



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:07 PM UTC

PDB ID : 3M4D / pdb_00003m4d
Title : Crystal structure of the M113N mutant of alpha-hemolysin
Authors : Montoya, M.; Gouaux, E.
Deposited on : 2010-03-10
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
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

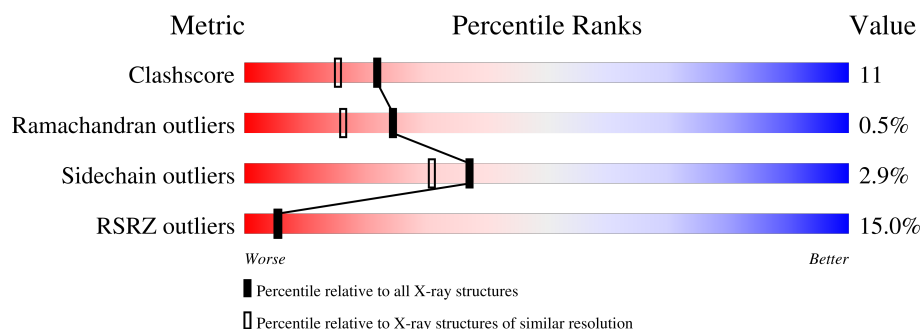
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	293	17% 79% 19% .
1	B	293	17% 77% 21% .
1	C	293	16% 79% 18% .
1	D	293	14% 75% 23% .
1	E	293	13% 80% 17% .
1	F	293	15% 81% 16% .
1	G	293	13% 77% 20% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16762 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 Alpha-hemolysin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	41	0	0
			2338	1465	402	465	6			
1	B	293	Total	C	N	O	S	45	0	0
			2345	1471	402	466	6			
1	C	293	Total	C	N	O	S	59	0	0
			2345	1471	402	466	6			
1	D	293	Total	C	N	O	S	66	0	0
			2345	1471	402	466	6			
1	E	293	Total	C	N	O	S	49	0	0
			2341	1467	402	466	6			
1	F	293	Total	C	N	O	S	62	0	0
			2345	1471	402	466	6			
1	G	293	Total	C	N	O	S	52	0	0
			2345	1471	402	466	6			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	113	ASN	MET	engineered mutation	UNP P09616
B	113	ASN	MET	engineered mutation	UNP P09616
C	113	ASN	MET	engineered mutation	UNP P09616
D	113	ASN	MET	engineered mutation	UNP P09616
E	113	ASN	MET	engineered mutation	UNP P09616
F	113	ASN	MET	engineered mutation	UNP P09616
G	113	ASN	MET	engineered mutation	UNP P09616

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	45	Total	O	0	0
			45	45		
2	B	52	Total	O	0	0
			52	52		

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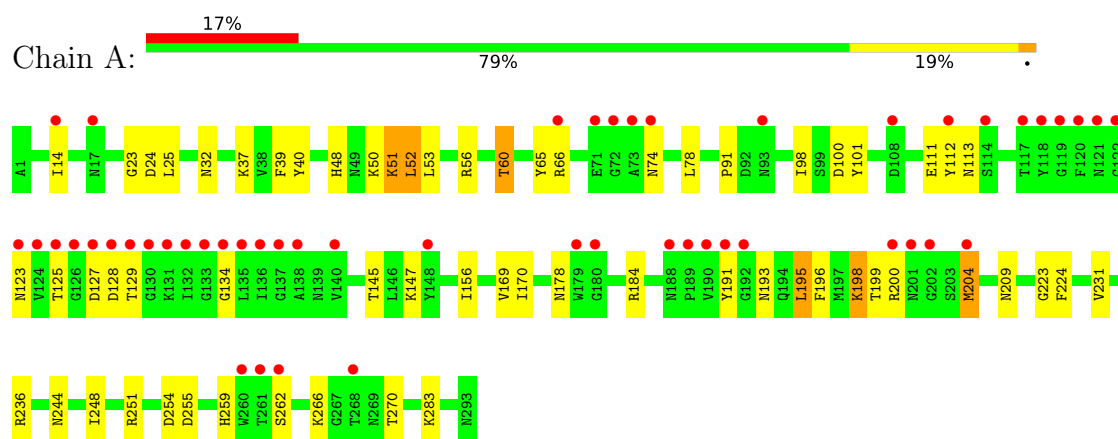
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	52	Total 52	O 52	0	0
2	D	48	Total 48	O 48	0	0
2	E	46	Total 46	O 46	0	0
2	F	54	Total 54	O 54	0	0
2	G	61	Total 61	O 61	0	0

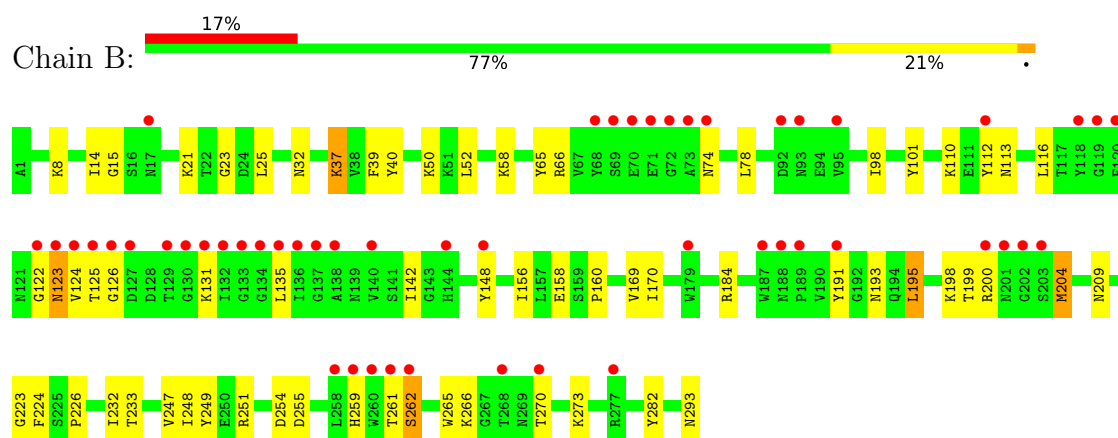
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

