



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:55 PM UTC

PDB ID : 8D7I / pdb_00008d7i
Title : Bifunctional Inhibition of Neutrophil Elastase and Cathepsin G by Eap1 from *S. aureus*
Authors : Gido, C.D.; Herdendorf, T.J.; Geisbrecht, B.V.
Deposited on : 2022-06-07
Resolution : 3.63 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

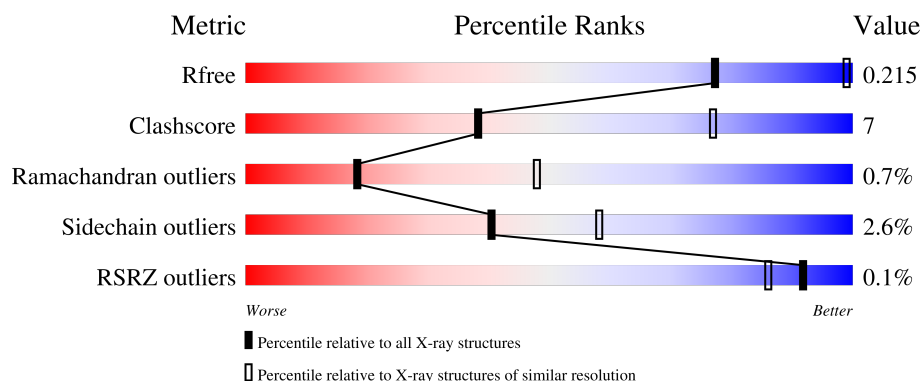
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.63 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	1132 (3.76-3.52)
Clashscore	190562	1014 (3.74-3.54)
Ramachandran outliers	187476	1123 (3.76-3.52)
Sidechain outliers	187428	1121 (3.76-3.52)
RSRZ outliers	180081	1130 (3.76-3.52)

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	218	88% 12%
1	D	218	88% 11%
1	G	218	84% 15%
1	J	218	88% 11%
1	M	218	85% 15%

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Mol	Chain	Length	Quality of chain
1	P	218	 79% 20% .
2	B	100	 77% 21% ..
2	E	100	 79% 16% . . .
2	H	100	 76% 21% ...
2	K	100	 82% 14% . . .
2	N	100	 79% 15% . . .
2	Q	100	 74% 17% 7% ..
3	C	223	 82% 17% .
3	F	223	 77% 22% .
3	I	223	 78% 21%
3	L	223	 82% 16% .
3	O	223	 83% 15% .
3	R	223	 83% 16% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25188 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 Neutrophil elastase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	0	0
			1635	1026	316	282	11			
1	D	218	Total	C	N	O	S	0	0	0
			1635	1026	316	282	11			
1	G	218	Total	C	N	O	S	0	0	0
			1635	1026	316	282	11			
1	J	218	Total	C	N	O	S	0	0	0
			1635	1026	316	282	11			
1	M	218	Total	C	N	O	S	0	0	0
			1635	1026	316	282	11			
1	P	218	Total	C	N	O	S	0	0	0
			1635	1026	316	282	11			

- Molecule 2 is a protein called Extracellular Adherence Protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	0	0	0
			783	494	133	156			
2	E	99	Total	C	N	O	0	0	0
			783	494	133	156			
2	H	99	Total	C	N	O	0	0	0
			783	494	133	156			
2	K	99	Total	C	N	O	0	0	0
			783	494	133	156			
2	N	99	Total	C	N	O	0	0	0
			783	494	133	156			
2	Q	99	Total	C	N	O	0	0	0
			783	494	133	156			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	46	GLY	-	expression tag	UNP Q99QS1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	47	SER	-	expression tag	UNP Q99QS1
B	48	THR	-	expression tag	UNP Q99QS1
E	46	GLY	-	expression tag	UNP Q99QS1
E	47	SER	-	expression tag	UNP Q99QS1
E	48	THR	-	expression tag	UNP Q99QS1
H	46	GLY	-	expression tag	UNP Q99QS1
H	47	SER	-	expression tag	UNP Q99QS1
H	48	THR	-	expression tag	UNP Q99QS1
K	46	GLY	-	expression tag	UNP Q99QS1
K	47	SER	-	expression tag	UNP Q99QS1
K	48	THR	-	expression tag	UNP Q99QS1
N	46	GLY	-	expression tag	UNP Q99QS1
N	47	SER	-	expression tag	UNP Q99QS1
N	48	THR	-	expression tag	UNP Q99QS1
Q	46	GLY	-	expression tag	UNP Q99QS1
Q	47	SER	-	expression tag	UNP Q99QS1
Q	48	THR	-	expression tag	UNP Q99QS1

- Molecule 3 is a protein called Cathepsin G, C-terminal truncated form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	223	Total	C	N	O	S	0	0	0
			1780	1093	369	308	10			
3	F	223	Total	C	N	O	S	0	0	0
			1780	1093	369	308	10			
3	I	223	Total	C	N	O	S	0	0	0
			1780	1093	369	308	10			
3	L	223	Total	C	N	O	S	0	0	0
			1780	1093	369	308	10			
3	O	223	Total	C	N	O	S	0	0	0
			1780	1093	369	308	10			
3	R	223	Total	C	N	O	S	0	0	0
			1780	1093	369	308	10			

3 Residue-property plots

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: Neutrophil elastase

Chain A: 



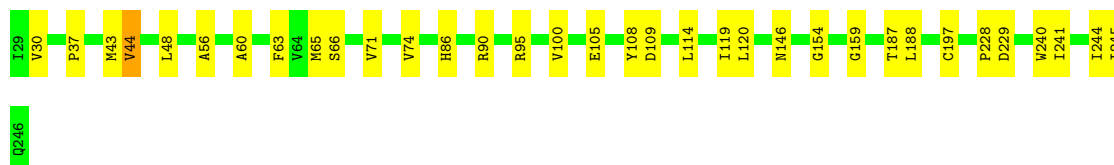
- Molecule 1: Neutrophil elastase

Chain D: 



- Molecule 1: Neutrophil elastase

Chain G: 



- Molecule 1: Neutrophil elastase

Chain J: 



- Molecule 1: Neutrophil elastase

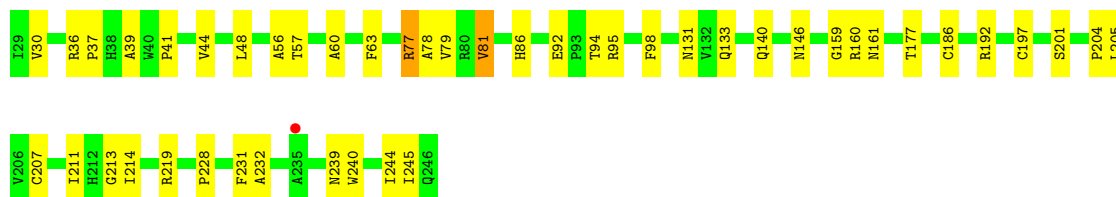
Chain M: 





