



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:49 AM UTC

PDB ID : 3VGV / pdb_00003vgv
Title : E134A mutant nucleoside diphosphate kinase derived from Halomonas sp. 593
Authors : Okazaki, N.; Yonezawa, Y.; Arai, S.; Matsumoto, F.; Tamada, T.; Tokunaga, H.; Ishibashi, M.; Tokunaga, M.; Kuroki, R.
Deposited on : 2011-08-21
Resolution : 2.50 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
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

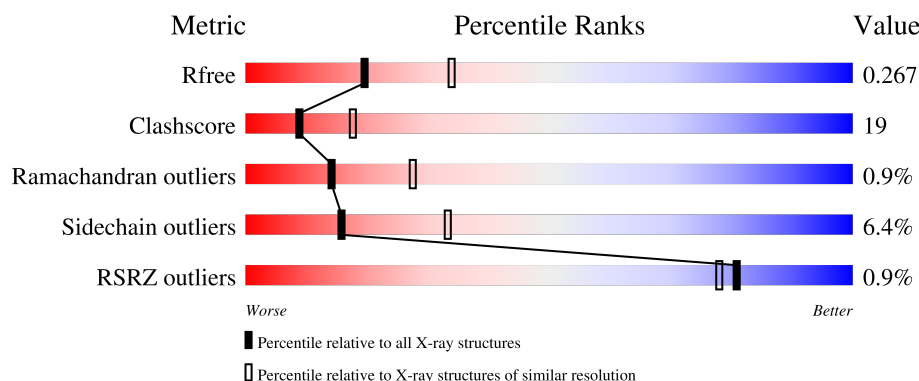
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 $\leq 5\%$. 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	A	141	% 60% 35% ..
1	B	141	69% 29% ..
1	C	141	70% 26% ..
1	D	141	% 57% 35% ..
1	E	141	63% 34% ..

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Mol	Chain	Length	Quality of chain
1	F	141	 66% 31% ..
1	G	141	 66% 32% ..
1	H	141	 65% 32% ..
1	I	141	 % 60% 38% ..
1	J	141	 % 55% 32% 5% 9%
1	K	141	 60% 37% ..
1	L	141	 % 67% 30% ..
1	M	141	 65% 32% ...
1	N	141	 7% 48% 28% 20%
1	O	141	 2% 60% 35% ..
1	P	141	 69% 27% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16777 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 Nucleoside diphosphate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	136	Total	C	N	O	S	0	0	0
			1024	639	174	207	4			
1	B	140	Total	C	N	O	S	0	0	0
			1060	661	182	213	4			
1	C	140	Total	C	N	O	S	0	0	0
			1060	661	182	213	4			
1	D	137	Total	C	N	O	S	0	0	0
			1033	645	176	208	4			
1	E	140	Total	C	N	O	S	0	0	0
			1060	661	182	213	4			
1	F	140	Total	C	N	O	S	0	0	0
			1060	661	182	213	4			
1	G	140	Total	C	N	O	S	0	0	0
			1060	661	182	213	4			
1	H	140	Total	C	N	O	S	0	0	0
			1060	661	182	213	4			
1	I	140	Total	C	N	O	S	0	0	0
			1060	661	182	213	4			
1	J	129	Total	C	N	O	S	0	0	0
			974	607	167	196	4			
1	K	140	Total	C	N	O	S	0	0	0
			1060	661	182	213	4			
1	L	140	Total	C	N	O	S	0	0	0
			1060	661	182	213	4			
1	M	140	Total	C	N	O	S	0	0	0
			1060	661	182	213	4			
1	N	113	Total	C	N	O	S	0	0	0
			840	520	146	171	3			
1	O	138	Total	C	N	O	S	0	0	0
			1038	643	180	211	4			
1	P	140	Total	C	N	O	S	0	0	0
			1060	661	182	213	4			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	134	ALA	GLU	engineered mutation	UNP Q83WH5
B	134	ALA	GLU	engineered mutation	UNP Q83WH5
C	134	ALA	GLU	engineered mutation	UNP Q83WH5
D	134	ALA	GLU	engineered mutation	UNP Q83WH5
E	134	ALA	GLU	engineered mutation	UNP Q83WH5
F	134	ALA	GLU	engineered mutation	UNP Q83WH5
G	134	ALA	GLU	engineered mutation	UNP Q83WH5
H	134	ALA	GLU	engineered mutation	UNP Q83WH5
I	134	ALA	GLU	engineered mutation	UNP Q83WH5
J	134	ALA	GLU	engineered mutation	UNP Q83WH5
K	134	ALA	GLU	engineered mutation	UNP Q83WH5
L	134	ALA	GLU	engineered mutation	UNP Q83WH5
M	134	ALA	GLU	engineered mutation	UNP Q83WH5
N	134	ALA	GLU	engineered mutation	UNP Q83WH5
O	134	ALA	GLU	engineered mutation	UNP Q83WH5
P	134	ALA	GLU	engineered mutation	UNP Q83WH5

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	15	Total O 15 15	0	0
2	B	23	Total O 23 23	0	0
2	C	13	Total O 13 13	0	0
2	D	13	Total O 13 13	0	0
2	E	12	Total O 12 12	0	0
2	F	8	Total O 8 8	0	0
2	G	15	Total O 15 15	0	0
2	H	18	Total O 18 18	0	0
2	I	13	Total O 13 13	0	0
2	J	8	Total O 8 8	0	0
2	K	14	Total O 14 14	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	L	14	Total 14	O 14	0	0
2	M	9	Total 9	O 9	0	0
2	N	9	Total 9	O 9	0	0
2	O	11	Total 11	O 11	0	0
2	P	13	Total 13	O 13	0	0



- Molecule 1: Nucleoside diphosphate kinase

Chain E: 63% 34% ..



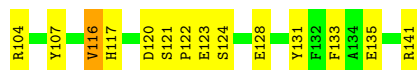
- Molecule 1: Nucleoside diphosphate kinase

Chain F: 66% 31% ..



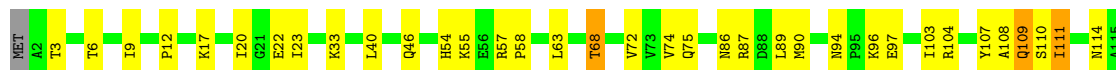
- Molecule 1: Nucleoside diphosphate kinase

Chain G: 66% 32% ..



- Molecule 1: Nucleoside diphosphate kinase

Chain H: 65% 32% ..



- Molecule 1: Nucleoside diphosphate kinase

Chain I: 60% 38% ..





