



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 03:21 AM EDT

PDB ID : 8D7I
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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

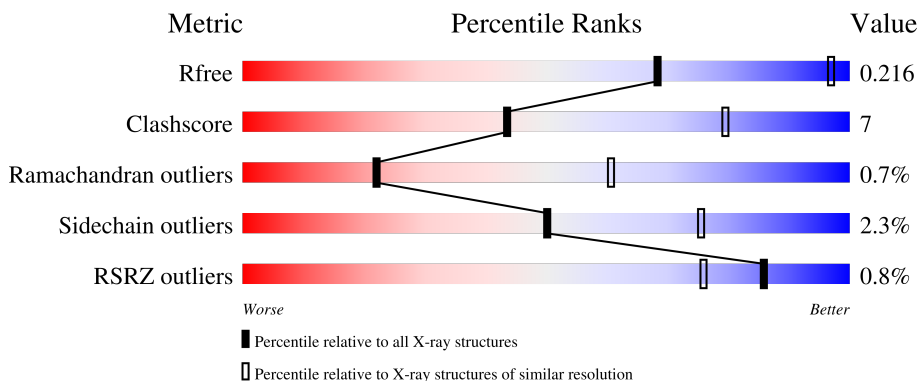
1 Overall quality at a glance

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}	130704	1341 (3.78-3.50)
Clashscore	141614	1439 (3.78-3.50)
Ramachandran outliers	138981	1391 (3.78-3.50)
Sidechain outliers	138945	1391 (3.78-3.50)
RSRZ outliers	127900	1242 (3.78-3.50)

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	218	88% 12%
1	D	218	88% 11%
1	G	218	85% 14%
1	J	218	88% 12%
1	M	218	86% 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	P	218	 2% 78% 21% .
2	B	100	 78% 21% .
2	E	100	 79% 17% ...
2	H	100	 76% 22% ..
2	K	100	 2% 82% 14% ...
2	N	100	 2% 79% 15% ...
2	Q	100	 % 73% 19% 7% .
3	C	223	 83% 16% .
3	F	223	 79% 20% .
3	I	223	 79% 20%
3	L	223	 2% 82% 17% .
3	O	223	 83% 15% .
3	R	223	 4% 82% 16% .

2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	A	218	Total 1635	C 1026	N 316	O 282	S 11	0	0	0
1	D	218	Total 1635	C 1026	N 316	O 282	S 11	0	0	0
1	G	218	Total 1635	C 1026	N 316	O 282	S 11	0	0	0
1	J	218	Total 1635	C 1026	N 316	O 282	S 11	0	0	0
1	M	218	Total 1635	C 1026	N 316	O 282	S 11	0	0	0
1	P	218	Total 1635	C 1026	N 316	O 282	S 11	0	0	0

- Molecule 2 is a protein called Extracellular Adherence Protein.

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

There are 18 discrepancies between the modelled and reference sequences:

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

Continued on next page...

Continued from previous page...

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
			Total	C	N	O	S			
3	C	223	1780	1093	369	308	10	0	0	0
3	F	223	1780	1093	369	308	10	0	0	0
3	I	223	1780	1093	369	308	10	0	0	0
3	L	223	1780	1093	369	308	10	0	0	0
3	O	223	1780	1093	369	308	10	0	0	0
3	R	223	1780	1093	369	308	10	0	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: Neutrophil elastase