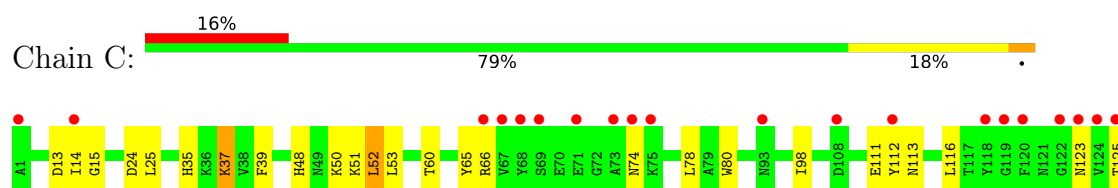
• Molecule 1: Alpha-hemolysin

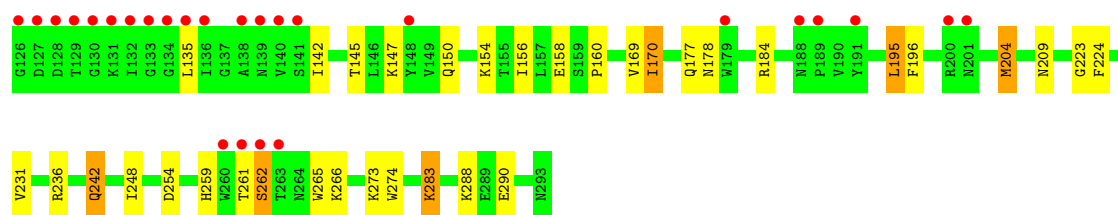


• Molecule 1: Alpha-hemolysin

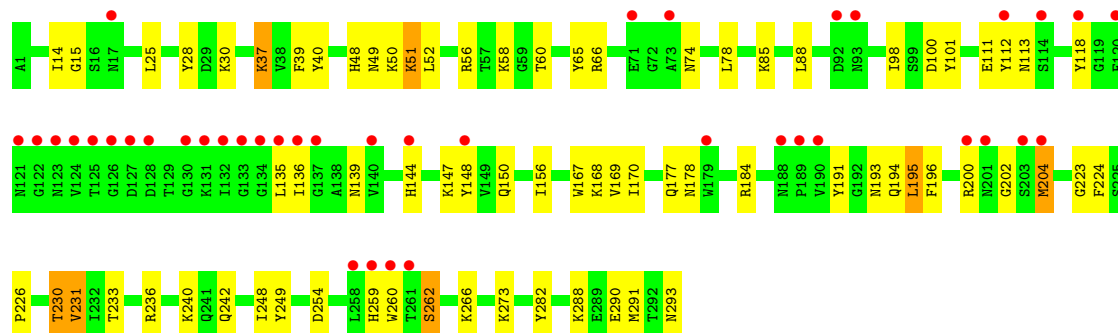
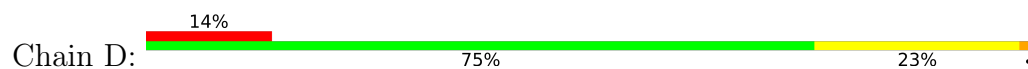


• Molecule 1: Alpha-hemolysin

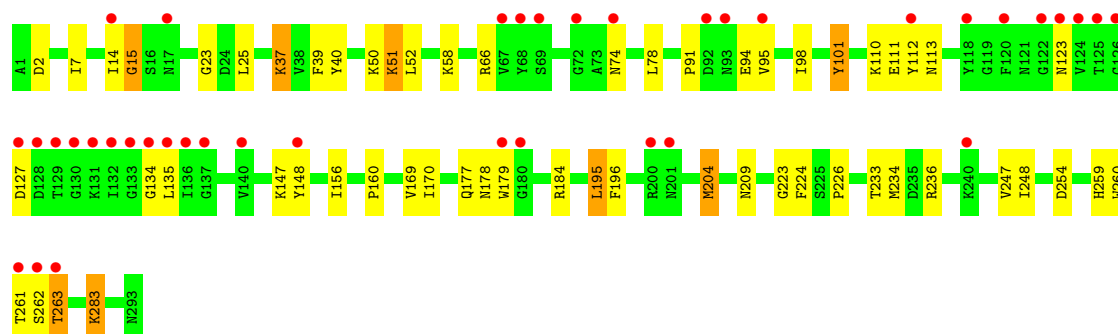
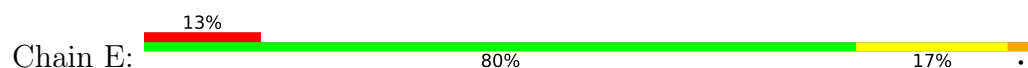




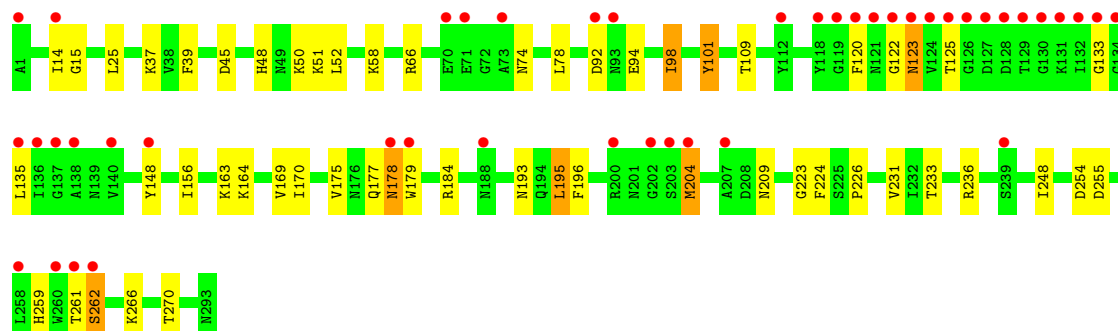
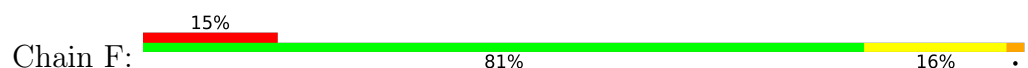
● Molecule 1: Alpha-hemolysin



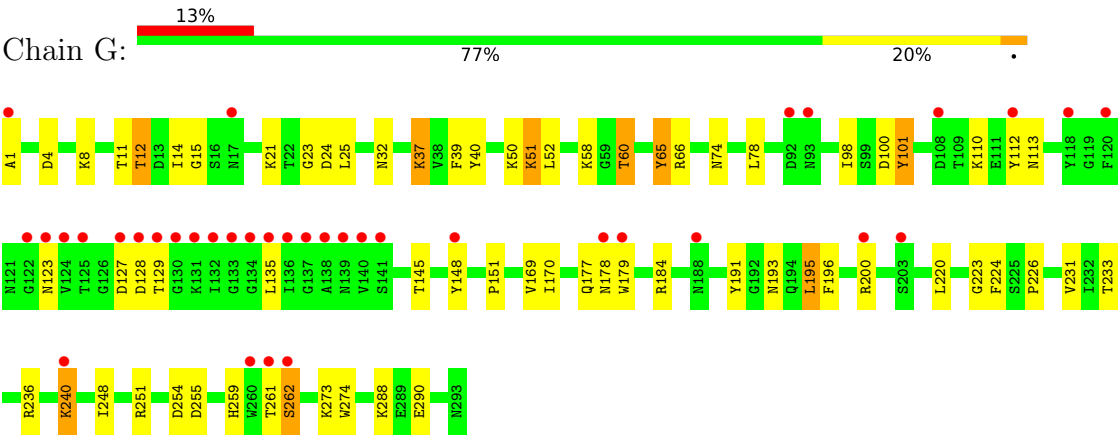
● Molecule 1: Alpha-hemolysin



● Molecule 1: Alpha-hemolysin



● Molecule 1: Alpha-hemolysin



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	151.15Å 134.59Å 132.90Å 90.00° 90.78° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 20.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.90) 99.0 (20.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 1.87Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.240 , 0.265 0.236 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.007 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16762	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.41% 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

5.1 Standard geometry

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	0.34	0/2389	0.84	5/3233 (0.2%)
1	B	0.34	0/2397	0.85	6/3244 (0.2%)
1	C	0.35	0/2397	0.85	4/3244 (0.1%)
1	D	0.35	0/2397	0.84	6/3244 (0.2%)
1	E	0.34	0/2393	0.84	6/3238 (0.2%)
1	F	0.35	0/2397	0.83	5/3244 (0.2%)
1	G	0.34	0/2397	0.84	4/3244 (0.1%)
All	All	0.34	0/16767	0.84	36/22691 (0.2%)