- Molecule 1: Nucleoside diphosphate kinase



- Molecule 1: Nucleoside diphosphate kinase



- Molecule 1: Nucleoside diphosphate kinase

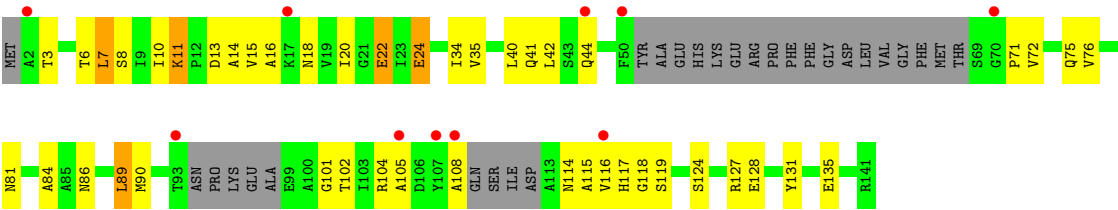


- Molecule 1: Nucleoside diphosphate kinase

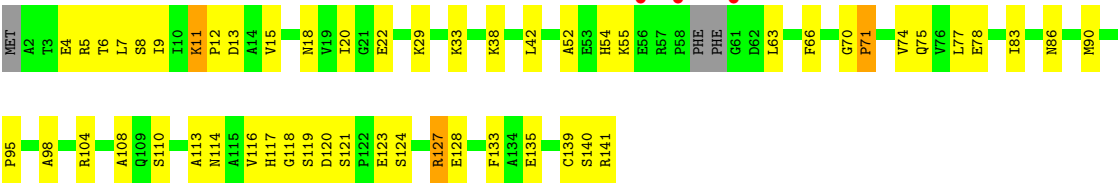


- Molecule 1: Nucleoside diphosphate kinase

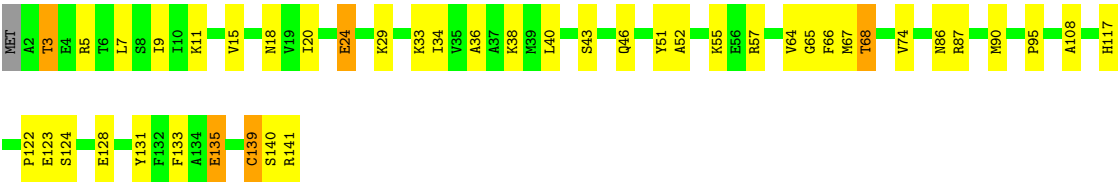




● Molecule 1: Nucleoside diphosphate kinase



● Molecule 1: Nucleoside diphosphate kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	112.17Å 92.02Å 113.61Å 90.00° 94.72° 90.00°	Depositor
Resolution (Å)	42.95 – 2.50 42.95 – 2.50	Depositor EDS
% Data completeness (in resolution range)	91.8 (42.95-2.50) 91.9 (42.95-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.216 , 0.269 0.215 , 0.267	Depositor DCC
R_{free} test set	3697 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å ²)	28.1	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.026 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16777	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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	A	0.88	0/1038	1.03	1/1398 (0.1%)
1	B	1.04	0/1076	1.08	1/1450 (0.1%)
1	C	0.93	0/1076	1.06	2/1450 (0.1%)
1	D	0.91	0/1047	0.96	2/1409 (0.1%)
1	E	0.89	0/1076	1.01	0/1450
1	F	1.03	0/1076	1.09	1/1450 (0.1%)
1	G	0.89	0/1076	1.06	0/1450
1	H	0.97	0/1076	1.10	4/1450 (0.3%)
1	I	0.93	0/1076	1.09	1/1450 (0.1%)
1	J	0.84	0/985	1.02	1/1324 (0.1%)
1	K	0.93	0/1076	1.06	2/1450 (0.1%)
1	L	0.92	0/1076	1.04	0/1450
1	M	0.91	0/1076	0.97	1/1450 (0.1%)
1	N	0.93	0/846	0.99	1/1135 (0.1%)
1	O	0.87	0/1051	1.03	0/1415
1	P	0.93	0/1076	1.01	0/1450
All	All	0.93	0/16803	1.04	17/22631 (0.1%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	121	SER	N-CA-C	7.85	115.29	108.22
1	K	121	SER	N-CA-C	7.00	114.30	108.07
1	M	72	VAL	CB-CA-C	-5.75	103.28	111.34
1	H	111	ILE	N-CA-C	-5.70	106.21	113.22
1	H	116	VAL	N-CA-C	5.68	118.32	108.90
1	N	75	GLN	N-CA-C	5.63	116.83	108.60
1	C	116	VAL	N-CA-C	5.61	118.22	108.90
1	J	93	THR	N-CA-C	-5.59	106.50	113.15
1	H	110	SER	N-CA-C	5.55	115.45	108.45
1	A	116	VAL	N-CA-C	5.54	116.83	108.96
1	C	68	THR	N-CA-C	-5.38	106.59	114.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	116	VAL	N-CA-C	5.35	116.61	108.80
1	K	104	ARG	N-CA-C	-5.29	105.51	111.28
1	D	121	SER	N-CA-C	5.28	112.88	108.13
1	H	75	GLN	N-CA-C	5.08	116.57	108.79
1	B	82	ALA	N-CA-C	5.06	116.80	111.28
1	F	116	VAL	N-CA-C	5.03	116.14	108.80

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	1024	0	995	40	0
1	B	1060	0	1035	30	0
1	C	1060	0	1035	40	0
1	D	1033	0	1008	44	0
1	E	1060	0	1035	46	0
1	F	1060	0	1035	36	0
1	G	1060	0	1035	38	0
1	H	1060	0	1035	46	0
1	I	1060	0	1035	48	0
1	J	974	0	953	40	0
1	K	1060	0	1035	49	0
1	L	1060	0	1035	37	0
1	M	1060	0	1035	36	0
1	N	840	0	828	37	0
1	O	1038	0	1016	47	0
1	P	1060	0	1035	34	0
2	A	15	0	0	8	0
2	B	23	0	0	7	0
2	C	13	0	0	4	0
2	D	13	0	0	10	0
2	E	12	0	0	8	0
2	F	8	0	0	6	0
2	G	15	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	18	0	0	12	0
2	I	13	0	0	7	0
2	J	8	0	0	2	0
2	K	14	0	0	9	0
2	L	14	0	0	9	0
2	M	9	0	0	5	0
2	N	9	0	0	3	0
2	O	11	0	0	7	0
2	P	13	0	0	6	0
All	All	16777	0	16185	609	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 19.

