Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:51 AM GMT

PDB ID	:	3Q84
Title	:	Crystal structure of human PACSIN 1 F-BAR domain
Authors	:	Bai, X.
Deposited on	:	2011-01-06
Resolution	:	2.80 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:

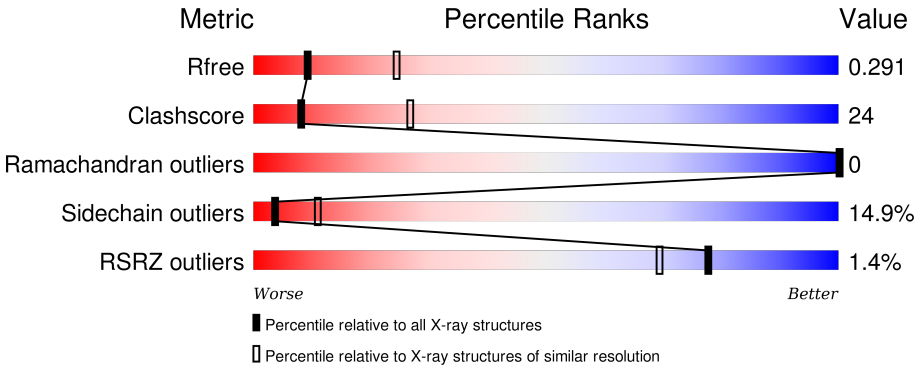
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	295	60% 30% 7% •
1	B	295	% 64% 27% 5% •
1	G	295	% 66% 23% 7% •
1	H	295	% 61% 28% 8% ••
1	M	295	2% 51% 36% 5% 8%

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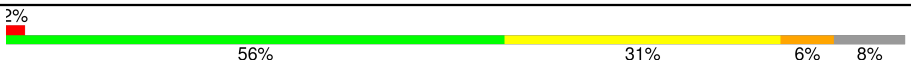
Mol	Chain	Length	Quality of chain
1	N	295	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14091 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 kinase C and casein kinase substrate in neurons protein 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	Se	0	0	0
			2350	1478	415	442	5	10			
1	B	285	Total	C	N	O	S	Se	0	0	0
			2353	1475	418	445	5	10			
1	G	287	Total	C	N	O	S	Se	0	0	0
			2353	1475	419	444	5	10			
1	H	288	Total	C	N	O	S	Se	0	0	0
			2375	1492	421	447	5	10			
1	M	271	Total	C	N	O	S	Se	0	0	0
			2227	1401	395	418	5	8			
1	N	272	Total	C	N	O	S	Se	0	0	0
			2216	1390	395	418	5	8			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		
2	N	1	Total	Ca	0	0
			1	1		
2	M	1	Total	Ca	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	44	Total	O	0	0
			44	44		
3	B	44	Total	O	0	0
			44	44		

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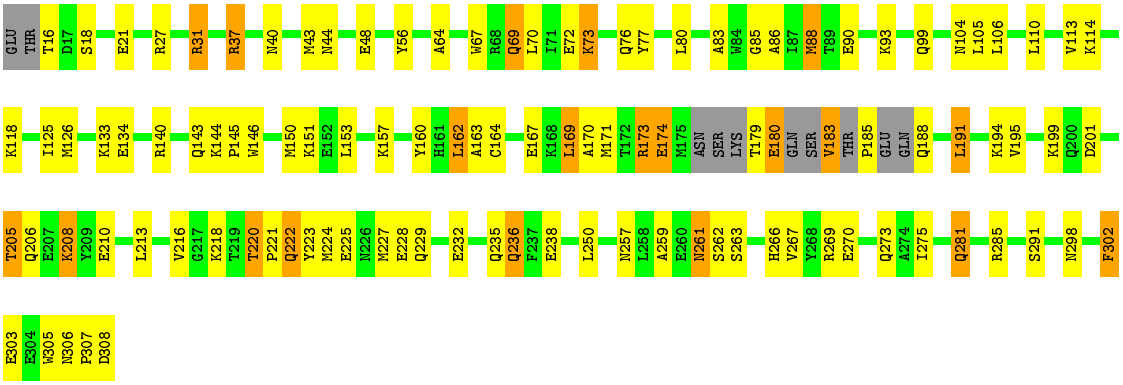
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	40	Total O 40 40	0	0
3	H	32	Total O 32 32	0	0
3	M	23	Total O 23 23	0	0
3	N	30	Total O 30 30	0	0

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.

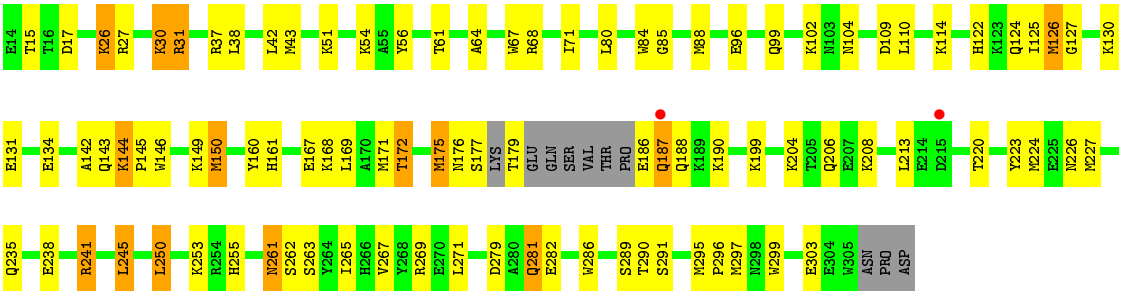
- Molecule 1: Protein kinase C and casein kinase substrate in neurons protein 1

Chain A:



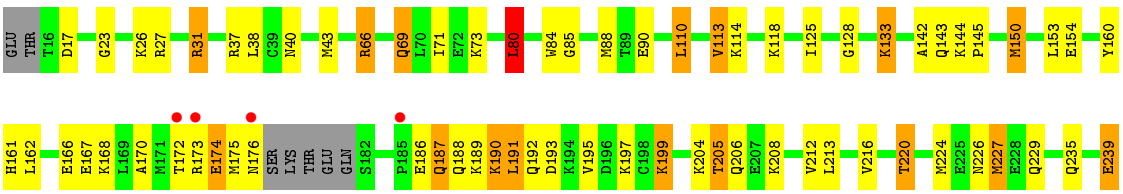
- Molecule 1: Protein kinase C and casein kinase substrate in neurons protein 1

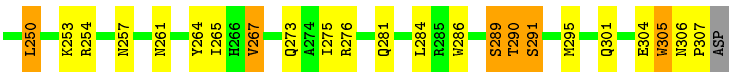
Chain B:



- Molecule 1: Protein kinase C and casein kinase substrate in neurons protein 1

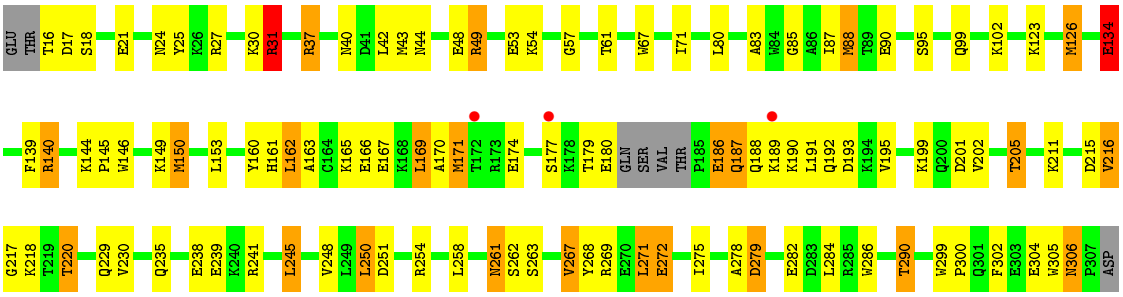
Chain G:





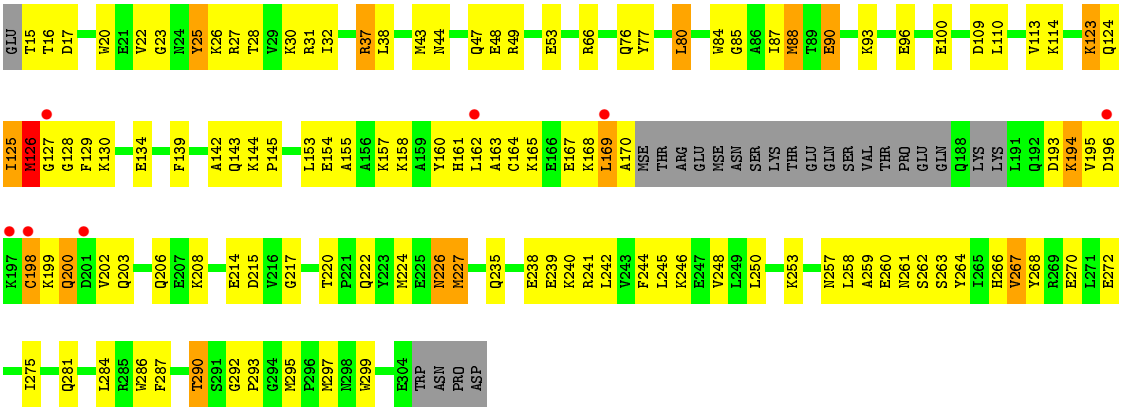
• Molecule 1: Protein kinase C and casein kinase substrate in neurons protein 1

Chain H:



