



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 15, 2026 – 04:07 PM EDT

PDB ID : 9OMD / pdb_00009omd
Title : Crystal structure of Protease IV in complex with its propeptide
Authors : Neupane, T.; Daboor, S.; Cheng, Z.; Langelaan, D.N.
Deposited on : 2025-05-13
Resolution : 3.30 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

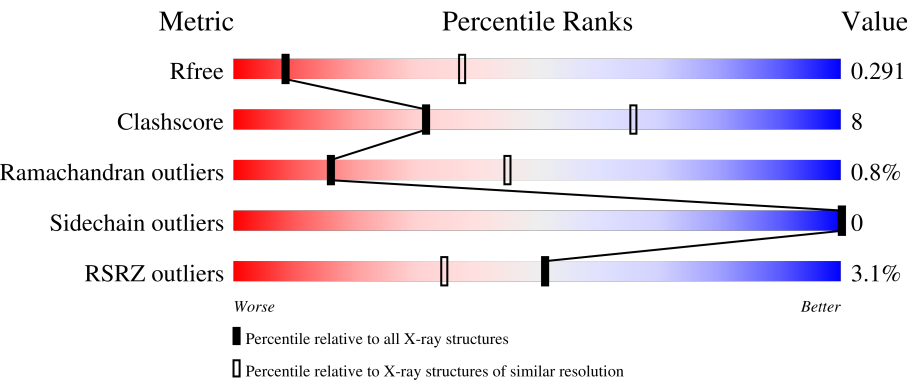
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	251	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>82%18%</div></div>
1	B	251	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>82%17%</div><div></div></div>
1	C	251	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>82%18%</div></div>
1	D	251	<div><div>5%</div><div><div></div><div></div><div></div><div></div></div><div>76%21%</div><div></div></div>
1	E	251	<div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>80%19%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	251	
1	G	251	
1	H	251	
2	I	186	
2	J	186	
2	K	186	
2	L	186	
2	M	186	
2	N	186	
2	O	186	
2	P	186	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23795 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 Lysyl endopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1852	1150	326	369	7			
1	B	249	Total	C	N	O	S	0	0	0
			1845	1145	325	368	7			
1	C	250	Total	C	N	O	S	0	0	0
			1852	1150	326	369	7			
1	D	244	Total	C	N	O	S	0	0	0
			1805	1120	318	360	7			
1	E	250	Total	C	N	O	S	0	0	0
			1852	1150	326	369	7			
1	F	234	Total	C	N	O	S	0	0	0
			1749	1090	307	345	7			
1	G	247	Total	C	N	O	S	0	0	0
			1826	1136	320	363	7			
1	H	145	Total	C	N	O	S	0	0	0
			1052	647	187	213	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	198	ALA	SER	engineered mutation	UNP Q02SZ7
B	198	ALA	SER	engineered mutation	UNP Q02SZ7
C	198	ALA	SER	engineered mutation	UNP Q02SZ7
D	198	ALA	SER	engineered mutation	UNP Q02SZ7
E	198	ALA	SER	engineered mutation	UNP Q02SZ7
F	198	ALA	SER	engineered mutation	UNP Q02SZ7
G	198	ALA	SER	engineered mutation	UNP Q02SZ7
H	198	ALA	SER	engineered mutation	UNP Q02SZ7

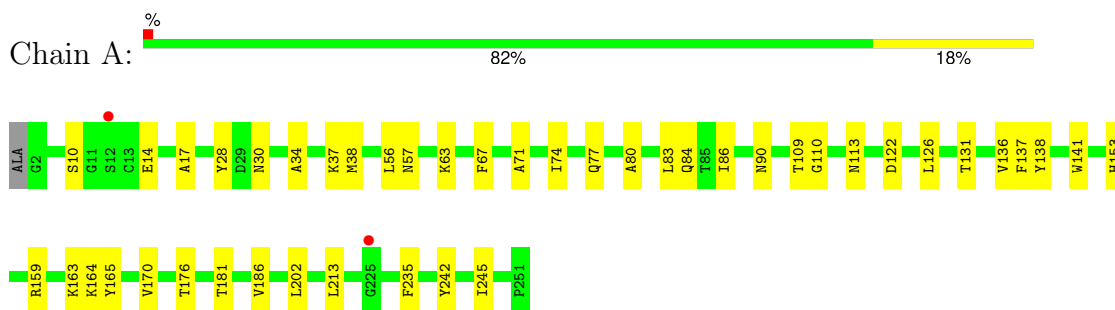
- Molecule 2 is a protein called Lysyl endopeptidase propeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	172	Total	C	N	O	S	0	0	0
			1273	806	225	241	1			
2	J	170	Total	C	N	O	S	0	0	0
			1263	800	223	239	1			
2	K	168	Total	C	N	O		0	0	0
			1248	792	221	235				
2	L	166	Total	C	N	O		0	0	0
			1231	782	217	232				
2	M	167	Total	C	N	O	S	0	0	0
			1238	785	218	234	1			
2	N	173	Total	C	N	O	S	0	0	0
			1282	811	226	244	1			
2	O	164	Total	C	N	O		0	0	0
			1210	769	210	231				
2	P	165	Total	C	N	O		0	0	0
			1217	774	211	232				

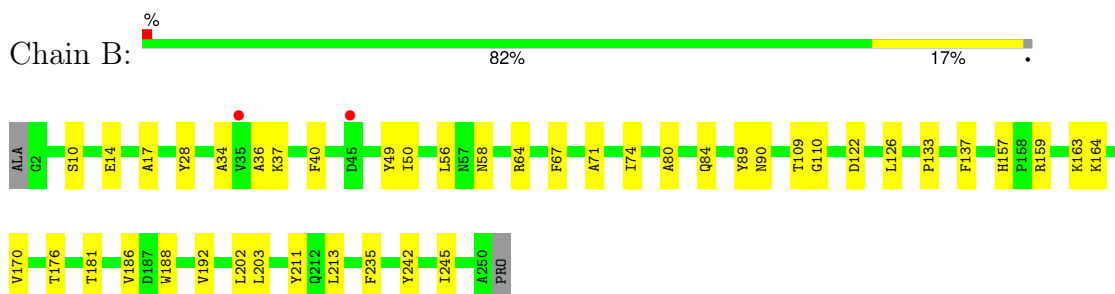
3 Residue-property plots [i](#)

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.