All (609) 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:D:74:VAL:HB	2:D:152:HOH:O	1.24	1.28
1:I:114:ASN:HB3	2:I:149:HOH:O	1.36	1.24
1:A:87:ARG:HG2	2:A:150:HOH:O	1.40	1.21
1:H:17:LYS:HB3	2:H:150:HOH:O	1.60	1.02
1:H:68:THR:HG23	2:H:148:HOH:O	1.63	0.98
1:K:95:PRO:HG2	1:K:96:LYS:NZ	1.81	0.96
1:K:81:ASN:HB2	2:K:173:HOH:O	1.65	0.96
1:P:3:THR:HB	2:P:197:HOH:O	1.68	0.93
1:G:18:ASN:HD21	1:H:141:ARG:HH22	1.16	0.93
1:P:57:ARG:HD2	2:P:142:HOH:O	1.68	0.92
1:O:90:MET:HB2	2:O:144:HOH:O	1.69	0.92
1:A:44:GLN:HG2	2:A:149:HOH:O	1.69	0.92
1:H:109:GLN:H	1:H:109:GLN:HE21	1.11	0.91
1:H:139:CYS:HB3	2:H:145:HOH:O	1.70	0.90
1:E:44:GLN:HG3	2:E:147:HOH:O	1.72	0.90
1:F:12:PRO:HD3	1:F:72:VAL:HG12	1.55	0.88
1:E:90:MET:HE1	1:E:118:GLY:HA3	1.55	0.87
1:O:75:GLN:HE21	1:O:77:LEU:HD21	1.38	0.87
1:A:26:ARG:NH2	1:A:101:GLY:O	2.07	0.87
1:O:5:ARG:HG2	1:O:78:GLU:HG3	1.56	0.87
1:G:38:LYS:HD2	2:G:148:HOH:O	1.76	0.84
1:K:104:ARG:HD3	1:K:114:ASN:HB2	1.59	0.82
1:E:11:LYS:HD3	1:E:67:MET:SD	2.20	0.82
1:L:22:GLU:HG2	1:L:107:TYR:OH	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:95:PRO:HG2	1:K:96:LYS:HZ2	1.42	0.81
1:I:124:SER:O	1:I:128:GLU:HG3	1.81	0.80
1:D:24:GLU:HG3	1:D:34:ILE:HD11	1.65	0.79
1:H:108:ALA:HA	2:H:175:HOH:O	1.83	0.78
1:L:12:PRO:HD3	1:L:72:VAL:HG12	1.64	0.78
1:H:108:ALA:HB1	1:H:114:ASN:HA	1.66	0.77
1:J:44:GLN:HB2	2:J:143:HOH:O	1.84	0.77
1:I:104:ARG:HE	1:I:114:ASN:HB2	1.49	0.77
1:G:54:HIS:HE1	2:G:208:HOH:O	1.68	0.77
1:L:4:GLU:CD	1:L:81:ASN:HA	2.09	0.77
1:A:87:ARG:HD3	2:A:160:HOH:O	1.84	0.76
1:L:136:SER:HB2	2:L:145:HOH:O	1.84	0.76
1:K:3:THR:HB	2:K:162:HOH:O	1.85	0.75
1:F:12:PRO:HA	2:F:142:HOH:O	1.87	0.75
1:D:9:ILE:HB	1:D:117:HIS:HB3	1.67	0.75
1:C:68:THR:HG21	2:C:147:HOH:O	1.86	0.74
1:H:22:GLU:HG2	1:H:107:TYR:OH	1.87	0.74
1:J:124:SER:O	1:J:128:GLU:HG3	1.87	0.74
1:O:140:SER:HB3	2:O:196:HOH:O	1.87	0.74
1:C:54:HIS:HA	1:C:57:ARG:HD3	1.69	0.74
1:H:109:GLN:HE21	1:H:109:GLN:N	1.85	0.73
1:A:87:ARG:CD	2:A:160:HOH:O	2.36	0.73
1:L:46:GLN:CG	2:L:182:HOH:O	2.36	0.73
1:P:124:SER:O	1:P:128:GLU:HG3	1.88	0.73
1:D:94:ASN:HD22	1:D:97:GLU:HG2	1.53	0.72
1:J:90:MET:O	1:J:104:ARG:HB2	1.88	0.72
1:O:98:ALA:HA	2:O:145:HOH:O	1.89	0.72
1:K:95:PRO:HG2	1:K:96:LYS:HZ1	1.55	0.71
1:K:139:CYS:SG	2:K:166:HOH:O	2.38	0.71
1:O:127:ARG:HH11	1:O:127:ARG:HB2	1.54	0.71
1:E:90:MET:CE	1:E:118:GLY:HA3	2.20	0.71
1:M:131:TYR:N	2:M:149:HOH:O	2.23	0.71
1:H:63:LEU:CD1	2:H:171:HOH:O	2.39	0.70
1:N:15:VAL:HG11	2:N:144:HOH:O	1.89	0.70
1:I:26:ARG:HD2	2:I:177:HOH:O	1.92	0.70
1:O:9:ILE:HG12	1:O:74:VAL:HG12	1.74	0.70
1:H:94:ASN:ND2	1:H:111:ILE:HB	2.06	0.70
1:B:25:SER:HB3	1:B:29:LYS:HE2	1.73	0.70
1:L:46:GLN:HG3	2:L:182:HOH:O	1.92	0.70
1:L:87:ARG:HA	1:L:90:MET:HE3	1.74	0.70
1:L:12:PRO:HD3	1:L:72:VAL:CG1	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:55:LYS:HB2	2:P:150:HOH:O	1.92	0.69
1:A:135:GLU:HB2	1:C:131:TYR:HA	1.72	0.69
1:I:104:ARG:O	1:I:108:ALA:HB3	1.93	0.69
1:O:90:MET:HE1	1:O:118:GLY:HA3	1.75	0.69
1:N:24:GLU:HG3	1:N:34:ILE:HD11	1.72	0.69
1:D:109:GLN:HB2	2:D:146:HOH:O	1.93	0.69
1:F:94:ASN:HB3	1:F:97:GLU:HG2	1.74	0.68
1:H:109:GLN:H	1:H:109:GLN:NE2	1.89	0.68
1:H:55:LYS:HB2	2:H:154:HOH:O	1.93	0.68
1:N:131:TYR:HA	1:P:135:GLU:HB2	1.76	0.68
1:L:87:ARG:HD2	2:L:147:HOH:O	1.94	0.67
1:B:89:LEU:HD23	1:F:101:GLY:HA3	1.75	0.67
1:E:44:GLN:NE2	1:E:64:VAL:HG12	2.09	0.67
1:G:104:ARG:O	2:G:194:HOH:O	2.13	0.67
1:M:15:VAL:HG21	1:M:71:PRO:O	1.95	0.66
1:F:5:ARG:HG2	1:F:78:GLU:HB2	1.76	0.66
1:L:4:GLU:OE1	1:L:81:ASN:HA	1.95	0.66
1:N:90:MET:HE1	1:N:118:GLY:HA3	1.76	0.66
1:J:29:LYS:HE2	1:N:22:GLU:OE2	1.94	0.66
1:N:86:ASN:O	1:N:90:MET:HG3	1.95	0.66
1:O:140:SER:CB	2:O:196:HOH:O	2.43	0.66
1:I:139:CYS:HB3	2:I:144:HOH:O	1.96	0.66
1:I:110:SER:HB3	2:I:148:HOH:O	1.96	0.66
1:E:44:GLN:NE2	1:E:64:VAL:CG1	2.59	0.66
1:C:104:ARG:HG2	1:C:114:ASN:HB2	1.78	0.65
1:I:9:ILE:HB	1:I:117:HIS:HB3	1.78	0.65
1:P:64:VAL:O	1:P:68:THR:HB	1.97	0.65
1:N:124:SER:O	1:N:128:GLU:HG3	1.96	0.65
1:E:83:ILE:HD13	1:E:122:PRO:HA	1.79	0.65
1:L:9:ILE:HB	1:L:117:HIS:HB3	1.77	0.65
1:F:57:ARG:HD2	1:F:59:PHE:HE2	1.62	0.64
1:J:104:ARG:O	1:J:108:ALA:HB3	1.96	0.64
1:D:62:ASP:HB3	2:D:147:HOH:O	1.98	0.64
1:D:124:SER:O	1:D:128:GLU:HG3	1.98	0.64
1:N:81:ASN:OD1	1:N:84:ALA:HB3	1.97	0.64
1:G:18:ASN:HD21	1:H:141:ARG:NH2	1.93	0.64
1:O:33:LYS:HB3	1:O:141:ARG:HH12	1.62	0.64
1:P:20:ILE:O	1:P:24:GLU:HB2	1.97	0.64
1:A:117:HIS:CD2	1:A:118:GLY:N	2.65	0.64
1:N:11:LYS:HB2	1:N:13:ASP:OD1	1.97	0.64
1:G:38:LYS:HE3	1:G:133:PHE:CE1	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:123:GLU:CD	1:I:123:GLU:H	2.05	0.63
1:H:94:ASN:HB3	1:H:97:GLU:OE1	1.99	0.63
1:L:12:PRO:CD	1:L:72:VAL:HG12	2.29	0.63
1:M:13:ASP:HA	2:M:146:HOH:O	1.98	0.63
1:J:86:ASN:O	1:J:90:MET:HG3	1.98	0.63
1:A:18:ASN:ND2	1:B:141:ARG:HH12	1.97	0.63
1:N:104:ARG:NE	1:N:114:ASN:HD22	1.97	0.63
1:I:38:LYS:HD2	2:I:147:HOH:O	1.98	0.63
1:I:7:LEU:HD22	1:I:128:GLU:HB3	1.80	0.63
1:A:23:ILE:O	1:A:26:ARG:HB2	1.98	0.63
1:J:24:GLU:HG3	1:J:34:ILE:HD11	1.81	0.62
1:J:63:LEU:HD23	1:J:63:LEU:O	1.99	0.62
1:M:9:ILE:HB	1:M:117:HIS:HB3	1.81	0.62
1:O:13:ASP:HA	2:O:142:HOH:O	1.98	0.62
1:B:44:GLN:HG2	2:B:172:HOH:O	1.99	0.62
1:F:108:ALA:HB1	1:F:114:ASN:HA	1.80	0.62
1:K:15:VAL:HG22	2:K:142:HOH:O	1.98	0.62
1:M:90:MET:HE1	1:M:118:GLY:HA3	1.80	0.62
1:E:44:GLN:CG	2:E:147:HOH:O	2.40	0.62
1:K:3:THR:HG23	1:K:3:THR:O	2.01	0.61
1:K:120:ASP:HA	2:K:143:HOH:O	2.00	0.61
1:E:5:ARG:HH21	1:E:140:SER:HB2	1.64	0.61
1:I:114:ASN:CB	2:I:149:HOH:O	2.15	0.61
1:K:22:GLU:HG2	1:K:107:TYR:OH	2.00	0.61
1:O:127:ARG:HB2	1:O:127:ARG:NH1	2.16	0.61
1:G:7:LEU:HD22	1:G:128:GLU:HB3	1.83	0.61
1:G:57:ARG:HG2	1:L:97:GLU:HG2	1.83	0.61
1:K:9:ILE:HB	1:K:117:HIS:HB3	1.82	0.61
1:K:68:THR:HG21	2:K:150:HOH:O	2.01	0.61
1:D:104:ARG:O	1:D:108:ALA:HB3	2.01	0.61
1:K:121:SER:HB2	1:K:122:PRO:HD2	1.83	0.61
1:O:75:GLN:NE2	1:O:77:LEU:HD21	2.11	0.61
1:E:9:ILE:HG12	1:E:74:VAL:HG12	1.83	0.60
1:C:124:SER:O	1:C:128:GLU:HG3	2.01	0.60
1:A:86:ASN:O	1:A:90:MET:HG3	2.02	0.60
1:F:42:LEU:HD21	1:F:132:PHE:HE1	1.65	0.60
1:D:94:ASN:ND2	1:D:97:GLU:HG2	2.16	0.60
1:E:135:GLU:HB2	1:G:131:TYR:HA	1.82	0.60
1:N:104:ARG:HE	1:N:114:ASN:HD22	1.48	0.60
1:B:131:TYR:HA	1:D:135:GLU:HB2	1.84	0.60
1:K:43:SER:OG	1:K:46:GLN:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:95:PRO:HB3	1:M:108:ALA:HB3	1.84	0.59
1:P:51:TYR:CE2	1:P:67:MET:HG3	2.36	0.59
1:D:86:ASN:O	1:D:90:MET:HG3	2.02	0.59
1:O:66:PHE:CZ	1:O:113:ALA:HA	2.36	0.59
1:F:93:THR:HA	1:F:104:ARG:HH11	1.67	0.59
1:K:15:VAL:CG2	2:K:142:HOH:O	2.49	0.59
1:P:95:PRO:HB3	1:P:108:ALA:HB3	1.85	0.59
1:O:7:LEU:HG	1:O:8:SER:N	2.16	0.59
1:C:53:GLU:HG3	1:C:54:HIS:CD2	2.37	0.59
1:F:42:LEU:HD21	1:F:132:PHE:CE1	2.37	0.59
1:N:104:ARG:O	1:N:108:ALA:HB3	2.03	0.59
1:H:87:ARG:HA	1:H:90:MET:HE3	1.84	0.58
1:O:7:LEU:HG	1:O:8:SER:H	1.68	0.58
1:D:32:LEU:HD13	1:D:77:LEU:HD13	1.85	0.58
1:O:4:GLU:OE1	1:O:83:ILE:HD12	2.02	0.58
1:I:91:GLY:O	1:I:104:ARG:HD2	2.01	0.58
1:K:127:ARG:NH2	2:K:169:HOH:O	2.36	0.58
1:I:87:ARG:NH2	1:I:120:ASP:HB2	2.19	0.58
1:A:104:ARG:O	1:A:108:ALA:HB3	2.03	0.58
1:K:104:ARG:CD	1:K:114:ASN:HB2	2.32	0.58
1:K:15:VAL:HG21	1:K:71:PRO:O	2.04	0.58
1:C:15:VAL:HG21	1:C:71:PRO:O	2.04	0.58
1:G:9:ILE:HB	1:G:117:HIS:HB3	1.85	0.58
1:O:90:MET:O	1:O:104:ARG:CG	2.52	0.58
1:P:33:LYS:HB3	1:P:141:ARG:NH1	2.18	0.57
1:D:51:TYR:HE2	1:D:67:MET:HG3	1.68	0.57
1:E:57:ARG:HD3	2:E:149:HOH:O	2.04	0.57
1:F:135:GLU:HB2	1:H:131:TYR:HA	1.85	0.57
1:J:7:LEU:HD22	1:J:128:GLU:HB3	1.86	0.57
1:B:45:GLU:HG2	2:B:154:HOH:O	2.03	0.57
1:D:104:ARG:HG2	1:D:114:ASN:ND2	2.19	0.57
1:F:12:PRO:HD3	1:F:72:VAL:CG1	2.31	0.57
1:H:109:GLN:HB2	2:H:142:HOH:O	2.04	0.57
1:N:135:GLU:HB2	1:P:131:TYR:HA	1.87	0.57
1:I:94:ASN:HD22	1:I:97:GLU:HG2	1.69	0.56
1:J:131:TYR:HA	1:L:135:GLU:HB2	1.88	0.56
1:E:71:PRO:HD2	2:E:145:HOH:O	2.04	0.56
1:N:71:PRO:HB2	2:N:144:HOH:O	2.06	0.56
1:B:9:ILE:HB	1:B:117:HIS:HB3	1.87	0.56
1:F:86:ASN:HB3	2:F:144:HOH:O	2.04	0.56
1:I:87:ARG:HH21	1:I:120:ASP:HB2	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:18:ASN:ND2	1:H:141:ARG:HH22	1.96	0.56
1:G:44:GLN:O	1:G:48:GLU:HG3	2.06	0.56
1:P:51:TYR:HE2	1:P:67:MET:HG3	1.71	0.56
1:E:7:LEU:HD22	1:E:128:GLU:HB3	1.86	0.56
1:I:11:LYS:HD3	1:I:67:MET:SD	2.46	0.56
1:D:109:GLN:HG2	1:D:113:ALA:HB3	1.86	0.56
1:I:95:PRO:HG2	1:I:96:LYS:HD2	1.88	0.56
1:N:119:SER:OG	1:N:128:GLU:OE1	2.10	0.56
1:P:9:ILE:HB	1:P:117:HIS:HB3	1.87	0.56
1:E:2:ALA:HA	1:L:44:GLN:NE2	2.21	0.56
1:A:85:ALA:O	1:A:89:LEU:HB2	2.07	0.55
1:F:109:GLN:HB2	2:F:147:HOH:O	2.05	0.55
1:L:42:LEU:HD12	1:L:67:MET:O	2.07	0.55
1:E:55:LYS:CB	2:E:191:HOH:O	2.53	0.55
1:E:55:LYS:HB3	2:E:191:HOH:O	2.06	0.55
1:O:7:LEU:HD22	1:O:128:GLU:HB3	1.88	0.55
1:E:8:SER:HB3	1:E:75:GLN:HG3	1.88	0.55
1:M:109:GLN:HA	2:M:144:HOH:O	2.06	0.55
1:E:44:GLN:HE22	1:E:64:VAL:HG12	1.72	0.55
1:L:87:ARG:CD	2:L:204:HOH:O	2.54	0.55