Chain A:  88% 12%



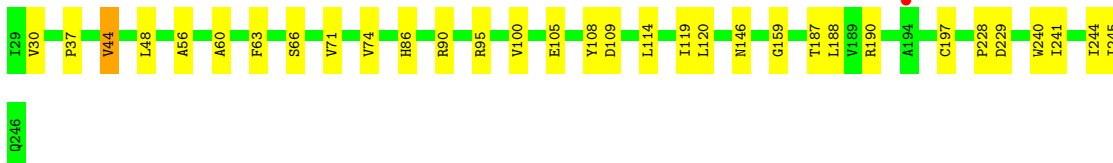
- Molecule 1: Neutrophil elastase

Chain D:  88% 11%




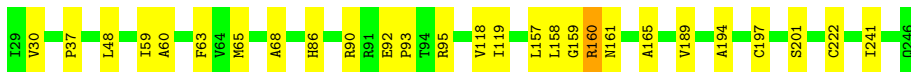
- Molecule 1: Neutrophil elastase

Chain G:  85% 14%




- Molecule 1: Neutrophil elastase

Chain J:  88% 12%



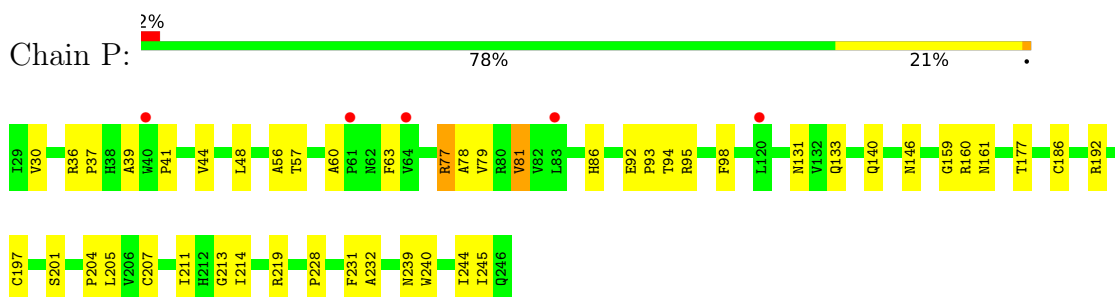
- Molecule 1: Neutrophil elastase

Chain M:  86% 14%

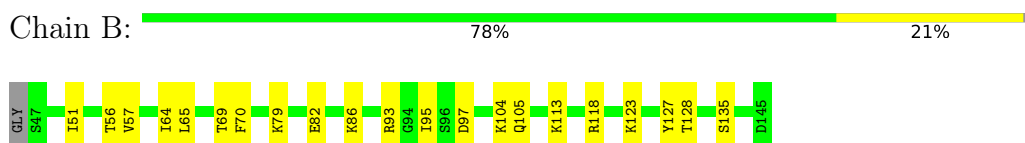


0246

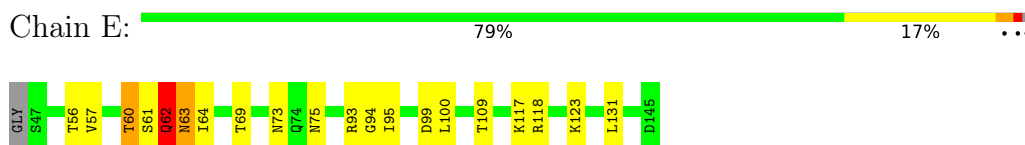
- Molecule 1: Neutrophil elastase



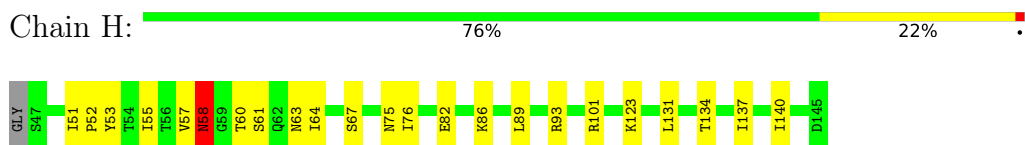
- Molecule 2: Extracellular Adherence Protein



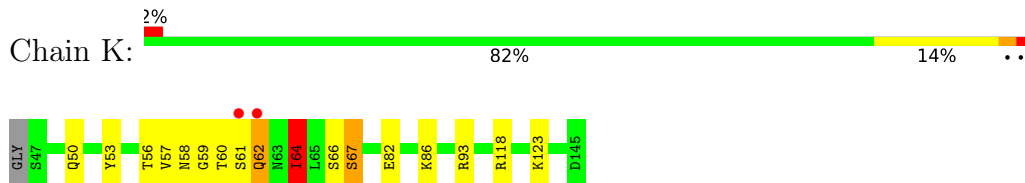
- Molecule 2: Extracellular Adherence Protein