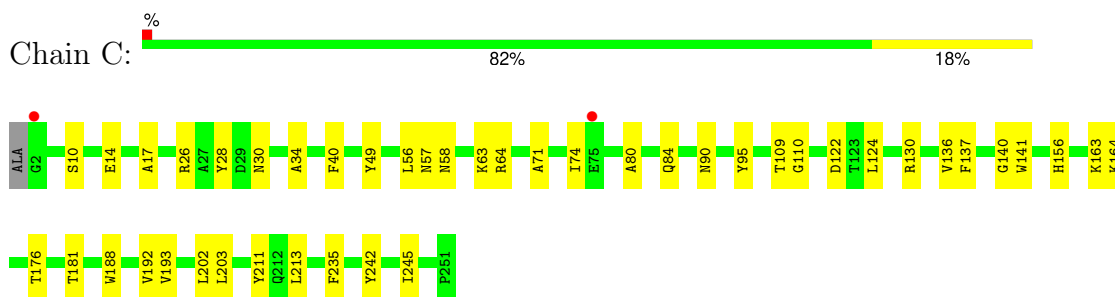
- Molecule 1: Lysyl endopeptidase



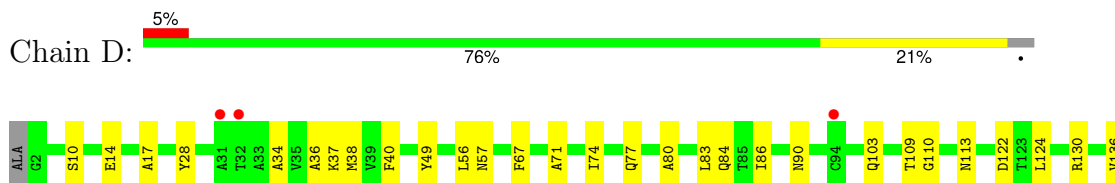
- Molecule 1: Lysyl endopeptidase

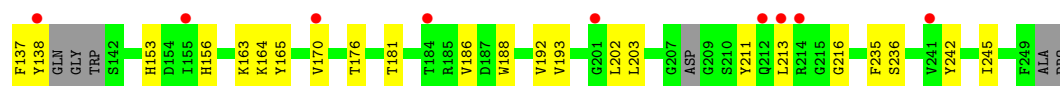


- Molecule 1: Lysyl endopeptidase

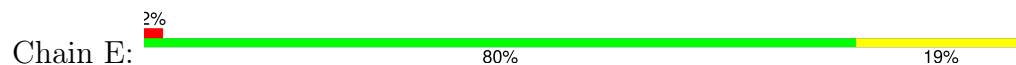


- Molecule 1: Lysyl endopeptidase

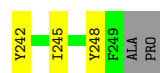
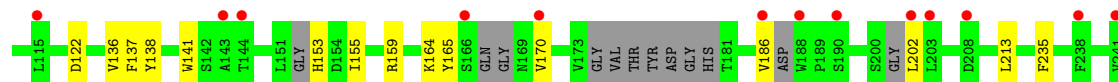
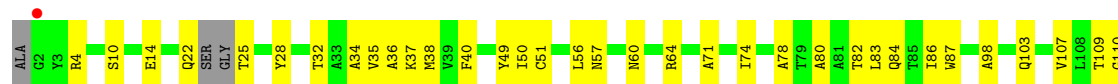




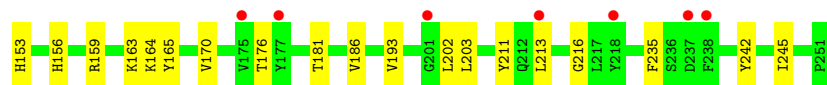
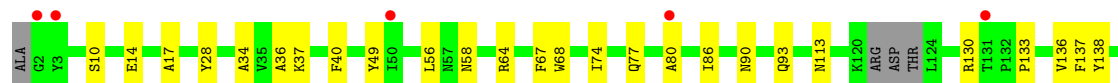
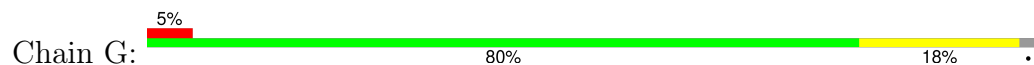
- Molecule 1: Lysyl endopeptidase



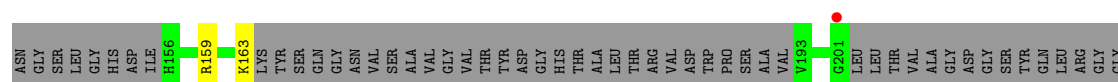
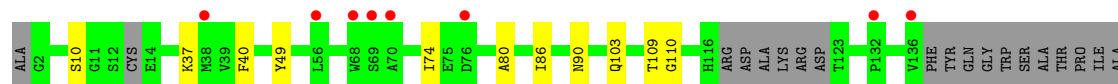
- Molecule 1: Lysyl endopeptidase



- Molecule 1: Lysyl endopeptidase



- Molecule 1: Lysyl endopeptidase



LEU TYR GLY GLY PRO SER TYR CYS GLY ALA PRO THR SER GLN ARG ASN ASP TYR PHE SER ASP PHE SER SER VAL TYR SER GLN ILE SER ARG TYR PHE ALA PRO

• Molecule 2: Lysyl endopeptidase propeptide



PRO GLY ALA SER GLU M31 A32 G33 D34 V35 A36 V37 I38 Q39 A40 S44 H63 F64 A65 A66 P67 A69 R70 R71 VAL ARG ALA ALA PRO LEU ALA PRO K81 I99 S121 R129 R133 R137 D144 V145 L146 L147 F148 F149 A150 G151 E155 R168

P169 V174 I175 L180 E183 L184 V185 L186 P187 Q191 P192 R196 V199 P200 K211

• Molecule 2: Lysyl endopeptidase propeptide



PRO GLY ALA SER GLU M31 A32 G33 D34 V35 A36 V37 I38 Q39 A40 S44 A43 N52 A55 S58 ALA A61 G61 I62 H63 P67 P68 A69 R70 R71 VAL ALA ARG ALA ALA PRO LEU ALA PRO K81 E98 I99 T115 A116 R117 A122 R129 R137 D144

H148 G151 E155 R168 P169 V174 I175 L180 E183 L184 P187 Q191 P192 R196 V199 S208 K211

• Molecule 2: Lysyl endopeptidase propeptide



PRO GLY ALA SER MET GLU ALA GLY ASP V35 A36 V37 S41 A42 A43 S44 T45 G46 N52 H63 P67 P68 A69 R70 R71 VAL ARG ALA ALA PRO K81 L92 E98 I99 T115 S121 I128 R129 A130 R133 L134 F135 T136 G139

P142 D143 D144 L147 H148 E155 I156 F157 E158 L164 P169 V174 I175 L180 P187 L190 Q191 P192 R196 V199 P200 Y210 K211

• Molecule 2: Lysyl endopeptidase propeptide

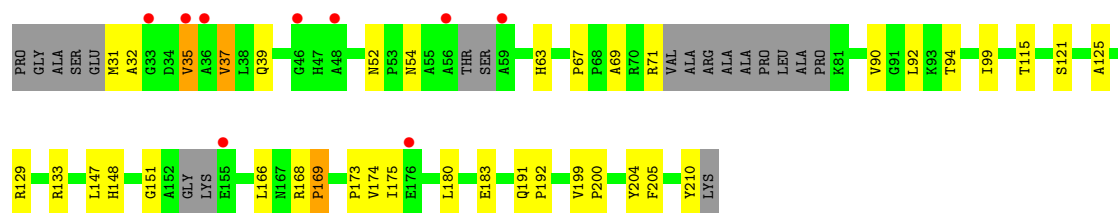


PRO GLY ALA SER MET GLU ALA GLY ASP V35 A36 V37 A46 N52 A65 P68 A69 R70 R71 VAL ARG ALA ALA PRO LEU ALA PRO LYS P82 I99 D108 D111 G112 R113 H114 T115 R129 A130 A131 I132 R133 R137 S138 P142 D143 D144 V145 L146 L147

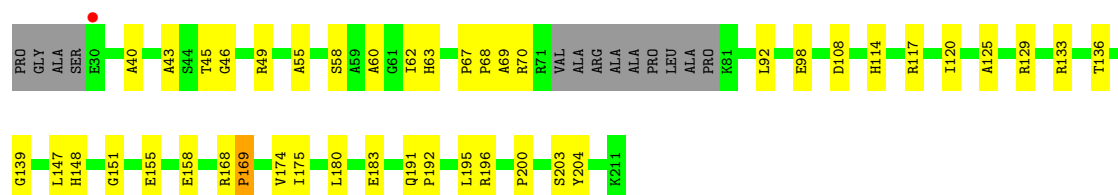
H148 F149 G151 E155 L166 ASN R168 P169 P173 V174 I175 L180 E183 L184 V185 L186 P187 L197 S198 V199 P200 L209 Y210 K211