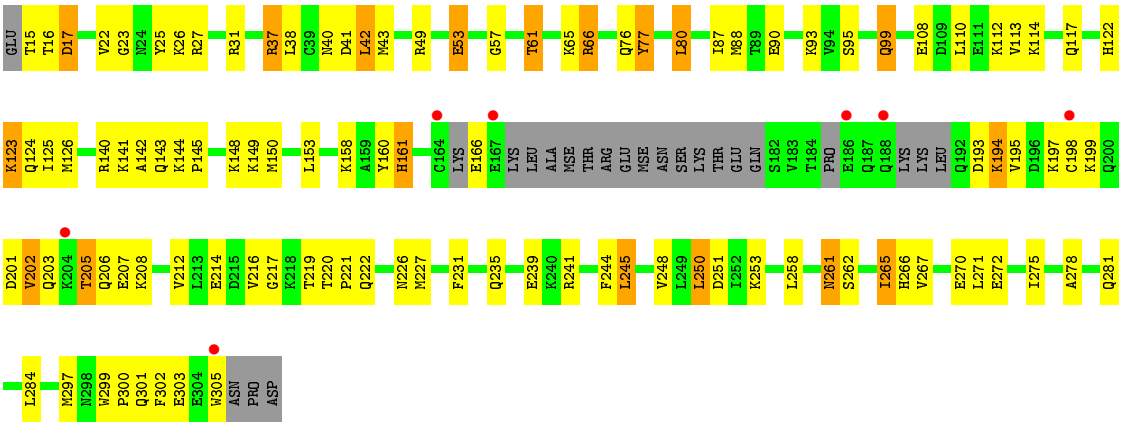
• Molecule 1: Protein kinase C and casein kinase substrate in neurons protein 1

Chain M:



• Molecule 1: Protein kinase C and casein kinase substrate in neurons protein 1

Chain N:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	86.35Å 154.29Å 215.45Å 90.00° 90.34° 90.00°	Depositor
Resolution (Å)	29.06 – 2.80 29.06 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.2 (29.06-2.80) 94.6 (29.06-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.33 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.221 , 0.294 0.234 , 0.291	Depositor DCC
R_{free} test set	3358 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	53.5	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 21.0	EDS
Estimated twinning fraction	0.008 for -1/2*h-1/2*k,-3/2*h+1/2*k,-l 0.012 for -1/2*h+1/2*k,3/2*h+1/2*k,-l 0.003 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.005 for 1/2*h+1/2*k,3/2*h-1/2*k,-l 0.447 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 66712 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	14091	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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: CA

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	1.17	1/2384 (0.0%)	0.91	1/3178 (0.0%)
1	B	1.02	0/2387	0.87	0/3184
1	G	1.05	0/2386	0.86	4/3180 (0.1%)
1	H	1.09	1/2411 (0.0%)	0.89	2/3215 (0.1%)
1	M	1.06	1/2261 (0.0%)	0.86	1/3019 (0.0%)
1	N	0.84	0/2247	0.80	0/2998
All	All	1.05	3/14076 (0.0%)	0.87	8/18774 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	164	CYS	CB-SG	-5.70	1.72	1.81
1	H	134	GLU	CG-CD	5.68	1.60	1.51
1	M	268	TYR	CE2-CZ	-5.00	1.32	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	80	LEU	CA-CB-CG	-5.73	102.12	115.30
1	G	66	ARG	NE-CZ-NH1	-5.53	117.54	120.30
1	M	126	MSE	N-CA-C	-5.35	96.55	111.00
1	G	305	TRP	N-CA-C	-5.34	96.59	111.00
1	H	31	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	G	276	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	H	279	ASP	CB-CG-OD1	5.24	123.02	118.30
1	A	73	LYS	N-CA-C	-5.01	97.47	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2350	0	2286	125	1
1	B	2353	0	2288	104	1
1	G	2353	0	2285	145	1
1	H	2375	0	2313	101	1
1	M	2227	0	2171	147	0
1	N	2216	0	2134	110	0
2	B	1	0	0	0	0
2	G	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
3	A	44	0	0	0	0
3	B	44	0	0	1	0
3	G	40	0	0	2	0
3	H	32	0	0	1	0
3	M	23	0	0	0	0
3	N	30	0	0	2	0
All	All	14091	0	13477	669	2

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 24.