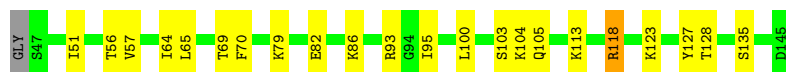
- Molecule 1: Neutrophil elastase

Chain P: 79% 20%



- Molecule 2: Extracellular Adherence Protein

Chain B: 77% 21%



- Molecule 2: Extracellular Adherence Protein

Chain E: 79% 16%



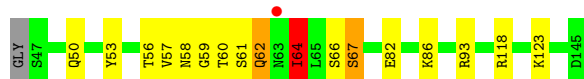
- Molecule 2: Extracellular Adherence Protein

Chain H: 76% 21%



- Molecule 2: Extracellular Adherence Protein

Chain K: 82% 14%

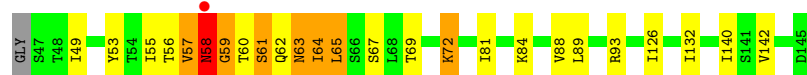
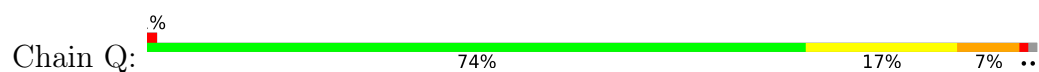


- Molecule 2: Extracellular Adherence Protein

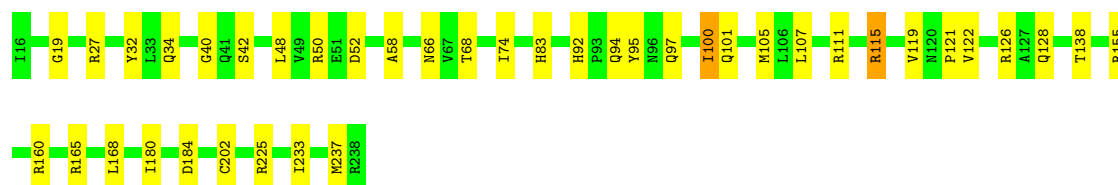
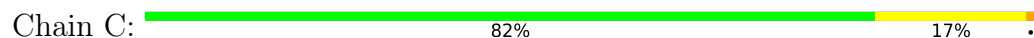
Chain N: 79% 15%



- Molecule 2: Extracellular Adherence Protein



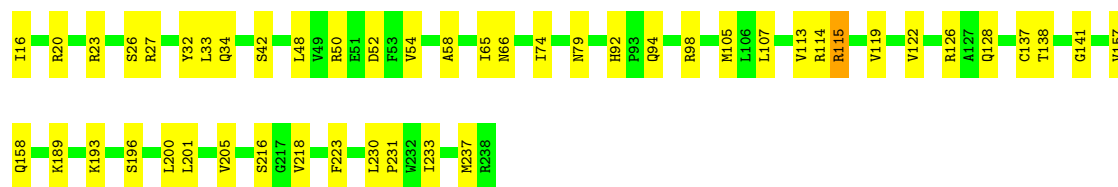
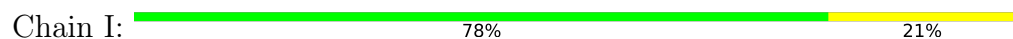
- Molecule 3: Cathepsin G, C-terminal truncated form



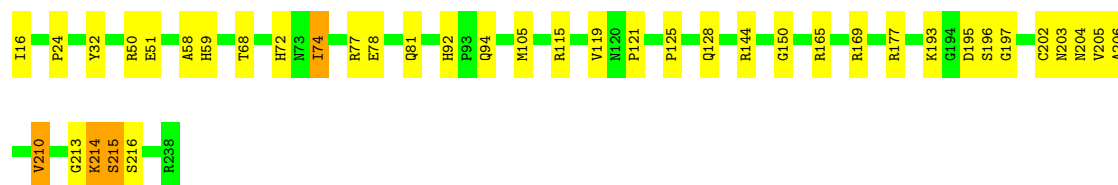
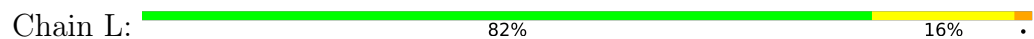
- Molecule 3: Cathepsin G, C-terminal truncated form



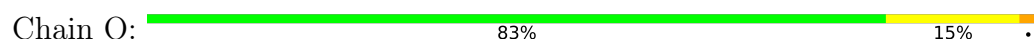
- Molecule 3: Cathepsin G, C-terminal truncated form

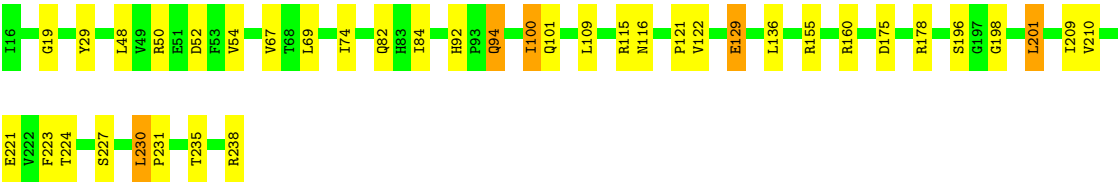


- Molecule 3: Cathepsin G, C-terminal truncated form

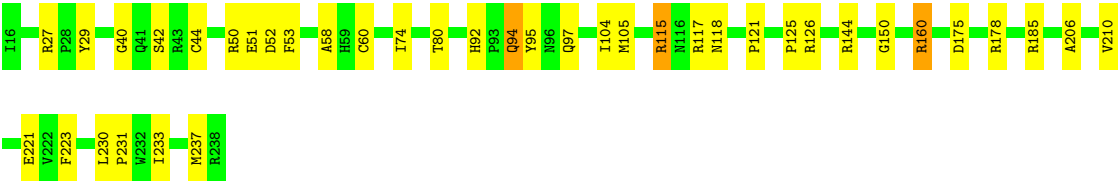
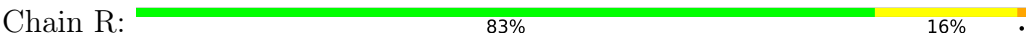