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	223	GLY	N-CA-C	9.68	121.86	112.08
1	D	223	GLY	N-CA-C	9.27	121.49	112.04
1	F	223	GLY	N-CA-C	8.94	121.16	112.04
1	A	223	GLY	N-CA-C	8.74	120.95	112.04
1	E	223	GLY	N-CA-C	7.88	121.78	111.70
1	C	223	GLY	N-CA-C	7.85	121.27	111.85
1	B	223	GLY	N-CA-C	7.43	120.77	111.85
1	B	98	ILE	N-CA-C	-6.61	101.04	109.30
1	B	170	ILE	N-CA-C	6.33	117.72	108.53
1	E	156	ILE	N-CA-C	6.24	116.84	108.11
1	F	170	ILE	N-CA-C	6.16	117.46	108.53
1	D	98	ILE	N-CA-C	-6.13	100.80	108.89
1	C	156	ILE	N-CA-C	5.96	117.07	108.48
1	G	51	LYS	N-CA-C	-5.78	101.92	110.48
1	A	170	ILE	N-CA-C	5.75	117.27	108.71
1	C	98	ILE	N-CA-C	-5.67	101.40	108.89
1	A	156	ILE	N-CA-C	5.54	115.86	108.11
1	F	156	ILE	N-CA-C	5.50	115.81	108.11
1	A	98	ILE	N-CA-C	-5.50	101.64	108.89
1	B	249	TYR	N-CA-C	-5.48	100.25	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	98	ILE	N-CA-C	-5.42	101.74	108.89
1	D	156	ILE	N-CA-C	5.37	116.21	108.48
1	C	170	ILE	N-CA-C	5.34	116.27	108.53
1	D	51	LYS	N-CA-C	-5.25	102.71	110.48
1	G	65	TYR	N-CA-C	-5.25	102.14	109.96
1	B	15	GLY	N-CA-C	5.24	120.71	114.48
1	E	15	GLY	N-CA-C	5.24	120.97	114.37
1	A	51	LYS	N-CA-C	-5.13	103.26	110.50
1	D	170	ILE	N-CA-C	5.12	116.67	108.89
1	F	92	ASP	N-CA-C	5.10	117.57	111.71
1	B	156	ILE	N-CA-C	5.09	115.82	108.48
1	G	98	ILE	N-CA-C	-5.08	102.18	108.89
1	E	51	LYS	N-CA-C	-5.05	103.01	110.48
1	E	98	ILE	N-CA-C	-5.04	102.23	108.89
1	D	249	TYR	N-CA-C	-5.02	100.99	109.07
1	E	170	ILE	N-CA-C	5.01	116.50	108.89

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	2338	0	2260	50	0
1	B	2345	0	2267	58	0
1	C	2345	0	2267	65	0
1	D	2345	0	2267	66	0
1	E	2341	0	2257	40	0
1	F	2345	0	2267	45	0
1	G	2345	0	2267	69	0
2	A	45	0	0	4	0
2	B	52	0	0	2	0
2	C	52	0	0	1	0
2	D	48	0	0	2	0
2	E	46	0	0	1	0
2	F	54	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	61	0	0	1	0
All	All	16762	0	15852	336	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 11.