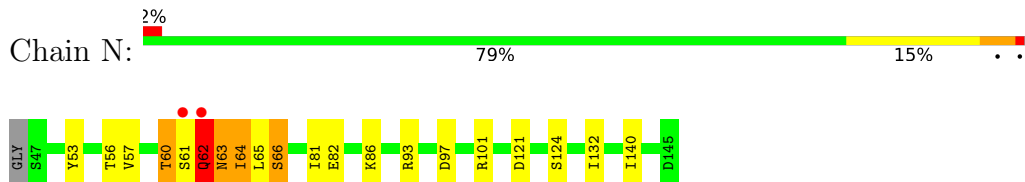
- Molecule 2: Extracellular Adherence Protein



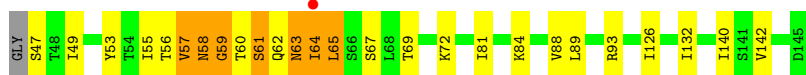
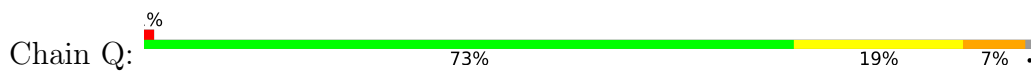
- Molecule 2: Extracellular Adherence Protein



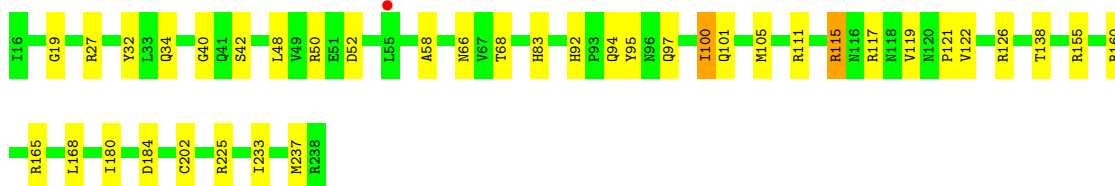
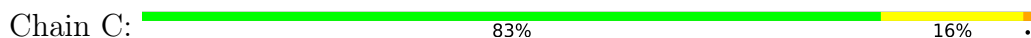
- Molecule 2: Extracellular Adherence Protein



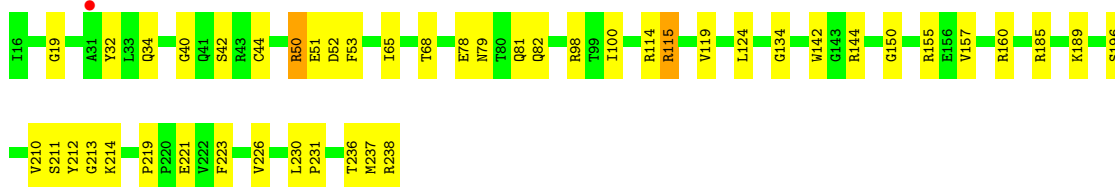
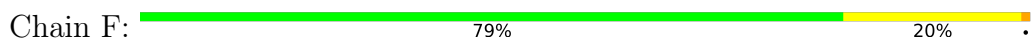
- Molecule 2: Extracellular Adherence Protein



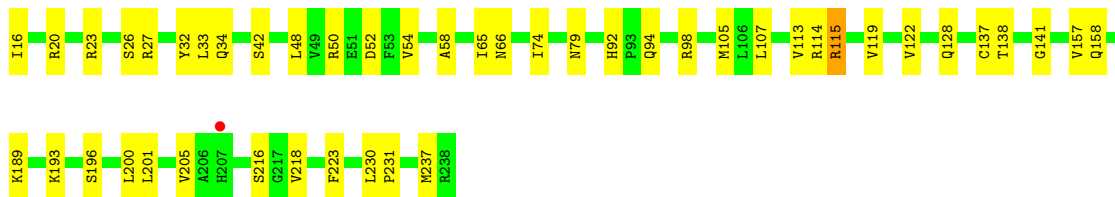
- Molecule 3: Cathepsin G, C-terminal truncated form