1:K:26:ARG:NH2	1:K:106:ASP:OD1	2.39	0.55
1:F:93:THR:HA	1:F:104:ARG:NH1	2.22	0.55
1:E:64:VAL:O	1:E:68:THR:HG22	2.07	0.55
1:I:11:LYS:HB3	1:I:12:PRO:CD	2.38	0.54
1:I:18:ASN:ND2	1:J:141:ARG:HH11	2.06	0.54
1:C:8:SER:HB3	1:C:75:GLN:HG3	1.90	0.54
1:C:44:GLN:OE1	2:C:147:HOH:O	2.18	0.54
1:C:18:ASN:ND2	1:D:141:ARG:HH11	2.06	0.54
1:L:74:VAL:HG12	1:L:133:PHE:CE2	2.43	0.54
1:A:83:ILE:O	1:A:87:ARG:HG3	2.07	0.54
1:H:94:ASN:HD22	1:H:111:ILE:HB	1.70	0.54
1:B:20:ILE:O	1:B:24:GLU:HB2	2.08	0.54
1:N:104:ARG:HE	1:N:114:ASN:ND2	2.06	0.54
1:G:27:PHE:CE1	1:G:86:ASN:ND2	2.76	0.53
1:O:90:MET:HE3	2:O:144:HOH:O	2.08	0.53
1:A:89:LEU:HD22	1:A:103:ILE:HD11	1.90	0.53
1:L:4:GLU:HG2	1:L:82:ALA:H	1.73	0.53
1:P:52:ALA:O	1:P:55:LYS:HB3	2.08	0.53
1:I:6:THR:HB	1:I:83:ILE:HG12	1.91	0.53
1:L:7:LEU:HD22	1:L:128:GLU:HB3	1.89	0.53
1:M:29:LYS:C	1:M:31:GLY:H	2.15	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:26:ARG:NH2	1:G:101:GLY:O	2.42	0.53
1:A:12:PRO:HD3	1:A:72:VAL:HG12	1.91	0.53
1:C:57:ARG:HG2	1:C:57:ARG:HH21	1.74	0.53
1:H:9:ILE:HB	1:H:117:HIS:HB3	1.89	0.53
1:D:11:LYS:HE3	1:D:116:VAL:O	2.09	0.52
1:D:43:SER:OG	1:D:46:GLN:HG3	2.09	0.52
1:B:50:PHE:HB2	1:B:131:TYR:CE2	2.44	0.52
1:B:89:LEU:CD2	1:F:101:GLY:HA3	2.38	0.52
1:A:134:ALA:HB3	1:A:137:GLU:HG3	1.91	0.52
1:D:8:SER:HB3	1:D:75:GLN:HG3	1.90	0.52
1:G:12:PRO:HG3	1:G:72:VAL:CG1	2.39	0.52
1:H:94:ASN:HB2	1:H:111:ILE:HD12	1.92	0.52
1:L:90:MET:HG2	1:L:116:VAL:HG21	1.91	0.52
1:C:108:ALA:CB	1:C:114:ASN:HA	2.39	0.52
1:M:130:ALA:HB3	2:M:149:HOH:O	2.09	0.52
1:F:20:ILE:O	1:F:24:GLU:HB2	2.10	0.52
1:L:45:GLU:CD	1:L:45:GLU:H	2.17	0.52
1:F:131:TYR:HA	1:H:135:GLU:HB2	1.92	0.52
1:I:11:LYS:HE2	1:I:117:HIS:HB2	1.90	0.52
1:K:86:ASN:O	1:K:90:MET:HG3	2.09	0.52
1:M:39:MET:HE1	1:N:34:ILE:O	2.09	0.52
1:N:11:LYS:HD3	1:N:115:ALA:O	2.10	0.52
1:P:40:LEU:C	1:P:40:LEU:HD12	2.35	0.52
1:O:5:ARG:CG	1:O:78:GLU:HG3	2.35	0.52
1:D:20:ILE:O	1:D:24:GLU:HB2	2.10	0.52
1:L:17:LYS:NZ	2:L:198:HOH:O	2.32	0.52
1:K:94:ASN:HA	1:K:111:ILE:HG12	1.92	0.52
1:I:13:ASP:OD2	1:I:115:ALA:HA	2.10	0.52
1:E:11:LYS:HB3	1:E:12:PRO:HD2	1.92	0.51
1:B:141:ARG:HD3	2:B:183:HOH:O	2.09	0.51
1:J:13:ASP:OD2	1:J:115:ALA:N	2.43	0.51
1:O:120:ASP:HB2	2:O:146:HOH:O	2.11	0.51
1:F:9:ILE:HB	1:F:117:HIS:HB3	1.92	0.51
1:M:131:TYR:HA	1:O:135:GLU:HB2	1.91	0.51
1:J:90:MET:HE1	1:J:118:GLY:HA3	1.91	0.51
1:K:23:ILE:HG23	1:K:103:ILE:HD13	1.93	0.51
1:J:40:LEU:HD21	1:J:42:LEU:HD23	1.93	0.51
1:I:24:GLU:OE1	1:I:34:ILE:HD13	2.11	0.51
1:I:68:THR:HG21	2:I:145:HOH:O	2.09	0.51
1:O:95:PRO:HG2	1:O:110:SER:O	2.10	0.51
1:P:43:SER:OG	1:P:46:GLN:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:104:ARG:O	1:H:108:ALA:HB3	2.11	0.51
1:B:114:ASN:O	1:B:116:VAL:N	2.42	0.51
1:F:13:ASP:OD1	1:F:13:ASP:N	2.44	0.51
1:A:131:TYR:HA	1:C:135:GLU:HB2	1.93	0.51
1:L:90:MET:HE1	1:L:118:GLY:HA3	1.93	0.50
1:O:86:ASN:O	1:O:90:MET:HG3	2.11	0.50
1:E:11:LYS:HB3	1:E:12:PRO:CD	2.41	0.50
1:F:111:ILE:HG23	1:F:112:ASP:N	2.26	0.50
1:I:90:MET:HE1	1:I:118:GLY:HA3	1.93	0.50
1:K:24:GLU:OE1	1:K:75:GLN:NE2	2.33	0.50
1:C:66:PHE:C	1:C:68:THR:H	2.17	0.50
1:E:57:ARG:CD	2:E:149:HOH:O	2.60	0.50
1:J:66:PHE:C	1:J:68:THR:H	2.19	0.50
1:J:93:THR:HA	1:J:104:ARG:HH11	1.75	0.50
1:K:54:HIS:HD2	1:K:57:ARG:NH2	2.09	0.50
1:N:7:LEU:HD22	1:N:128:GLU:HB3	1.94	0.50
1:O:33:LYS:NZ	1:P:18:ASN:HD21	2.10	0.50
1:C:64:VAL:O	1:C:68:THR:HB	2.11	0.50
1:E:44:GLN:HE21	1:E:64:VAL:CG1	2.24	0.50
1:O:38:LYS:HG2	1:O:133:PHE:CE1	2.47	0.49
1:C:54:HIS:CA	1:C:57:ARG:HD3	2.41	0.49
1:G:51:TYR:CE2	1:G:67:MET:HG3	2.46	0.49
1:I:104:ARG:HA	1:I:108:ALA:HB2	1.94	0.49
1:F:94:ASN:OD1	1:F:96:LYS:HG2	2.12	0.49
1:L:2:ALA:HB1	2:L:143:HOH:O	2.12	0.49
1:F:24:GLU:HG3	1:F:34:ILE:CD1	2.42	0.49
1:I:15:VAL:HG21	1:I:71:PRO:O	2.13	0.49
1:E:9:ILE:HB	1:E:117:HIS:HB3	1.95	0.49
1:I:86:ASN:O	1:I:90:MET:HG3	2.13	0.49
1:N:41:GLN:HA	1:N:41:GLN:NE2	2.28	0.49
1:A:118:GLY:O	1:A:119:SER:C	2.54	0.49
1:B:7:LEU:HD22	1:B:128:GLU:HB3	1.94	0.49
1:O:108:ALA:HB1	1:O:114:ASN:HA	1.94	0.49
1:C:114:ASN:O	1:C:116:VAL:N	2.41	0.49
1:D:30:ALA:CB	1:D:89:LEU:HD11	2.42	0.49
1:E:86:ASN:O	1:E:90:MET:HG3	2.12	0.49
1:G:51:TYR:OH	1:G:67:MET:HE2	2.12	0.49
1:I:90:MET:HG2	1:I:116:VAL:HG21	1.94	0.49
1:C:57:ARG:HG2	2:C:144:HOH:O	2.13	0.49
1:F:95:PRO:HG2	1:F:110:SER:O	2.13	0.49
1:N:11:LYS:HD3	1:N:115:ALA:C	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:SER:HB3	1:C:131:TYR:CE2	2.48	0.49
1:C:111:ILE:C	1:C:111:ILE:HD13	2.38	0.49
1:H:63:LEU:HD13	2:H:171:HOH:O	2.10	0.49
1:L:4:GLU:O	1:L:78:GLU:HA	2.13	0.49
1:G:87:ARG:HD3	2:G:151:HOH:O	2.13	0.49
1:M:90:MET:HG2	1:M:116:VAL:HG21	1.95	0.49
1:H:124:SER:HA	2:H:146:HOH:O	2.13	0.48
1:H:139:CYS:C	2:H:145:HOH:O	2.56	0.48
1:A:54:HIS:C	2:A:146:HOH:O	2.56	0.48
1:E:121:SER:HB2	1:E:122:PRO:HD2	1.95	0.48
1:G:121:SER:HB2	1:G:122:PRO:HD2	1.96	0.48
1:I:26:ARG:NH2	1:I:107:TYR:HE2	2.11	0.48
1:D:24:GLU:HA	1:D:24:GLU:OE2	2.13	0.48
1:G:124:SER:O	1:G:128:GLU:HG3	2.13	0.48
1:A:39:MET:HE1	1:B:34:ILE:O	2.13	0.48
1:D:52:ALA:N	2:D:150:HOH:O	2.46	0.48
1:J:45:GLU:CD	1:J:45:GLU:H	2.22	0.48
1:M:9:ILE:HG12	1:M:74:VAL:HG12	1.95	0.48
1:P:87:ARG:HA	1:P:90:MET:HE3	1.96	0.48
1:F:74:VAL:HG12	1:F:133:PHE:CE2	2.49	0.48
1:F:108:ALA:CB	1:F:114:ASN:HA	2.43	0.48
1:H:57:ARG:HB3	1:H:58:PRO:HD2	1.95	0.48
1:I:104:ARG:NE	1:I:114:ASN:HB2	2.23	0.48
1:A:84:ALA:HA	1:A:87:ARG:HD3	1.96	0.48
1:I:131:TYR:HA	1:K:135:GLU:HB2	1.95	0.48
1:M:11:LYS:HE3	1:M:117:HIS:HB2	1.95	0.48
1:G:51:TYR:CD1	1:G:63:LEU:HD21	2.48	0.48
1:I:94:ASN:HB3	1:I:97:GLU:HG2	1.95	0.48
1:A:12:PRO:HA	2:A:142:HOH:O	2.14	0.48
1:D:51:TYR:C	2:D:150:HOH:O	2.57	0.48
1:E:57:ARG:HA	2:E:149:HOH:O	2.12	0.48
1:K:87:ARG:CB	1:K:87:ARG:HH11	2.26	0.48
1:O:33:LYS:HB3	1:O:141:ARG:NH1	2.29	0.48
1:C:11:LYS:HE3	1:C:116:VAL:C	2.39	0.47
1:N:13:ASP:OD1	1:N:115:ALA:HA	2.14	0.47
1:A:59:PHE:O	1:A:62:ASP:HB2	2.14	0.47
1:H:108:ALA:CB	1:H:114:ASN:HA	2.41	0.47
1:J:36:ALA:HB3	1:J:76:VAL:HB	1.96	0.47
1:M:29:LYS:C	1:M:31:GLY:N	2.72	0.47
1:O:12:PRO:HG3	1:O:70:GLY:O	2.14	0.47
1:E:11:LYS:O	1:E:15:VAL:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:PHE:CE1	1:E:128:GLU:HG2	2.48	0.47
1:G:33:LYS:HB3	1:G:141:ARG:HH12	1.79	0.47
1:H:6:THR:OG1	1:H:119:SER:HB2	2.14	0.47
1:M:24:GLU:OE1	1:M:34:ILE:HD13	2.14	0.47
1:N:20:ILE:O	1:N:24:GLU:HB2	2.14	0.47
1:H:22:GLU:CG	1:H:107:TYR:OH	2.61	0.47
1:K:11:LYS:HE2	1:K:117:HIS:HB2	1.96	0.47
1:B:43:SER:H	1:B:46:GLN:HB2	1.80	0.47
1:E:98:ALA:HB3	1:E:105:ALA:HB2	1.97	0.47
1:J:11:LYS:HB3	1:J:12:PRO:CD	2.44	0.47
1:J:89:LEU:HD23	1:N:101:GLY:HA3	1.96	0.47
1:J:52:ALA:O	1:J:55:LYS:HG3	2.15	0.47
1:M:87:ARG:HA	1:M:90:MET:HE3	1.97	0.47
1:O:11:LYS:HE3	1:O:116:VAL:O	2.15	0.47
1:L:96:LYS:H	1:L:96:LYS:HD2	1.79	0.47
1:N:102:THR:H	1:N:105:ALA:HB3	1.80	0.47
1:A:15:VAL:HG13	1:A:20:ILE:HD11	1.96	0.47
1:D:45:GLU:HG3	2:D:176:HOH:O	2.14	0.47
1:H:54:HIS:HD2	1:H:57:ARG:HE	1.62	0.47
1:L:46:GLN:CD	2:L:182:HOH:O	2.58	0.47
1:B:33:LYS:HE3	2:B:144:HOH:O	2.14	0.46
1:B:54:HIS:HD2	1:B:57:ARG:HH11	1.62	0.46
1:D:81:ASN:O	1:D:82:ALA:C	2.58	0.46
1:F:7:LEU:HG	1:F:8:SER:N	2.30	0.46
1:I:42:LEU:O	1:I:68:THR:HG23	2.15	0.46
1:P:74:VAL:HG12	1:P:133:PHE:CE2	2.50	0.46
1:H:96:LYS:HG2	1:H:97:GLU:OE1	2.15	0.46
1:M:53:GLU:HG3	1:M:54:HIS:CD2	2.51	0.46
1:M:68:THR:HG22	1:M:68:THR:O	2.14	0.46
1:F:24:GLU:HG3	1:F:34:ILE:HD11	1.96	0.46
1:E:114:ASN:O	1:E:116:VAL:N	2.44	0.46
1:H:139:CYS:CA	2:H:145:HOH:O	2.63	0.46
1:K:87:ARG:HH11	1:K:87:ARG:HB3	1.80	0.46
1:M:104:ARG:O	1:M:108:ALA:HB3	2.15	0.46
1:A:124:SER:O	1:A:128:GLU:HG3	2.15	0.46
1:C:11:LYS:O	1:C:15:VAL:HG13	2.15	0.46
1:G:12:PRO:HG3	1:G:72:VAL:HG12	1.97	0.46
1:M:130:ALA:C	2:M:149:HOH:O	2.58	0.46
1:K:24:GLU:O	1:K:28:GLU:HG3	2.16	0.46
1:J:13:ASP:OD1	1:J:66:PHE:HZ	1.99	0.46
1:M:123:GLU:O	1:M:126:ALA:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:43:SER:OG	1:G:46:GLN:HG3	2.16	0.46
1:K:109:GLN:NE2	1:K:110:SER:HB3	2.30	0.46
1:A:95:PRO:HB3	1:A:108:ALA:HB3	1.98	0.46
1:B:45:GLU:CG	2:B:154:HOH:O	2.62	0.46
1:J:92:ALA:C	1:J:94:ASN:H	2.23	0.46
1:K:26:ARG:HH12	1:K:106:ASP:HB2	1.78	0.46
1:O:22:GLU:OE2	1:P:29:LYS:NZ	2.48	0.46
1:O:108:ALA:CB	1:O:114:ASN:HA	2.46	0.46
1:D:55:LYS:HA	1:D:60:PHE:CD1	2.51	0.46
1:E:131:TYR:HA	1:G:135:GLU:HB2	1.97	0.46
1:F:121:SER:HB2	1:F:122:PRO:HD2	1.98	0.46
1:N:89:LEU:O	1:N:102:THR:HB	2.16	0.46
1:O:38:LYS:HG2	1:O:133:PHE:HE1	1.79	0.46
1:E:51:TYR:O	1:E:60:PHE:HE1	1.99	0.45
1:G:8:SER:HB2	1:G:77:LEU:HD11	1.98	0.45
1:G:120:ASP:OD2	1:G:120:ASP:C	2.58	0.45
1:H:139:CYS:CB	2:H:145:HOH:O	2.47	0.45
1:K:121:SER:HB2	1:K:122:PRO:CD	2.45	0.45
1:D:89:LEU:HD21	2:D:149:HOH:O	2.16	0.45
1:H:23:ILE:HG23	1:H:103:ILE:HD13	1.98	0.45
1:O:90:MET:CE	1:O:118:GLY:HA3	2.44	0.45
1:A:95:PRO:C	1:A:97:GLU:H	2.24	0.45
1:A:51:TYR:HE2	1:A:67:MET:HG3	1.80	0.45
1:H:89:LEU:O	1:H:103:ILE:HG13	2.17	0.45
1:J:109:GLN:HG2	1:J:110:SER:H	1.81	0.45
1:H:90:MET:CE	1:H:118:GLY:HA3	2.46	0.45
1:B:124:SER:O	1:B:128:GLU:HG3	2.16	0.45
