:SER:H	3:A:290:ARG:HB3	1.86	0.40
3:M:314:ILE:HD13	3:M:314:ILE:HG23	1.78	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	B	132/206 (64%)	127 (96%)	5 (4%)	0	100	100
1	C	136/206 (66%)	132 (97%)	4 (3%)	0	100	100
2	D	17/28 (61%)	16 (94%)	1 (6%)	0	100	100
2	E	15/28 (54%)	14 (93%)	1 (7%)	0	100	100
3	A	252/266 (95%)	241 (96%)	11 (4%)	0	100	100
3	M	252/266 (95%)	246 (98%)	6 (2%)	0	100	100
All	All	804/1000 (80%)	776 (96%)	28 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	B	122/169 (72%)	107 (88%)	15 (12%)	4	15
1	C	125/169 (74%)	103 (82%)	22 (18%)	2	6
2	D	12/20 (60%)	9 (75%)	3 (25%)	0	2
2	E	10/20 (50%)	6 (60%)	4 (40%)	0	0
3	A	234/237 (99%)	196 (84%)	38 (16%)	2	8
3	M	234/237 (99%)	192 (82%)	42 (18%)	2	6
All	All	737/852 (86%)	613 (83%)	124 (17%)	2	7

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	20	MSE
1	C	58	LEU
1	C	61	GLN
1	C	62	GLU
1	C	64	GLU
1	C	66	VAL
1	C	71	THR
1	C	72	PRO
1	C	77	ARG
1	C	87	LEU
1	C	88	SER
1	C	91	LEU
1	C	97	LEU
1	C	98	GLU
1	C	101	ILE
1	C	106	ARG
1	C	107	GLN
1	C	110	LEU
1	C	123	ASP
1	C	125	GLN
1	C	151	ASP
1	C	178	ARG

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Mol	Chain	Res	Type
2	D	315	ARG
2	D	328	SER
2	D	330	GLN
2	E	315	ARG
2	E	316	LYS
2	E	326	SER
2	E	328	SER
1	B	59	GLU
1	B	61	GLN
1	B	71	THR
1	B	72	PRO
1	B	77	ARG
1	B	80	THR
1	B	87	LEU
1	B	91	LEU
1	B	93	GLU
1	B	94	LYS
1	B	97	LEU
1	B	114	ILE
1	B	125	GLN
1	B	146	VAL
1	B	184	ARG
3	A	161	SER
3	A	164	ILE
3	A	176	ILE
3	A	181	LEU
3	A	182	LEU
3	A	197	SER
3	A	207	MSE
3	A	209	GLU
3	A	227	LYS
3	A	229	LYS
3	A	231	VAL
3	A	234	GLU
3	A	250	ASP
3	A	256	ILE
3	A	259	ASP
3	A	263	GLU
3	A	269	LEU
3	A	270	ASN
3	A	272	HIS
3	A	281	SER

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Mol	Chain	Res	Type
3	A	283	ILE
3	A	286	HIS
3	A	287	SER
3	A	291	ILE
3	A	295	VAL
3	A	306	THR
3	A	310	VAL
3	A	318	ASN
3	A	321	ASP
3	A	331	SER
3	A	355	LEU
3	A	357	ARG
3	A	376	ILE
3	A	378	VAL
3	A	392	VAL
3	A	400	LYS
3	A	401	SER
3	A	421	ARG
3	M	160	ARG
3	M	161	SER
3	M	164	ILE
3	M	167	ARG
3	M	173	LEU
3	M	181	LEU
3	M	182	LEU
3	M	210	LEU
3	M	216	ASP
3	M	219	LEU
3	M	227	LYS
3	M	231	VAL
3	M	237	LYS
3	M	250	ASP
3	M	261	GLU
3	M	269	LEU
3	M	271	THR
3	M	272	HIS
3	M	284	GLU
3	M	295	VAL
3	M	310	VAL
3	M	314	ILE
3	M	324	LYS
3	M	325	PHE

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Mol	Chain	Res	Type
3	M	326	LYS
3	M	328	THR
3	M	329	VAL
3	M	332	VAL
3	M	337	GLU
3	M	355	LEU
3	M	357	ARG
3	M	373	LYS
3	M	378	VAL
3	M	387	THR
3	M	392	VAL
3	M	398	ILE
3	M	399	GLU
3	M	400	LYS
3	M	401	SER
3	M	403	TYR
3	M	420	LEU
3	M	422	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	89	HIS
1	C	116	HIS
1	C	199	HIS
2	E	322	GLN
1	B	102	HIS
1	B	193	HIS
3	A	186	ASN
3	A	286	HIS
3	A	288	HIS
3	A	300	GLN
3	A	308	ASN
3	A	338	ASN
3	A	423	GLN
3	M	249	ASN
3	M	286	HIS

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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

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, 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	B	136/206 (66%)	0.58	7 (5%) 33 26	86, 122, 195, 256	0
1	C	140/206 (67%)	0.57	12 (8%) 16 13	72, 113, 176, 201	0
2	D	19/28 (67%)	0.38	0 100 100	71, 94, 139, 149	0
2	E	17/28 (60%)	0.52	0 100 100	86, 102, 148, 151	0
3	A	250/266 (93%)	0.33	8 (3%) 50 41	52, 115, 170, 236	1 (0%)
3	M	250/266 (93%)	0.14	4 (1%) 70 62	53, 104, 148, 182	1 (0%)
All	All	812/1000 (81%)	0.36	31 (3%) 44 36	52, 113, 168, 256	2 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	159	TRP	4.2
1	B	23	ALA	3.7
3	A	362	LEU	3.3
1	C	202	TYR	3.1
3	A	159	TRP	3.0
1	B	204	LYS	3.0
1	B	138	THR	3.0
1	C	149	GLU	2.8
1	C	23	ALA	2.8
1	B	149	GLU	2.7
1	C	10	VAL	2.7
3	A	360	PHE	2.7
1	C	180	VAL	2.7
1	C	189	LEU	2.6
3	A	288	HIS	2.5
1	B	10	VAL	2.4
1	B	5	TRP	2.4
1	C	204	LYS	2.4
1	C	183	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
3	A	285	LYS	2.3
1	C	185	PHE	2.3
1	B	150	PRO	2.3
3	M	237	LYS	2.2
3	M	272	HIS	2.2
1	C	193	HIS	2.1
1	C	192	HIS	2.0
3	A	233	LEU	2.0
1	C	90	PHE	2.0
3	A	161	SER	2.0
3	M	357	ARG	2.0
3	A	283	ILE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.