- Molecule 3: Cathepsin G, C-terminal truncated form





• Molecule 3: Cathepsin G, C-terminal truncated form



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	102.23Å 152.27Å 296.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	96.64 – 3.63 96.64 – 3.63	Depositor EDS
% Data completeness (in resolution range)	96.3 (96.64-3.63) 96.3 (96.64-3.63)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.02 (at 3.67Å)	Xtriage
Refinement program	PHENIX v1.9.2	Depositor
R, R_{free}	0.186 , 0.217 0.189 , 0.215	Depositor DCC
R_{free} test set	2000 reflections (3.76%)	wwPDB-VP
Wilson B-factor (Å ²)	84.5	Xtriage
Anisotropy	0.539	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 72.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	25188	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% 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	0.16	0/1665	0.35	0/2263
1	D	0.16	0/1665	0.38	0/2263
1	G	0.14	0/1665	0.37	0/2263
1	J	0.16	0/1665	0.39	0/2263
1	M	0.16	0/1665	0.38	0/2263
1	P	0.17	0/1665	0.42	0/2263
2	B	0.16	0/792	0.30	0/1071
2	E	0.14	0/792	0.33	0/1071
2	H	0.15	0/792	0.33	0/1071
2	K	0.17	0/792	0.33	0/1071
2	N	0.17	0/792	0.42	0/1071
2	Q	0.20	0/792	0.64	2/1071 (0.2%)
3	C	0.15	0/1814	0.38	0/2447
3	F	0.15	0/1814	0.43	0/2447
3	I	0.16	0/1814	0.41	0/2447
3	L	0.15	0/1814	0.40	0/2447
3	O	0.15	0/1814	0.36	0/2447
3	R	0.15	0/1814	0.39	0/2447
All	All	0.16	0/25626	0.39	2/34686 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	58	ASN	N-CA-C	-10.33	98.11	113.61
2	Q	57	VAL	N-CA-C	-7.26	94.23	109.34

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	1635	0	1652	15	0
1	D	1635	0	1652	18	0
1	G	1635	0	1652	19	0
1	J	1635	0	1652	15	0
1	M	1635	0	1652	21	0
1	P	1635	0	1652	32	0
2	B	783	0	801	15	0
2	E	783	0	801	27	0
2	H	783	0	801	15	0
2	K	783	0	801	17	0
2	N	783	0	801	15	0
2	Q	783	0	801	23	0
3	C	1780	0	1793	24	0
3	F	1780	0	1793	33	0
3	I	1780	0	1793	28	0
3	L	1780	0	1793	29	0
3	O	1780	0	1793	27	0
3	R	1780	0	1793	27	0
All	All	25188	0	25476	349	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 7.