1:C:36:ALA:HB3	1:C:76:VAL:HB	1.97	0.45
1:E:36:ALA:HB3	1:E:76:VAL:HB	1.98	0.45
1:G:34:ILE:HD12	1:H:20:ILE:HD12	1.99	0.45
1:K:20:ILE:O	1:K:24:GLU:HG2	2.16	0.45
1:C:59:PHE:CD1	1:C:59:PHE:C	2.95	0.45
1:D:94:ASN:HD21	1:D:96:LYS:HB2	1.82	0.45
1:P:15:VAL:HG13	1:P:20:ILE:HD11	1.98	0.45
1:B:26:ARG:NH2	1:B:106:ASP:OD1	2.49	0.45
1:I:35:VAL:HG11	1:I:140:SER:HA	1.99	0.45
1:K:40:LEU:HD21	1:K:74:VAL:HG22	1.98	0.45
1:K:51:TYR:CD1	1:K:63:LEU:HD21	2.51	0.45
1:M:48:GLU:HG2	1:M:60:PHE:CZ	2.51	0.45
1:A:24:GLU:OE1	1:A:34:ILE:HD13	2.17	0.45
1:B:12:PRO:HA	2:B:153:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:26:ARG:NH1	1:K:103:ILE:HA	2.32	0.45
1:E:87:ARG:HG2	1:E:87:ARG:HH11	1.81	0.44
1:E:90:MET:HG2	1:E:116:VAL:HG21	1.99	0.44
1:O:18:ASN:HD21	1:P:141:ARG:HH22	1.64	0.44
1:D:51:TYR:CE2	1:D:67:MET:HG3	2.50	0.44
1:E:43:SER:OG	1:E:46:GLN:HG3	2.16	0.44
1:M:87:ARG:HH11	1:M:87:ARG:HG2	1.82	0.44
1:M:109:GLN:HB2	1:M:110:SER:H	1.67	0.44
1:I:17:LYS:HE3	1:I:109:GLN:NE2	2.32	0.44
1:M:10:ILE:HD11	1:M:24:GLU:OE2	2.17	0.44
1:O:121:SER:OG	1:O:124:SER:HB2	2.17	0.44
1:J:40:LEU:HD21	1:J:42:LEU:CD2	2.48	0.44
1:J:54:HIS:O	1:J:60:PHE:HB2	2.16	0.44
1:J:92:ALA:O	1:J:104:ARG:HD2	2.17	0.44
1:K:81:ASN:ND2	1:K:84:ALA:HB3	2.32	0.44
1:L:87:ARG:NH1	1:L:120:ASP:O	2.50	0.44
1:O:29:LYS:HG3	2:P:144:HOH:O	2.16	0.44
1:E:90:MET:HE1	1:E:118:GLY:CA	2.36	0.44
1:N:11:LYS:HE3	1:N:116:VAL:C	2.42	0.44
1:N:117:HIS:CE1	1:N:118:GLY:O	2.71	0.44
1:A:109:GLN:OE1	1:A:109:GLN:HA	2.18	0.44
1:G:44:GLN:HA	1:G:44:GLN:OE1	2.17	0.44
1:J:79:GLY:O	1:J:82:ALA:HB2	2.17	0.44
1:O:22:GLU:HG3	2:P:148:HOH:O	2.16	0.44
1:P:11:LYS:O	1:P:15:VAL:HG23	2.18	0.44
1:K:11:LYS:HB3	1:K:12:PRO:CD	2.48	0.44
1:O:6:THR:OG1	1:O:119:SER:HB2	2.17	0.44
1:A:18:ASN:HD21	1:B:141:ARG:HH12	1.64	0.44
1:G:22:GLU:O	1:G:26:ARG:HG2	2.18	0.44
1:H:12:PRO:HD3	1:H:72:VAL:HG12	2.00	0.44
1:I:123:GLU:CD	1:I:123:GLU:N	2.74	0.44
1:J:9:ILE:HB	1:J:117:HIS:HB3	2.00	0.44
1:P:66:PHE:C	1:P:68:THR:H	2.26	0.44
1:A:4:GLU:HG3	1:A:83:ILE:HG13	2.00	0.43
1:N:7:LEU:HG	1:N:8:SER:N	2.33	0.43
1:E:59:PHE:CD1	1:E:59:PHE:C	2.96	0.43
1:E:134:ALA:O	1:E:135:GLU:C	2.60	0.43
1:F:131:TYR:O	1:H:134:ALA:HB1	2.18	0.43
1:G:9:ILE:O	1:G:116:VAL:HA	2.18	0.43
1:M:54:HIS:HA	1:M:57:ARG:HD3	1.99	0.43
1:P:140:SER:HB3	2:P:145:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:87:ARG:HA	1:H:90:MET:CE	2.47	0.43
1:N:10:ILE:HG23	1:N:14:ALA:HB3	2.00	0.43
1:C:44:GLN:HB3	1:C:45:GLU:OE1	2.19	0.43
1:H:90:MET:HE1	1:H:118:GLY:HA3	1.98	0.43
1:I:9:ILE:O	1:I:116:VAL:HA	2.19	0.43
1:I:94:ASN:HD21	1:I:96:LYS:HB2	1.83	0.43
1:L:20:ILE:O	1:L:21:GLY:C	2.61	0.43
1:P:7:LEU:HD22	1:P:128:GLU:HB3	1.99	0.43
1:A:108:ALA:HB1	1:A:114:ASN:HA	2.00	0.43
1:C:55:LYS:HA	1:C:60:PHE:CD1	2.53	0.43
1:C:108:ALA:HB1	1:C:114:ASN:HA	2.00	0.43
1:G:27:PHE:HE1	1:G:86:ASN:ND2	2.17	0.43
1:K:50:PHE:CE1	1:K:128:GLU:HG2	2.53	0.43
1:M:12:PRO:HD3	1:M:72:VAL:HG12	2.00	0.43
1:M:15:VAL:CG2	1:M:71:PRO:O	2.66	0.43
1:M:83:ILE:HD13	1:M:122:PRO:HA	2.00	0.43
1:M:108:ALA:HB1	1:M:114:ASN:HA	1.99	0.43
1:O:124:SER:O	1:O:128:GLU:HG3	2.18	0.43
1:D:51:TYR:CA	2:D:150:HOH:O	2.66	0.43
1:K:6:THR:HB	1:K:83:ILE:HG12	2.01	0.43
1:K:103:ILE:O	1:K:104:ARG:C	2.61	0.43
1:M:38:LYS:HG3	1:M:40:LEU:HD12	1.99	0.43
1:A:51:TYR:CE2	1:A:67:MET:HG3	2.54	0.43
1:C:27:PHE:HE1	1:C:86:ASN:ND2	2.17	0.43
1:E:45:GLU:CD	1:E:45:GLU:H	2.27	0.43
1:E:104:ARG:O	1:E:108:ALA:HB3	2.18	0.43
1:G:8:SER:HB3	1:G:75:GLN:HG3	1.99	0.43
1:L:111:ILE:O	1:L:114:ASN:ND2	2.52	0.43
1:G:83:ILE:CD1	1:G:122:PRO:HA	2.49	0.43
1:I:25:SER:HB3	1:I:29:LYS:HE2	2.01	0.43
1:P:33:LYS:HB3	1:P:141:ARG:HH12	1.82	0.43
1:B:98:ALA:HB1	1:B:102:THR:OG1	2.19	0.43
1:J:104:ARG:HG2	1:J:114:ASN:HB2	2.01	0.43
1:L:74:VAL:HG11	1:L:132:PHE:CG	2.54	0.43
1:C:110:SER:HB2	2:C:148:HOH:O	2.19	0.42
1:F:86:ASN:O	1:F:90:MET:HG3	2.18	0.42
1:P:86:ASN:O	1:P:90:MET:HG3	2.18	0.42
1:F:12:PRO:CD	1:F:72:VAL:HG12	2.37	0.42
1:I:26:ARG:HH22	1:I:106:ASP:HB2	1.84	0.42
1:O:71:PRO:HG3	1:P:139:CYS:HB2	2.01	0.42
1:A:94:ASN:O	1:A:97:GLU:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:44:GLN:HE21	1:E:64:VAL:HG11	1.84	0.42
1:H:124:SER:O	1:H:128:GLU:HG3	2.19	0.42
1:G:45:GLU:CD	1:G:45:GLU:H	2.27	0.42
1:N:35:VAL:HG23	1:N:76:VAL:HB	2.01	0.42
1:D:11:LYS:HE3	1:D:116:VAL:C	2.45	0.42
1:G:26:ARG:HD2	1:G:26:ARG:HA	1.87	0.42
1:I:7:LEU:HG	1:I:8:SER:N	2.33	0.42
1:I:68:THR:O	1:I:68:THR:HG22	2.19	0.42
1:J:87:ARG:HA	1:J:90:MET:CE	2.49	0.42
1:J:90:MET:CE	1:J:118:GLY:HA3	2.50	0.42
1:M:33:LYS:NZ	1:N:18:ASN:HD21	2.18	0.42
1:A:87:ARG:NH1	2:A:150:HOH:O	2.52	0.42
1:B:134:ALA:O	1:B:135:GLU:C	2.61	0.42
1:C:95:PRO:HG2	1:C:110:SER:O	2.19	0.42
1:F:109:GLN:CB	2:F:147:HOH:O	2.65	0.42
1:D:51:TYR:HA	2:D:150:HOH:O	2.19	0.42
1:I:11:LYS:HB3	1:I:12:PRO:HD2	2.02	0.42
1:I:135:GLU:HB2	1:K:131:TYR:HA	2.01	0.42
1:L:87:ARG:HD2	2:L:204:HOH:O	2.17	0.42
1:K:33:LYS:HD2	1:K:141:ARG:O	2.20	0.42
1:L:66:PHE:C	1:L:68:THR:H	2.27	0.42
1:N:41:GLN:HE21	1:N:42:LEU:N	2.18	0.42
1:O:52:ALA:C	1:O:54:HIS:N	2.77	0.42
1:C:51:TYR:HE2	1:C:67:MET:HG3	1.85	0.42
1:O:9:ILE:HB	1:O:117:HIS:HB3	2.02	0.42
1:P:122:PRO:O	1:P:123:GLU:C	2.62	0.42
1:C:51:TYR:CE2	1:C:67:MET:HG3	2.55	0.42
1:D:109:GLN:HG3	1:D:110:SER:N	2.34	0.42
1:D:141:ARG:HG2	1:D:141:ARG:HH21	1.85	0.42
1:G:8:SER:HB2	1:G:77:LEU:CD1	2.50	0.42
1:J:5:ARG:NH1	1:J:135:GLU:OE1	2.52	0.42
1:A:11:LYS:CE	2:A:200:HOH:O	2.68	0.41
1:C:94:ASN:HA	1:C:95:PRO:HD3	1.93	0.41
1:F:111:ILE:HG23	1:F:112:ASP:H	1.85	0.41
1:F:127:ARG:NH1	2:F:146:HOH:O	2.52	0.41
1:L:124:SER:O	1:L:128:GLU:HG3	2.20	0.41
1:A:12:PRO:CD	1:A:72:VAL:HG12	2.49	0.41
1:E:44:GLN:O	1:E:48:GLU:HG3	2.20	0.41
1:H:86:ASN:O	1:H:90:MET:HG3	2.20	0.41
1:A:117:HIS:CD2	1:A:117:HIS:C	2.99	0.41
1:G:17:LYS:HE3	1:G:107:TYR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:42:LEU:HD23	1:O:42:LEU:HA	1.85	0.41
1:C:11:LYS:HD3	1:C:67:MET:SD	2.61	0.41
1:J:40:LEU:HD22	1:J:40:LEU:C	2.45	0.41
1:L:83:ILE:HD13	1:L:122:PRO:HA	2.01	0.41
1:B:63:LEU:O	1:B:64:VAL:C	2.63	0.41
1:N:15:VAL:HG21	1:N:72:VAL:HA	2.02	0.41
1:C:27:PHE:CE1	1:C:86:ASN:ND2	2.89	0.41
1:H:74:VAL:HG11	1:H:132:PHE:CG	2.56	0.41
1:M:141:ARG:NH1	1:N:16:ALA:HA	2.36	0.41
1:O:52:ALA:O	1:O:55:LYS:HG2	2.20	0.41
1:B:11:LYS:HB3	1:B:12:PRO:CD	2.50	0.41
1:C:7:LEU:HD22	1:C:128:GLU:HB3	2.03	0.41
1:C:66:PHE:C	1:C:68:THR:N	2.79	0.41
1:D:50:PHE:HE1	1:D:128:GLU:HB3	1.86	0.41
1:E:11:LYS:HB2	1:E:13:ASP:OD1	2.20	0.41
1:I:43:SER:OG	1:I:46:GLN:HG3	2.20	0.41
1:J:66:PHE:CZ	1:J:113:ALA:HA	2.56	0.41
1:B:81:ASN:ND2	2:B:152:HOH:O	2.53	0.41
1:D:52:ALA:C	1:D:54:HIS:N	2.79	0.41
1:J:104:ARG:HD3	1:J:114:ASN:ND2	2.35	0.41
1:K:81:ASN:HD21	1:K:84:ALA:HB3	1.86	0.41
1:B:7:LEU:HG	1:B:8:SER:N	2.36	0.41
1:B:98:ALA:HB3	1:B:105:ALA:HB2	2.03	0.41
1:J:60:PHE:N	2:J:144:HOH:O	2.53	0.41
1:K:11:LYS:HG2	1:K:67:MET:SD	2.60	0.41
1:K:53:GLU:HB2	2:K:149:HOH:O	2.21	0.41
1:K:120:ASP:OD2	1:K:120:ASP:C	2.63	0.41
1:M:124:SER:O	1:M:128:GLU:HG3	2.21	0.41
1:O:20:ILE:HD12	1:P:34:ILE:HD12	2.02	0.41
1:F:33:LYS:HE3	2:F:143:HOH:O	2.20	0.41
1:J:74:VAL:HG12	1:J:133:PHE:CE2	2.56	0.41
1:B:40:LEU:C	1:B:40:LEU:HD12	2.47	0.40
1:C:9:ILE:HB	1:C:117:HIS:HB3	2.02	0.40
1:C:94:ASN:OD1	1:C:94:ASN:C	2.65	0.40
1:D:74:VAL:CB	2:D:152:HOH:O	2.12	0.40
1:D:86:ASN:HD22	1:D:86:ASN:HA	1.72	0.40
1:C:18:ASN:HD22	1:D:141:ARG:HH11	1.68	0.40
1:D:43:SER:OG	1:D:45:GLU:HG2	2.21	0.40
1:I:94:ASN:HB3	1:I:97:GLU:CG	2.51	0.40
1:K:54:HIS:HD2	1:K:57:ARG:HH21	1.69	0.40
1:N:15:VAL:CG1	2:N:144:HOH:O	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:65:GLY:O	1:P:68:THR:HG22	2.21	0.40
1:D:6:THR:OG1	1:D:119:SER:HB2	2.22	0.40
1:D:12:PRO:HB3	1:D:70:GLY:HA3	2.04	0.40
1:D:44:GLN:O	1:D:48:GLU:HG3	2.21	0.40
1:J:108:ALA:HB1	1:J:114:ASN:HA	2.01	0.40
1:L:90:MET:O	1:L:104:ARG:HD2	2.21	0.40
1:J:30:ALA:HB2	1:J:89:LEU:HD21	2.04	0.40
1:M:24:GLU:CD	1:M:75:GLN:HE22	2.28	0.40
1:N:90:MET:HG2	1:N:116:VAL:HG21	2.03	0.40
1:P:38:LYS:HG3	1:P:38:LYS:O	2.21	0.40
1:P:95:PRO:HB3	1:P:108:ALA:CB	2.51	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	132/141 (94%)	120 (91%)	8 (6%)	4 (3%)	3	5
1	B	138/141 (98%)	130 (94%)	8 (6%)	0	100	100
1	C	138/141 (98%)	131 (95%)	7 (5%)	0	100	100
1	D	133/141 (94%)	118 (89%)	13 (10%)	2 (2%)	8	16
1	E	138/141 (98%)	128 (93%)	10 (7%)	0	100	100
1	F	138/141 (98%)	128 (93%)	10 (7%)	0	100	100
1	G	138/141 (98%)	128 (93%)	10 (7%)	0	100	100
1	H	138/141 (98%)	129 (94%)	9 (6%)	0	100	100
1	I	138/141 (98%)	124 (90%)	13 (9%)	1 (1%)	18	34
1	J	123/141 (87%)	113 (92%)	6 (5%)	4 (3%)	3	4
1	K	138/141 (98%)	130 (94%)	8 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	138/141 (98%)	120 (87%)	16 (12%)	2 (1%)	9	17
1	M	138/141 (98%)	124 (90%)	11 (8%)	3 (2%)	5	9
1	N	105/141 (74%)	92 (88%)	12 (11%)	1 (1%)	12	24
1	O	134/141 (95%)	123 (92%)	10 (8%)	1 (1%)	18	34
1	P	138/141 (98%)	130 (94%)	6 (4%)	2 (1%)	9	17
All	All	2145/2256 (95%)	1968 (92%)	157 (7%)	20 (1%)	14	27