All (336) 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:G:123:ASN:HB3	1:G:135:LEU:HB3	1.39	1.01
1:F:123:ASN:HB3	1:F:135:LEU:HB3	1.45	0.96
1:C:160:PRO:HD2	1:D:60:THR:HG21	1.51	0.93
1:B:123:ASN:HB3	1:B:135:LEU:HB3	1.52	0.90
1:A:56:ARG:NH2	1:G:12:THR:HG21	1.87	0.88
1:C:242:GLN:HB2	1:C:283:LYS:HE3	1.56	0.88
1:B:8:LYS:HD2	1:C:13:ASP:HB2	1.59	0.85
1:C:14:ILE:HD11	1:D:39:PHE:HE1	1.41	0.85
1:B:160:PRO:HD2	1:C:60:THR:HG21	1.58	0.84
1:G:24:ASP:C	1:G:25:LEU:HD12	2.02	0.84
1:B:160:PRO:CG	1:C:60:THR:HG21	2.07	0.84
1:A:56:ARG:HH22	1:G:12:THR:HG21	1.41	0.84
1:B:160:PRO:HG2	1:C:60:THR:HG21	1.60	0.83
1:A:14:ILE:HD11	1:B:39:PHE:HE1	1.41	0.83
1:B:199:THR:H	1:B:209:ASN:HD21	1.24	0.82
1:C:160:PRO:CD	1:D:60:THR:HG21	2.08	0.82
1:E:14:ILE:HD11	1:F:39:PHE:HE1	1.44	0.82
1:B:160:PRO:CD	1:C:60:THR:HG21	2.11	0.81
1:C:160:PRO:CG	1:D:60:THR:HG21	2.13	0.79
1:C:123:ASN:HB3	1:C:135:LEU:HB3	1.65	0.79
1:C:125:THR:HG22	1:D:135:LEU:HD13	1.63	0.79
1:A:39:PHE:HE1	1:G:14:ILE:HD11	1.46	0.78
1:D:14:ILE:HD11	1:E:39:PHE:HE1	1.48	0.77
1:E:52:LEU:CD2	1:E:233:THR:HG22	2.16	0.76
1:B:255:ASP:HB3	1:B:270:THR:OG1	1.84	0.76
1:F:125:THR:HG22	1:G:135:LEU:HD13	1.67	0.75
2:B:307:HOH:O	1:C:24:ASP:HB3	1.89	0.73
1:D:100:ASP:HB3	1:D:231:VAL:CG1	2.20	0.72
1:A:100:ASP:HB3	1:A:231:VAL:HG11	1.70	0.71
1:D:100:ASP:HB3	1:D:231:VAL:HG11	1.71	0.71
1:A:100:ASP:HB3	1:A:231:VAL:CG1	2.21	0.70
1:G:51:LYS:HE3	1:G:236:ARG:HG2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:GLN:CB	1:C:283:LYS:HE3	2.22	0.69
1:A:24:ASP:HB3	2:A:310:HOH:O	1.92	0.69
1:B:160:PRO:HG2	1:C:60:THR:CG2	2.23	0.69
1:D:52:LEU:CD2	1:D:233:THR:HG22	2.23	0.69
1:G:240:LYS:HB2	1:G:240:LYS:NZ	2.07	0.69
1:A:204:MET:HE1	1:A:209:ASN:OD1	1.94	0.68
1:B:199:THR:H	1:B:209:ASN:ND2	1.91	0.68
1:E:123:ASN:HB3	1:E:135:LEU:HB3	1.74	0.68
1:F:123:ASN:HD21	1:G:135:LEU:HD11	1.58	0.68
1:F:14:ILE:HD11	1:G:39:PHE:HE1	1.60	0.67
1:B:112:TYR:C	1:B:113:ASN:HD22	2.03	0.67
1:D:112:TYR:C	1:D:113:ASN:HD22	2.03	0.66
1:F:123:ASN:ND2	1:G:135:LEU:HD11	2.10	0.66
1:B:52:LEU:CD2	1:B:233:THR:HG22	2.26	0.66
1:C:160:PRO:HG2	1:D:60:THR:HG21	1.77	0.65
1:B:52:LEU:HD23	1:B:233:THR:HG22	1.77	0.65
1:B:204:MET:HE2	1:B:204:MET:H	1.61	0.65
1:G:25:LEU:HD11	1:G:40:TYR:HE1	1.62	0.65
1:D:52:LEU:HD23	1:D:233:THR:HG22	1.79	0.65
1:E:52:LEU:HD23	1:E:233:THR:HG22	1.78	0.64
1:D:148:TYR:OH	1:E:178:ASN:ND2	2.30	0.64
1:F:178:ASN:HD22	1:F:178:ASN:N	1.95	0.64
1:B:14:ILE:HD11	1:C:39:PHE:HE1	1.63	0.63
1:F:204:MET:HE1	1:F:209:ASN:OD1	1.97	0.63
1:B:199:THR:N	1:B:209:ASN:HD21	1.97	0.62
1:B:191:TYR:CE2	1:B:200:ARG:HB3	2.34	0.62
1:G:240:LYS:HB2	1:G:240:LYS:HZ2	1.63	0.62
1:C:204:MET:HE1	1:C:265:TRP:HE1	1.65	0.62
1:D:167:TRP:HH2	1:D:230:THR:HG22	1.63	0.62
1:F:184:ARG:HD2	1:F:254:ASP:OD2	2.00	0.61
1:B:184:ARG:HD2	1:B:254:ASP:OD2	2.01	0.61
1:B:122:GLY:O	1:B:123:ASN:HB2	2.00	0.61
1:F:123:ASN:OD1	1:G:135:LEU:HD11	2.00	0.61
1:F:14:ILE:HD11	1:F:48:HIS:CE1	2.36	0.60
1:C:50:LYS:NZ	2:C:311:HOH:O	2.34	0.60
1:B:125:THR:HG22	1:B:126:GLY:N	2.16	0.60
1:G:52:LEU:HD23	1:G:233:THR:HG22	1.83	0.60
1:C:170:ILE:O	1:C:170:ILE:HD12	2.01	0.59
1:A:178:ASN:N	1:A:178:ASN:HD22	2.01	0.59
1:A:50:LYS:NZ	2:A:313:HOH:O	2.35	0.59
1:A:184:ARG:HD2	1:A:254:ASP:OD2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:288:LYS:HE2	1:C:290:GLU:OE1	2.02	0.59
1:G:52:LEU:CD2	1:G:233:THR:HG22	2.33	0.59
1:F:148:TYR:OH	1:G:178:ASN:ND2	2.36	0.58
1:D:184:ARG:HD2	1:D:254:ASP:OD2	2.02	0.58
1:F:14:ILE:HG22	1:F:15:GLY:N	2.19	0.58
1:G:74:ASN:O	1:G:259:HIS:HA	2.04	0.58
1:D:135:LEU:HD12	1:D:136:ILE:H	1.68	0.58
1:A:178:ASN:ND2	1:G:148:TYR:OH	2.37	0.58
1:B:259:HIS:CE1	1:B:266:LYS:HB3	2.39	0.58
1:G:191:TYR:CE2	1:G:200:ARG:HB3	2.39	0.58
1:F:122:GLY:O	1:F:123:ASN:HB2	2.02	0.57
1:D:191:TYR:CE2	1:D:200:ARG:HB3	2.39	0.57
1:D:259:HIS:CE1	1:D:266:LYS:HB3	2.39	0.57
1:E:148:TYR:OH	1:F:178:ASN:ND2	2.37	0.57
1:G:100:ASP:HB3	1:G:231:VAL:CG1	2.35	0.57
1:A:244:ASN:OD1	1:A:283:LYS:HE2	2.04	0.57
1:D:88:LEU:HD13	1:D:230:THR:HG21	1.87	0.56
1:F:123:ASN:CG	1:G:135:LEU:HD11	2.30	0.56
1:B:148:TYR:OH	1:C:178:ASN:ND2	2.37	0.56
1:F:74:ASN:O	1:F:259:HIS:HA	2.06	0.56
1:E:177:GLN:O	1:E:179:TRP:HD1	1.88	0.56
1:G:24:ASP:O	1:G:25:LEU:HD12	2.06	0.56
1:C:184:ARG:HD2	1:C:254:ASP:OD2	2.05	0.56
1:C:112:TYR:C	1:C:113:ASN:HD22	2.14	0.56
1:F:259:HIS:CE1	1:F:266:LYS:HB3	2.40	0.56
1:B:255:ASP:HB3	1:B:270:THR:HG1	1.70	0.56
1:G:184:ARG:HD2	1:G:254:ASP:OD2	2.05	0.56
1:C:14:ILE:HD11	1:D:39:PHE:CE1	2.31	0.55
1:E:248:ILE:N	1:E:248:ILE:HD12	2.22	0.55
1:C:52:LEU:HD13	1:C:53:LEU:N	2.22	0.55
1:A:111:GLU:HB3	1:A:147:LYS:HB2	1.88	0.55
1:E:184:ARG:HD2	1:E:254:ASP:OD2	2.05	0.55
1:C:261:THR:O	1:C:262:SER:HB3	2.06	0.55
1:F:169:VAL:HG21	1:F:224:PHE:CZ	2.41	0.55
1:C:204:MET:HE3	1:C:209:ASN:HB2	1.88	0.55
1:F:261:THR:O	1:F:262:SER:CB	2.55	0.55
1:G:112:TYR:C	1:G:113:ASN:HD22	2.15	0.55
1:G:100:ASP:HB3	1:G:231:VAL:HG11	1.89	0.54
1:A:113:ASN:HB2	1:A:145:THR:HB	1.88	0.54
1:E:14:ILE:HD11	1:F:39:PHE:CE1	2.34	0.54
