



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 07:49 PM UTC

PDB ID : 8G25 / pdb_00008g25
Title : Crystal Structure of Cathepsin-G and Neutrophil Elastase Inhibited by S. aureus EapH2 at pH 7.5
Authors : Mishra, N.B.; Geisbrecht, B.V.
Deposited on : 2023-02-03
Resolution : 1.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

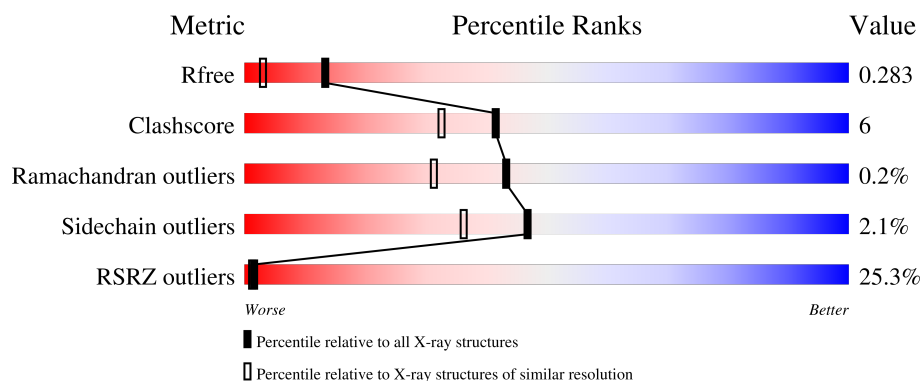
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	223	
1	F	223	
1	I	223	
2	B	218	
2	E	218	

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Mol	Chain	Length	Quality of chain
2	H	218	69% 76% 23%
3	C	117	4% 74% 14% 12%
3	D	117	25% 75% 13% 12%
3	G	117	12% 72% 15% 12%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13335 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 Cathepsin-G.

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

- Molecule 2 is a protein called Neutrophil elastase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total	C	N	O	S	0	0	0
			1635	1026	316	282	11			
2	E	218	Total	C	N	O	S	0	0	0
			1635	1026	316	282	11			
2	H	218	Total	C	N	O	S	0	0	0
			1635	1026	316	282	11			

- Molecule 3 is a protein called MAP domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	103	Total	C	N	O	S	0	0	0
			819	520	136	161	2			
3	D	103	Total	C	N	O	S	0	0	0
			819	520	136	161	2			
3	G	103	Total	C	N	O	S	0	0	0
			819	520	136	161	2			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	28	GLY	-	expression tag	UNP A0A0H3JUK5
C	29	SER	-	expression tag	UNP A0A0H3JUK5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	30	THR	-	expression tag	UNP A0A0H3JUK5
D	28	GLY	-	expression tag	UNP A0A0H3JUK5
D	29	SER	-	expression tag	UNP A0A0H3JUK5
D	30	THR	-	expression tag	UNP A0A0H3JUK5
G	28	GLY	-	expression tag	UNP A0A0H3JUK5
G	29	SER	-	expression tag	UNP A0A0H3JUK5
G	30	THR	-	expression tag	UNP A0A0H3JUK5

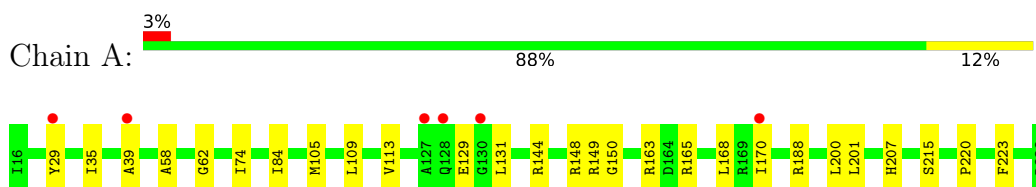
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	134	Total 134	O 134	0	0
4	B	93	Total 93	O 93	0	0
4	C	65	Total 65	O 65	0	0
4	D	34	Total 34	O 34	0	0
4	E	20	Total 20	O 20	0	0
4	F	85	Total 85	O 85	0	0
4	G	47	Total 47	O 47	0	0
4	H	30	Total 30	O 30	0	0
4	I	125	Total 125	O 125	0	0

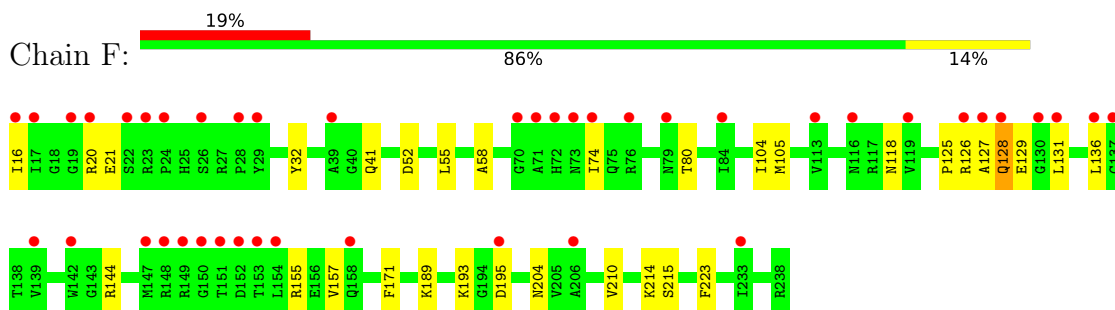
3 Residue-property plots

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.