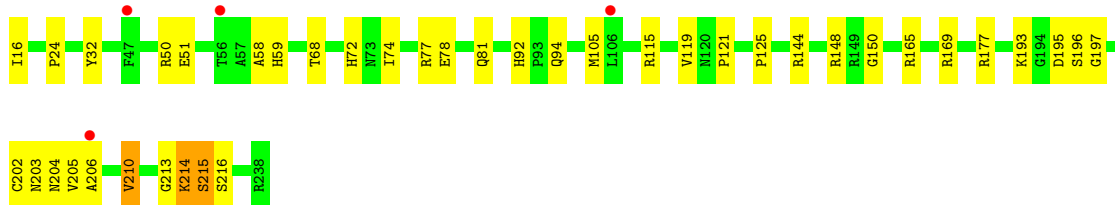
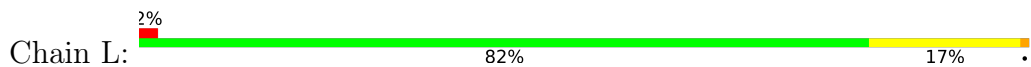
- Molecule 3: Cathepsin G, C-terminal truncated form




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



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




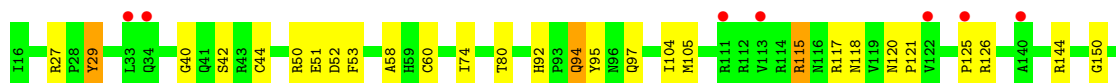
- Molecule 3: Cathepsin G, C-terminal truncated form

Chain O:  83% 15%



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

Chain R:  4% 82% 16%



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)	Xtrriage
Refinement program	PHENIX v1.9.2	Depositor
R, R_{free}	0.186 , 0.217 0.185 , 0.216	Depositor DCC
R_{free} test set	1998 reflections (3.90%)	wwPDB-VP
Wilson B-factor (Å ²)	84.5	Xtrriage
Anisotropy	0.539	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	25188	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtrriage'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	0.28	0/1665	0.57	0/2263
1	D	0.27	0/1665	0.56	0/2263
1	G	0.26	0/1665	0.56	0/2263
1	J	0.27	0/1665	0.58	0/2263
1	M	0.27	0/1665	0.56	0/2263
1	P	0.28	0/1665	0.57	0/2263
2	B	0.25	0/792	0.49	0/1071
2	E	0.26	0/792	0.48	0/1071
2	H	0.25	0/792	0.50	0/1071
2	K	0.26	0/792	0.49	0/1071
2	N	0.27	0/792	0.52	0/1071
2	Q	0.27	0/792	0.60	1/1071 (0.1%)
3	C	0.27	0/1814	0.61	0/2447
3	F	0.26	0/1814	0.63	0/2447
3	I	0.27	0/1814	0.63	0/2447
3	L	0.27	0/1814	0.62	0/2447
3	O	0.26	0/1814	0.61	0/2447
3	R	0.27	0/1814	0.63	0/2447
All	All	0.27	0/25626	0.58	1/34686 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	57	VAL	N-CA-C	-6.21	94.23	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1635	0	1652	15	0
1	D	1635	0	1652	18	0
1	G	1635	0	1652	17	0
1	J	1635	0	1652	15	0
1	M	1635	0	1652	20	0
1	P	1635	0	1652	30	0
2	B	783	0	801	14	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	14	0
2	Q	783	0	801	23	0
3	C	1780	0	1793	22	0
3	F	1780	0	1793	32	0
3	I	1780	0	1793	27	0
3	L	1780	0	1793	29	0
3	O	1780	0	1793	26	0
3	R	1780	0	1793	27	0
All	All	25188	0	25476	338	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 (338) 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

Continued on next page...

Continued from previous page...