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	92	ALA
1	I	55	LYS
1	L	53	GLU
1	M	115	ALA
1	P	135	GLU
1	A	96	LYS
1	D	89	LEU
1	J	53	GLU
1	J	67	MET
1	M	109	GLN
1	M	30	ALA
1	P	36	ALA
1	A	53	GLU
1	D	88	ASP
1	J	88	ASP
1	L	20	ILE
1	N	44	GLN
1	A	67	MET
1	A	119	SER
1	O	71	PRO

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	A	104/109 (95%)	98 (94%)	6 (6%)	18	38
1	B	108/109 (99%)	101 (94%)	7 (6%)	15	32
1	C	108/109 (99%)	101 (94%)	7 (6%)	15	32
1	D	105/109 (96%)	95 (90%)	10 (10%)	8	17
1	E	108/109 (99%)	101 (94%)	7 (6%)	15	32
1	F	108/109 (99%)	98 (91%)	10 (9%)	8	18
1	G	108/109 (99%)	101 (94%)	7 (6%)	15	32
1	H	108/109 (99%)	101 (94%)	7 (6%)	15	32
1	I	108/109 (99%)	102 (94%)	6 (6%)	19	39
1	J	100/109 (92%)	94 (94%)	6 (6%)	17	36
1	K	108/109 (99%)	104 (96%)	4 (4%)	30	57
1	L	108/109 (99%)	103 (95%)	5 (5%)	24	48
1	M	108/109 (99%)	102 (94%)	6 (6%)	19	39
1	N	85/109 (78%)	76 (89%)	9 (11%)	6	14
1	O	106/109 (97%)	100 (94%)	6 (6%)	18	39
1	P	108/109 (99%)	103 (95%)	5 (5%)	24	48
All	All	1688/1744 (97%)	1580 (94%)	108 (6%)	16	33