• Molecule 2: Lysyl endopeptidase propeptide

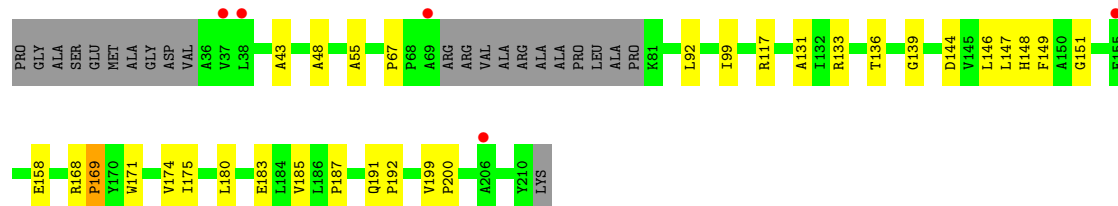




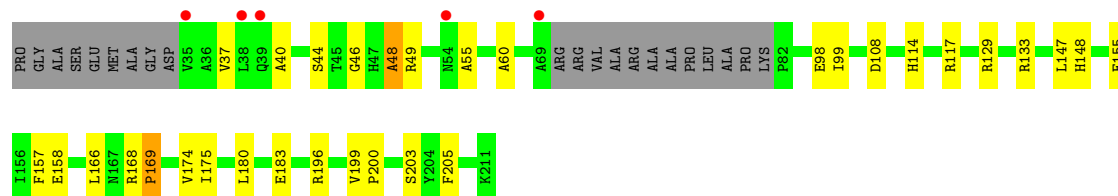
• Molecule 2: Lysyl endopeptidase propeptide



• Molecule 2: Lysyl endopeptidase propeptide



• Molecule 2: Lysyl endopeptidase propeptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	192.12Å 192.12Å 231.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.41 – 3.30 48.41 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.41-3.30) 95.9 (48.41-3.30)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.65 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.262 , 0.291 0.262 , 0.291	Depositor DCC
R_{free} test set	2000 reflections (1.95%)	wwPDB-VP
Wilson B-factor (Å ²)	71.5	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	23795	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.26% 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	0.07	0/1896	0.20	0/2582
1	B	0.06	0/1888	0.19	0/2570
1	C	0.07	0/1896	0.20	0/2582
1	D	0.06	0/1844	0.18	0/2506
1	E	0.07	0/1896	0.20	0/2582
1	F	0.06	0/1784	0.19	0/2420
1	G	0.06	0/1869	0.19	0/2544
1	H	0.06	0/1068	0.17	0/1447
2	I	0.12	0/1303	0.33	0/1780
2	J	0.14	0/1292	0.37	0/1763
2	K	0.11	0/1278	0.33	0/1747
2	L	0.16	0/1260	0.36	0/1721
2	M	0.12	0/1266	0.38	0/1729
2	N	0.10	0/1312	0.31	0/1792
2	O	0.12	0/1240	0.36	0/1698
2	P	0.11	0/1247	0.32	0/1707
All	All	0.09	0/24339	0.27	0/33170

There are no bond length outliers.

There are no bond angle outliers.

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	1852	0	1737	35	0
1	B	1845	0	1730	25	0
1	C	1852	0	1737	30	0
1	D	1805	0	1698	32	0
1	E	1852	0	1737	35	0
1	F	1749	0	1648	33	0
1	G	1826	0	1712	29	0
1	H	1052	0	994	7	0
2	I	1273	0	1269	29	0
2	J	1263	0	1258	26	0
2	K	1248	0	1248	25	0
2	L	1231	0	1229	28	0
2	M	1238	0	1226	31	0
2	N	1282	0	1275	29	0
2	O	1210	0	1200	17	0
2	P	1217	0	1210	25	0
All	All	23795	0	22908	378	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 8.