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: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
2:K:82:GLU:HG2	2:K:86:LYS:HD3	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:I:92:HIS:CE1	3:I:94:GLN:HG2	2.41	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
2:K:61:SER:H	3:L:213:GLY:C	2.10	0.55
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
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
2:E:61:SER:HB2	3:F:214:LYS:C	2.29	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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:E:61:SER:C	2:E:63:ASN:H	2.13	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:K:61:SER:HB2	3:L:214:LYS:C	2.36	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: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
2:Q:47:SER:N	2:Q:72:LYS:HZ2	2.15	0.45
3:F:32:TYR:HB3	3:F:68:THR:HB	1.97	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
3:R:50:ARG:C	3:R:52:ASP:H	2.20	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
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:62:ASN:OD1	1:M:62:ASN:N	2.50	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: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
2:Q:61:SER:C	2:Q:63:ASN:H	2.21	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
2:Q:59:GLY:C	2:Q:61:SER:H	2.21	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
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
3:C:48:LEU:O	3:C:122:VAL:HG12	2.21	0.41
3:F:236:THR:C	3:F:238:ARG:H	2.23	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:122:VAL:HG21	3:I:201:LEU:HD21	2.02	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	216/218 (99%)	204 (94%)	12 (6%)	0	100	100
1	D	216/218 (99%)	204 (94%)	11 (5%)	1 (0%)	29	67
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%)	17	56
2	B	97/100 (97%)	93 (96%)	4 (4%)	0	100	100
2	E	97/100 (97%)	89 (92%)	6 (6%)	2 (2%)	7	39
2	H	97/100 (97%)	94 (97%)	2 (2%)	1 (1%)	15	54
2	K	97/100 (97%)	90 (93%)	5 (5%)	2 (2%)	7	39
2	N	97/100 (97%)	89 (92%)	6 (6%)	2 (2%)	7	39
2	Q	97/100 (97%)	87 (90%)	5 (5%)	5 (5%)	2	19
3	C	221/223 (99%)	207 (94%)	12 (5%)	2 (1%)	17	56
3	F	221/223 (99%)	207 (94%)	13 (6%)	1 (0%)	29	67
3	I	221/223 (99%)	204 (92%)	16 (7%)	1 (0%)	29	67
3	L	221/223 (99%)	204 (92%)	15 (7%)	2 (1%)	17	56
3	O	221/223 (99%)	211 (96%)	9 (4%)	1 (0%)	29	67
3	R	221/223 (99%)	207 (94%)	13 (6%)	1 (0%)	29	67
All	All	3204/3246 (99%)	3002 (94%)	179 (6%)	23 (1%)	22	61

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 [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	172/172 (100%)	172 (100%)	0	100	100
1	D	172/172 (100%)	169 (98%)	3 (2%)	60	81
1	G	172/172 (100%)	167 (97%)	5 (3%)	42	71
1	J	172/172 (100%)	169 (98%)	3 (2%)	60	81
1	M	172/172 (100%)	169 (98%)	3 (2%)	60	81
1	P	172/172 (100%)	167 (97%)	5 (3%)	42	71

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	92/92 (100%)	89 (97%)	3 (3%)	38	68
2	E	92/92 (100%)	89 (97%)	3 (3%)	38	68
2	H	92/92 (100%)	91 (99%)	1 (1%)	73	87
2	K	92/92 (100%)	87 (95%)	5 (5%)	22	56
2	N	92/92 (100%)	87 (95%)	5 (5%)	22	56
2	Q	92/92 (100%)	91 (99%)	1 (1%)	73	87
3	C	190/190 (100%)	187 (98%)	3 (2%)	62	82
3	F	190/190 (100%)	186 (98%)	4 (2%)	53	77
3	I	190/190 (100%)	187 (98%)	3 (2%)	62	82
3	L	190/190 (100%)	185 (97%)	5 (3%)	46	73
3	O	190/190 (100%)	185 (97%)	5 (3%)	46	73
3	R	190/190 (100%)	185 (97%)	5 (3%)	46	73
All	All	2724/2724 (100%)	2662 (98%)	62 (2%)	50	75