1:D:195:LEU:HD13	1:D:196:PHE:CE2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ASP:N	1:A:231:VAL:HG13	2.23	0.54
1:D:135:LEU:HD12	1:D:136:ILE:N	2.22	0.54
1:A:100:ASP:H	1:A:231:VAL:HG13	1.73	0.54
1:C:273:LYS:HD2	1:C:274:TRP:CE2	2.43	0.54
1:C:160:PRO:HG2	1:D:60:THR:CG2	2.37	0.54
1:E:112:TYR:C	1:E:113:ASN:HD22	2.16	0.54
1:B:74:ASN:O	1:B:259:HIS:HA	2.08	0.53
1:F:178:ASN:N	1:F:178:ASN:ND2	2.55	0.53
1:D:248:ILE:HD12	1:D:248:ILE:N	2.23	0.53
1:F:51:LYS:HG3	1:F:236:ARG:HG2	1.89	0.53
1:A:32:ASN:O	1:A:251:ARG:NH1	2.39	0.53
1:C:204:MET:HE1	1:C:265:TRP:NE1	2.24	0.53
1:A:65:TYR:CE1	1:A:78:LEU:HD21	2.44	0.53
1:G:273:LYS:HD3	1:G:274:TRP:CH2	2.44	0.53
1:C:51:LYS:HE3	1:C:236:ARG:HG2	1.91	0.53
1:G:110:LYS:HD3	1:G:110:LYS:N	2.24	0.53
1:B:8:LYS:HD2	1:C:13:ASP:CB	2.36	0.52
1:B:125:THR:HG22	1:B:126:GLY:H	1.74	0.52
1:B:123:ASN:CG	1:C:135:LEU:HD11	2.34	0.52
1:C:169:VAL:HG21	1:C:224:PHE:CZ	2.44	0.52
1:C:195:LEU:HD13	1:C:196:PHE:CE2	2.45	0.52
1:D:28:TYR:CE1	1:D:30:LYS:HG2	2.44	0.52
1:E:204:MET:HE1	1:E:209:ASN:OD1	2.09	0.52
1:C:51:LYS:HG3	1:C:236:ARG:HG3	1.90	0.52
1:G:261:THR:O	1:G:262:SER:HB2	2.09	0.52
1:B:169:VAL:HG21	1:B:224:PHE:CZ	2.44	0.52
1:B:248:ILE:HD12	1:B:248:ILE:N	2.25	0.52
1:F:248:ILE:N	1:F:248:ILE:HD12	2.24	0.52
1:B:261:THR:O	1:B:262:SER:HB3	2.10	0.52
1:D:100:ASP:N	1:D:231:VAL:HG13	2.25	0.52
1:F:14:ILE:HG23	1:F:45:ASP:OD1	2.10	0.52
1:C:125:THR:CG2	1:D:135:LEU:HD13	2.35	0.51
1:D:74:ASN:O	1:D:259:HIS:HA	2.10	0.51
1:D:193:ASN:OD1	1:D:195:LEU:HB2	2.10	0.51
1:B:65:TYR:CE2	1:B:78:LEU:HD21	2.45	0.51
1:A:125:THR:HG22	1:B:135:LEU:HD13	1.92	0.51
1:F:52:LEU:HD22	1:F:231:VAL:HG13	1.92	0.51
1:B:232:ILE:N	1:B:232:ILE:HD12	2.25	0.51
1:D:66:ARG:C	1:D:78:LEU:HD12	2.36	0.51
1:E:50:LYS:NZ	2:E:300:HOH:O	2.44	0.51
1:D:14:ILE:HD11	1:D:48:HIS:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ASN:OD1	1:B:135:LEU:HD11	2.11	0.51
1:C:14:ILE:HD11	1:C:48:HIS:CE1	2.46	0.51
1:A:100:ASP:CB	1:A:231:VAL:CG1	2.88	0.50
1:D:260:TRP:NE1	1:D:262:SER:HA	2.26	0.50
1:F:50:LYS:NZ	2:F:332:HOH:O	2.41	0.50
1:D:240:LYS:CE	1:D:242:GLN:HE21	2.24	0.50
1:A:51:LYS:HG3	1:A:236:ARG:HG2	1.93	0.50
1:A:127:ASP:C	1:A:129:THR:H	2.19	0.50
1:C:116:LEU:HB3	1:D:144:HIS:CE1	2.46	0.50
1:D:100:ASP:H	1:D:231:VAL:HG13	1.77	0.50
1:D:240:LYS:HD2	1:D:242:GLN:NE2	2.26	0.50
1:D:56:ARG:NH2	2:D:305:HOH:O	2.44	0.50
1:D:240:LYS:HE3	1:D:242:GLN:HB2	1.94	0.50
1:A:248:ILE:N	1:A:248:ILE:HD12	2.27	0.49
1:D:111:GLU:HB3	1:D:147:LYS:HB2	1.94	0.49
1:E:91:PRO:HD2	1:E:94:GLU:HG3	1.93	0.49
1:F:193:ASN:OD1	1:F:195:LEU:HB2	2.11	0.49
1:G:248:ILE:HD12	1:G:248:ILE:N	2.27	0.49
1:C:158:GLU:O	1:C:160:PRO:HD3	2.11	0.49
1:D:167:TRP:CH2	1:D:230:THR:HG22	2.44	0.49
1:E:177:GLN:O	1:E:178:ASN:HB2	2.11	0.49
1:D:51:LYS:HG3	1:D:236:ARG:HG2	1.93	0.49
1:A:169:VAL:HG21	1:A:224:PHE:CZ	2.48	0.49
1:C:74:ASN:O	1:C:259:HIS:HA	2.11	0.49
1:E:95:VAL:HG13	1:E:234:MET:SD	2.52	0.49
1:D:85:LYS:HE2	1:D:168:LYS:HB3	1.94	0.49
1:A:14:ILE:HD11	1:B:39:PHE:CE1	2.32	0.49
1:A:259:HIS:CE1	1:A:266:LYS:HB3	2.48	0.49
1:F:125:THR:CG2	1:G:135:LEU:HD13	2.41	0.48
1:G:50:LYS:HD3	1:G:233:THR:HB	1.95	0.48
1:D:202:GLY:HA3	1:D:204:MET:CE	2.43	0.48
1:D:282:TYR:CD1	1:D:293:ASN:HB3	2.48	0.48
1:D:169:VAL:HG21	1:D:224:PHE:CZ	2.48	0.48
1:B:37:LYS:HD2	1:B:37:LYS:C	2.38	0.48
1:E:261:THR:O	1:E:262:SER:HB2	2.13	0.48
1:D:65:TYR:CE2	1:D:78:LEU:HD21	2.49	0.48
1:E:261:THR:OG1	1:E:263:THR:HG23	2.14	0.48
1:E:52:LEU:HD21	1:E:233:THR:HG22	1.95	0.48
1:A:178:ASN:N	1:A:178:ASN:ND2	2.62	0.47
1:B:158:GLU:O	1:B:160:PRO:HD3	2.14	0.47
1:F:58:LYS:HA	1:F:226:PRO:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:195:LEU:HD13	1:F:196:PHE:CE2	2.49	0.47
1:G:288:LYS:HE2	1:G:290:GLU:CD	2.39	0.47
1:A:195:LEU:HD13	1:A:196:PHE:CE2	2.49	0.47
1:D:50:LYS:NZ	2:D:302:HOH:O	2.47	0.47
1:A:112:TYR:C	1:A:113:ASN:HD22	2.22	0.47
1:E:74:ASN:O	1:E:259:HIS:HA	2.14	0.47
1:C:35:HIS:HB3	1:C:60:THR:HG22	1.96	0.47
1:C:52:LEU:HD11	1:C:231:VAL:HG13	1.96	0.47
1:C:160:PRO:HD2	1:D:60:THR:CG2	2.36	0.47
1:C:259:HIS:CE1	1:C:266:LYS:HB3	2.50	0.47
1:D:37:LYS:C	1:D:37:LYS:HD2	2.39	0.47
1:E:260:TRP:CD1	1:E:262:SER:H	2.31	0.47
1:F:101:TYR:OH	1:G:60:THR:CG2	2.63	0.47
1:A:14:ILE:HD11	1:A:48:HIS:CE1	2.50	0.47
1:G:240:LYS:NZ	1:G:240:LYS:CB	2.78	0.47
1:A:66:ARG:C	1:A:78:LEU:HD12	2.40	0.47
1:A:100:ASP:CB	1:A:231:VAL:HG11	2.41	0.47
1:D:100:ASP:CB	1:D:231:VAL:CG1	2.92	0.47
1:C:177:GLN:O	1:C:178:ASN:HB2	2.15	0.47
1:G:261:THR:O	1:G:262:SER:CB	2.63	0.47
1:C:48:HIS:O	1:C:236:ARG:NH2	2.36	0.46
1:C:116:LEU:HD13	1:C:142:ILE:HG12	1.96	0.46
1:C:248:ILE:N	1:C:248:ILE:HD12	2.30	0.46
1:A:193:ASN:OD1	1:A:195:LEU:HB2	2.16	0.46
1:G:58:LYS:HA	1:G:226:PRO:O	2.16	0.46
1:A:39:PHE:CE1	1:G:14:ILE:HD11	2.38	0.46
1:B:124:VAL:O	1:C:135:LEU:HD12	2.16	0.46
1:G:127:ASP:C	1:G:129:THR:H	2.24	0.46
1:G:231:VAL:HG13	1:G:231:VAL:O	2.15	0.46
1:C:116:LEU:HD23	1:D:144:HIS:HE1	1.81	0.46
1:D:14:ILE:HD11	1:E:39:PHE:CE1	2.38	0.46
1:G:100:ASP:N	1:G:231:VAL:CG1	2.79	0.46
1:B:50:LYS:NZ	2:B:324:HOH:O	2.49	0.46
1:F:14:ILE:CG2	1:F:15:GLY:N	2.79	0.46
1:G:66:ARG:C	1:G:78:LEU:HD12	2.40	0.46