All (378) 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:C:140:GLY:HA2	2:I:33:GLY:HA3	1.61	0.82
1:B:37:LYS:HE3	1:B:50:ILE:HD11	1.64	0.79
2:M:71:ARG:HD3	2:M:90:VAL:HG11	1.64	0.78
1:C:95:TYR:HB2	2:J:70:ARG:HG2	1.67	0.76
1:A:159:ARG:HH21	2:M:210:TYR:HA	1.51	0.74
1:E:130:ARG:HH21	2:J:41:SER:HB2	1.55	0.72
1:A:131:THR:HG21	2:M:39:GLN:HB2	1.72	0.70
2:L:68:PRO:O	2:L:70:ARG:N	2.26	0.69
1:H:103:GLN:NE2	2:J:151:GLY:O	2.27	0.68
1:C:130:ARG:HG2	2:I:44:SER:HB3	1.75	0.67
1:C:34:ALA:HB2	1:C:137:PHE:HB3	1.78	0.66
1:A:77:GLN:HE22	1:A:113:ASN:HA	1.61	0.66
1:D:77:GLN:HE22	1:D:113:ASN:HA	1.60	0.65
2:K:68:PRO:O	2:K:70:ARG:N	2.30	0.64
1:C:57:ASN:HD22	2:I:33:GLY:HA2	1.63	0.64
1:E:34:ALA:HB2	1:E:137:PHE:HB3	1.79	0.64
2:I:39:GLN:HG3	2:I:40:ALA:H	1.63	0.63
1:F:103:GLN:NE2	2:I:151:GLY:O	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:34:ALA:HB2	1:F:137:PHE:HB3	1.81	0.62
2:P:55:ALA:HB3	2:P:117:ARG:HH11	1.64	0.62
1:E:77:GLN:HE22	1:E:113:ASN:HA	1.65	0.62
1:G:93:GLN:HG3	2:I:70:ARG:HH12	1.64	0.62
2:K:147:LEU:HD12	2:K:164:LEU:HD21	1.81	0.62
2:M:133:ARG:HH21	2:M:200:PRO:HG3	1.64	0.61
1:C:63:LYS:HE3	2:I:35:VAL:HG21	1.82	0.61
2:I:133:ARG:HH21	2:I:200:PRO:HG3	1.67	0.60
2:J:67:PRO:HG2	2:J:71:ARG:HE	1.68	0.59
1:A:34:ALA:HB2	1:A:137:PHE:HB3	1.85	0.59
2:M:52:ASN:HB2	2:M:115:THR:HG21	1.84	0.59
2:O:99:ILE:HD11	2:O:199:VAL:HG12	1.84	0.59
2:P:148:HIS:HB2	2:P:183:GLU:HB3	1.83	0.59
2:I:63:HIS:ND1	2:I:121:SER:OG	2.36	0.59
2:N:43:ALA:HB1	2:N:158:GLU:HB3	1.83	0.59
1:B:242:TYR:HA	1:B:245:ILE:HG12	1.85	0.58
2:J:31:MET:HG3	2:J:33:GLY:H	1.68	0.58
1:D:84:GLN:HE22	2:K:174:VAL:H	1.51	0.58
1:E:138:TYR:CE2	2:J:37:VAL:HG22	2.39	0.58
2:L:71:ARG:HD2	2:L:209:LEU:HD11	1.85	0.58
2:M:129:ARG:HD2	2:M:174:VAL:HG12	1.84	0.58
2:N:98:GLU:OE2	2:N:196:ARG:NH1	2.37	0.58
2:O:55:ALA:HB3	2:O:117:ARG:HH11	1.69	0.58
2:K:175:ILE:HG13	2:K:180:LEU:HD13	1.86	0.58
1:B:34:ALA:HB2	1:B:137:PHE:HB3	1.86	0.58
1:C:140:GLY:CA	2:I:33:GLY:HA3	2.34	0.57
1:D:34:ALA:HB2	1:D:137:PHE:HB3	1.86	0.57
1:G:77:GLN:HE22	1:G:113:ASN:HA	1.69	0.57
2:N:55:ALA:HB3	2:N:117:ARG:HH11	1.67	0.57
2:N:175:ILE:HG13	2:N:180:LEU:HD13	1.86	0.57
1:F:38:MET:HB3	1:F:83:LEU:HD11	1.86	0.57
2:L:151:GLY:H	2:L:175:ILE:HD12	1.69	0.57
2:P:175:ILE:HG13	2:P:180:LEU:HD13	1.87	0.57
2:J:98:GLU:OE2	2:J:196:ARG:NH1	2.37	0.57
2:L:52:ASN:HB2	2:L:115:THR:HG21	1.87	0.57
1:A:71:ALA:N	1:A:122:ASP:OD1	2.39	0.56
1:B:71:ALA:N	1:B:122:ASP:OD1	2.38	0.56
2:I:67:PRO:O	2:I:71:ARG:NH2	2.38	0.56
2:P:108:ASP:OD1	2:P:114:HIS:ND1	2.34	0.56
1:A:242:TYR:HA	1:A:245:ILE:HG12	1.88	0.56
1:D:56:LEU:HD21	1:D:213:LEU:HD22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:ILE:HG21	1:B:80:ALA:HB2	1.88	0.56
1:F:84:GLN:HE22	2:L:173:PRO:HB3	1.71	0.56
1:B:14:GLU:HB3	1:B:164:LYS:HG2	1.87	0.55
1:D:203:LEU:HB3	1:D:211:TYR:HB3	1.88	0.55
2:J:52:ASN:HB2	2:J:115:THR:HG21	1.88	0.55
1:A:14:GLU:HB3	1:A:164:LYS:HG2	1.89	0.55
1:D:103:GLN:NE2	2:M:151:GLY:O	2.40	0.55
2:M:148:HIS:HB2	2:M:183:GLU:HB3	1.89	0.55
1:E:137:PHE:CZ	2:J:34:ASP:HA	2.42	0.55
2:L:99:ILE:HD11	2:L:199:VAL:HG12	1.88	0.55
1:D:242:TYR:HA	1:D:245:ILE:HG12	1.89	0.55
1:E:242:TYR:HA	1:E:245:ILE:HG12	1.88	0.55
1:F:86:ILE:HG13	1:F:107:VAL:HG22	1.89	0.55
1:A:138:TYR:CE2	2:M:37:VAL:HG22	2.41	0.54
1:D:170:VAL:HA	1:D:186:VAL:HA	1.89	0.54
1:A:84:GLN:HE22	2:M:173:PRO:HA	1.71	0.54
2:N:67:PRO:HG3	2:N:92:LEU:HD21	1.90	0.54
2:O:136:THR:OG1	2:O:139:GLY:O	2.23	0.54
1:C:14:GLU:HB3	1:C:164:LYS:HG2	1.90	0.54
1:D:14:GLU:HB3	1:D:164:LYS:HG2	1.90	0.54
1:G:136:VAL:HG23	2:P:37:VAL:HG21	1.90	0.54
1:C:84:GLN:NE2	2:I:174:VAL:H	2.06	0.54
1:F:136:VAL:HG23	2:L:37:VAL:HG21	1.90	0.54
2:L:175:ILE:HG13	2:L:180:LEU:HD13	1.89	0.54
2:P:55:ALA:HB3	2:P:117:ARG:NH1	2.23	0.54
1:D:71:ALA:N	1:D:122:ASP:OD1	2.40	0.53
1:D:74:ILE:HG21	1:D:80:ALA:HB2	1.89	0.53
2:L:129:ARG:HD2	2:L:174:VAL:HG12	1.90	0.53
2:I:129:ARG:HD2	2:I:174:VAL:HG12	1.91	0.53
2:M:67:PRO:HB3	2:M:92:LEU:HD21	1.90	0.53
2:O:55:ALA:HB3	2:O:117:ARG:NH1	2.24	0.53
2:P:98:GLU:OE2	2:P:196:ARG:NH1	2.41	0.53
1:A:176:THR:HG22	1:A:181:THR:HA	1.89	0.53
1:A:109:THR:HG21	2:M:173:PRO:HG3	1.90	0.53
2:I:168:ARG:HB3	2:I:169:PRO:HD3	1.91	0.53
2:J:148:HIS:HB2	2:J:183:GLU:HB3	1.90	0.53
1:D:84:GLN:NE2	2:K:174:VAL:H	2.06	0.53
1:E:77:GLN:NE2	1:E:113:ASN:OD1	2.41	0.53
2:K:155:GLU:HB2	2:K:157:PHE:CZ	2.43	0.53
2:N:168:ARG:HB3	2:N:169:PRO:HD3	1.91	0.53
1:F:138:TYR:CE2	2:L:37:VAL:HG22	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:17:ALA:O	1:G:28:TYR:OH	2.26	0.53
1:E:71:ALA:N	1:E:122:ASP:OD1	2.40	0.53
2:K:52:ASN:HB2	2:K:115:THR:HG21	1.91	0.52
1:G:56:LEU:HD21	1:G:213:LEU:HD22	1.91	0.52
1:C:242:TYR:HA	1:C:245:ILE:HG12	1.90	0.52
2:J:168:ARG:HB2	2:J:169:PRO:HD3	1.90	0.52
1:B:56:LEU:HD21	1:B:213:LEU:HD22	1.91	0.52
1:F:71:ALA:N	1:F:122:ASP:OD1	2.41	0.52
1:F:242:TYR:HA	1:F:245:ILE:HG12	1.90	0.52
2:M:35:VAL:HG12	2:M:37:VAL:H	1.73	0.52
2:M:168:ARG:HB3	2:M:169:PRO:HD3	1.91	0.52
1:F:60:ASN:ND2	1:F:248:TYR:O	2.40	0.52
2:N:46:GLY:HA3	2:N:155:GLU:HG3	1.92	0.52
1:C:74:ILE:HG21	1:C:80:ALA:HB2	1.90	0.52
1:F:14:GLU:HB3	1:F:164:LYS:HG2	1.92	0.52
1:F:74:ILE:HG21	1:F:80:ALA:HB2	1.92	0.52
1:G:242:TYR:HA	1:G:245:ILE:HG12	1.92	0.52
2:L:142:PRO:HG2	2:L:145:VAL:HG23	1.90	0.52
2:O:133:ARG:HH21	2:O:200:PRO:HG3	1.75	0.51
1:E:10:SER:HB2	1:E:14:GLU:HG3	1.91	0.51
2:O:168:ARG:HB3	2:O:169:PRO:HD3	1.93	0.51
1:D:153:HIS:HB3	1:D:165:TYR:HE1	1.76	0.51
2:N:133:ARG:HH21	2:N:200:PRO:HG3	1.73	0.51
1:C:203:LEU:HB3	1:C:211:TYR:HB3	1.92	0.51
1:G:93:GLN:HB2	2:I:70:ARG:HH22	1.76	0.51
1:A:159:ARG:NH2	2:M:210:TYR:HA	2.23	0.50
1:C:84:GLN:HE22	2:I:174:VAL:H	1.58	0.50
1:A:109:THR:HG22	1:A:110:GLY:H	1.75	0.50
2:L:151:GLY:HA3	2:L:175:ILE:HG23	1.92	0.50
1:A:57:ASN:ND2	2:M:32:ALA:O	2.38	0.50
1:C:26:ARG:HH21	2:L:108:ASP:HB2	1.77	0.50
1:C:71:ALA:N	1:C:122:ASP:OD1	2.44	0.50