All (349) 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)
2:H:64:ILE:HD11	3:I:42:SER:HB3	1.52	0.90
2:N:93:ARG:HH12	3:O:100:ILE:HD11	1.42	0.83
2:N:61:SER:O	2:N:63:ASN:N	2.12	0.81
2:Q:64:ILE:HG12	3:R:42:SER:HB3	1.61	0.81
1:A:77:ARG:HH12	3:R:160:ARG:HH21	1.28	0.81
2:E:93:ARG:HH12	3:F:100:ILE:HD11	1.50	0.77
1:A:76:VAL:HG21	1:A:103:ILE:HD11	1.66	0.76
2:E:64:ILE:HG21	3:F:42:SER:HB3	1.66	0.76
2:Q:58:ASN:H	2:Q:93:ARG:HH22	1.32	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:144:ARG:HA	3:L:150:GLY:HA2	1.68	0.74
2:K:61:SER:HA	3:L:215:SER:HA	1.70	0.72
1:P:77:ARG:O	1:P:79:VAL:N	2.21	0.72
3:O:196:SER:HA	3:O:210:VAL:HB	1.72	0.70
2:E:61:SER:O	2:E:63:ASN:N	2.21	0.70
1:P:60:ALA:HB3	1:P:63:PHE:HB2	1.73	0.70
2:B:57:VAL:HB	2:B:93:ARG:HE	1.56	0.70
2:Q:57:VAL:H	2:Q:59:GLY:H	1.40	0.70
1:D:36:ARG:HB2	1:D:39:ALA:HB2	1.73	0.70
3:F:78:GLU:HB2	3:F:81:GLN:HG3	1.72	0.69
2:Q:69:THR:HG23	3:R:40:GLY:HA2	1.74	0.69
2:B:93:ARG:HH12	3:C:100:ILE:HD11	1.59	0.67
3:I:34:GLN:HB2	3:I:66:ASN:HB2	1.76	0.67
3:C:83:HIS:O	3:C:111:ARG:NH2	2.28	0.67
1:A:36:ARG:HB2	1:A:39:ALA:HB2	1.77	0.67
3:R:175:ASP:OD2	3:R:178:ARG:NH1	2.27	0.66
3:L:32:TYR:HB3	3:L:68:THR:HB	1.76	0.66
2:Q:56:THR:HA	2:Q:59:GLY:HA2	1.76	0.66
3:C:34:GLN:HB2	3:C:66:ASN:HB2	1.79	0.65
2:N:57:VAL:HB	2:N:93:ARG:HH21	1.60	0.65
3:C:180:ILE:HG12	3:C:225:ARG:HE	1.63	0.63
3:L:115:ARG:HA	3:L:119:VAL:O	1.98	0.63
1:P:205:LEU:HD23	1:P:231:PHE:CG	2.34	0.62
3:C:184:ASP:OD2	1:M:102:ARG:NH1	2.32	0.62
3:L:197:GLY:H	3:L:210:VAL:HG23	1.65	0.62
1:G:60:ALA:HB3	1:G:63:PHE:HB2	1.82	0.62
3:R:27:ARG:NH1	3:R:29:TYR:OH	2.33	0.62
1:J:30:VAL:HG22	1:J:159:GLY:HA2	1.80	0.61
1:M:88:LEU:HA	1:M:95:ARG:HH22	1.65	0.61
1:P:205:LEU:HD23	1:P:231:PHE:CD2	2.36	0.61
1:P:205:LEU:HG	1:P:213:GLY:HA3	1.83	0.60
2:E:61:SER:H	3:F:213:GLY:H	1.47	0.60
1:P:36:ARG:HB2	1:P:39:ALA:HB2	1.82	0.60
2:E:56:THR:HA	2:E:60:THR:HG23	1.82	0.60
2:K:61:SER:H	3:L:213:GLY:C	2.10	0.60
2:E:60:THR:OG1	2:E:63:ASN:OD1	2.16	0.59
3:O:54:VAL:HG21	3:O:67:VAL:HG11	1.84	0.59
2:E:93:ARG:NH1	3:F:100:ILE:HD11	2.17	0.59
2:K:62:GLN:HE22	3:L:196:SER:HA	1.66	0.59
2:E:62:GLN:O	3:F:196:SER:OG	2.21	0.58
1:A:246:GLN:HB2	3:L:177:ARG:HH22	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:61:SER:HB2	3:F:214:LYS:C	2.29	0.57
2:K:82:GLU:HG2	2:K:86:LYS:HD3	1.85	0.57
2:Q:64:ILE:HD12	3:R:60:CYS:HA	1.85	0.57
1:M:44:VAL:HG21	1:M:81:VAL:HG13	1.87	0.57
2:Q:64:ILE:HG13	3:R:44:CYS:SG	2.45	0.57
1:G:37:PRO:HA	1:G:86:HIS:CD2	2.40	0.56
2:H:61:SER:OG	3:I:193:LYS:NZ	2.38	0.56
1:P:160:ARG:O	1:P:161:ASN:HB3	2.04	0.56
1:J:59:ILE:HD13	1:J:65:MET:HB2	1.85	0.56
2:E:61:SER:C	2:E:63:ASN:H	2.13	0.56
3:I:92:HIS:CE1	3:I:94:GLN:HG2	2.41	0.56
3:F:30:MET:HE2	3:F:154:LEU:HD11	1.87	0.56
1:P:57:THR:OG1	1:P:204:PRO:HB3	2.05	0.56
1:P:63:PHE:HD2	1:P:245:ILE:HG22	1.71	0.56
1:G:119:ILE:HD11	1:G:241:ILE:HG12	1.87	0.56
2:N:56:THR:HA	2:N:60:THR:HG23	1.87	0.56
3:R:58:ALA:HA	3:R:105:MET:HB2	1.88	0.55
3:L:214:LYS:O	3:L:216:SER:N	2.39	0.55
1:P:205:LEU:HD12	1:P:205:LEU:O	2.06	0.55
3:O:122:VAL:HG21	3:O:201:LEU:HD21	1.88	0.55
1:P:30:VAL:HG22	1:P:159:GLY:HA2	1.89	0.55
3:O:82:GLN:NE2	3:O:116:ASN:HD21	2.05	0.55
2:N:62:GLN:NE2	3:O:221:GLU:OE1	2.40	0.55
1:D:151:LEU:HD11	1:D:170:GLU:HB2	1.90	0.54
1:P:140:GLN:NE2	1:P:239:ASN:H	2.05	0.54
3:C:50:ARG:HB2	3:C:237:MET:HE1	1.89	0.54
1:G:30:VAL:HG23	1:G:197:CYS:HB2	1.89	0.54
3:R:92:HIS:CE1	3:R:94:GLN:HG2	2.42	0.54
1:P:37:PRO:HA	1:P:86:HIS:CD2	2.42	0.54
2:H:57:VAL:HG22	2:H:93:ARG:NH2	2.23	0.54
1:J:90:ARG:O	1:J:95:ARG:NH2	2.41	0.54
2:B:93:ARG:NH1	3:C:100:ILE:HD11	2.24	0.53
3:O:84:ILE:HG21	3:O:109:LEU:HB3	1.89	0.53
1:D:162:ARG:HB3	1:D:162:ARG:HH11	1.74	0.53
3:I:48:LEU:HD21	3:I:113:VAL:HG21	1.90	0.53
1:M:30:VAL:HG22	1:M:159:GLY:HA2	1.91	0.53
3:C:92:HIS:CE1	3:C:94:GLN:HG2	2.44	0.52
1:M:88:LEU:HA	1:M:95:ARG:NH2	2.24	0.52
3:O:92:HIS:CE1	3:O:94:GLN:HG2	2.44	0.52
2:Q:49:ILE:HG23	2:Q:72:LYS:HG2	1.91	0.52
1:A:189:VAL:HG11	1:A:194:ALA:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:77:ARG:C	1:P:79:VAL:H	2.15	0.52
1:D:37:PRO:HA	1:D:86:HIS:CD2	2.45	0.52
1:M:139:ALA:HB3	1:M:142:ARG:HG3	1.92	0.52
2:B:118:ARG:NH2	2:B:128:THR:OG1	2.39	0.52
1:M:143:ARG:CZ	1:M:182:ARG:HD2	2.40	0.51
3:O:19:GLY:O	3:O:155:ARG:NH2	2.43	0.51
2:Q:81:ILE:HD11	2:Q:132:ILE:HD11	1.93	0.51
3:L:115:ARG:HH11	3:L:121:PRO:HD2	1.76	0.51
3:C:19:GLY:O	3:C:155:ARG:NH2	2.43	0.51
1:D:49:ARG:HD3	2:E:73:ASN:HD21	1.75	0.51
2:K:62:GLN:NE2	3:L:210:VAL:HB	2.26	0.51
1:P:44:VAL:HB	1:P:56:ALA:HB3	1.93	0.51
2:Q:63:ASN:O	2:Q:65:LEU:N	2.42	0.51
2:K:50:GLN:OE1	2:K:67:SER:OG	2.28	0.51
2:E:99:ASP:OD2	3:F:98:ARG:NH2	2.44	0.51
1:G:100:VAL:HG13	1:G:120:LEU:HB3	1.93	0.51
2:E:69:THR:OG1	3:F:40:GLY:HA2	2.10	0.51
2:K:61:SER:HB2	3:L:214:LYS:C	2.36	0.50
1:M:143:ARG:HH22	1:M:182:ARG:HH11	1.58	0.50
1:A:30:VAL:HG23	1:A:197:CYS:HB2	1.93	0.50
3:I:54:VAL:HB	3:I:107:LEU:HB2	1.93	0.50
1:P:214:ILE:HB	1:P:232:ALA:HB3	1.93	0.50
3:F:50:ARG:HD2	3:F:52:ASP:OD1	2.11	0.50
3:C:160:ARG:HD2	1:M:102:ARG:CZ	2.42	0.50
3:L:92:HIS:CE1	3:L:94:GLN:HG2	2.46	0.50
3:O:50:ARG:HD2	3:O:52:ASP:OD1	2.12	0.50
2:E:60:THR:HB	2:E:93:ARG:HH12	1.77	0.50
2:H:55:ILE:HD13	2:H:89:LEU:HD23	1.92	0.50
3:I:16:ILE:HD11	3:I:141:GLY:N	2.27	0.50
1:P:41:PRO:HG2	1:P:133:GLN:HB2	1.94	0.50
3:F:144:ARG:HA	3:F:150:GLY:HA2	1.93	0.50
3:R:50:ARG:C	3:R:52:ASP:H	2.20	0.50