1:A:74:ASN:O	1:A:259:HIS:HA	2.16	0.46
1:F:101:TYR:OH	1:G:60:THR:HG23	2.16	0.46
1:G:32:ASN:O	1:G:251:ARG:NH1	2.42	0.46
1:A:60:THR:CG2	1:G:101:TYR:OH	2.64	0.46
1:B:282:TYR:CD1	1:B:293:ASN:HB3	2.51	0.46
1:G:1:ALA:HB3	1:G:4:ASP:OD1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:14:ILE:HG22	1:E:15:GLY:N	2.30	0.46
1:B:126:GLY:HA2	1:B:131:LYS:O	2.16	0.45
1:E:195:LEU:HD13	1:E:196:PHE:CE2	2.52	0.45
1:A:125:THR:CG2	1:B:135:LEU:HD13	2.46	0.45
1:B:14:ILE:HD11	1:C:39:PHE:CE1	2.47	0.45
1:E:101:TYR:CZ	1:E:160:PRO:HG3	2.51	0.45
1:F:66:ARG:C	1:F:78:LEU:HD12	2.40	0.45
1:E:66:ARG:C	1:E:78:LEU:HD12	2.42	0.45
1:C:204:MET:CE	1:C:265:TRP:NE1	2.80	0.45
1:A:191:TYR:CE2	1:A:200:ARG:HB3	2.51	0.45
1:B:247:VAL:C	1:B:248:ILE:HD12	2.41	0.45
1:B:66:ARG:C	1:B:78:LEU:HD12	2.42	0.45
1:E:127:ASP:HA	1:F:133:GLY:HA2	1.99	0.45
1:G:273:LYS:HD3	1:G:274:TRP:CZ2	2.51	0.45
1:C:65:TYR:CE2	1:C:78:LEU:HD21	2.52	0.45
1:E:110:LYS:HD3	1:F:175:VAL:HG23	1.99	0.44
1:G:12:THR:O	1:G:12:THR:CG2	2.65	0.44
1:D:118:TYR:HA	1:D:139:ASN:O	2.18	0.44
1:G:37:LYS:HD2	1:G:37:LYS:C	2.42	0.44
1:E:195:LEU:HD22	1:E:196:PHE:CE1	2.53	0.44
1:F:52:LEU:CD2	1:F:233:THR:HG22	2.47	0.44
1:F:109:THR:HG22	1:G:151:PRO:HA	2.00	0.44
1:A:23:GLY:HA3	1:A:40:TYR:CE1	2.53	0.44
1:C:14:ILE:HG22	1:C:15:GLY:N	2.33	0.44
1:D:40:TYR:CE1	1:D:291:MET:HB3	2.53	0.44
1:D:58:LYS:HA	1:D:226:PRO:O	2.18	0.44
1:B:32:ASN:O	1:B:251:ARG:NH1	2.40	0.44
1:G:100:ASP:CB	1:G:231:VAL:CG1	2.95	0.44
1:C:65:TYR:C	1:C:66:ARG:HG3	2.43	0.43
1:F:94:GLU:O	1:F:163:LYS:NZ	2.46	0.43
1:C:204:MET:CE	1:C:265:TRP:HE1	2.28	0.43
1:E:51:LYS:HG3	1:E:236:ARG:HG2	2.00	0.43
1:F:98:ILE:HD12	1:F:164:LYS:N	2.34	0.43
1:A:198:LYS:HD2	1:A:199:THR:HG23	1.99	0.43
1:A:23:GLY:HA3	1:A:40:TYR:CZ	2.52	0.43
1:B:204:MET:HE1	1:B:265:TRP:HE1	1.83	0.43
1:F:204:MET:HE1	1:F:209:ASN:HA	2.01	0.43
1:G:251:ARG:NH1	2:G:299:HOH:O	2.52	0.43
1:G:177:GLN:O	1:G:178:ASN:HB2	2.17	0.43
1:A:56:ARG:NH2	2:A:303:HOH:O	2.51	0.43
1:D:60:THR:HG23	1:D:60:THR:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:111:GLU:HB3	1:E:147:LYS:HB2	2.01	0.43
1:G:51:LYS:HG3	1:G:236:ARG:CG	2.49	0.43
1:A:24:ASP:CB	2:A:310:HOH:O	2.61	0.42
1:B:110:LYS:HD3	1:C:150:GLN:O	2.18	0.42
1:E:2:ASP:HB3	1:E:7:ILE:HB	2.01	0.42
1:B:125:THR:CG2	1:B:126:GLY:N	2.82	0.42
1:G:14:ILE:HG22	1:G:15:GLY:N	2.34	0.42
1:G:193:ASN:OD1	1:G:195:LEU:HB2	2.18	0.42
1:G:195:LEU:HD22	1:G:196:PHE:CE1	2.54	0.42
1:B:116:LEU:HD13	1:B:142:ILE:HG12	2.01	0.42
1:C:52:LEU:HD21	1:C:231:VAL:CG1	2.49	0.42
1:C:111:GLU:HB3	1:C:147:LYS:HB2	2.00	0.42
1:E:283:LYS:HA	1:E:283:LYS:HE3	2.01	0.42
1:G:170:ILE:HD12	1:G:170:ILE:O	2.19	0.42
1:D:49:ASN:O	1:D:50:LYS:HG3	2.19	0.42
1:D:177:GLN:O	1:D:178:ASN:HB2	2.19	0.42
1:E:169:VAL:HG21	1:E:224:PHE:CZ	2.54	0.42
1:F:177:GLN:O	1:F:179:TRP:HD1	2.02	0.42
1:G:25:LEU:HD12	1:G:25:LEU:N	2.33	0.42
1:G:65:TYR:CE2	1:G:78:LEU:HD21	2.54	0.42
1:C:154:LYS:HB2	1:C:170:ILE:HD11	2.01	0.42
1:A:60:THR:HG23	1:G:101:TYR:OH	2.20	0.42
1:G:51:LYS:HG3	1:G:236:ARG:HG2	2.01	0.42
1:B:193:ASN:OD1	1:B:195:LEU:HB2	2.19	0.42
1:D:202:GLY:C	1:D:204:MET:HE3	2.45	0.42
1:G:113:ASN:HB2	1:G:145:THR:HB	2.02	0.42
1:G:65:TYR:HB2	1:G:220:LEU:O	2.19	0.41
1:A:123:ASN:O	1:A:134:GLY:HA2	2.21	0.41
1:B:23:GLY:HA3	1:B:40:TYR:CZ	2.55	0.41
1:C:37:LYS:HD2	1:C:37:LYS:C	2.45	0.41
1:D:14:ILE:HG22	1:D:15:GLY:N	2.34	0.41
1:D:112:TYR:C	1:D:113:ASN:ND2	2.76	0.41
1:E:58:LYS:HA	1:E:226:PRO:O	2.20	0.41
1:A:255:ASP:HB3	1:A:270:THR:HB	2.01	0.41
1:G:169:VAL:HG21	1:G:224:PHE:CZ	2.56	0.41
1:E:23:GLY:HA3	1:E:40:TYR:CE1	2.55	0.41
1:C:80:TRP:CE2	1:C:254:ASP:HB2	2.56	0.41
1:C:113:ASN:HB2	1:C:145:THR:HB	2.02	0.41
1:F:255:ASP:HB3	1:F:270:THR:HB	2.01	0.41
1:B:58:LYS:HA	1:B:226:PRO:O	2.20	0.41
1:B:66:ARG:HG3	1:B:66:ARG:HH11	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:LEU:HD13	1:A:53:LEU:N	2.35	0.41
1:B:204:MET:HE3	1:B:209:ASN:HB2	2.02	0.41
1:D:28:TYR:HE1	1:D:30:LYS:HG2	1.86	0.41
1:D:202:GLY:HA3	1:D:204:MET:HE2	2.01	0.41
1:G:8:LYS:HB2	1:G:11:THR:OG1	2.21	0.41
1:E:37:LYS:HD2	1:E:37:LYS:C	2.46	0.41
1:G:255:ASP:HB2	1:G:273:LYS:HD2	2.03	0.41
1:G:100:ASP:CB	1:G:231:VAL:HG11	2.50	0.40
1:A:123:ASN:HD21	1:B:135:LEU:CD1	2.34	0.40
1:D:194:GLN:O	1:D:195:LEU:C	2.64	0.40
1:B:198:LYS:HB3	1:B:209:ASN:ND2	2.37	0.40
1:D:148:TYR:HE2	1:D:150:GLN:OE1	2.03	0.40
1:D:288:LYS:HB2	1:D:290:GLU:HG2	2.03	0.40
1:E:247:VAL:C	1:E:248:ILE:HD12	2.45	0.40
1:E:123:ASN:O	1:E:134:GLY:HA2	2.22	0.40
1:F:45:ASP:O	1:F:236:ARG:NH1	2.55	0.40
1:G:23:GLY:HA3	1:G:40:TYR:CZ	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	291/293 (99%)	280 (96%)	9 (3%)	2 (1%)	18	10
1	B	291/293 (99%)	276 (95%)	13 (4%)	2 (1%)	18	10
1	C	291/293 (99%)	281 (97%)	9 (3%)	1 (0%)	36	29
1	D	291/293 (99%)	279 (96%)	11 (4%)	1 (0%)	36	29
1	E	291/293 (99%)	280 (96%)	11 (4%)	0	100	100
1	F	291/293 (99%)	278 (96%)	11 (4%)	2 (1%)	18	10
1	G	291/293 (99%)	277 (95%)	12 (4%)	2 (1%)	18	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2037/2051 (99%)	1951 (96%)	76 (4%)	10 (0%)	24	16