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	29	LYS
1	A	38	LYS
1	A	46	GLN
1	A	89	LEU
1	A	139	CYS
1	B	5	ARG
1	B	24	GLU
1	B	33	LYS
1	B	56	GLU
1	B	110	SER
1	B	139	CYS
1	B	140	SER
1	C	7	LEU
1	C	15	VAL
1	C	40	LEU

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Mol	Chain	Res	Type
1	C	46	GLN
1	C	68	THR
1	C	81	ASN
1	C	111	ILE
1	D	3	THR
1	D	24	GLU
1	D	29	LYS
1	D	40	LEU
1	D	45	GLU
1	D	111	ILE
1	D	112	ASP
1	D	114	ASN
1	D	139	CYS
1	D	141	ARG
1	E	15	VAL
1	E	40	LEU
1	E	45	GLU
1	E	57	ARG
1	E	109	GLN
1	E	111	ILE
1	E	139	CYS
1	F	3	THR
1	F	12	PRO
1	F	24	GLU
1	F	40	LEU
1	F	45	GLU
1	F	55	LYS
1	F	56	GLU
1	F	81	ASN
1	F	89	LEU
1	F	127	ARG
1	G	5	ARG
1	G	15	VAL
1	G	29	LYS
1	G	40	LEU
1	G	45	GLU
1	G	116	VAL
1	G	123	GLU
1	H	3	THR
1	H	33	LYS
1	H	40	LEU
1	H	46	GLN