2:Q:53:TYR:HA	2:Q:140:ILE:O	2.11	0.50
2:B:82:GLU:HG2	2:B:86:LYS:HD3	1.94	0.50
2:H:51:ILE:HD13	2:H:137:ILE:HB	1.94	0.50
3:F:82:GLN:NE2	3:F:114:ARG:HB3	2.26	0.50
1:P:186:CYS:HB3	1:P:228:PRO:HB2	1.92	0.50
2:Q:60:THR:O	2:Q:63:ASN:N	2.45	0.50
2:B:93:ARG:HA	3:C:97:GLN:HB2	1.94	0.49
2:E:64:ILE:HG23	3:F:44:CYS:SG	2.52	0.49
3:I:50:ARG:NH2	3:I:237:MET:HB3	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:16:ILE:N	3:L:144:ARG:O	2.45	0.49
3:O:209:ILE:HB	3:O:224:THR:HB	1.94	0.49
1:P:205:LEU:HG	1:P:213:GLY:CA	2.42	0.49
1:D:53:PHE:HA	2:E:131:LEU:HD12	1.94	0.49
1:G:188:LEU:HB2	1:G:228:PRO:HB3	1.94	0.49
1:J:158:LEU:HD21	1:J:165:ALA:HB2	1.94	0.49
1:D:44:VAL:HB	1:D:56:ALA:HB3	1.93	0.49
1:G:187:THR:HG22	1:G:229:ASP:HB2	1.94	0.49
3:I:20:ARG:HH22	3:I:158:GLN:HG3	1.77	0.49
3:O:82:GLN:HE22	3:O:116:ASN:HD21	1.59	0.49
2:N:62:GLN:O	3:O:196:SER:OG	2.31	0.48
1:M:104:PHE:HB2	1:M:119:ILE:HB	1.94	0.48
3:O:129:GLU:H	3:O:227:SER:HB2	1.79	0.48
3:F:134:GLY:O	3:F:160:ARG:NH1	2.47	0.48
3:R:144:ARG:HA	3:R:150:GLY:HA2	1.95	0.48
1:A:160:ARG:O	1:A:161:ASN:HB3	2.13	0.48
1:D:96:GLN:HE21	1:D:132:VAL:HG21	1.79	0.48
1:A:68:ALA:HA	1:A:118:VAL:HB	1.96	0.48
1:J:60:ALA:HB3	1:J:63:PHE:HB2	1.95	0.48
2:B:113:LYS:NZ	2:B:135:SER:O	2.43	0.48
2:Q:58:ASN:N	2:Q:93:ARG:HH22	2.08	0.48
2:Q:59:GLY:C	2:Q:61:SER:H	2.21	0.48
2:K:53:TYR:CE1	2:K:66:SER:HB3	2.48	0.48
2:K:61:SER:HB2	3:L:214:LYS:O	2.14	0.48
1:G:240:TRP:O	1:G:244:ILE:HG12	2.14	0.47
2:H:58:ASN:HD21	3:I:98:ARG:HH21	1.62	0.47
1:J:160:ARG:HG2	1:J:222:CYS:HB2	1.96	0.47
1:P:30:VAL:HG23	1:P:197:CYS:HB2	1.96	0.47
1:G:108:TYR:O	3:R:117:ARG:NH2	2.47	0.47
3:R:104:ILE:HD11	3:R:233:ILE:HD11	1.95	0.47
3:L:78:GLU:OE1	3:L:81:GLN:NE2	2.45	0.47
3:C:32:TYR:HB3	3:C:68:THR:HB	1.97	0.47
2:N:121:ASP:HB3	2:N:124:SER:HB3	1.97	0.47
1:G:90:ARG:O	1:G:95:ARG:NH2	2.47	0.47
1:M:60:ALA:HB3	1:M:63:PHE:HB2	1.97	0.47
1:P:204:PRO:HB2	1:P:211:ILE:HD12	1.96	0.47
3:F:185:ARG:HA	3:F:219:PRO:HG2	1.97	0.47
3:F:196:SER:HA	3:F:210:VAL:HB	1.96	0.47
1:M:214:ILE:HB	1:M:232:ALA:HB3	1.97	0.47
3:F:32:TYR:HD1	3:F:142:TRP:CE3	2.33	0.47
1:J:37:PRO:HA	1:J:86:HIS:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:197:GLY:N	3:L:210:VAL:HG23	2.30	0.47
1:P:63:PHE:HE2	1:P:245:ILE:HA	1.80	0.47
2:K:62:GLN:OE1	3:L:195:ASP:HB2	2.15	0.47
2:Q:55:ILE:HD13	2:Q:142:VAL:HB	1.97	0.46
2:Q:61:SER:C	2:Q:63:ASN:H	2.21	0.46
1:J:30:VAL:HG23	1:J:197:CYS:HB2	1.96	0.46
3:L:32:TYR:CE1	3:L:74:ILE:HD13	2.51	0.46
1:D:162:ARG:HB3	1:D:162:ARG:NH1	2.29	0.46
3:I:115:ARG:HA	3:I:119:VAL:O	2.16	0.46
1:J:160:ARG:O	1:J:161:ASN:HB3	2.15	0.46
2:N:57:VAL:HB	2:N:93:ARG:NH2	2.28	0.46
1:P:146:ASN:ND2	1:P:177:THR:HG22	2.29	0.46
1:P:205:LEU:HD13	1:P:207:CYS:SG	2.55	0.46
1:J:189:VAL:HG11	1:J:194:ALA:HB3	1.98	0.46
1:P:92:GLU:HB2	1:P:95:ARG:HE	1.80	0.46
1:P:94:THR:HB	1:P:131:ASN:ND2	2.30	0.46
1:G:30:VAL:HG22	1:G:159:GLY:HA2	1.98	0.46
1:J:92:GLU:HB2	1:J:95:ARG:NE	2.31	0.46
3:O:210:VAL:HG22	3:O:223:PHE:CE2	2.50	0.46
2:B:57:VAL:HG11	2:B:95:ILE:HD11	1.98	0.46
3:L:50:ARG:HG2	3:L:51:GLU:H	1.80	0.46
2:Q:62:GLN:NE2	3:R:221:GLU:OE1	2.49	0.46
2:E:75:ASN:HB3	2:E:131:LEU:HB3	1.97	0.46
2:E:109:THR:HG21	2:E:117:LYS:HD2	1.97	0.46
1:A:30:VAL:HG22	1:A:159:GLY:HA2	1.97	0.45
3:C:105:MET:HE3	3:C:107:LEU:HD21	1.98	0.45
3:I:34:GLN:O	3:I:65:ILE:HA	2.16	0.45
2:N:53:TYR:HA	2:N:140:ILE:O	2.15	0.45
3:F:32:TYR:HB3	3:F:68:THR:HB	1.97	0.45
3:F:236:THR:C	3:F:238:ARG:H	2.23	0.45
1:G:56:ALA:HB2	1:G:66:SER:HB2	1.99	0.45
3:I:92:HIS:HE1	3:I:94:GLN:HG2	1.81	0.45
1:M:143:ARG:HH12	1:M:182:ARG:NH1	2.14	0.45
2:E:95:ILE:HD13	3:F:98:ARG:HE	1.81	0.45
3:F:34:GLN:O	3:F:65:ILE:HA	2.17	0.45
3:O:48:LEU:HD13	3:O:69:LEU:HD11	1.99	0.45
1:P:240:TRP:O	1:P:244:ILE:HG12	2.15	0.45
3:R:50:ARG:HD2	3:R:52:ASP:HB3	1.98	0.45
1:P:219:ARG:HG2	2:Q:126:ILE:HG12	1.99	0.45
1:G:30:VAL:HG13	1:G:159:GLY:HA2	1.99	0.45
3:I:137:CYS:O	3:I:158:GLN:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:61:SER:O	3:L:193:LYS:HE2	2.17	0.45
1:A:240:TRP:O	1:A:244:ILE:HG12	2.17	0.45
2:E:100:LEU:HA	2:E:100:LEU:HD23	1.84	0.45
1:G:43:MET:HE2	1:G:154:GLY:HA2	1.98	0.45
3:O:29:TYR:CG	3:O:122:VAL:HB	2.52	0.45
1:J:119:ILE:HD11	1:J:241:ILE:HG23	1.98	0.44
1:M:37:PRO:HA	1:M:86:HIS:CD2	2.52	0.44
3:I:157:VAL:HG22	3:I:189:LYS:HE3	1.98	0.44
1:M:62:ASN:OD1	1:M:62:ASN:N	2.50	0.44
2:Q:59:GLY:C	2:Q:61:SER:N	2.76	0.44
2:B:123:LYS:HB3	2:B:123:LYS:HE2	1.83	0.44
2:K:57:VAL:HB	2:K:93:ARG:NH2	2.32	0.44
3:O:230:LEU:N	3:O:231:PRO:HD2	2.33	0.44
1:P:205:LEU:HD12	1:P:205:LEU:C	2.41	0.44
1:J:68:ALA:HA	1:J:118:VAL:HB	1.98	0.44
2:K:64:ILE:HG23	3:L:59:HIS:CD2	2.52	0.44
3:R:51:GLU:OE2	3:R:115:ARG:HD3	2.17	0.44
2:K:53:TYR:CZ	2:K:66:SER:HB3	2.53	0.44
2:H:53:TYR:HA	2:H:140:ILE:O	2.18	0.44
2:N:63:ASN:HB3	2:N:64:ILE:HG12	1.99	0.44
1:A:186:CYS:HB3	1:A:228:PRO:HB2	2.00	0.43
3:C:50:ARG:HD2	3:C:52:ASP:OD1	2.18	0.43
2:E:94:GLY:O	3:F:98:ARG:NH2	2.51	0.43
3:L:125:PRO:HD3	3:L:206:ALA:O	2.18	0.43
3:L:165:ARG:HE	3:L:169:ARG:NH2	2.16	0.43
2:N:63:ASN:O	3:O:196:SER:HB2	2.18	0.43
1:P:219:ARG:HH22	1:P:228:PRO:HG2	1.82	0.43
3:C:27:ARG:NH2	3:C:138:THR:HG21	2.33	0.43
3:F:210:VAL:HG22	3:F:223:PHE:CE2	2.53	0.43
1:G:63:PHE:CD2	1:G:245:ILE:HG22	2.53	0.43
3:L:115:ARG:NH1	3:L:121:PRO:HD2	2.33	0.43
3:L:203:ASN:O	3:L:205:VAL:HG23	2.19	0.43
3:R:50:ARG:HA	3:R:121:PRO:HB3	2.01	0.43
1:D:179:LEU:HD23	1:D:179:LEU:HA	1.87	0.43