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	262	SER
1	B	262	SER
1	C	262	SER
1	B	123	ASN
1	F	262	SER
1	G	262	SER
1	A	128	ASP
1	D	262	SER
1	F	123	ASN
1	G	128	ASP

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	258/259 (100%)	249 (96%)	9 (4%)	32	24
1	B	259/259 (100%)	252 (97%)	7 (3%)	39	34
1	C	259/259 (100%)	252 (97%)	7 (3%)	39	34
1	D	259/259 (100%)	251 (97%)	8 (3%)	35	29
1	E	258/259 (100%)	251 (97%)	7 (3%)	39	34
1	F	259/259 (100%)	252 (97%)	7 (3%)	39	34
1	G	259/259 (100%)	251 (97%)	8 (3%)	35	29
All	All	1811/1813 (100%)	1758 (97%)	53 (3%)	37	31

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU

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Mol	Chain	Res	Type
1	A	37	LYS
1	A	52	LEU
1	A	60	THR
1	A	91	PRO
1	A	101	TYR
1	A	195	LEU
1	A	198	LYS
1	A	204	MET
1	B	21	LYS
1	B	25	LEU
1	B	37	LYS
1	B	101	TYR
1	B	195	LEU
1	B	204	MET
1	B	273	LYS
1	C	25	LEU
1	C	37	LYS
1	C	52	LEU
1	C	195	LEU
1	C	204	MET
1	C	242	GLN
1	C	283	LYS
1	D	25	LEU
1	D	37	LYS
1	D	101	TYR
1	D	195	LEU
1	D	204	MET
1	D	230	THR
1	D	231	VAL
1	D	273	LYS
1	E	25	LEU
1	E	37	LYS
1	E	101	TYR
1	E	195	LEU
1	E	204	MET
1	E	263	THR
1	E	283	LYS
1	F	25	LEU
1	F	37	LYS
1	F	101	TYR
1	F	120	PHE
1	F	178	ASN

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Mol	Chain	Res	Type
1	F	195	LEU
1	F	204	MET
1	G	12	THR
1	G	21	LYS
1	G	37	LYS
1	G	60	THR
1	G	101	TYR
1	G	179	TRP
1	G	195	LEU
1	G	240	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	64	GLN
1	A	74	ASN
1	A	113	ASN
1	A	177	GLN
1	A	178	ASN
1	A	242	GLN
1	A	257	GLN
1	A	259	HIS
1	B	17	ASN
1	B	64	GLN
1	B	74	ASN
1	B	89	GLN
1	B	113	ASN
1	B	178	ASN
1	B	209	ASN
1	B	242	GLN
1	B	259	HIS
1	C	74	ASN
1	C	89	GLN
1	C	113	ASN
1	C	178	ASN
1	C	259	HIS
1	D	17	ASN
1	D	64	GLN
1	D	74	ASN
1	D	89	GLN
1	D	113	ASN

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Mol	Chain	Res	Type
1	D	144	HIS
1	D	201	ASN
1	D	242	GLN
1	D	244	ASN
1	D	259	HIS
1	E	64	GLN
1	E	74	ASN
1	E	89	GLN
1	E	113	ASN
1	E	178	ASN
1	E	259	HIS
1	F	74	ASN
1	F	89	GLN
1	F	113	ASN
1	F	144	HIS
1	F	178	ASN
1	F	242	GLN
1	F	259	HIS
1	G	17	ASN
1	G	64	GLN
1	G	74	ASN
1	G	89	GLN
1	G	113	ASN
1	G	144	HIS
1	G	150	GLN
1	G	178	ASN
1	G	259	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no 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	293/293 (100%)	0.78	50 (17%) 4 4	10, 24, 49, 69	13 (4%)
1	B	292/293 (99%)	0.73	51 (17%) 4 4	13, 24, 49, 65	12 (4%)
1	C	293/293 (100%)	0.63	46 (15%) 5 5	9, 23, 47, 64	16 (5%)
1	D	292/293 (99%)	0.65	40 (13%) 6 7	12, 23, 45, 56	19 (6%)
1	E	293/293 (100%)	0.64	39 (13%) 7 7	13, 23, 43, 61	17 (5%)
1	F	293/293 (100%)	0.69	44 (15%) 5 5	13, 23, 47, 62	19 (6%)
1	G	292/293 (99%)	0.57	37 (12%) 8 8	10, 22, 43, 64	16 (5%)
All	All	2048/2051 (99%)	0.67	307 (14%) 5 5	9, 24, 46, 69	112 (5%)

All (307) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	127	ASP	9.3
1	A	132	ILE	8.0
1	A	135	LEU	7.7
1	F	132	ILE	7.6
1	F	127	ASP	7.4
1	F	135	LEU	7.4
1	G	127	ASP	7.4
1	B	129	THR	7.2
1	G	179	TRP	6.9
1	D	128	ASP	6.5
1	G	132	ILE	6.5
1	D	179	TRP	6.5
1	F	118	TYR	6.4
1	B	132	ILE	6.4
1	C	126	GLY	6.4
1	F	126	GLY	6.2
1	F	179	TRP	6.1