All (669) 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:H:177:SER:CB	1:H:191:LEU:HD13	1.51	1.40
1:N:43:MSE:HE1	1:N:114:LYS:CB	1.53	1.38
1:A:169:LEU:HD13	1:A:170:ALA:N	1.41	1.33
1:M:160:TYR:HE1	1:M:206:GLN:NE2	1.28	1.29
1:N:43:MSE:CE	1:N:114:LYS:HB2	1.62	1.28
1:G:191:LEU:HD12	1:G:192:GLN:N	1.45	1.28
1:B:110:LEU:HD23	1:B:110:LEU:O	1.33	1.27
1:M:161:HIS:CD2	1:M:164:CYS:SG	2.29	1.25
1:H:85:GLY:HA2	1:H:88:MSE:CE	1.68	1.24
1:G:43:MSE:HE1	1:G:114:LYS:CA	1.66	1.24
1:H:169:LEU:HD23	1:H:169:LEU:C	1.54	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:43:MSE:HE3	1:N:114:LYS:N	1.52	1.23
1:N:43:MSE:HE1	1:N:114:LYS:CA	1.67	1.22
1:G:128:GLY:HA3	1:G:133:LYS:CE	1.70	1.19
1:H:177:SER:CB	1:H:191:LEU:CD1	2.20	1.19
1:A:162:LEU:HD23	1:A:162:LEU:C	1.60	1.19
1:M:125:ILE:H	1:M:125:ILE:CD1	1.49	1.18
1:G:174:GLU:HB3	1:G:191:LEU:CD2	1.73	1.18
1:A:169:LEU:O	1:A:169:LEU:HD22	1.39	1.17
1:B:110:LEU:HD23	1:B:110:LEU:C	1.54	1.17
1:M:43:MSE:CE	1:M:114:LYS:HB2	1.74	1.16
1:N:43:MSE:CE	1:N:114:LYS:CB	2.22	1.15
1:N:194:LYS:HD3	1:N:194:LYS:N	1.57	1.13
1:G:128:GLY:CA	1:G:133:LYS:HE2	1.79	1.13
1:B:43:MSE:HE1	1:B:114:LYS:CA	1.78	1.13
1:H:169:LEU:HD23	1:H:170:ALA:N	1.61	1.12
1:A:223:TYR:HE1	1:A:227:MSE:HE3	1.05	1.12
1:H:85:GLY:HA2	1:H:88:MSE:HE1	1.30	1.11
1:M:123:LYS:NZ	1:M:127:GLY:HA2	1.65	1.11
1:G:43:MSE:CE	1:G:114:LYS:N	2.14	1.10
1:G:174:GLU:CB	1:G:191:LEU:HD21	1.81	1.10
1:G:167:GLU:OE1	1:G:199:LYS:HE3	1.52	1.10
1:A:37:ARG:HH21	1:A:37:ARG:HG2	1.00	1.10
1:M:125:ILE:HD12	1:M:125:ILE:N	1.56	1.10
1:G:43:MSE:HE1	1:G:114:LYS:HA	1.14	1.09
1:A:143:GLN:HB2	1:A:227:MSE:HE1	1.11	1.08
1:M:43:MSE:HE1	1:M:114:LYS:CB	1.84	1.08
1:A:169:LEU:C	1:A:169:LEU:HD13	1.73	1.08
1:M:155:ALA:HA	1:M:158:LYS:HE2	1.26	1.08
1:M:160:TYR:CE1	1:M:206:GLN:NE2	2.21	1.07
1:B:43:MSE:HE1	1:B:114:LYS:HA	1.26	1.07
1:B:43:MSE:CE	1:B:114:LYS:CA	2.32	1.07
1:N:43:MSE:CE	1:N:114:LYS:CA	2.30	1.07
1:A:223:TYR:CE1	1:A:227:MSE:HE3	1.91	1.05
1:N:43:MSE:HE2	1:N:114:LYS:HB2	1.34	1.05
1:N:43:MSE:CE	1:N:114:LYS:N	2.19	1.05
1:G:43:MSE:CE	1:G:114:LYS:CA	2.36	1.02
1:G:43:MSE:HE3	1:G:113:VAL:HG22	1.38	1.02
1:A:162:LEU:HD23	1:A:162:LEU:O	1.56	1.02
1:M:162:LEU:C	1:M:162:LEU:HD23	1.79	1.01
1:M:154:GLU:O	1:M:158:LYS:HG2	1.60	1.01
1:M:198:CYS:SG	1:M:199:LYS:N	2.34	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:85:GLY:HA2	1:G:88:MSE:CE	1.90	1.00
1:H:171:MSE:N	1:H:171:MSE:SE	2.45	1.00
1:G:128:GLY:HA3	1:G:133:LYS:HE2	1.01	0.99
1:M:43:MSE:CE	1:M:114:LYS:CB	2.37	0.99
1:B:175:MSE:SE	1:B:176:ASN:OD1	2.29	0.99
1:A:162:LEU:C	1:A:162:LEU:CD2	2.30	0.99
1:G:191:LEU:C	1:G:191:LEU:CD1	2.30	0.99
1:B:43:MSE:HE3	1:B:114:LYS:N	1.76	0.98
1:H:126:MSE:H	1:H:126:MSE:SE	1.96	0.98
1:A:37:ARG:HH21	1:A:37:ARG:CG	1.76	0.98
1:G:85:GLY:HA2	1:G:88:MSE:HE2	1.41	0.98
1:H:160:TYR:HA	1:H:205:THR:HG23	1.42	0.97
1:B:43:MSE:CE	1:B:114:LYS:N	2.27	0.97
1:G:190:LYS:HZ2	1:G:190:LYS:HA	1.28	0.97
1:M:264:TYR:O	1:M:267:VAL:HG13	1.64	0.96
1:M:169:LEU:O	1:M:169:LEU:HD13	1.64	0.96
1:B:110:LEU:C	1:B:110:LEU:CD2	2.30	0.96
1:A:169:LEU:HD13	1:A:170:ALA:CA	1.95	0.96
1:H:169:LEU:CD2	1:H:170:ALA:N	2.30	0.95
1:A:169:LEU:CD1	1:A:170:ALA:N	2.29	0.94
1:G:191:LEU:CD1	1:G:192:GLN:N	2.30	0.94
1:B:43:MSE:HE2	1:B:114:LYS:HB2	1.49	0.94
1:A:143:GLN:CB	1:A:227:MSE:HE1	1.95	0.94
1:H:169:LEU:CD2	1:H:169:LEU:C	2.30	0.93
1:B:31:ARG:HH22	1:B:235:GLN:HE22	1.07	0.93
1:G:186:GLU:CD	1:G:187:GLN:HA	1.88	0.93
1:H:216:VAL:O	1:H:220:THR:HG22	1.69	0.93
1:M:43:MSE:HE1	1:M:114:LYS:CG	1.98	0.93
1:M:170:ALA:HB1	1:M:195:VAL:HG22	1.50	0.92
1:G:191:LEU:C	1:G:191:LEU:HD12	1.89	0.91
1:M:160:TYR:HE1	1:M:206:GLN:HE21	0.93	0.91
1:M:155:ALA:O	1:M:158:LYS:HG3	1.70	0.90
1:M:43:MSE:HE1	1:M:114:LYS:HG3	1.51	0.90
1:M:80:LEU:HD22	1:N:245:LEU:HD13	1.53	0.90
1:M:161:HIS:O	1:M:164:CYS:SG	2.29	0.90
1:A:143:GLN:HB2	1:A:227:MSE:CE	2.00	0.90
1:M:123:LYS:HZ1	1:M:127:GLY:HA2	1.36	0.89
1:M:275:ILE:HG21	1:N:250:LEU:HD13	1.52	0.89
1:A:169:LEU:C	1:A:169:LEU:HD22	1.85	0.89
1:A:43:MSE:CG	1:A:113:VAL:HG21	2.04	0.88
1:B:85:GLY:HA2	1:B:88:MSE:HE2	1.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:186:GLU:OE1	1:G:187:GLN:HB2	1.73	0.87
1:H:170:ALA:HB1	1:H:195:VAL:HG22	1.56	0.87
1:B:85:GLY:HA2	1:B:88:MSE:CE	2.04	0.87
1:A:223:TYR:HE1	1:A:227:MSE:CE	1.86	0.86
1:N:194:LYS:CD	1:N:194:LYS:N	2.38	0.86
1:A:37:ARG:NH2	1:A:37:ARG:HG2	1.81	0.86
1:N:43:MSE:HE1	1:N:114:LYS:HA	1.55	0.85
1:B:142:ALA:HB3	1:B:227:MSE:HE2	1.57	0.85
1:M:161:HIS:NE2	1:M:164:CYS:SG	2.48	0.85
1:H:160:TYR:HA	1:H:205:THR:CG2	2.07	0.85
1:N:43:MSE:HE3	1:N:114:LYS:H	1.40	0.85
1:G:189:LYS:C	1:G:190:LYS:NZ	2.30	0.85
1:A:43:MSE:CG	1:A:113:VAL:CG2	2.55	0.85
1:A:305:TRP:CG	1:A:305:TRP:O	2.30	0.84
1:G:31:ARG:HH22	1:G:235:GLN:HE22	1.25	0.84
1:B:43:MSE:CE	1:B:114:LYS:HB2	2.07	0.84
1:M:93:LYS:HE3	1:M:270:GLU:OE2	1.78	0.84
1:A:206:GLN:O	1:A:210:GLU:HG3	1.78	0.84
1:M:125:ILE:H	1:M:125:ILE:HD12	0.72	0.84
1:G:142:ALA:HB3	1:G:227:MSE:HE1	1.58	0.84
1:G:190:LYS:HZ3	1:G:190:LYS:N	1.76	0.83
1:A:31:ARG:NH2	1:A:235:GLN:HE21	1.75	0.83
1:B:43:MSE:CE	1:B:114:LYS:HA	2.01	0.83
1:A:85:GLY:O	1:A:88:MSE:HG2	1.77	0.83
1:B:43:MSE:CE	1:B:114:LYS:CB	2.56	0.83
1:G:174:GLU:HB3	1:G:191:LEU:HD21	0.89	0.82
1:G:187:GLN:HG2	1:G:187:GLN:O	1.76	0.82
1:G:190:LYS:HA	1:G:190:LYS:NZ	1.94	0.82
1:H:254:ARG:HD2	3:H:335:HOH:O	1.79	0.82
1:G:43:MSE:HE3	1:G:114:LYS:N	1.92	0.82
1:A:43:MSE:HG2	1:A:113:VAL:CG2	2.09	0.82
1:A:170:ALA:HB1	1:A:195:VAL:HG22	1.62	0.82
1:M:161:HIS:HE1	1:N:305:TRP:CB	1.93	0.82
1:M:167:GLU:HG3	1:M:198:CYS:SG	2.20	0.82
1:H:169:LEU:HD23	1:H:170:ALA:CA	2.10	0.81
1:A:167:GLU:OE1	1:A:199:LYS:HG2	1.80	0.81
1:M:250:LEU:HD23	1:N:275:ILE:HG21	1.63	0.81
1:G:189:LYS:C	1:G:190:LYS:HZ3	1.83	0.80
1:B:43:MSE:HE1	1:B:114:LYS:CB	2.10	0.80
1:G:190:LYS:N	1:G:190:LYS:NZ	2.30	0.80
1:M:264:TYR:O	1:M:267:VAL:CG1	2.30	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:SER:HA	1:B:295:MSE:HE2	1.64	0.80
1:H:179:THR:O	1:H:180:GLU:CB	2.30	0.80
1:M:169:LEU:O	1:M:169:LEU:CD1	2.30	0.79
1:B:175:MSE:CE	1:B:176:ASN:OD1	2.30	0.79
1:A:43:MSE:HG2	1:A:113:VAL:HG21	1.63	0.79
1:B:142:ALA:HB3	1:B:227:MSE:CE	2.12	0.79
1:B:142:ALA:HB1	1:B:226:ASN:HB3	1.64	0.79
1:G:186:GLU:OE1	1:G:187:GLN:CB	2.30	0.78
1:G:142:ALA:HB3	1:G:227:MSE:CE	2.13	0.78
1:H:261:ASN:ND2	1:H:263:SER:H	1.82	0.78
1:B:261:ASN:C	1:B:261:ASN:HD22	1.85	0.78
1:A:174:GLU:OE1	1:A:191:LEU:HD21	1.84	0.78
1:B:261:ASN:ND2	1:B:263:SER:H	1.82	0.78
1:B:68:ARG:HD2	3:B:318:HOH:O	1.83	0.78
1:N:202:VAL:CG2	1:N:203:GLN:N	2.47	0.77
1:A:261:ASN:C	1:A:261:ASN:HD22	1.88	0.77
1:A:169:LEU:CD1	1:A:169:LEU:C	2.43	0.77
1:G:224:MSE:HE2	1:H:299:TRP:CZ2	2.18	0.77
1:H:85:GLY:HA2	1:H:88:MSE:HE2	1.64	0.77
1:G:253:LYS:HG3	1:H:271:LEU:HD13	1.67	0.76
1:B:175:MSE:HE3	1:B:176:ASN:OD1	1.85	0.76
1:A:305:TRP:CD1	1:A:305:TRP:O	2.38	0.76
1:A:67:TRP:HB2	1:A:88:MSE:HE1	1.66	0.76
1:M:43:MSE:HE3	1:M:114:LYS:HB2	1.66	0.76
1:G:43:MSE:HE3	1:G:113:VAL:CG2	2.13	0.75
1:G:187:GLN:CG	1:G:187:GLN:O	2.34	0.75
1:M:123:LYS:NZ	1:M:127:GLY:CA	2.47	0.75
1:M:245:LEU:HD23	1:N:80:LEU:HD22	1.68	0.75
1:M:76:GLN:HE21	1:M:77:TYR:H	1.35	0.74
1:G:142:ALA:CB	1:G:227:MSE:HE1	2.15	0.74
1:M:169:LEU:C	1:M:169:LEU:CD1	2.55	0.74
1:H:169:LEU:HD23	1:H:169:LEU:O	1.87	0.74
1:A:134:GLU:HA	1:A:134:GLU:OE2	1.87	0.74
1:G:190:LYS:HZ2	1:G:190:LYS:CA	2.01	0.74
1:H:201:ASP:O	1:H:205:THR:HB	1.87	0.74
1:G:186:GLU:CD	1:G:187:GLN:CA	2.55	0.73
1:G:227:MSE:HE2	1:G:227:MSE:HA	1.70	0.73
1:M:49:ARG:NH1	1:M:53:GLU:OE1	2.20	0.73
1:N:194:LYS:H	1:N:194:LYS:HD3	1.54	0.73
1:A:27:ARG:HD2	1:B:291:SER:HB3	1.70	0.73
1:H:85:GLY:CA	1:H:88:MSE:CE	2.60	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:186:GLU:OE1	1:G:187:GLN:HA	1.88	0.72
1:A:236:GLN:HE21	1:A:236:GLN:HA	1.54	0.72
1:G:190:LYS:CA	1:G:190:LYS:NZ	2.52	0.72
1:H:177:SER:CB	1:H:191:LEU:HD11	2.18	0.72
1:M:163:ALA:HB1	1:M:202:VAL:HG22	1.70	0.72
1:M:161:HIS:CG	1:M:164:CYS:SG	2.82	0.72
1:M:195:VAL:O	1:M:198:CYS:SG	2.48	0.71
1:N:149:LYS:HE3	1:N:219:THR:HG21	1.71	0.71
1:B:175:MSE:HG3	1:B:176:ASN:N	2.05	0.71
1:N:43:MSE:HE1	1:N:114:LYS:CG	2.20	0.71
1:G:142:ALA:CB	1:G:227:MSE:CE	2.68	0.71
1:A:167:GLU:O	1:A:171:MSE:HG3	1.91	0.71
1:G:17:ASP:O	1:G:27:ARG:NH2	2.23	0.71
1:N:193:ASP:C	1:N:194:LYS:HD3	2.10	0.70
1:G:85:GLY:CA	1:G:88:MSE:HE2	2.21	0.70
1:B:175:MSE:C	1:B:177:SER:H	1.94	0.70
1:G:216:VAL:O	1:G:220:THR:HG22	1.90	0.70
1:M:250:LEU:CD2	1:N:275:ILE:HG21	2.22	0.70
1:A:146:TRP:HZ3	1:A:220:THR:HG22	1.57	0.69
1:A:67:TRP:HB2	1:A:88:MSE:CE	2.21	0.69
1:M:272:GLU:HB2	1:N:253:LYS:HE3	1.75	0.69
1:H:146:TRP:CE2	1:H:150:MSE:HE3	2.28	0.69
1:G:191:LEU:C	1:G:191:LEU:HD13	2.09	0.69
1:M:126:MSE:HE2	1:M:126:MSE:HA	1.75	0.69
1:A:205:THR:O	1:A:208:LYS:HD2	1.94	0.68
1:G:43:MSE:HE1	1:G:114:LYS:CB	2.23	0.68
1:G:161:HIS:CD2	1:H:305:TRP:HA	2.29	0.68
1:N:31:ARG:HH22	1:N:235:GLN:HE22	1.39	0.68
1:M:43:MSE:HE1	1:M:114:LYS:CA	2.23	0.68
1:A:99:GLN:HA	1:A:99:GLN:NE2	2.09	0.68
1:G:143:GLN:HG2	3:G:321:HOH:O	1.93	0.68
1:M:162:LEU:C	1:M:162:LEU:CD2	2.57	0.68
1:B:31:ARG:HH22	1:B:235:GLN:NE2	1.89	0.68
1:A:43:MSE:SE	1:A:113:VAL:HG23	2.43	0.68
1:A:43:MSE:HG3	1:A:113:VAL:HG21	1.74	0.68
1:N:31:ARG:HH22	1:N:235:GLN:NE2	1.90	0.68
1:M:43:MSE:HG2	1:M:110:LEU:CD2	2.23	0.68
1:A:307:PRO:O	1:A:308:ASP:C	2.31	0.68
1:N:93:LYS:NZ	1:N:270:GLU:OE1	2.26	0.68
1:G:191:LEU:HD12	1:G:192:GLN:CA	2.25	0.67
1:M:164:CYS:SG	1:M:165:LYS:N	2.67	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:186:GLU:OE1	1:G:187:GLN:CA	2.41	0.67
1:M:123:LYS:HZ1	1:M:127:GLY:CA	2.08	0.67
1:N:57:GLY:O	1:N:61:THR:HG23	1.95	0.67
1:A:173:ARG:NH1	1:A:194:LYS:NZ	2.43	0.67
1:N:301:GLN:HG2	1:N:302:PHE:N	2.08	0.67
1:B:130:LYS:O	1:B:134:GLU:HG3	1.94	0.67