3:I:216:SER:OG	3:I:218:VAL:HG12	2.19	0.43
2:N:82:GLU:HG2	2:N:86:LYS:HD3	2.00	0.43
2:E:57:VAL:HB	2:E:93:ARG:HH21	1.84	0.43
3:O:221:GLU:HG3	3:O:223:PHE:HE1	1.83	0.43
3:R:80:THR:HB	3:R:118:ASN:ND2	2.33	0.43
3:C:233:ILE:O	3:C:237:MET:HG3	2.19	0.43
1:D:44:VAL:HG13	1:D:83:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:57:VAL:HB	2:E:93:ARG:NH2	2.34	0.43
1:D:81:VAL:O	1:D:97:VAL:HA	2.19	0.43
3:F:230:LEU:N	3:F:231:PRO:HD2	2.33	0.43
1:M:160:ARG:O	1:M:161:ASN:CG	2.62	0.43
2:B:64:ILE:HD11	3:C:42:SER:HB3	2.00	0.42
2:H:63:ASN:O	3:I:196:SER:HB2	2.18	0.42
1:D:30:VAL:HG23	1:D:197:CYS:HB2	2.00	0.42
3:F:124:LEU:HD22	3:F:226:VAL:HG11	2.00	0.42
2:K:56:THR:HG23	2:K:59:GLY:H	1.84	0.42
3:R:230:LEU:N	3:R:231:PRO:HD2	2.34	0.42
2:E:62:GLN:HE21	3:F:221:GLU:HB3	1.84	0.42
3:F:157:VAL:HG22	3:F:189:LYS:HE3	2.01	0.42
1:G:71:VAL:HA	1:G:74:VAL:HG12	2.01	0.42
2:N:64:ILE:HG13	2:N:66:SER:HB2	2.02	0.42
3:O:48:LEU:HB3	3:O:121:PRO:HA	2.00	0.42
2:B:51:ILE:HD12	2:B:70:PHE:CD1	2.54	0.42
3:F:19:GLY:O	3:F:155:ARG:NH2	2.52	0.42
2:H:75:ASN:HB3	2:H:131:LEU:HD23	2.01	0.42
3:I:200:LEU:HB2	3:I:223:PHE:CE2	2.54	0.42
3:R:74:ILE:H	3:R:74:ILE:HG13	1.67	0.42
3:C:58:ALA:HA	3:C:105:MET:HB2	2.00	0.42
1:D:49:ARG:HD3	2:E:73:ASN:ND2	2.35	0.42
3:F:100:ILE:HD12	3:F:212:TYR:CG	2.54	0.42
3:I:23:ARG:HE	3:I:26:SER:HB3	1.85	0.42
1:J:157:LEU:HD12	1:J:197:CYS:SG	2.60	0.42
3:O:136:LEU:HD13	3:O:160:ARG:NH1	2.34	0.42
3:I:32:TYR:CZ	3:I:74:ILE:HD13	2.54	0.42
2:K:123:LYS:HB3	2:K:123:LYS:HE2	1.82	0.42
1:M:58:LEU:HD12	1:M:83:LEU:HD22	2.01	0.42
1:M:100:VAL:HG13	1:M:120:LEU:HB3	2.01	0.42
3:O:52:ASP:OD1	3:O:52:ASP:N	2.49	0.42
3:R:126:ARG:HD2	3:R:126:ARG:HA	1.92	0.42
1:A:37:PRO:HA	1:A:86:HIS:CD2	2.55	0.42
1:A:106:ASN:HB2	1:A:240:TRP:CE2	2.54	0.42
1:D:70:CYS:SG	1:D:201:SER:HB3	2.59	0.42
1:D:190:ARG:HA	1:D:190:ARG:HD2	1.79	0.42
2:H:57:VAL:HG22	2:H:93:ARG:CZ	2.50	0.42
2:H:82:GLU:HG2	2:H:86:LYS:HD3	2.02	0.42
3:I:27:ARG:NH2	3:I:138:THR:HG21	2.34	0.42
2:B:104:LYS:O	2:B:105:GLN:HG3	2.19	0.42
3:L:24:PRO:HA	3:L:72:HIS:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:158:LEU:HB2	1:D:162:ARG:NH1	2.34	0.42
3:C:115:ARG:HA	3:C:119:VAL:O	2.20	0.41
3:I:33:LEU:HD21	3:I:107:LEU:HD11	2.00	0.41
1:M:219:ARG:NH2	1:M:228:PRO:HG2	2.34	0.41
2:N:97:ASP:O	2:N:101:ARG:HG3	2.20	0.41
2:E:123:LYS:HE2	2:E:123:LYS:HB3	1.87	0.41
3:L:58:ALA:HA	3:L:105:MET:HB2	2.01	0.41
3:C:48:LEU:HB3	3:C:121:PRO:HA	2.03	0.41
3:C:95:TYR:HA	3:C:101:GLN:O	2.20	0.41
3:C:165:ARG:HA	3:C:168:LEU:HD12	2.02	0.41
3:F:53:PHE:CZ	3:F:237:MET:HA	2.56	0.41
2:H:76:ILE:HD13	2:H:134:THR:HG22	2.02	0.41
3:I:50:ARG:HD2	3:I:52:ASP:OD1	2.20	0.41
3:I:114:ARG:O	3:I:115:ARG:HG2	2.20	0.41
3:O:84:ILE:HB	3:O:109:LEU:HD22	2.02	0.41
3:O:175:ASP:OD2	3:O:178:ARG:HD2	2.20	0.41
2:E:61:SER:N	3:F:213:GLY:O	2.53	0.41
1:G:65:MET:HE2	1:G:65:MET:HB3	1.98	0.41
2:H:60:THR:OG1	2:H:93:ARG:NH2	2.50	0.41
2:H:101:ARG:O	2:H:123:LYS:NZ	2.53	0.41
2:N:81:ILE:HD11	2:N:132:ILE:HD11	2.01	0.41
3:O:198:GLY:O	3:O:210:VAL:HG23	2.20	0.41
1:D:30:VAL:HG22	1:D:159:GLY:HA2	2.02	0.41
1:G:109:ASP:HB3	1:G:114:LEU:HB2	2.02	0.41
3:I:58:ALA:HA	3:I:105:MET:HB2	2.02	0.41
3:I:233:ILE:HG22	3:I:237:MET:HE2	2.03	0.41
2:Q:67:SER:O	3:R:40:GLY:HA3	2.20	0.41
3:R:210:VAL:HG22	3:R:223:PHE:CE2	2.56	0.41
2:B:69:THR:OG1	3:C:40:GLY:HA2	2.20	0.41
1:M:138:PRO:HA	1:M:210:LEU:HD13	2.03	0.41
2:H:52:PRO:HA	2:H:67:SER:HA	2.02	0.41
1:M:186:CYS:HB3	1:M:228:PRO:HB2	2.02	0.41
2:Q:84:LYS:O	2:Q:88:VAL:HG22	2.21	0.41
3:R:125:PRO:HD3	3:R:206:ALA:O	2.20	0.41
1:A:204:PRO:HB2	1:A:211:ILE:HD12	2.02	0.41
2:B:100:LEU:O	2:B:103:SER:OG	2.31	0.41
3:C:48:LEU:O	3:C:122:VAL:HG12	2.21	0.41
2:Q:60:THR:O	2:Q:62:GLN:N	2.54	0.41
1:G:44:VAL:CG2	1:G:56:ALA:HB3	2.51	0.41
3:I:230:LEU:N	3:I:231:PRO:HD2	2.36	0.41
3:O:235:THR:HA	3:O:238:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:81:VAL:HG13	1:P:98:PHE:HB2	2.01	0.41
2:K:64:ILE:HG23	3:L:59:HIS:HD2	1.85	0.40
1:J:92:GLU:HA	1:J:93:PRO:HD3	1.96	0.40
2:Q:89:LEU:HD23	2:Q:89:LEU:HA	1.87	0.40
3:R:115:ARG:HD2	3:R:121:PRO:HD2	2.03	0.40
2:B:79:LYS:HD3	2:B:127:TYR:CE1	2.57	0.40
1:A:164:ILE:HG13	1:A:165:ALA:N	2.35	0.40
3:F:115:ARG:HA	3:F:119:VAL:O	2.21	0.40
1:P:214:ILE:O	1:P:232:ALA:N	2.39	0.40
3:R:53:PHE:CE2	3:R:237:MET:HA	2.56	0.40
3:R:95:TYR:CE2	3:R:97:GLN:HB3	2.57	0.40
3:I:122:VAL:HG21	3:I:201:LEU:HD21	2.02	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	216/218 (99%)	204 (94%)	12 (6%)	0	100	100
1	D	216/218 (99%)	204 (94%)	11 (5%)	1 (0%)	24	55
1	G	216/218 (99%)	206 (95%)	10 (5%)	0	100	100
1	J	216/218 (99%)	203 (94%)	13 (6%)	0	100	100
1	M	216/218 (99%)	205 (95%)	11 (5%)	0	100	100
1	P	216/218 (99%)	198 (92%)	16 (7%)	2 (1%)	14	43
2	B	97/100 (97%)	93 (96%)	4 (4%)	0	100	100
2	E	97/100 (97%)	89 (92%)	6 (6%)	2 (2%)	5	27
2	H	97/100 (97%)	94 (97%)	2 (2%)	1 (1%)	12	41
2	K	97/100 (97%)	90 (93%)	5 (5%)	2 (2%)	5	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	97/100 (97%)	89 (92%)	6 (6%)	2 (2%)	5	27
2	Q	97/100 (97%)	87 (90%)	5 (5%)	5 (5%)	1	13
3	C	221/223 (99%)	207 (94%)	12 (5%)	2 (1%)	14	43
3	F	221/223 (99%)	207 (94%)	13 (6%)	1 (0%)	24	55
3	I	221/223 (99%)	204 (92%)	16 (7%)	1 (0%)	24	55
3	L	221/223 (99%)	204 (92%)	15 (7%)	2 (1%)	14	43
3	O	221/223 (99%)	211 (96%)	9 (4%)	1 (0%)	24	55
3	R	221/223 (99%)	207 (94%)	13 (6%)	1 (0%)	24	55
All	All	3204/3246 (99%)	3002 (94%)	179 (6%)	23 (1%)	18	48