2:L:149:PHE:HB3	2:L:180:LEU:HD11	1.93	0.50
1:C:90:ASN:HB3	1:C:163:LYS:HB2	1.94	0.50
1:A:77:GLN:NE2	1:A:113:ASN:OD1	2.45	0.50
2:I:39:GLN:CG	2:I:40:ALA:H	2.25	0.50
1:B:17:ALA:O	1:B:28:TYR:OH	2.29	0.49
2:P:133:ARG:HH21	2:P:200:PRO:HG3	1.76	0.49
1:E:63:LYS:HE3	2:J:35:VAL:HG21	1.94	0.49
1:F:4:ARG:HD2	1:F:98:ALA:HB1	1.94	0.49
2:M:63:HIS:ND1	2:M:121:SER:OG	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:168:ARG:HB3	2:P:169:PRO:HD3	1.93	0.49
1:A:56:LEU:HD21	1:A:213:LEU:HD22	1.94	0.49
1:E:10:SER:HA	1:E:159:ARG:HG3	1.93	0.49
1:F:35:VAL:HG21	1:F:155:ILE:HB	1.94	0.49
1:G:170:VAL:HA	1:G:186:VAL:HA	1.95	0.49
1:A:136:VAL:HG23	2:M:37:VAL:HG21	1.94	0.49
1:G:34:ALA:HB2	1:G:137:PHE:HB3	1.94	0.49
1:B:202:LEU:HB2	1:B:235:PHE:CD2	2.48	0.49
1:G:74:ILE:HG21	1:G:80:ALA:HB2	1.94	0.49
1:D:136:VAL:HG23	2:K:37:VAL:HG21	1.94	0.49
2:I:146:LEU:HB2	2:I:185:VAL:HB	1.94	0.49
1:A:131:THR:HG21	2:M:39:GLN:CB	2.43	0.48
1:E:74:ILE:HG21	1:E:80:ALA:HB2	1.94	0.48
2:L:146:LEU:HB2	2:L:185:VAL:HB	1.95	0.48
2:N:58:SER:O	2:N:60:ALA:N	2.44	0.48
1:H:74:ILE:HG21	1:H:80:ALA:HB2	1.96	0.48
1:A:84:GLN:NE2	1:A:109:THR:HG23	2.28	0.48
2:K:63:HIS:ND1	2:K:121:SER:OG	2.46	0.48
2:K:144:ASP:HB2	2:K:187:PRO:HG3	1.95	0.48
1:G:138:TYR:CE2	2:P:37:VAL:HG22	2.49	0.48
2:J:129:ARG:HD2	2:J:174:VAL:HG12	1.96	0.48
2:M:99:ILE:HD11	2:M:199:VAL:HG12	1.96	0.48
1:A:37:LYS:HD2	1:A:86:ILE:HD13	1.95	0.48
1:A:90:ASN:HB3	1:A:163:LYS:HB2	1.95	0.48
1:B:90:ASN:HB3	1:B:163:LYS:HB2	1.95	0.48
1:F:57:ASN:O	1:F:141:TRP:NE1	2.37	0.48
1:D:216:GLY:O	1:D:236:SER:N	2.44	0.48
1:B:84:GLN:NE2	2:N:174:VAL:H	2.11	0.47
2:J:175:ILE:HG13	2:J:180:LEU:HD13	1.96	0.47
2:I:175:ILE:HG13	2:I:180:LEU:HD13	1.96	0.47
2:J:137:ARG:HG2	2:J:196:ARG:HG3	1.94	0.47
1:A:74:ILE:HG21	1:A:80:ALA:HB2	1.97	0.47
1:C:202:LEU:HB2	1:C:235:PHE:CD2	2.50	0.47
1:E:56:LEU:HD21	1:E:213:LEU:HD22	1.95	0.47
2:P:129:ARG:HD2	2:P:174:VAL:HG12	1.97	0.47
1:B:84:GLN:HE22	2:N:174:VAL:H	1.63	0.47
2:I:144:ASP:HB2	2:I:187:PRO:HG3	1.96	0.47
2:N:55:ALA:HB3	2:N:117:ARG:NH1	2.30	0.47
2:N:148:HIS:HB2	2:N:183:GLU:HB3	1.97	0.47
2:O:174:VAL:O	2:O:175:ILE:HD12	2.14	0.47
1:B:67:PHE:HB3	1:B:126:LEU:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:140:GLY:HA2	2:J:33:GLY:HA3	1.97	0.47
1:G:14:GLU:HB3	1:G:164:LYS:HG2	1.96	0.47
2:I:148:HIS:HB2	2:I:183:GLU:HB3	1.96	0.47
1:C:136:VAL:HG23	2:I:37:VAL:HG21	1.97	0.47
1:E:176:THR:HG22	1:E:181:THR:HA	1.97	0.47
2:I:99:ILE:HD11	2:I:199:VAL:HG12	1.97	0.47
1:A:38:MET:HB3	1:A:83:LEU:HD11	1.97	0.46
1:A:202:LEU:HB2	1:A:235:PHE:CD2	2.50	0.46
1:H:37:LYS:HD2	1:H:86:ILE:HD13	1.97	0.46
1:C:56:LEU:HD21	1:C:213:LEU:HD22	1.95	0.46
1:G:153:HIS:HB3	1:G:165:TYR:HE1	1.81	0.46
2:L:144:ASP:HB2	2:L:187:PRO:HG3	1.97	0.46
2:N:62:ILE:HD12	2:N:120:ILE:HG12	1.97	0.46
1:G:133:PRO:HA	2:P:40:ALA:HB2	1.98	0.46
2:J:55:ALA:HB3	2:J:117:ARG:HH11	1.81	0.46
1:D:202:LEU:HB2	1:D:235:PHE:CD2	2.50	0.46
1:E:14:GLU:HB3	1:E:164:LYS:HG2	1.98	0.46
1:E:56:LEU:HD11	1:E:213:LEU:HD23	1.97	0.46
1:E:202:LEU:HB2	1:E:235:PHE:CD2	2.50	0.46
1:G:202:LEU:HB2	1:G:235:PHE:CD2	2.50	0.46
1:A:170:VAL:HA	1:A:186:VAL:HA	1.98	0.46
1:H:109:THR:OG1	1:H:110:GLY:N	2.49	0.46
2:O:131:ALA:HB2	2:O:171:TRP:CE2	2.51	0.46
2:O:175:ILE:HG12	2:O:180:LEU:HD13	1.98	0.46
1:A:153:HIS:HB3	1:A:165:TYR:HE1	1.80	0.46
1:E:153:HIS:HB3	1:E:165:TYR:HE1	1.81	0.46
2:M:175:ILE:HG13	2:M:180:LEU:HD13	1.98	0.46
1:E:90:ASN:HB3	1:E:163:LYS:HB2	1.97	0.46
2:O:148:HIS:HB2	2:O:183:GLU:HB3	1.98	0.46
1:B:10:SER:HA	1:B:159:ARG:HG3	1.98	0.46
1:D:36:ALA:HB3	1:D:67:PHE:HZ	1.81	0.46
1:E:40:PHE:CE2	1:E:49:TYR:HB2	2.52	0.45
1:F:78:ALA:O	1:F:82:THR:HG23	2.15	0.45
2:K:129:ARG:HD2	2:K:174:VAL:HG12	1.97	0.45
1:B:40:PHE:CE2	1:B:49:TYR:HB2	2.52	0.45
1:F:40:PHE:CE2	1:F:49:TYR:HB2	2.51	0.45
1:F:153:HIS:HB3	1:F:165:TYR:HE1	1.81	0.45
2:I:150:ALA:O	2:I:175:ILE:HD12	2.17	0.45
1:B:203:LEU:HB3	1:B:211:TYR:HB3	1.99	0.45
2:K:136:THR:OG1	2:K:139:GLY:O	2.35	0.45
1:C:17:ALA:O	1:C:28:TYR:OH	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:134:ALA:HB2	2:J:39:GLN:O	2.16	0.45
1:F:170:VAL:HA	1:F:186:VAL:HA	1.98	0.45
1:A:56:LEU:HD11	1:A:213:LEU:HD23	1.98	0.45
1:C:40:PHE:CE2	1:C:49:TYR:HB2	2.51	0.45
2:L:148:HIS:HB2	2:L:183:GLU:HB3	1.98	0.45
1:D:90:ASN:HB3	1:D:163:LYS:HB2	1.98	0.45
2:M:129:ARG:HG2	2:M:205:PHE:HE1	1.81	0.45
1:C:176:THR:HG22	1:C:181:THR:HA	1.99	0.45
2:K:99:ILE:HD11	2:K:199:VAL:HG12	1.98	0.45
2:N:49:ARG:HH12	2:P:40:ALA:HB3	1.82	0.45
1:D:138:TYR:CE2	2:K:37:VAL:HG22	2.51	0.45
1:F:40:PHE:HE1	1:F:51:CYS:HB2	1.82	0.45
1:F:202:LEU:HB2	1:F:235:PHE:CD2	2.52	0.45
2:P:46:GLY:HA3	2:P:155:GLU:HG3	1.99	0.45
1:E:84:GLN:NE2	2:J:174:VAL:H	2.16	0.44
1:E:117:ARG:HH12	1:E:119:ALA:HB2	1.82	0.44
1:E:137:PHE:CE2	2:J:34:ASP:HA	2.52	0.44
1:G:10:SER:HB2	1:G:14:GLU:HG3	1.99	0.44
2:L:168:ARG:HB2	2:L:169:PRO:HD3	1.98	0.44
1:F:28:TYR:O	1:F:32:THR:HG23	2.16	0.44
1:G:130:ARG:HG2	2:P:44:SER:HB2	1.99	0.44
2:M:35:VAL:C	2:M:37:VAL:H	2.24	0.44
1:G:77:GLN:NE2	1:G:113:ASN:OD1	2.51	0.44
2:J:99:ILE:HD11	2:J:199:VAL:HG12	1.99	0.44
2:L:111:ASP:OD2	2:L:113:ARG:HG3	2.18	0.44
1:B:176:THR:HG22	1:B:181:THR:HA	1.98	0.44
1:F:159:ARG:HE	1:F:159:ARG:HB3	1.68	0.44
2:P:166:LEU:HD23	2:P:166:LEU:HA	1.89	0.44
1:A:30:ASN:HB3	1:A:137:PHE:CD2	2.53	0.44
1:A:63:LYS:HE2	2:M:35:VAL:HG21	1.98	0.44
1:E:30:ASN:HB3	1:E:137:PHE:CD2	2.53	0.44
2:N:125:ALA:HB2	2:N:204:TYR:CE2	2.52	0.44
2:P:129:ARG:HG2	2:P:205:PHE:HE1	1.83	0.44
1:H:10:SER:HA	1:H:159:ARG:HG3	1.98	0.44
2:I:69:ALA:H	2:I:71:ARG:HH21	1.65	0.44
1:B:89:TYR:HB3	1:B:157:HIS:HE1	1.83	0.44
1:E:37:LYS:HD2	1:E:86:ILE:HD13	2.00	0.44
1:B:188:TRP:HB2	1:B:192:VAL:HG12	2.00	0.43
1:E:156:HIS:CE1	1:E:193:VAL:HG12	2.53	0.43
2:M:147:LEU:HD23	2:M:147:LEU:HA	1.85	0.43
2:N:191:GLN:HG3	2:N:192:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:146:LEU:HB2	2:O:185:VAL:HB	1.99	0.43