1:H:261:ASN:HD22	1:H:263:SER:H	1.41	0.67
1:A:162:LEU:CD2	1:A:163:ALA:N	2.58	0.66
1:G:43:MSE:CE	1:G:113:VAL:HG22	2.22	0.66
1:A:169:LEU:HD13	1:A:170:ALA:HA	1.77	0.66
1:B:71:ILE:HD12	1:B:88:MSE:HE1	1.76	0.66
1:H:174:GLU:HA	1:H:191:LEU:HD21	1.78	0.66
1:M:43:MSE:CE	1:M:114:LYS:CA	2.73	0.66
1:M:142:ALA:HB1	1:M:226:ASN:HB3	1.77	0.66
1:M:17:ASP:O	1:M:27:ARG:NH2	2.29	0.65
1:G:43:MSE:HE2	1:G:114:LYS:HB2	1.77	0.65
1:A:257:ASN:HD21	1:A:259:ALA:HB3	1.61	0.65
1:A:169:LEU:O	1:A:169:LEU:CD2	2.30	0.65
1:H:85:GLY:CA	1:H:88:MSE:HE1	2.19	0.65
1:A:143:GLN:CB	1:A:227:MSE:CE	2.70	0.65
1:M:162:LEU:HD23	1:M:163:ALA:N	2.12	0.65
1:A:305:TRP:CZ2	1:A:307:PRO:HG3	2.31	0.65
1:A:275:ILE:HG21	1:B:250:LEU:HD13	1.78	0.65
1:M:292:GLY:O	1:M:295:MSE:HB2	1.96	0.65
1:H:166:GLU:O	1:H:169:LEU:HB3	1.97	0.65
1:N:193:ASP:H	1:N:194:LYS:NZ	1.95	0.65
1:N:202:VAL:HG22	1:N:203:GLN:N	2.11	0.65
1:B:124:GLN:O	1:B:127:GLY:HA3	1.97	0.64
1:B:142:ALA:CB	1:B:227:MSE:HE2	2.26	0.64
1:G:186:GLU:CG	1:G:187:GLN:HA	2.27	0.64
1:B:175:MSE:HG3	1:B:176:ASN:H	1.63	0.64
1:A:216:VAL:O	1:A:220:THR:HG23	1.98	0.64
1:A:225:GLU:O	1:A:229:GLN:HG2	1.98	0.64
1:M:80:LEU:HD22	1:N:245:LEU:CD1	2.26	0.63
1:M:169:LEU:C	1:M:169:LEU:HD13	2.10	0.63
1:N:49:ARG:NH1	1:N:53:GLU:OE2	2.31	0.63
1:A:160:TYR:HA	1:A:205:THR:CG2	2.29	0.63
1:N:158:LYS:HA	1:N:161:HIS:HB2	1.80	0.63
1:H:192:GLN:HA	1:H:195:VAL:HB	1.80	0.62
1:B:261:ASN:ND2	1:B:263:SER:N	2.47	0.62
1:B:238:GLU:OE2	1:B:241:ARG:NH2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:LYS:HE2	1:A:270:GLU:OE2	1.99	0.62
1:A:69:GLN:HG3	1:A:73:LYS:HE2	1.80	0.62
1:M:253:LYS:HE3	1:N:272:GLU:HB2	1.81	0.62
1:A:223:TYR:CE1	1:A:227:MSE:CE	2.71	0.62
1:A:31:ARG:NH2	1:A:235:GLN:NE2	2.47	0.62
1:G:43:MSE:CE	1:G:114:LYS:CB	2.77	0.62
1:B:261:ASN:HD21	1:B:263:SER:H	1.46	0.62
1:G:275:ILE:HG21	1:H:250:LEU:HD13	1.81	0.62
1:B:17:ASP:O	1:B:27:ARG:NH2	2.31	0.62
1:N:227:MSE:HA	1:N:227:MSE:HE2	1.80	0.62
1:G:43:MSE:CE	1:G:114:LYS:HB2	2.29	0.62
1:B:175:MSE:CG	1:B:176:ASN:N	2.62	0.62
1:H:140:ARG:HH11	1:H:140:ARG:HG3	1.65	0.62
1:A:261:ASN:ND2	1:A:263:SER:H	1.98	0.61
1:H:267:VAL:HG22	1:H:268:TYR:CD2	2.34	0.61
1:G:261:ASN:O	1:G:265:ILE:HD13	1.99	0.61
1:M:123:LYS:HZ2	1:M:127:GLY:HA2	1.59	0.61
1:M:37:ARG:HG3	1:M:38:LEU:N	2.10	0.61
1:H:54:LYS:HB2	1:H:102:LYS:HD3	1.82	0.61
1:H:126:MSE:N	1:H:126:MSE:SE	2.78	0.61
1:G:212:VAL:O	1:G:216:VAL:HG23	2.00	0.61
1:G:191:LEU:HD12	1:G:192:GLN:H	1.60	0.61
1:M:170:ALA:HB1	1:M:195:VAL:CG2	2.29	0.61
1:G:167:GLU:OE1	1:G:199:LYS:CE	2.40	0.61
1:M:157:LYS:NZ	1:N:303:GLU:CB	2.64	0.61
1:G:239:GLU:HG3	1:H:284:LEU:HD11	1.83	0.61
1:M:43:MSE:HE3	1:M:114:LYS:N	2.15	0.60
1:G:253:LYS:CD	1:H:272:GLU:HG3	2.31	0.60
1:G:43:MSE:HE2	1:G:114:LYS:N	2.16	0.60
1:G:162:LEU:HD23	1:G:162:LEU:O	2.01	0.60
1:N:123:LYS:HD2	1:N:124:GLN:O	2.00	0.60
1:A:99:GLN:HE21	1:A:99:GLN:HA	1.64	0.60
1:M:90:GLU:OE2	1:N:49:ARG:NH2	2.28	0.60
1:A:266:HIS:CE1	1:A:269:ARG:NH1	2.69	0.60
1:M:275:ILE:CG2	1:N:250:LEU:HD13	2.30	0.60
1:M:155:ALA:HA	1:M:158:LYS:CE	2.16	0.60
1:M:43:MSE:HE2	1:M:114:LYS:HB2	1.80	0.60
1:B:142:ALA:CB	1:B:227:MSE:CE	2.80	0.60
1:G:153:LEU:HD11	1:G:213:LEU:CD1	2.32	0.60
1:N:122:HIS:HE1	3:N:321:HOH:O	1.83	0.60
1:B:261:ASN:HD22	1:B:262:SER:N	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:PHE:C	1:A:302:PHE:CD2	2.75	0.60
1:N:37:ARG:O	1:N:40:ASN:HB2	2.02	0.59
1:A:162:LEU:HD23	1:A:163:ALA:N	2.12	0.59
1:H:169:LEU:HD23	1:H:170:ALA:HA	1.84	0.59
1:N:43:MSE:CE	1:N:114:LYS:H	2.02	0.59
1:A:261:ASN:HD22	1:A:262:SER:N	2.00	0.59
1:A:44:ASN:O	1:A:48:GLU:HG3	2.03	0.59
1:G:304:GLU:O	1:G:305:TRP:C	2.37	0.59
1:B:172:THR:O	1:B:175:MSE:HG3	2.02	0.59
1:H:261:ASN:C	1:H:261:ASN:HD22	2.06	0.59
1:M:241:ARG:HH12	1:N:76:GLN:HE22	1.50	0.59
1:B:261:ASN:C	1:B:261:ASN:ND2	2.56	0.59
1:M:226:ASN:HD22	1:M:226:ASN:N	2.00	0.59
1:A:160:TYR:HA	1:A:205:THR:HG23	1.84	0.59
1:A:80:LEU:HD12	1:B:245:LEU:HD13	1.85	0.59
1:G:43:MSE:CE	1:G:114:LYS:H	2.14	0.59
1:M:162:LEU:HD23	1:M:162:LEU:O	2.02	0.59
1:M:87:ILE:O	1:M:90:GLU:HG3	2.02	0.58
1:M:31:ARG:NH2	1:M:235:GLN:HE21	2.01	0.58
1:M:85:GLY:O	1:M:88:MSE:HG2	2.04	0.58
1:M:239:GLU:HG3	1:N:284:LEU:HD11	1.86	0.58
1:A:305:TRP:O	1:A:306:ASN:C	2.40	0.58
1:M:49:ARG:NH2	1:N:90:GLU:OE2	2.26	0.58
1:M:245:LEU:CD2	1:N:80:LEU:HD22	2.33	0.58
1:A:169:LEU:C	1:A:169:LEU:CD2	2.51	0.58
1:N:216:VAL:HA	1:N:219:THR:HG22	1.86	0.58
1:M:109:ASP:O	1:M:113:VAL:HG13	2.04	0.58
1:M:25:TYR:CD2	1:M:139:PHE:CB	2.87	0.58
1:G:69:GLN:NE2	1:G:73:LYS:HG3	2.19	0.57
1:H:85:GLY:CA	1:H:88:MSE:HE2	2.33	0.57
1:M:281:GLN:NE2	1:M:281:GLN:H	2.01	0.57
1:G:144:LYS:HB3	1:G:145:PRO:HD3	1.86	0.57
1:G:153:LEU:HD11	1:G:213:LEU:HD12	1.85	0.57
1:G:160:TYR:HE1	1:G:206:GLN:HE21	1.52	0.57
1:H:87:ILE:O	1:H:90:GLU:HG3	2.04	0.57
1:M:242:LEU:HD22	1:N:80:LEU:HD13	1.86	0.57
1:B:64:ALA:HA	1:B:88:MSE:HG3	1.87	0.57
1:H:44:ASN:O	1:H:48:GLU:HG3	2.04	0.57
1:M:170:ALA:CB	1:M:195:VAL:HG22	2.29	0.57
1:B:179:THR:HG22	1:B:179:THR:O	2.05	0.57
1:G:150:MSE:HE1	1:H:300:PRO:HG3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:ILE:HD11	1:B:84:TRP:CE2	2.39	0.57
1:M:286:TRP:O	1:M:290:THR:HB	2.05	0.57
1:M:48:GLU:OE2	1:N:66:ARG:NH2	2.38	0.57
1:G:254:ARG:HD3	3:G:312:HOH:O	2.04	0.57
1:G:189:LYS:C	1:G:190:LYS:HZ2	2.09	0.57
1:H:261:ASN:HD22	1:H:263:SER:N	2.01	0.56
1:N:250:LEU:O	1:N:251:ASP:C	2.43	0.56
1:B:43:MSE:CE	1:B:114:LYS:H	2.16	0.56
1:B:175:MSE:O	1:B:177:SER:N	2.30	0.56
1:M:284:LEU:HD11	1:N:239:GLU:HB2	1.86	0.56
1:G:71:ILE:HD12	1:G:88:MSE:CE	2.35	0.56
1:M:84:TRP:O	1:M:88:MSE:HE3	2.05	0.56
1:M:22:VAL:HA	1:M:143:GLN:HE22	1.70	0.56
1:H:279:ASP:OD2	1:H:282:GLU:HB2	2.05	0.56
1:H:302:PHE:HE1	1:H:304:GLU:OE1	1.87	0.56
1:G:286:TRP:O	1:G:290:THR:HB	2.05	0.56
1:M:257:ASN:OD1	1:M:260:GLU:HG3	2.06	0.56
1:M:44:ASN:O	1:M:48:GLU:HG3	2.06	0.55
1:H:31:ARG:HH22	1:H:235:GLN:HE22	1.53	0.55
1:B:126:MSE:N	1:B:127:GLY:HA2	2.22	0.55
1:A:298:ASN:ND2	1:B:15:THR:HG23	2.21	0.55
1:H:238:GLU:HG3	1:H:238:GLU:O	2.05	0.55
1:M:80:LEU:CD2	1:N:245:LEU:HD13	2.30	0.55
1:N:160:TYR:CB	3:N:6:HOH:O	2.55	0.55
1:A:307:PRO:HD2	1:A:308:ASP:H	1.72	0.55
1:G:220:THR:OG1	1:G:224:MSE:HE3	2.06	0.55
1:H:146:TRP:CD2	1:H:150:MSE:HE3	2.41	0.55
1:N:258:LEU:O	1:N:261:ASN:CB	2.54	0.55
1:A:185:PRO:N	1:A:188:GLN:HG2	2.22	0.55
1:H:83:ALA:HB2	1:H:278:ALA:HB2	1.87	0.55
1:G:253:LYS:HD2	1:H:272:GLU:HG3	1.88	0.54
1:A:216:VAL:O	1:A:220:THR:CG2	2.56	0.54
1:G:304:GLU:CA	1:H:161:HIS:NE2	2.70	0.54
1:A:261:ASN:C	1:A:261:ASN:ND2	2.57	0.54
1:B:125:ILE:HG23	1:B:126:MSE:SE	2.57	0.54
1:A:281:GLN:H	1:A:281:GLN:NE2	2.05	0.54
1:B:235:GLN:HE21	1:B:235:GLN:HA	1.73	0.54
1:A:146:TRP:CZ3	1:A:220:THR:HG22	2.41	0.54
1:A:153:LEU:HD23	1:A:153:LEU:C	2.26	0.54
1:H:169:LEU:CD2	1:H:170:ALA:CA	2.82	0.54
1:A:303:GLU:O	1:B:161:HIS:HE1	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:264:TYR:OH	1:H:258:LEU:HB2	2.08	0.54
1:M:93:LYS:CE	1:M:270:GLU:OE2	2.55	0.54
1:N:17:ASP:O	1:N:27:ARG:NH2	2.41	0.54
1:A:43:MSE:CG	1:A:113:VAL:HG23	2.38	0.54
1:M:227:MSE:CE	1:M:227:MSE:HA	2.38	0.54
1:A:275:ILE:CG2	1:B:250:LEU:HD13	2.38	0.53
1:A:76:GLN:HE21	1:A:77:TYR:H	1.56	0.53
1:G:43:MSE:HE3	1:G:113:VAL:C	2.28	0.53
1:G:162:LEU:HD23	1:G:162:LEU:C	2.28	0.53
1:B:175:MSE:C	1:B:177:SER:N	2.58	0.53
1:G:128:GLY:C	1:G:133:LYS:HE2	2.29	0.53
1:M:124:GLN:O	1:M:126:MSE:O	2.26	0.53
1:G:161:HIS:HD2	1:H:305:TRP:HA	1.74	0.53
1:M:241:ARG:NH1	1:N:76:GLN:HE22	2.06	0.53
1:M:25:TYR:CE2	1:M:139:PHE:CB	2.92	0.53
1:G:190:LYS:HA	1:G:190:LYS:CE	2.39	0.53
1:H:305:TRP:C	1:H:306:ASN:HD22	2.11	0.52
1:A:266:HIS:ND1	1:A:269:ARG:NH1	2.57	0.52
1:H:31:ARG:HH12	1:H:235:GLN:HE21	1.56	0.52
1:B:143:GLN:NE2	1:B:223:TYR:OH	2.42	0.52
1:G:31:ARG:HH22	1:G:235:GLN:NE2	2.02	0.52
1:M:76:GLN:NE2	1:M:77:TYR:H	2.03	0.52
1:M:43:MSE:HE3	1:M:114:LYS:CA	2.40	0.52
1:A:266:HIS:CE1	1:A:269:ARG:HH12	2.27	0.52
1:A:173:ARG:NH1	1:A:194:LYS:HZ3	2.06	0.52
1:A:31:ARG:HH22	1:A:235:GLN:HE21	1.53	0.52
1:H:305:TRP:O	1:H:306:ASN:ND2	2.30	0.52
1:B:109:ASP:OD2	1:B:255:HIS:ND1	2.31	0.51
1:H:37:ARG:O	1:H:40:ASN:HB2	2.10	0.51
1:M:123:LYS:NZ	1:M:128:GLY:N	2.58	0.51
1:B:71:ILE:HD12	1:B:88:MSE:CE	2.39	0.51
1:M:257:ASN:HD21	1:M:259:ALA:HB3	1.76	0.51
1:N:194:LYS:CD	1:N:194:LYS:H	2.15	0.51
1:G:186:GLU:CD	1:G:187:GLN:CB	2.79	0.51
1:N:108:GLU:O	1:N:112:LYS:HB2	2.10	0.51
1:G:80:LEU:HD22	1:H:245:LEU:HD13	1.92	0.51
1:H:171:MSE:H	1:H:171:MSE:SE	2.40	0.51
1:G:43:MSE:CE	1:G:114:LYS:HA	2.06	0.51
1:B:126:MSE:N	1:B:127:GLY:CA	2.73	0.51
1:H:67:TRP:O	1:H:71:ILE:HG13	2.11	0.51
1:M:196:ASP:O	1:M:200:GLN:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:258:LEU:O	1:N:261:ASN:HB2	2.11	0.51
1:A:174:GLU:OE1	1:A:191:LEU:HD11	2.11	0.51
1:B:31:ARG:NH2	1:B:235:GLN:HE22	1.91	0.51
1:M:25:TYR:CD2	1:M:139:PHE:CG	3.00	0.50
1:N:87:ILE:O	1:N:90:GLU:HG3	2.12	0.50
1:M:238:GLU:O	1:M:238:GLU:HG3	2.11	0.50
1:N:193:ASP:H	1:N:194:LYS:HZ3	1.59	0.50
1:A:134:GLU:OE2	1:A:134:GLU:CA	2.54	0.50
1:G:69:GLN:HE22	1:G:73:LYS:HD2	1.76	0.50
1:H:286:TRP:O	1:H:290:THR:OG1	2.30	0.50
1:B:281:GLN:HE21	1:B:281:GLN:HA	1.76	0.50
1:H:167:GLU:OE2	1:H:199:LYS:HG2	2.12	0.50
1:G:154:GLU:OE2	1:G:154:GLU:HA	2.11	0.50
1:N:197:LYS:O	1:N:201:ASP:OD2	2.30	0.50
1:B:146:TRP:O	1:B:150:MSE:HB2	2.11	0.50
1:A:162:LEU:HD22	1:A:163:ALA:N	2.27	0.50
1:N:202:VAL:HG23	1:N:203:GLN:N	2.23	0.50
1:A:76:GLN:NE2	1:A:77:TYR:H	2.10	0.50
1:M:125:ILE:CD1	1:M:125:ILE:N	2.30	0.49
1:G:227:MSE:CE	1:G:227:MSE:HA	2.40	0.49
1:N:205:THR:O	1:N:208:LYS:HB3	2.12	0.49
1:B:176:ASN:O	1:B:177:SER:CB	2.60	0.49
1:G:187:GLN:OE1	1:G:187:GLN:O	2.30	0.49
1:G:304:GLU:O	1:G:306:ASN:O	2.30	0.49
1:G:71:ILE:HD11	1:G:84:TRP:CE2	2.47	0.49
1:A:307:PRO:O	1:A:308:ASP:O	2.30	0.49
1:M:43:MSE:CE	1:M:114:LYS:CG	2.81	0.49