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	63	ASN
2	H	58	ASN
2	N	62	GLN
2	Q	61	SER
2	Q	63	ASN
2	Q	64	ILE
2	Q	65	LEU
3	C	115	ARG
2	E	62	GLN
3	F	115	ARG
3	I	115	ARG
3	L	204	ASN
3	L	215	SER
2	N	63	ASN
3	R	115	ARG
3	O	115	ARG
2	K	58	ASN
1	P	78	ALA
2	Q	59	GLY
1	D	161	ASN
1	P	77	ARG
2	K	64	ILE
3	C	100	ILE

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	172/172 (100%)	172 (100%)	0	100	100
1	D	172/172 (100%)	168 (98%)	4 (2%)	44	61
1	G	172/172 (100%)	168 (98%)	4 (2%)	44	61
1	J	172/172 (100%)	170 (99%)	2 (1%)	63	70
1	M	172/172 (100%)	169 (98%)	3 (2%)	53	65
1	P	172/172 (100%)	168 (98%)	4 (2%)	44	61
2	B	92/92 (100%)	89 (97%)	3 (3%)	33	54
2	E	92/92 (100%)	88 (96%)	4 (4%)	26	49
2	H	92/92 (100%)	90 (98%)	2 (2%)	45	61
2	K	92/92 (100%)	87 (95%)	5 (5%)	20	44
2	N	92/92 (100%)	87 (95%)	5 (5%)	20	44
2	Q	92/92 (100%)	90 (98%)	2 (2%)	45	61
3	C	190/190 (100%)	186 (98%)	4 (2%)	47	62
3	F	190/190 (100%)	182 (96%)	8 (4%)	26	49
3	I	190/190 (100%)	186 (98%)	4 (2%)	47	62
3	L	190/190 (100%)	184 (97%)	6 (3%)	34	54
3	O	190/190 (100%)	183 (96%)	7 (4%)	30	52
3	R	190/190 (100%)	187 (98%)	3 (2%)	55	65
All	All	2724/2724 (100%)	2654 (97%)	70 (3%)	40	58