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	56	THR
2	B	65	LEU
2	B	97	ASP
3	C	117	ARG
3	C	126	ARG
3	C	202	CYS
1	D	143	ARG
1	D	162	ARG
1	D	201	SER
2	E	60	THR
2	E	62	GLN
2	E	118	ARG
3	F	50	ARG
3	F	51	GLU
3	F	79	ASN
3	F	211	SER
1	G	44	VAL
1	G	48	LEU
1	G	105	GLU
1	G	146	ASN
1	G	190	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	58	ASN
3	I	79	ASN
3	I	128	GLN
3	I	205	VAL
1	J	48	LEU
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	77	ARG
3	L	148	ARG
3	L	202	CYS
3	L	210	VAL
3	L	214	LYS
1	M	44	VAL
1	M	125	SER
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	94	GLN
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	93	PRO
1	P	192	ARG
1	P	201	SER
2	Q	58	ASN
3	R	29	TYR
3	R	94	GLN
3	R	120	ASN
3	R	160	ARG
3	R	185	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such

sidechains are listed below:

Mol	Chain	Res	Type
1	D	131	ASN
3	I	102	ASN
2	K	62	GLN
3	L	118	ASN
3	O	116	ASN
1	P	140	GLN

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 monosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	0.06	0 100 100	59, 77, 100, 135	0
1	D	218/218 (100%)	0.09	0 100 100	59, 79, 108, 138	0
1	G	218/218 (100%)	0.14	1 (0%) 91 84	65, 87, 119, 137	0
1	J	218/218 (100%)	0.08	0 100 100	61, 79, 114, 140	0
1	M	218/218 (100%)	0.10	1 (0%) 91 84	69, 86, 110, 156	0
1	P	218/218 (100%)	0.34	5 (2%) 60 44	81, 121, 161, 182	0
2	B	99/100 (99%)	0.03	0 100 100	59, 73, 94, 105	0
2	E	99/100 (99%)	0.15	0 100 100	54, 80, 108, 160	0
2	H	99/100 (99%)	0.15	0 100 100	63, 79, 102, 111	0
2	K	99/100 (99%)	0.20	2 (2%) 65 50	64, 80, 104, 189	0
2	N	99/100 (99%)	0.23	2 (2%) 65 50	65, 82, 108, 161	0
2	Q	99/100 (99%)	0.16	1 (1%) 82 71	65, 97, 127, 175	0
3	C	223/223 (100%)	0.10	1 (0%) 92 87	61, 89, 125, 145	0
3	F	223/223 (100%)	0.20	1 (0%) 92 87	79, 110, 155, 176	0
3	I	223/223 (100%)	0.17	1 (0%) 92 87	67, 96, 122, 150	0
3	L	223/223 (100%)	0.29	4 (1%) 68 53	78, 104, 141, 173	0
3	O	223/223 (100%)	0.15	0 100 100	59, 87, 113, 143	0
3	R	223/223 (100%)	0.32	8 (3%) 42 29	83, 116, 150, 183	0
All	All	3240/3246 (99%)	0.17	27 (0%) 86 76	54, 91, 137, 189	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	64	VAL	3.5
2	K	62	GLN	3.4
2	N	61	SER	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	R	125	PRO	3.0
3	L	56	THR	2.9
2	K	61	SER	2.8
2	N	62	GLN	2.7
3	R	140	ALA	2.6
3	R	122	VAL	2.5
3	I	207	HIS	2.4
3	R	113	VAL	2.3
1	P	120	LEU	2.3
1	P	83	LEU	2.3
1	P	61	PRO	2.2
2	Q	64	ILE	2.2
3	L	106	LEU	2.2
3	F	31	ALA	2.2
3	R	207	HIS	2.1
3	R	34	GLN	2.1
1	M	211	ILE	2.1
1	P	40	TRP	2.1
1	G	194	ALA	2.0
3	L	47	PHE	2.0
3	R	33	LEU	2.0
3	L	206	ALA	2.0
3	C	55	LEU	2.0
3	R	111	ARG	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 monosaccharides 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.