1:N:301:GLN:CG	1:N:302:PHE:N	2.73	0.49
1:H:170:ALA:HB1	1:H:195:VAL:CG2	2.36	0.49
1:A:173:ARG:NH1	1:A:194:LYS:HZ2	2.10	0.49
1:N:202:VAL:O	1:N:205:THR:OG1	2.30	0.49
1:A:201:ASP:O	1:A:205:THR:HB	2.13	0.49
1:M:25:TYR:CE2	1:M:139:PHE:HB2	2.48	0.49
1:M:25:TYR:HD1	1:M:25:TYR:H	1.56	0.49
1:M:194:LYS:HB3	1:M:194:LYS:NZ	2.28	0.49
1:N:299:TRP:HE3	1:N:300:PRO:HD2	1.77	0.49
1:A:37:ARG:NH2	1:A:37:ARG:CG	2.50	0.48
1:G:235:GLN:HE21	1:G:235:GLN:HA	1.78	0.48
1:M:250:LEU:CD2	1:N:275:ILE:CG2	2.91	0.48
1:M:222:GLN:HA	1:M:222:GLN:NE2	2.28	0.48
1:G:208:LYS:O	1:G:212:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:43:MSE:HE1	1:M:114:LYS:HA	1.95	0.48
1:A:104:ASN:O	1:A:105:LEU:C	2.47	0.48
1:B:286:TRP:O	1:B:290:THR:HB	2.14	0.48
1:N:144:LYS:O	1:N:148:LYS:HG3	2.13	0.48
1:G:142:ALA:HB1	1:G:226:ASN:HB3	1.94	0.48
1:M:43:MSE:HG2	1:M:110:LEU:HD23	1.95	0.47
1:B:176:ASN:O	1:B:177:SER:OG	2.30	0.47
1:G:142:ALA:HB1	1:G:227:MSE:CE	2.43	0.47
1:M:227:MSE:HE2	1:M:227:MSE:HA	1.95	0.47
1:A:76:GLN:OE1	1:B:241:ARG:NH1	2.47	0.47
1:M:161:HIS:CE1	1:M:164:CYS:SG	3.06	0.47
1:B:261:ASN:HD22	1:B:263:SER:N	2.12	0.47
1:G:37:ARG:O	1:G:40:ASN:HB2	2.14	0.47
1:G:197:LYS:HA	1:G:197:LYS:HD3	1.44	0.47
1:B:297:MSE:HG2	1:B:299:TRP:CE2	2.49	0.47
1:G:235:GLN:NE2	1:G:235:GLN:HA	2.30	0.47
1:G:216:VAL:O	1:G:220:THR:CG2	2.62	0.47
1:B:85:GLY:CA	1:B:88:MSE:HE2	2.38	0.47
1:M:217:GLY:O	1:M:220:THR:HG22	2.14	0.47
1:G:284:LEU:HD11	1:H:239:GLU:HG3	1.95	0.47
1:H:191:LEU:O	1:H:195:VAL:HG23	2.14	0.47
1:G:43:MSE:HE2	1:G:114:LYS:H	1.78	0.47
1:M:167:GLU:CG	1:M:198:CYS:SG	2.97	0.47
1:G:227:MSE:HE2	1:G:227:MSE:CA	2.40	0.47
1:N:142:ALA:HB1	1:N:226:ASN:HB3	1.96	0.47
1:A:180:GLU:HG2	1:A:183:VAL:HB	1.96	0.47
1:G:170:ALA:O	1:G:195:VAL:HG12	2.14	0.47
1:B:160:TYR:O	1:B:161:HIS:C	2.52	0.47
1:N:206:GLN:O	1:N:207:GLU:C	2.46	0.47
1:G:261:ASN:C	1:G:261:ASN:OD1	2.52	0.47
1:M:157:LYS:HZ1	1:N:303:GLU:CB	2.26	0.47
1:N:123:LYS:HB3	1:N:123:LYS:HE2	1.55	0.47
1:G:281:GLN:H	1:G:281:GLN:CD	2.17	0.47
1:G:253:LYS:NZ	1:H:272:GLU:HG3	2.29	0.46
1:N:140:ARG:HG3	1:N:141:LYS:N	2.30	0.46
1:H:162:LEU:O	1:H:166:GLU:HG2	2.14	0.46
1:N:142:ALA:HB3	1:N:227:MSE:HE3	1.96	0.46
1:M:25:TYR:CD2	1:M:139:PHE:HB3	2.50	0.46
1:A:222:GLN:HE21	1:A:222:GLN:HA	1.79	0.46
1:B:38:LEU:HD23	1:B:38:LEU:HA	1.74	0.46
1:N:201:ASP:O	1:N:205:THR:OG1	2.22	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:54:LYS:HB2	1:H:102:LYS:CD	2.46	0.46
1:H:267:VAL:HG22	1:H:268:TYR:CE2	2.51	0.46
1:H:40:ASN:HA	1:H:43:MSE:CE	2.44	0.46
1:G:281:GLN:H	1:G:281:GLN:NE2	2.14	0.46
1:A:144:LYS:HB3	1:A:145:PRO:HD3	1.97	0.46
1:H:261:ASN:HD22	1:H:262:SER:N	2.13	0.46
1:B:122:HIS:HD2	1:B:131:GLU:OE2	1.98	0.46
1:G:142:ALA:HB3	1:G:227:MSE:HE2	1.95	0.46
1:A:224:MSE:O	1:A:228:GLU:HB2	2.15	0.46
1:B:54:LYS:HB2	1:B:102:LYS:HD2	1.98	0.46
1:B:85:GLY:HA2	1:B:88:MSE:HE1	1.90	0.46
1:G:31:ARG:HH12	1:G:235:GLN:HE21	1.63	0.46
1:M:196:ASP:OD1	1:M:196:ASP:N	2.48	0.46
1:G:174:GLU:HG2	1:G:191:LEU:HD11	1.96	0.46
1:B:261:ASN:ND2	1:B:262:SER:N	2.62	0.46
1:A:257:ASN:ND2	1:A:259:ALA:H	2.14	0.46
1:G:90:GLU:OE2	1:H:49:ARG:NH2	2.48	0.46
1:G:275:ILE:CG2	1:H:250:LEU:HD13	2.45	0.45
1:A:224:MSE:HE3	1:B:299:TRP:CZ2	2.51	0.45
1:A:174:GLU:OE2	1:A:195:VAL:HG21	2.16	0.45
1:H:271:LEU:HD22	1:H:275:ILE:CD1	2.46	0.45
1:G:189:LYS:O	1:G:190:LYS:NZ	2.48	0.45
1:N:253:LYS:C	1:N:253:LYS:HD3	2.36	0.45
1:A:302:PHE:CD2	1:A:303:GLU:N	2.84	0.45
1:N:258:LEU:O	1:N:261:ASN:HB3	2.17	0.45
1:M:20:TRP:HB2	1:N:297:MSE:SE	2.67	0.45
1:A:83:ALA:O	1:A:86:ALA:HB3	2.17	0.45
1:N:244:PHE:O	1:N:248:VAL:HG23	2.16	0.45
1:H:31:ARG:HH22	1:H:235:GLN:NE2	2.15	0.45
1:N:38:LEU:HD13	1:N:241:ARG:NH1	2.31	0.45
1:A:99:GLN:HE21	1:A:99:GLN:CA	2.25	0.45
1:N:41:ASP:O	1:N:42:LEU:C	2.54	0.45
1:A:70:LEU:HA	1:A:70:LEU:HD23	1.73	0.45
1:M:258:LEU:HA	1:M:258:LEU:HD23	1.73	0.45
1:M:262:SER:O	1:M:266:HIS:CD2	2.69	0.45
1:G:71:ILE:CD1	1:G:88:MSE:HE1	2.46	0.45
1:A:224:MSE:HE3	1:B:299:TRP:HZ2	1.82	0.45
1:M:28:THR:O	1:M:32:ILE:HD12	2.15	0.45
1:G:175:MSE:O	1:G:176:ASN:CB	2.64	0.45
1:M:125:ILE:C	1:M:126:MSE:O	2.54	0.45
1:N:57:GLY:HA3	1:N:99:GLN:HE22	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:57:GLY:O	1:H:95:SER:OG	2.28	0.45
1:N:43:MSE:HE3	1:N:113:VAL:C	2.30	0.44
1:G:191:LEU:O	1:G:191:LEU:HD13	2.17	0.44
1:M:169:LEU:C	1:M:169:LEU:HD12	2.37	0.44
1:G:227:MSE:CE	1:G:227:MSE:CA	2.95	0.44
1:G:162:LEU:C	1:G:162:LEU:CD2	2.86	0.44
1:M:25:TYR:CE2	1:M:139:PHE:HB3	2.52	0.44
1:B:104:ASN:HB3	1:B:255:HIS:CG	2.53	0.44
1:B:51:LYS:HE3	1:M:127:GLY:H	1.82	0.44
1:N:141:LYS:HG3	1:N:142:ALA:N	2.32	0.44
1:A:56:TYR:CD1	1:B:56:TYR:HB2	2.52	0.44
1:N:77:TYR:CD1	1:N:77:TYR:N	2.85	0.44
1:A:232:GLU:O	1:A:236:GLN:HG2	2.17	0.44
1:H:169:LEU:CD2	1:H:170:ALA:HA	2.46	0.44
1:G:85:GLY:HA2	1:G:88:MSE:HE1	1.92	0.44
1:A:31:ARG:HH21	1:A:235:GLN:NE2	2.15	0.44
1:M:31:ARG:NH2	1:M:235:GLN:NE2	2.65	0.44
1:A:160:TYR:HA	1:A:205:THR:HG21	1.97	0.44
1:N:61:THR:HG22	1:N:95:SER:OG	2.18	0.44
1:M:157:LYS:HZ2	1:N:303:GLU:CB	2.31	0.44
1:H:49:ARG:HD2	1:H:53:GLU:OE2	2.18	0.44
1:G:289:SER:OG	1:G:289:SER:O	2.32	0.44
1:G:110:LEU:C	1:G:110:LEU:CD2	2.87	0.44
1:B:279:ASP:OD2	1:B:282:GLU:HB2	2.18	0.43
1:G:174:GLU:HG2	1:G:191:LEU:CD1	2.48	0.43
1:G:110:LEU:HD23	1:G:110:LEU:O	2.18	0.43
1:A:261:ASN:ND2	1:A:263:SER:HB2	2.33	0.43
1:G:160:TYR:HA	1:G:205:THR:CG2	2.48	0.43
1:H:18:SER:O	1:H:24:ASN:ND2	2.50	0.43
1:H:169:LEU:HD22	1:H:170:ALA:N	2.28	0.43
1:G:38:LEU:HD23	1:G:38:LEU:HA	1.76	0.43
1:H:25:TYR:C	1:H:25:TYR:CD1	2.91	0.43
1:N:199:LYS:O	1:N:202:VAL:HG22	2.18	0.43
1:H:144:LYS:HB3	1:H:145:PRO:HD3	2.01	0.43
1:A:220:THR:N	1:A:221:PRO:CD	2.82	0.43
1:B:167:GLU:OE2	1:B:199:LYS:HD2	2.19	0.43
1:H:85:GLY:O	1:H:88:MSE:HE2	2.18	0.43
1:G:291:SER:HB3	1:H:27:ARG:HD2	2.00	0.43
1:N:43:MSE:CE	1:N:114:LYS:HA	2.26	0.43
1:M:257:ASN:ND2	1:M:257:ASN:C	2.72	0.43
1:B:187:GLN:O	1:B:190:LYS:N	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:144:LYS:N	1:M:145:PRO:HD2	2.34	0.43
1:N:23:GLY:HA2	1:N:25:TYR:CE2	2.53	0.43
1:B:220:THR:O	1:B:224:MSE:HG3	2.18	0.43
1:G:128:GLY:HA3	1:G:133:LYS:NZ	2.26	0.43
1:N:261:ASN:HA	1:N:261:ASN:HD22	1.44	0.43
1:G:264:TYR:O	1:G:267:VAL:HG13	2.18	0.43
1:H:248:VAL:O	1:H:251:ASP:HB2	2.19	0.43
1:M:142:ALA:HB3	1:M:227:MSE:CE	2.49	0.42
1:H:85:GLY:C	1:H:88:MSE:HE2	2.39	0.42
1:N:216:VAL:CG2	1:N:217:GLY:N	2.82	0.42
1:G:304:GLU:C	1:G:306:ASN:O	2.57	0.42
1:M:224:MSE:HE2	1:N:299:TRP:CZ2	2.54	0.42
1:M:123:LYS:HZ1	1:M:128:GLY:H	1.67	0.42
1:A:27:ARG:CD	1:B:291:SER:HB3	2.43	0.42
1:A:106:LEU:HA	1:A:106:LEU:HD23	1.71	0.42
1:B:144:LYS:HB3	1:B:145:PRO:HD3	2.00	0.42
1:H:40:ASN:HA	1:H:43:MSE:HE3	2.02	0.42
1:N:265:ILE:HG22	1:N:266:HIS:N	2.33	0.42
1:H:139:PHE:CE2	1:H:230:VAL:HG23	2.54	0.42
1:M:123:LYS:HZ1	1:M:128:GLY:N	2.17	0.42
1:B:142:ALA:C	1:B:227:MSE:HE3	2.39	0.42
1:N:202:VAL:HG22	1:N:203:GLN:H	1.79	0.42
1:M:23:GLY:HA2	1:M:25:TYR:CE1	2.54	0.42
1:N:144:LYS:N	1:N:145:PRO:HD2	2.35	0.42
1:N:117:GLN:HE21	1:N:117:GLN:HB3	1.64	0.42
1:M:23:GLY:HA2	1:M:25:TYR:HE1	1.85	0.42
1:B:80:LEU:HD13	1:B:80:LEU:HA	1.89	0.42
1:G:71:ILE:HD12	1:G:88:MSE:HE1	2.01	0.42
1:G:23:GLY:O	1:G:26:LYS:HG2	2.20	0.42
1:M:297:MSE:HG2	1:M:299:TRP:CE2	2.55	0.42
1:M:130:LYS:O	1:M:134:GLU:HB2	2.20	0.42
1:M:244:PHE:O	1:M:248:VAL:HG23	2.20	0.42
1:B:27:ARG:HA	1:B:30:LYS:HD2	2.02	0.42
1:N:193:ASP:H	1:N:194:LYS:HZ2	1.64	0.42
1:B:142:ALA:CB	1:B:226:ASN:HB3	2.43	0.42
1:M:287:PHE:CD2	1:N:31:ARG:NH2	2.87	0.42
1:A:179:THR:HA	1:A:180:GLU:HA	1.80	0.42
1:M:155:ALA:O	1:M:158:LYS:CG	2.57	0.41
1:A:306:ASN:HA	1:A:307:PRO:HD3	1.70	0.41
1:B:67:TRP:O	1:B:71:ILE:HG13	2.20	0.41
1:M:293:PRO:HD2	1:N:231:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:220:THR:HB	1:N:221:PRO:HD3	2.01	0.41
1:G:174:GLU:HA	1:G:175:MSE:HA	1.69	0.41
1:M:264:TYR:HA	1:M:267:VAL:CG1	2.50	0.41
1:B:160:TYR:CE2	1:B:206:GLN:HG3	2.55	0.41
1:M:129:PHE:O	1:M:130:LYS:C	2.58	0.41
1:G:307:PRO:HG2	1:H:165:LYS:HG2	2.02	0.41
1:B:54:LYS:HB2	1:B:102:LYS:CD	2.51	0.41
1:N:22:VAL:HG13	1:N:143:GLN:OE1	2.19	0.41
1:M:43:MSE:HE2	1:M:110:LEU:HD23	2.03	0.41
1:G:173:ARG:O	1:G:191:LEU:CD2	2.69	0.41
1:H:261:ASN:C	1:H:261:ASN:ND2	2.74	0.41
1:B:208:LYS:HA	1:B:208:LYS:HD2	1.86	0.41
1:H:80:LEU:HA	1:H:80:LEU:HD13	1.91	0.41
1:B:235:GLN:NE2	1:B:235:GLN:HA	2.34	0.41
1:H:217:GLY:HA2	1:H:220:THR:CG2	2.51	0.41
1:A:64:ALA:HA	1:A:88:MSE:HE2	2.02	0.41
1:B:295:MSE:HA	1:B:296:PRO:HD3	1.97	0.41
1:H:261:ASN:ND2	1:H:263:SER:N	2.57	0.41
1:B:250:LEU:HD12	1:B:250:LEU:HA	1.83	0.41
1:A:80:LEU:HD13	1:A:80:LEU:HA	1.95	0.41
1:M:246:LYS:NZ	1:N:278:ALA:O	2.54	0.41
1:N:125:ILE:H	1:N:125:ILE:HD12	1.86	0.41
1:G:250:LEU:HD12	1:G:250:LEU:HA	1.93	0.41
1:G:160:TYR:HA	1:G:205:THR:HG23	2.02	0.41
1:B:31:ARG:HH12	1:B:235:GLN:NE2	2.19	0.40
1:G:253:LYS:HZ2	1:H:272:GLU:HG3	1.86	0.40
1:G:110:LEU:C	1:G:110:LEU:HD23	2.42	0.40
1:A:40:ASN:HA	1:A:43:MSE:HE3	2.03	0.40
1:N:216:VAL:HG23	1:N:217:GLY:N	2.37	0.40
1:B:26:LYS:HG2	1:B:27:ARG:N	2.36	0.40
1:A:238:GLU:O	1:A:238:GLU:HG3	2.20	0.40
1:M:47:GLN:HE21	1:M:47:GLN:HB2	1.60	0.40
1:N:43:MSE:HG2	1:N:110:LEU:HG	2.03	0.40
1:A:291:SER:HB3	1:B:27:ARG:HD2	2.03	0.40
1:N:222:GLN:NE2	1:N:226:ASN:HD21	2.20	0.40
1:H:163:ALA:HB3	1:H:205:THR:HG21	2.04	0.40
1:G:190:LYS:CA	1:G:190:LYS:CE	3.00	0.40
1:H:302:PHE:CE1	1:H:304:GLU:OE1	2.71	0.40
1:A:157:LYS:NZ	1:B:303:GLU:OE1	2.49	0.40
1:N:216:VAL:O	1:N:219:THR:N	2.54	0.40
1:M:87:ILE:HB	1:M:88:MSE:HE2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:186:GLU:OE1	1:H:187:GLN:HG2	2.21	0.40
1:M:96:GLU:O	1:M:100:GLU:HG3	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:125:ILE:O	1:H:134:GLU:OE1[3_445]	1.89	0.31
1:A:210:GLU:OE2	1:B:265:ILE:CD1[4_546]	2.01	0.19