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	56	THR
2	B	65	LEU
2	B	118	ARG
3	C	74	ILE
3	C	126	ARG
3	C	128	GLN

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Mol	Chain	Res	Type
3	C	202	CYS
1	D	103	ILE
1	D	143	ARG
1	D	162	ARG
1	D	201	SER
2	E	60	THR
2	E	62	GLN
2	E	64	ILE
2	E	118	ARG
3	F	50	ARG
3	F	51	GLU
3	F	79	ASN
3	F	100	ILE
3	F	101	GLN
3	F	126	ARG
3	F	201	LEU
3	F	211	SER
1	G	44	VAL
1	G	48	LEU
1	G	105	GLU
1	G	146	ASN
2	H	57	VAL
2	H	58	ASN
3	I	79	ASN
3	I	126	ARG
3	I	128	GLN
3	I	205	VAL
1	J	160	ARG
1	J	201	SER
2	K	60	THR
2	K	62	GLN
2	K	64	ILE
2	K	67	SER
2	K	118	ARG
3	L	74	ILE
3	L	77	ARG
3	L	128	GLN
3	L	202	CYS
3	L	210	VAL
3	L	214	LYS
1	M	44	VAL
1	M	125	SER

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Mol	Chain	Res	Type
1	M	201	SER
2	N	60	THR
2	N	62	GLN
2	N	64	ILE
2	N	65	LEU
2	N	66	SER
3	O	74	ILE
3	O	94	GLN
3	O	100	ILE
3	O	101	GLN
3	O	129	GLU
3	O	201	LEU
3	O	230	LEU
1	P	48	LEU
1	P	81	VAL
1	P	192	ARG
1	P	201	SER
2	Q	58	ASN
2	Q	72	LYS
3	R	94	GLN
3	R	160	ARG
3	R	185	ARG

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	38	HIS
1	A	149	GLN
1	A	236	GLN
1	A	239	ASN
2	B	75	ASN
2	B	105	GLN
2	B	143	ASN
3	C	34	GLN
3	C	101	GLN
3	C	118	ASN
3	C	158	GLN
1	D	75	ASN
1	D	131	ASN
1	D	149	GLN
1	D	212	HIS
2	E	73	ASN

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Mol	Chain	Res	Type
3	F	75	GLN
3	F	118	ASN
1	G	129	ASN
2	H	75	ASN
3	I	25	HIS
3	I	34	GLN
3	I	102	ASN
3	I	120	ASN
3	I	158	GLN
3	I	166	GLN
1	J	38	HIS
1	J	115	ASN
2	K	62	GLN
2	K	71	ASN
2	K	92	ASN
3	L	34	GLN
3	L	101	GLN
3	L	102	ASN
3	L	118	ASN
3	L	158	GLN
1	M	149	GLN
1	M	208	ASN
2	N	71	ASN
3	O	34	GLN
3	O	94	GLN
3	O	108	GLN
3	O	116	ASN
3	O	158	GLN
3	O	166	GLN
1	P	38	HIS
1	P	131	ASN
1	P	212	HIS
1	P	236	GLN
3	R	34	GLN
3	R	75	GLN
3	R	79	ASN
3	R	108	GLN
3	R	166	GLN
3	R	203	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	218/218 (100%)	-0.54	0 100 100	59, 77, 100, 135	0
1	D	218/218 (100%)	-0.51	0 100 100	59, 79, 108, 138	0
1	G	218/218 (100%)	-0.45	0 100 100	65, 87, 119, 137	0
1	J	218/218 (100%)	-0.54	0 100 100	61, 79, 114, 140	0
1	M	218/218 (100%)	-0.55	0 100 100	69, 86, 110, 156	0
1	P	218/218 (100%)	-0.38	1 (0%) 87 67	81, 121, 161, 182	0
2	B	99/100 (99%)	-0.66	0 100 100	59, 73, 94, 105	0
2	E	99/100 (99%)	-0.54	1 (1%) 79 54	54, 80, 108, 160	0
2	H	99/100 (99%)	-0.57	0 100 100	63, 79, 102, 111	0
2	K	99/100 (99%)	-0.49	1 (1%) 79 54	64, 80, 104, 189	0
2	N	99/100 (99%)	-0.39	0 100 100	65, 82, 108, 161	0
2	Q	99/100 (99%)	-0.37	1 (1%) 79 54	65, 97, 127, 175	0
3	C	223/223 (100%)	-0.48	0 100 100	61, 89, 125, 145	0
3	F	223/223 (100%)	-0.45	0 100 100	79, 110, 155, 176	0
3	I	223/223 (100%)	-0.47	0 100 100	67, 96, 122, 150	0
3	L	223/223 (100%)	-0.37	0 100 100	78, 104, 141, 173	0
3	O	223/223 (100%)	-0.49	0 100 100	59, 87, 113, 143	0
3	R	223/223 (100%)	-0.44	0 100 100	83, 116, 150, 183	0
All	All	3240/3246 (99%)	-0.48	4 (0%) 92 86	54, 91, 137, 189	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	63	ASN	3.1
2	Q	58	ASN	2.8
1	P	235	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
2	E	59	GLY	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 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.