2:P:48:ALA:O	2:P:49:ARG:HG3	2.18	0.43
1:D:57:ASN:HA	1:D:138:TYR:HB3	2.00	0.43
2:L:131:ALA:HB1	2:L:169:PRO:HB2	2.00	0.43
1:A:141:TRP:CE2	2:M:31:MET:HB2	2.54	0.43
1:D:10:SER:HB2	1:D:14:GLU:HG3	2.00	0.43
1:D:37:LYS:HD2	1:D:86:ILE:HD13	1.99	0.43
1:D:109:THR:OG1	1:D:110:GLY:N	2.51	0.43
1:D:156:HIS:CE1	1:D:193:VAL:HG12	2.53	0.43
1:E:30:ASN:HB3	1:E:137:PHE:CE2	2.54	0.43
1:A:10:SER:HB2	1:A:14:GLU:HG3	1.99	0.43
2:K:67:PRO:HB3	2:K:92:LEU:HD21	2.00	0.43
2:N:151:GLY:HA3	2:N:175:ILE:HG23	2.00	0.43
2:K:147:LEU:HD23	2:K:147:LEU:HA	1.81	0.43
2:P:148:HIS:CD2	2:P:158:GLU:HG3	2.53	0.43
1:A:10:SER:HA	1:A:159:ARG:HG3	2.00	0.43
1:B:58:ASN:ND2	1:B:64:ARG:O	2.52	0.43
1:C:156:HIS:CE1	1:C:193:VAL:HG12	2.54	0.43
2:K:98:GLU:OE2	2:K:196:ARG:NH1	2.52	0.43
2:O:147:LEU:HB3	2:O:149:PHE:CZ	2.53	0.43
2:P:155:GLU:HB3	2:P:157:PHE:CZ	2.54	0.43
1:E:109:THR:OG1	1:E:110:GLY:N	2.51	0.43
2:O:67:PRO:HD3	2:O:92:LEU:HD11	2.00	0.43
1:A:67:PHE:HB3	1:A:126:LEU:HB2	2.01	0.42
1:F:109:THR:OG1	1:F:110:GLY:N	2.52	0.42
2:N:68:PRO:O	2:N:70:ARG:N	2.52	0.42
2:N:136:THR:OG1	2:N:139:GLY:O	2.35	0.42
2:K:133:ARG:HH21	2:K:200:PRO:HG3	1.83	0.42
2:O:151:GLY:HA3	2:O:175:ILE:HG23	2.02	0.42
1:B:36:ALA:HB3	1:B:67:PHE:HZ	1.84	0.42
1:D:17:ALA:O	1:D:28:TYR:OH	2.30	0.42
1:E:93:GLN:CD	2:K:68:PRO:HB3	2.45	0.42
2:L:175:ILE:HD13	2:L:175:ILE:HA	1.87	0.42
2:N:55:ALA:HB3	2:N:117:ARG:HD2	2.01	0.42
1:D:130:ARG:HG2	2:K:44:SER:CB	2.49	0.42
1:G:159:ARG:HE	1:G:159:ARG:HB3	1.65	0.42
1:C:58:ASN:ND2	1:C:64:ARG:O	2.52	0.42
1:D:176:THR:HG22	1:D:181:THR:HA	2.02	0.42
1:E:58:ASN:ND2	1:E:64:ARG:O	2.52	0.42
2:K:130:ALA:HB1	2:K:199:VAL:HG21	2.02	0.42
2:K:148:HIS:CD2	2:K:158:GLU:HG3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:125:ALA:HB2	2:M:204:TYR:CE2	2.54	0.42
1:B:133:PRO:HA	2:N:40:ALA:HB2	2.02	0.42
1:C:10:SER:HB2	1:C:14:GLU:HG3	2.01	0.42
1:D:40:PHE:CE2	1:D:49:TYR:HB2	2.55	0.42
2:I:191:GLN:HG3	2:I:192:PRO:HD2	2.02	0.42
2:J:144:ASP:HB2	2:J:187:PRO:HG3	2.01	0.42
2:P:99:ILE:HD11	2:P:199:VAL:HG12	2.01	0.42
1:C:74:ILE:HB	1:C:124:LEU:HD21	2.01	0.42
1:C:188:TRP:HB2	1:C:192:VAL:HG12	2.02	0.42
1:F:10:SER:HA	1:F:159:ARG:HG3	2.00	0.42
1:G:90:ASN:HB3	1:G:163:LYS:HB2	2.01	0.42
2:J:191:GLN:HG3	2:J:192:PRO:HD2	2.01	0.42
2:L:151:GLY:HA3	2:L:175:ILE:CG2	2.49	0.42
2:N:136:THR:HA	2:N:195:LEU:HD23	2.02	0.42
2:O:43:ALA:HB1	2:O:158:GLU:HB3	2.02	0.42
2:P:147:LEU:HD23	2:P:147:LEU:HA	1.87	0.42
1:H:40:PHE:CE2	1:H:49:TYR:HB2	2.55	0.42
1:B:109:THR:OG1	1:B:110:GLY:N	2.52	0.42
1:D:74:ILE:HB	1:D:124:LEU:HD21	2.00	0.42
1:D:77:GLN:NE2	1:D:113:ASN:OD1	2.52	0.42
2:M:94:THR:C	2:P:60:ALA:HB1	2.45	0.42
2:O:144:ASP:HB2	2:O:187:PRO:HG3	2.01	0.42
1:H:90:ASN:HB3	1:H:163:LYS:HB2	2.00	0.42
2:M:166:LEU:HD23	2:M:166:LEU:HA	1.91	0.42
2:O:191:GLN:HG3	2:O:192:PRO:HD2	2.02	0.42
1:B:84:GLN:NE2	2:N:174:VAL:HG22	2.35	0.41
1:B:170:VAL:HA	1:B:186:VAL:HA	2.02	0.41
1:G:10:SER:HA	1:G:159:ARG:HG3	2.02	0.41
1:G:37:LYS:HD2	1:G:86:ILE:HD13	2.01	0.41
1:C:30:ASN:HB3	1:C:137:PHE:CD2	2.55	0.41
1:E:159:ARG:HE	1:E:159:ARG:HB3	1.72	0.41
1:G:203:LEU:HB3	1:G:211:TYR:HB3	2.01	0.41
2:J:175:ILE:HD13	2:J:175:ILE:HA	1.92	0.41
1:F:36:ALA:HB2	1:F:87:TRP:CE3	2.55	0.41
2:L:147:LEU:HD23	2:L:147:LEU:HA	1.86	0.41
1:F:10:SER:HB2	1:F:14:GLU:HG3	2.01	0.41
1:D:38:MET:HB3	1:D:83:LEU:HD11	2.01	0.41
1:F:37:LYS:HE2	1:F:50:ILE:HD11	2.02	0.41
2:N:108:ASP:OD2	2:N:114:HIS:ND1	2.50	0.41
1:C:109:THR:OG1	1:C:110:GLY:N	2.53	0.41
1:D:188:TRP:HB2	1:D:192:VAL:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:22:GLN:O	1:F:25:THR:N	2.54	0.41
1:G:40:PHE:CE2	1:G:49:TYR:HB2	2.55	0.41
2:J:63:HIS:CG	2:L:65:ALA:HB2	2.55	0.41
2:K:41:SER:HA	2:K:42:PRO:HD3	1.96	0.41
1:F:56:LEU:HD21	1:F:213:LEU:HD22	2.01	0.41
1:G:176:THR:HG22	1:G:181:THR:HA	2.02	0.41
2:K:191:GLN:HG3	2:K:192:PRO:HD2	2.03	0.41
2:M:191:GLN:HG3	2:M:192:PRO:HD2	2.02	0.41
1:A:84:GLN:NE2	2:M:173:PRO:HA	2.35	0.41
1:G:58:ASN:ND2	1:G:64:ARG:O	2.54	0.41
2:I:65:ALA:HB2	2:N:63:HIS:CG	2.56	0.41
1:A:17:ALA:O	1:A:28:TYR:OH	2.35	0.41
1:E:226:ALA:HB3	1:E:231:ARG:HG3	2.02	0.41
1:F:64:ARG:HH12	1:F:248:TYR:HD1	1.69	0.41
1:G:68:TRP:HE1	1:G:216:GLY:N	2.19	0.41
2:I:137:ARG:HH21	2:I:196:ARG:NH2	2.18	0.41
2:L:99:ILE:HG21	2:L:197:LEU:HD23	2.02	0.41
2:P:129:ARG:HG3	2:P:203:SER:HB3	2.02	0.41
1:G:36:ALA:HB3	1:G:67:PHE:HZ	1.86	0.41
1:G:156:HIS:CE1	1:G:193:VAL:HG12	2.56	0.41
2:J:71:ARG:HB2	2:J:208:SER:OG	2.21	0.41
2:L:133:ARG:HH21	2:L:200:PRO:HG3	1.86	0.41
2:K:142:PRO:HG2	2:K:190:LEU:HD22	2.02	0.40
2:N:175:ILE:HD13	2:N:175:ILE:HA	1.93	0.40
1:C:57:ASN:O	1:C:141:TRP:NE1	2.47	0.40
2:N:147:LEU:HD23	2:N:147:LEU:HA	1.87	0.40
2:I:150:ALA:HA	2:I:155:GLU:O	2.22	0.40
2:N:129:ARG:HG2	2:N:203:SER:HB3	2.04	0.40
2:P:175:ILE:HD13	2:P:175:ILE:HA	1.93	0.40
1:F:159:ARG:HH21	2:L:210:TYR:HA	1.86	0.40
1:E:188:TRP:HB2	1:E:192:VAL:HG12	2.04	0.40
1:F:159:ARG:NH2	2:L:210:TYR:HA	2.35	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	248/251 (99%)	236 (95%)	12 (5%)	0	100	100
1	B	247/251 (98%)	237 (96%)	10 (4%)	0	100	100
1	C	248/251 (99%)	237 (96%)	11 (4%)	0	100	100
1	D	238/251 (95%)	228 (96%)	10 (4%)	0	100	100
1	E	248/251 (99%)	237 (96%)	11 (4%)	0	100	100
1	F	220/251 (88%)	210 (96%)	10 (4%)	0	100	100
1	G	243/251 (97%)	232 (96%)	11 (4%)	0	100	100
1	H	135/251 (54%)	129 (96%)	6 (4%)	0	100	100
2	I	168/186 (90%)	150 (89%)	14 (8%)	4 (2%)	4	24
2	J	164/186 (88%)	144 (88%)	18 (11%)	2 (1%)	10	37
2	K	164/186 (88%)	147 (90%)	13 (8%)	4 (2%)	4	24
2	L	160/186 (86%)	143 (89%)	14 (9%)	3 (2%)	6	28
2	M	159/186 (86%)	133 (84%)	21 (13%)	5 (3%)	3	20
2	N	169/186 (91%)	149 (88%)	17 (10%)	3 (2%)	6	29
2	O	160/186 (86%)	141 (88%)	17 (11%)	2 (1%)	9	35
2	P	161/186 (87%)	146 (91%)	13 (8%)	2 (1%)	10	37
All	All	3132/3496 (90%)	2899 (93%)	208 (7%)	25 (1%)	16	45