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	277/295 (94%)	272 (98%)	5 (2%)	0	100	100
1	B	280/295 (95%)	274 (98%)	6 (2%)	0	100	100
1	G	283/295 (96%)	279 (99%)	4 (1%)	0	100	100
1	H	284/295 (96%)	281 (99%)	3 (1%)	0	100	100
1	M	266/295 (90%)	260 (98%)	6 (2%)	0	100	100
1	N	262/295 (89%)	249 (95%)	13 (5%)	0	100	100
All	All	1652/1770 (93%)	1615 (98%)	37 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	246/253 (97%)	208 (85%)	38 (15%)	3 10
1	B	247/253 (98%)	215 (87%)	32 (13%)	5 15
1	G	244/253 (96%)	210 (86%)	34 (14%)	4 13
1	H	248/253 (98%)	203 (82%)	45 (18%)	2 6
1	M	232/253 (92%)	201 (87%)	31 (13%)	5 14
1	N	228/253 (90%)	193 (85%)	35 (15%)	3 10
All	All	1445/1518 (95%)	1230 (85%)	215 (15%)	4 11

All (215) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	THR
1	A	21	GLU
1	A	31	ARG
1	A	37	ARG
1	A	69	GLN
1	A	72	GLU
1	A	88	MSE
1	A	90	GLU
1	A	110	LEU
1	A	114	LYS
1	A	118	LYS
1	A	125	ILE
1	A	126	MSE
1	A	133	LYS
1	A	140	ARG
1	A	150	MSE
1	A	151	LYS
1	A	162	LEU
1	A	169	LEU
1	A	173	ARG
1	A	174	GLU
1	A	180	GLU
1	A	183	VAL
1	A	191	LEU
1	A	205	THR
1	A	208	LYS
1	A	213	LEU