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Mol	Chain	Res	Type	RSRZ
1	D	123	ASN	6.1
1	C	132	ILE	6.1
1	A	127	ASP	6.1
1	B	127	ASP	6.1
1	B	118	TYR	5.9
1	C	118	TYR	5.8
1	E	126	GLY	5.7
1	A	179	TRP	5.7
1	B	120	PHE	5.6
1	A	129	THR	5.6
1	G	125	THR	5.6
1	F	128	ASP	5.5
1	G	135	LEU	5.5
1	E	124	VAL	5.5
1	G	128	ASP	5.5
1	D	144	HIS	5.4
1	A	133	GLY	5.4
1	A	136	ILE	5.3
1	C	130	GLY	5.3
1	E	179	TRP	5.2
1	D	112	TYR	5.2
1	G	129	THR	5.2
1	G	124	VAL	5.2
1	C	127	ASP	5.1
1	B	135	LEU	5.0
1	D	133	GLY	4.9
1	G	112	TYR	4.9
1	F	136	ILE	4.9
1	C	136	ILE	4.9
1	D	127	ASP	4.8
1	B	134	GLY	4.8
1	D	130	GLY	4.8
1	D	132	ILE	4.7
1	G	123	ASN	4.7
1	E	118	TYR	4.7
1	C	135	LEU	4.7
1	B	131	LYS	4.6
1	E	262	SER	4.6
1	E	125	THR	4.6
1	C	129	THR	4.6
1	B	124	VAL	4.6
1	D	126	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	179	TRP	4.5
1	G	137	GLY	4.5
1	D	135	LEU	4.5
1	G	136	ILE	4.4
1	B	136	ILE	4.4
1	E	122	GLY	4.4
1	A	112	TYR	4.4
1	E	136	ILE	4.4
1	G	93	ASN	4.3
1	A	118	TYR	4.3
1	C	148	TYR	4.3
1	F	133	GLY	4.3
1	F	134	GLY	4.3
1	G	133	GLY	4.3
1	D	124	VAL	4.3
1	C	123	ASN	4.3
1	F	123	ASN	4.2
1	A	131	LYS	4.2
1	G	131	LYS	4.2
1	F	200	ARG	4.2
1	A	130	GLY	4.2
1	C	134	GLY	4.2
1	G	134	GLY	4.1
1	B	74	ASN	4.1
1	E	129	THR	4.1
1	G	118	TYR	4.0
1	F	124	VAL	4.0
1	A	137	GLY	4.0
1	D	134	GLY	4.0
1	C	133	GLY	3.9
1	B	112	TYR	3.9
1	B	202	GLY	3.9
1	E	133	GLY	3.9
1	A	120	PHE	3.9
1	G	120	PHE	3.9
1	B	123	ASN	3.9
1	E	130	GLY	3.9
1	C	68	TYR	3.8
1	F	112	TYR	3.8
1	B	179	TRP	3.8
1	D	122	GLY	3.8
1	E	135	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	128	ASP	3.8
1	D	200	ARG	3.8
1	D	93	ASN	3.8
1	B	119	GLY	3.8
1	B	125	THR	3.8
1	B	261	THR	3.8
1	A	122	GLY	3.7
1	A	261	THR	3.7
1	A	188	ASN	3.7
1	B	73	ALA	3.7
1	C	138	ALA	3.7
1	F	130	GLY	3.7
1	A	123	ASN	3.7
1	F	129	THR	3.7
1	D	118	TYR	3.7
1	B	260	TRP	3.7
1	E	134	GLY	3.7
1	B	200	ARG	3.7
1	B	138	ALA	3.7
1	B	133	GLY	3.7
1	F	137	GLY	3.7
1	F	138	ALA	3.6
1	E	148	TYR	3.6
1	B	130	GLY	3.6
1	E	120	PHE	3.6
1	E	140	VAL	3.6
1	C	112	TYR	3.5
1	C	124	VAL	3.5
1	F	260	TRP	3.5
1	E	128	ASP	3.5
1	F	203	SER	3.4
1	A	124	VAL	3.4
1	C	128	ASP	3.4
1	E	67	VAL	3.3
1	D	120	PHE	3.3
1	F	120	PHE	3.3
1	A	93	ASN	3.3
1	D	131	LYS	3.3
1	G	130	GLY	3.3
1	G	148	TYR	3.3
1	E	123	ASN	3.2
1	A	72	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	258	LEU	3.2
1	D	121	ASN	3.2
1	E	68	TYR	3.2
1	G	138	ALA	3.2
1	C	74	ASN	3.2
1	A	134	GLY	3.2
1	C	120	PHE	3.1
1	C	141	SER	3.1
1	B	93	ASN	3.1
1	C	125	THR	3.1
1	A	126	GLY	3.1
1	D	203	SER	3.1
1	A	71	GLU	3.1
1	D	73	ALA	3.1
1	D	17	ASN	3.0
1	E	93	ASN	3.0
1	C	122	GLY	3.0
1	C	131	LYS	3.0
1	F	131	LYS	3.0
1	G	122	GLY	3.0
1	E	132	ILE	3.0
1	F	140	VAL	3.0
1	F	73	ALA	3.0
1	E	17	ASN	3.0
1	D	261	THR	2.9
1	F	125	THR	2.9
1	D	201	ASN	2.9
1	A	200	ARG	2.9
1	C	200	ARG	2.9
1	A	140	VAL	2.9
1	F	93	ASN	2.8
1	F	261	THR	2.8
1	F	71	GLU	2.8
1	A	260	TRP	2.8
1	G	262	SER	2.8
1	F	14	ILE	2.8
1	F	70	GLU	2.7
1	B	201	ASN	2.7
1	E	112	TYR	2.7
1	G	1	ALA	2.7
1	B	126	GLY	2.7
1	E	263	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	138	ALA	2.7
1	A	117	THR	2.7
1	A	121	ASN	2.7
1	D	136	ILE	2.7
1	E	14	ILE	2.7
1	D	204	MET	2.6
1	A	108	ASP	2.6
1	F	148	TYR	2.6
1	C	140	VAL	2.6
1	D	190	VAL	2.6
1	C	71	GLU	2.6
1	C	261	THR	2.6
1	D	114	SER	2.6
1	G	140	VAL	2.6
1	D	125	THR	2.6
1	A	189	PRO	2.6
1	G	200	ARG	2.6
1	E	137	GLY	2.6
1	A	190	VAL	2.6
1	A	74	ASN	2.6
1	B	270	THR	2.6
1	B	72	GLY	2.5
1	A	17	ASN	2.5
1	C	191	TYR	2.5
1	D	148	TYR	2.5
1	B	137	GLY	2.5
1	C	201	ASN	2.5
1	B	69	SER	2.5
1	B	203	SER	2.5
1	C	262	SER	2.5
1	G	203	SER	2.5
1	B	268	THR	2.5
1	B	68	TYR	2.5
1	C	139	ASN	2.5
1	E	201	ASN	2.5
1	A	66	ARG	2.5
1	C	14	ILE	2.5
1	F	262	SER	2.5
1	C	73	ALA	2.5
1	B	189	PRO	2.5
1	A	148	TYR	2.4
1	E	131	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	201	ASN	2.4
1	C	119	GLY	2.4
1	F	202	GLY	2.4
1	D	260	TRP	2.4
1	B	122	GLY	2.4
1	G	261	THR	2.4
1	D	71	GLU	2.4
1	A	180	GLY	2.4
1	D	140	VAL	2.4
1	E	72	GLY	2.4
1	F	119	GLY	2.4
1	C	69	SER	2.4
1	F	121	ASN	2.3
1	A	204	MET	2.3
1	C	75	LYS	2.3
1	G	240	LYS	2.3
1	E	95	VAL	2.3
1	F	239	SER	2.3
1	C	108	ASP	2.3
1	C	263	THR	2.3
1	B	259	HIS	2.3
1	F	188	ASN	2.3
1	E	69	SER	2.3
1	G	17	ASN	2.3
1	E	180	GLY	2.3
1	F	92	ASP	2.3
1	C	93	ASN	2.3
1	A	191	TYR	2.2
1	D	137	GLY	2.2
1	A	114	SER	2.2
1	A	262	SER	2.2
1	G	141	SER	2.2
1	B	188	ASN	2.2
1	E	74	ASN	2.2
1	C	189	PRO	2.2
1	G	92	ASP	2.2
1	B	148	TYR	2.2
1	B	187	TRP	2.2
1	B	17	ASN	2.2
1	E	240	LYS	2.2
1	A	125	THR	2.2
1	D	189	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	73	ALA	2.2
1	G	188	ASN	2.2
1	B	140	VAL	2.2
1	A	268	THR	2.2
1	B	262	SER	2.2
1	D	258	LEU	2.2
1	B	71	GLU	2.1
1	A	14	ILE	2.1
1	C	260	TRP	2.1
1	B	92	ASP	2.1
1	D	92	ASP	2.1
1	C	67	VAL	2.1
1	B	277	ARG	2.1
1	F	258	LEU	2.1
1	C	1	ALA	2.1
1	D	188	ASN	2.1
1	F	1	ALA	2.1
1	G	178	ASN	2.1
1	E	261	THR	2.1
1	D	259	HIS	2.1
1	C	188	ASN	2.1
1	G	139	ASN	2.1
1	B	191	TYR	2.1
1	F	122	GLY	2.1
1	F	204	MET	2.1
1	B	95	VAL	2.1
1	F	178	ASN	2.1
1	G	260	TRP	2.1
1	G	108	ASP	2.1
1	B	70	GLU	2.0
1	A	192	GLY	2.0
1	E	92	ASP	2.0
1	E	200	ARG	2.0
1	F	207	ALA	2.0
1	B	144	HIS	2.0
1	A	119	GLY	2.0
1	A	202	GLY	2.0
1	C	66	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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.