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	K	69	ALA
2	L	69	ALA
2	M	35	VAL
2	N	69	ALA
2	I	35	VAL
2	I	37	VAL
2	I	169	PRO
2	L	155	GLU
2	M	37	VAL
2	N	45	THR
2	K	46	GLY
2	O	169	PRO

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Mol	Chain	Res	Type
2	I	34	ASP
2	J	42	PRO
2	K	45	THR
2	M	69	ALA
2	M	169	PRO
2	N	169	PRO
2	O	48	ALA
2	P	169	PRO
2	J	169	PRO
2	K	169	PRO
2	M	54	ASN
2	P	48	ALA
2	L	169	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	190/190 (100%)	190 (100%)	0	100	100
1	B	189/190 (100%)	189 (100%)	0	100	100
1	C	190/190 (100%)	190 (100%)	0	100	100
1	D	186/190 (98%)	186 (100%)	0	100	100
1	E	190/190 (100%)	190 (100%)	0	100	100
1	F	181/190 (95%)	181 (100%)	0	100	100
1	G	187/190 (98%)	187 (100%)	0	100	100
1	H	108/190 (57%)	108 (100%)	0	100	100
2	I	131/139 (94%)	131 (100%)	0	100	100
2	J	131/139 (94%)	131 (100%)	0	100	100
2	K	129/139 (93%)	129 (100%)	0	100	100
2	L	127/139 (91%)	127 (100%)	0	100	100
2	M	127/139 (91%)	127 (100%)	0	100	100
2	N	132/139 (95%)	132 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	O	125/139 (90%)	125 (100%)	0	100	100
2	P	126/139 (91%)	126 (100%)	0	100	100
All	All	2449/2632 (93%)	2449 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	GLN
1	A	84	GLN
1	A	113	ASN
1	A	167	GLN
1	A	169	ASN
1	B	84	GLN
1	B	90	ASN
1	B	167	GLN
1	B	169	ASN
1	C	90	ASN
1	C	113	ASN
1	C	169	ASN
1	D	77	GLN
1	D	167	GLN
1	D	169	ASN
1	E	77	GLN
1	E	113	ASN
1	E	169	ASN
1	F	84	GLN
1	G	77	GLN
1	G	90	ASN
1	G	167	GLN
1	G	169	ASN
2	I	39	GLN
2	O	54	ASN
2	P	189	ASN