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Mol	Chain	Res	Type
1	A	218	LYS
1	A	220	THR
1	A	222	GLN
1	A	236	GLN
1	A	250	LEU
1	A	261	ASN
1	A	267	VAL
1	A	273	GLN
1	A	281	GLN
1	A	285	ARG
1	A	302	PHE
1	B	26	LYS
1	B	30	LYS
1	B	31	ARG
1	B	37	ARG
1	B	42	LEU
1	B	61	THR
1	B	96	GLU
1	B	99	GLN
1	B	126	MSE
1	B	144	LYS
1	B	149	LYS
1	B	150	MSE
1	B	168	LYS
1	B	169	LEU
1	B	171	MSE
1	B	172	THR
1	B	175	MSE
1	B	186	GLU
1	B	187	GLN
1	B	188	GLN
1	B	204	LYS
1	B	213	LEU
1	B	241	ARG
1	B	245	LEU
1	B	250	LEU
1	B	253	LYS
1	B	261	ASN
1	B	267	VAL
1	B	269	ARG
1	B	271	LEU
1	B	281	GLN

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Mol	Chain	Res	Type
1	B	289	SER
1	G	31	ARG
1	G	66	ARG
1	G	69	GLN
1	G	80	LEU
1	G	110	LEU
1	G	113	VAL
1	G	118	LYS
1	G	133	LYS
1	G	150	MSE
1	G	166	GLU
1	G	168	LYS
1	G	172	THR
1	G	174	GLU
1	G	187	GLN
1	G	188	GLN
1	G	190	LYS
1	G	191	LEU
1	G	193	ASP
1	G	199	LYS
1	G	204	LYS
1	G	205	THR
1	G	220	THR
1	G	227	MSE
1	G	229	GLN
1	G	239	GLU
1	G	250	LEU
1	G	257	ASN
1	G	267	VAL
1	G	273	GLN
1	G	289	SER
1	G	290	THR
1	G	291	SER
1	G	295	MSE
1	G	301	GLN
1	H	16	THR
1	H	17	ASP
1	H	21	GLU
1	H	30	LYS
1	H	31	ARG
1	H	37	ARG
1	H	42	LEU