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Mol	Chain	Res	Type
1	H	68	THR
1	H	109	GLN
1	H	123	GLU
1	I	29	LYS
1	I	33	LYS
1	I	55	LYS
1	I	74	VAL
1	I	81	ASN
1	I	123	GLU
1	J	5	ARG
1	J	24	GLU
1	J	40	LEU
1	J	45	GLU
1	J	68	THR
1	J	139	CYS
1	K	96	LYS
1	K	111	ILE
1	K	123	GLU
1	K	140	SER
1	L	12	PRO
1	L	40	LEU
1	L	45	GLU
1	L	56	GLU
1	L	119	SER
1	M	5	ARG
1	M	8	SER
1	M	40	LEU
1	M	54	HIS
1	M	81	ASN
1	M	109	GLN
1	N	3	THR
1	N	6	THR
1	N	7	LEU
1	N	11	LYS
1	N	22	GLU
1	N	24	GLU
1	N	40	LEU
1	N	89	LEU
1	N	127	ARG
1	O	11	LYS
1	O	15	VAL
1	O	63	LEU

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Mol	Chain	Res	Type
1	O	123	GLU
1	O	127	ARG
1	O	139	CYS
1	P	3	THR
1	P	5	ARG
1	P	24	GLU
1	P	68	THR
1	P	139	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	46	GLN
1	A	86	ASN
1	A	117	HIS
1	B	54	HIS
1	B	81	ASN
1	B	86	ASN
1	C	18	ASN
1	C	75	GLN
1	C	86	ASN
1	D	46	GLN
1	D	86	ASN
1	D	94	ASN
1	D	109	GLN
1	D	114	ASN
1	E	44	GLN
1	E	75	GLN
1	G	18	ASN
1	G	54	HIS
1	G	75	GLN
1	G	86	ASN
1	G	114	ASN
1	H	54	HIS
1	H	81	ASN
1	H	86	ASN
1	H	109	GLN
1	I	18	ASN
1	I	54	HIS
1	I	81	ASN
1	I	86	ASN

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Mol	Chain	Res	Type
1	I	94	ASN
1	I	109	GLN
1	J	54	HIS
1	K	18	ASN
1	K	54	HIS
1	K	81	ASN
1	K	86	ASN
1	K	109	GLN
1	L	54	HIS
1	L	114	ASN
1	M	44	GLN
1	M	54	HIS
1	M	86	ASN
1	M	109	GLN
1	N	18	ASN
1	N	75	GLN
1	N	86	ASN
1	O	18	ASN
1	O	75	GLN
1	O	86	ASN
1	O	109	GLN
1	P	18	ASN
1	P	81	ASN
1	P	86	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	136/141 (96%)	-0.21	1 (0%) 84 81	12, 32, 55, 65	0
1	B	140/141 (99%)	-0.53	0 100 100	9, 21, 36, 56	0
1	C	140/141 (99%)	-0.50	0 100 100	13, 25, 44, 51	0
1	D	137/141 (97%)	-0.15	1 (0%) 84 81	15, 33, 56, 60	0
1	E	140/141 (99%)	-0.26	0 100 100	14, 30, 50, 61	0
1	F	140/141 (99%)	-0.52	0 100 100	9, 22, 43, 54	0
1	G	140/141 (99%)	-0.28	0 100 100	12, 30, 52, 55	0
1	H	140/141 (99%)	-0.33	0 100 100	14, 27, 50, 66	0
1	I	140/141 (99%)	-0.16	1 (0%) 84 81	10, 34, 60, 64	0
1	J	129/141 (91%)	0.18	2 (1%) 70 67	19, 41, 57, 64	0
1	K	140/141 (99%)	-0.22	0 100 100	7, 32, 53, 63	0
1	L	140/141 (99%)	-0.35	1 (0%) 84 81	14, 27, 53, 66	0
1	M	140/141 (99%)	-0.11	0 100 100	13, 33, 61, 74	0
1	N	113/141 (80%)	0.76	10 (8%) 15 14	24, 48, 67, 73	0
1	O	138/141 (97%)	0.17	3 (2%) 62 58	22, 39, 57, 75	0
1	P	140/141 (99%)	-0.35	0 100 100	15, 27, 43, 59	0
All	All	2193/2256 (97%)	-0.19	19 (0%) 81 78	7, 31, 56, 75	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	116	VAL	3.4
1	O	61	GLY	3.3
1	N	93	THR	3.3
1	N	107	TYR	3.0
1	A	59	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	N	2	ALA	2.9
1	N	50	PHE	2.6
1	N	108	ALA	2.6
1	J	2	ALA	2.5
1	N	70	GLY	2.4
1	J	109	GLN	2.4
1	D	2	ALA	2.4
1	N	105	ALA	2.3
1	O	56	GLU	2.3
1	I	112	ASP	2.2
1	N	17	LYS	2.2
1	O	58	PRO	2.1
1	L	140	SER	2.1
1	N	44	GLN	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.