5.3.3 RNA ⓘ

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	250/251 (99%)	0.18	2 (0%) 82 68	57, 72, 91, 101	0
1	B	249/251 (99%)	0.27	2 (0%) 82 68	59, 76, 96, 106	0
1	C	250/251 (99%)	0.19	2 (0%) 82 68	59, 82, 103, 117	0
1	D	244/251 (97%)	0.54	12 (4%) 35 23	70, 103, 120, 132	0
1	E	250/251 (99%)	0.27	4 (1%) 70 52	57, 77, 93, 104	0
1	F	234/251 (93%)	0.61	14 (5%) 27 19	64, 99, 122, 133	0
1	G	247/251 (98%)	0.67	12 (4%) 35 23	74, 105, 129, 139	0
1	H	145/251 (57%)	0.77	9 (6%) 26 18	83, 109, 124, 128	0
2	I	172/186 (92%)	0.39	2 (1%) 76 58	56, 76, 105, 113	0
2	J	170/186 (91%)	0.57	8 (4%) 36 24	60, 85, 104, 111	0
2	K	168/186 (90%)	0.42	6 (3%) 46 31	63, 83, 115, 130	0
2	L	166/186 (89%)	0.49	6 (3%) 46 31	66, 89, 114, 123	0
2	M	167/186 (89%)	0.56	9 (5%) 31 21	62, 92, 120, 129	0
2	N	173/186 (93%)	0.27	1 (0%) 85 73	61, 78, 101, 115	0
2	O	164/186 (88%)	0.52	5 (3%) 52 35	66, 92, 122, 141	0
2	P	165/186 (88%)	0.65	5 (3%) 52 35	74, 96, 119, 136	0
All	All	3214/3496 (91%)	0.44	99 (3%) 51 35	56, 87, 118, 141	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	32	THR	4.5
1	G	80	ALA	4.4
2	L	48	ALA	4.3
2	M	56	ALA	4.2
2	P	38	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
2	O	69	ALA	4.1
2	K	155	GLU	4.0
2	P	69	ALA	3.8
1	F	115	LEU	3.4
2	O	37	VAL	3.4
1	E	2	GLY	3.4
1	H	69	SER	3.4
1	F	188	TRP	3.2
1	G	175	VAL	3.2
1	H	68	TRP	3.1
2	M	35	VAL	3.0
2	M	59	ALA	3.0
2	O	206	ALA	3.0
2	P	39	GLN	3.0
2	M	176	GLU	2.9
1	F	166	SER	2.9
1	G	201	GLY	2.9
1	G	237	ASP	2.9
1	H	70	ALA	2.8
1	G	2	GLY	2.8
1	H	56	LEU	2.8
1	B	45	ASP	2.8
1	G	50	ILE	2.8
1	F	238	PHE	2.7
2	P	35	VAL	2.7
2	M	155	GLU	2.7
1	D	241	VAL	2.7
2	I	71	ARG	2.6
2	L	169	PRO	2.6
1	A	225	GLY	2.6
2	J	71	ARG	2.6
2	J	68	PRO	2.6
1	E	155	ILE	2.6
2	K	35	VAL	2.6
1	F	2	GLY	2.5
1	E	103	GLN	2.5
2	L	35	VAL	2.5
1	D	94	CYS	2.5
1	B	35	VAL	2.5
1	F	208	ASP	2.4
2	J	58	SER	2.4
1	G	238	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
2	J	61	GLY	2.4
2	N	30	GLU	2.4
1	D	31	ALA	2.4
1	F	144	THR	2.3
1	G	218	TYR	2.3
2	K	128	LEU	2.3
2	J	184	LEU	2.3
1	A	12	SER	2.3
1	D	184	THR	2.3
1	H	136	VAL	2.3
1	C	2	GLY	2.3
1	D	201	GLY	2.3
2	I	33	GLY	2.3
1	E	3	TYR	2.3
1	G	3	TYR	2.3
1	F	170	VAL	2.3
1	D	214	ARG	2.2
1	D	212	GLN	2.2
1	F	186	VAL	2.2
2	K	37	VAL	2.2
2	J	155	GLU	2.2
1	F	202	LEU	2.2
1	F	190	SER	2.2
1	H	76	ASP	2.2
1	H	201	GLY	2.2
2	J	43	ALA	2.2
1	D	138	TYR	2.2
2	J	122	ALA	2.2
1	D	155	ILE	2.1
1	F	143	ALA	2.1
2	M	48	ALA	2.1
2	L	137	ARG	2.1
1	G	213	LEU	2.1
2	L	138	SER	2.1
1	F	241	VAL	2.1
1	F	203	LEU	2.1
2	K	210	TYR	2.1
2	M	36	ALA	2.1
2	M	46	GLY	2.1
1	D	170	VAL	2.1
1	G	131	THR	2.1
1	H	38	MET	2.1

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Mol	Chain	Res	Type	RSRZ
2	L	36	ALA	2.1
2	K	135	GLU	2.1
1	C	75	GLU	2.0
2	O	155	GLU	2.0
1	D	213	LEU	2.0
2	O	38	LEU	2.0
2	P	54	ASN	2.0
1	G	177	TYR	2.0
2	M	33	GLY	2.0
1	H	132	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.