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Mol	Chain	Res	Type
1	H	49	ARG
1	H	61	THR
1	H	88	MSE
1	H	99	GLN
1	H	123	LYS
1	H	126	MSE
1	H	134	GLU
1	H	140	ARG
1	H	149	LYS
1	H	150	MSE
1	H	153	LEU
1	H	162	LEU
1	H	169	LEU
1	H	171	MSE
1	H	186	GLU
1	H	187	GLN
1	H	188	GLN
1	H	189	LYS
1	H	190	LYS
1	H	193	ASP
1	H	202	VAL
1	H	205	THR
1	H	211	LYS
1	H	215	ASP
1	H	216	VAL
1	H	218	LYS
1	H	220	THR
1	H	229	GLN
1	H	241	ARG
1	H	245	LEU
1	H	250	LEU
1	H	261	ASN
1	H	267	VAL
1	H	269	ARG
1	H	271	LEU
1	H	272	GLU
1	H	290	THR
1	H	306	ASN
1	M	15	THR
1	M	16	THR
1	M	25	TYR
1	M	26	LYS

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Mol	Chain	Res	Type
1	M	30	LYS
1	M	37	ARG
1	M	66	ARG
1	M	80	LEU
1	M	88	MSE
1	M	90	GLU
1	M	123	LYS
1	M	125	ILE
1	M	126	MSE
1	M	153	LEU
1	M	168	LYS
1	M	169	LEU
1	M	193	ASP
1	M	194	LYS
1	M	198	CYS
1	M	200	GLN
1	M	203	GLN
1	M	208	LYS
1	M	214	GLU
1	M	215	ASP
1	M	226	ASN
1	M	227	MSE
1	M	240	LYS
1	M	261	ASN
1	M	263	SER
1	M	267	VAL
1	M	290	THR
1	N	15	THR
1	N	16	THR
1	N	17	ASP
1	N	26	LYS
1	N	37	ARG
1	N	42	LEU
1	N	53	GLU
1	N	61	THR
1	N	65	LYS
1	N	66	ARG
1	N	77	TYR
1	N	80	LEU
1	N	88	MSE
1	N	99	GLN
1	N	123	LYS

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Mol	Chain	Res	Type
1	N	126	MSE
1	N	150	MSE
1	N	153	LEU
1	N	161	HIS
1	N	166	GLU
1	N	194	LYS
1	N	195	VAL
1	N	198	CYS
1	N	202	VAL
1	N	205	THR
1	N	212	VAL
1	N	214	GLU
1	N	245	LEU
1	N	250	LEU
1	N	261	ASN
1	N	262	SER
1	N	265	ILE
1	N	267	VAL
1	N	271	LEU
1	N	281	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	99	GLN
1	A	107	ASN
1	A	222	GLN
1	A	226	ASN
1	A	235	GLN
1	A	236	GLN
1	A	257	ASN
1	A	261	ASN
1	A	281	GLN
1	A	298	ASN
1	B	58	GLN
1	B	103	ASN
1	B	104	ASN
1	B	117	GLN
1	B	122	HIS
1	B	124	GLN
1	B	161	HIS

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Mol	Chain	Res	Type
1	B	188	GLN
1	B	226	ASN
1	B	233	GLN
1	B	235	GLN
1	B	236	GLN
1	B	261	ASN
1	B	281	GLN
1	G	24	ASN
1	G	44	ASN
1	G	69	GLN
1	G	99	GLN
1	G	103	ASN
1	G	124	GLN
1	G	161	HIS
1	G	187	GLN
1	G	200	GLN
1	G	203	GLN
1	G	206	GLN
1	G	226	ASN
1	G	235	GLN
1	G	257	ASN
1	G	301	GLN
1	H	69	GLN
1	H	104	ASN
1	H	122	HIS
1	H	188	GLN
1	H	206	GLN
1	H	226	ASN
1	H	235	GLN
1	H	236	GLN
1	H	261	ASN
1	M	44	ASN
1	M	47	GLN
1	M	76	GLN
1	M	99	GLN
1	M	107	ASN
1	M	143	GLN
1	M	161	HIS
1	M	222	GLN
1	M	226	ASN
1	M	235	GLN
1	M	257	ASN

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Mol	Chain	Res	Type
1	M	261	ASN
1	M	266	HIS
1	M	273	GLN
1	M	281	GLN
1	N	69	GLN
1	N	76	GLN
1	N	99	GLN
1	N	103	ASN
1	N	104	ASN
1	N	117	GLN
1	N	122	HIS
1	N	200	GLN
1	N	203	GLN
1	N	222	GLN
1	N	226	ASN
1	N	235	GLN
1	N	236	GLN
1	N	261	ASN
1	N	273	GLN
1	N	281	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 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	275/295 (93%)	0.04	0 100 100	25, 44, 101, 123	0
1	B	275/295 (93%)	0.09	2 (0%) 89 84	25, 45, 95, 115	0
1	G	277/295 (93%)	0.14	4 (1%) 78 69	25, 43, 106, 114	0
1	H	278/295 (94%)	0.20	3 (1%) 82 74	23, 44, 111, 132	0
1	M	263/295 (89%)	0.22	7 (2%) 58 45	34, 58, 115, 121	0
1	N	264/295 (89%)	0.17	7 (2%) 58 45	36, 58, 105, 125	0
All	All	1632/1770 (92%)	0.14	23 (1%) 78 69	23, 48, 106, 132	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	187	GLN	3.6
1	G	176	ASN	3.4
1	M	127	GLY	3.4
1	M	169	LEU	3.3
1	H	189	LYS	3.1
1	M	162	LEU	3.0
1	G	185	PRO	3.0
1	G	172	THR	2.9
1	M	198	CYS	2.9
1	N	164	CYS	2.8
1	H	172	THR	2.6
1	M	201	ASP	2.5
1	N	186	GLU	2.4
1	N	198	CYS	2.4
1	N	204	LYS	2.4
1	N	167	GLU	2.4
1	B	215	ASP	2.4
1	N	188	GLN	2.4
1	N	305	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	177	SER	2.3
1	G	173	ARG	2.2
1	M	196	ASP	2.1
1	M	197	LYS	2.1

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	CA	B	400	1/1	0.92	0.25	1.10	87,87,87,87	0
2	CA	G	400	1/1	0.87	0.21	-0.19	91,91,91,91	0
2	CA	N	400	1/1	0.71	0.12	-	92,92,92,92	0
2	CA	M	400	1/1	0.88	0.14	-	85,85,85,85	0

6.5 Other polymers (i)

There are no such residues in this entry.