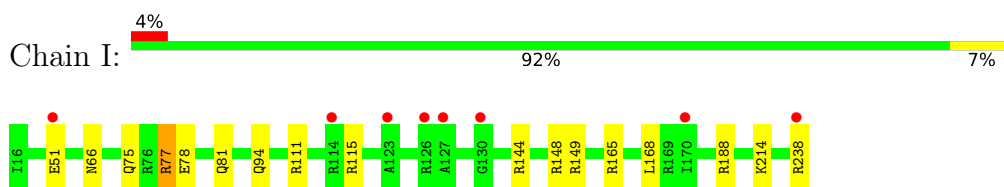
- Molecule 1: Cathepsin-G



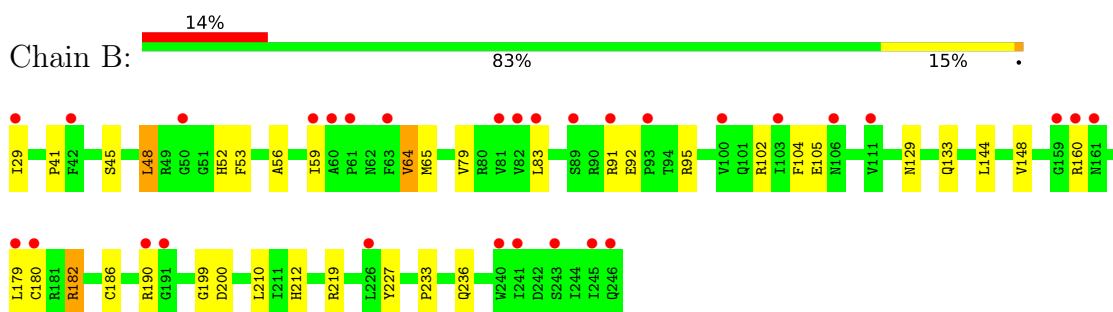
- Molecule 1: Cathepsin-G



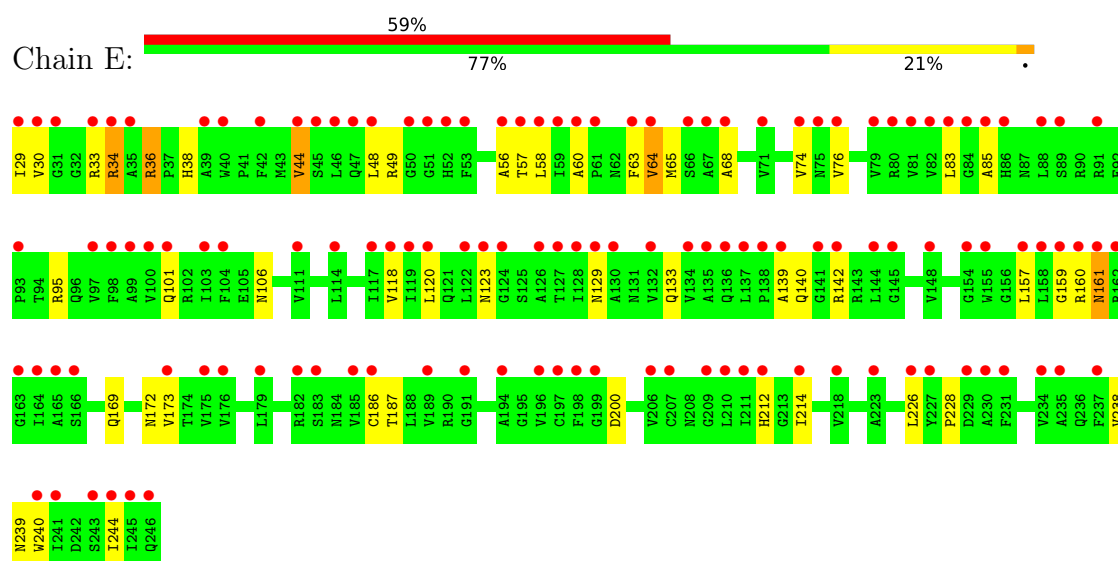
- Molecule 1: Cathepsin-G



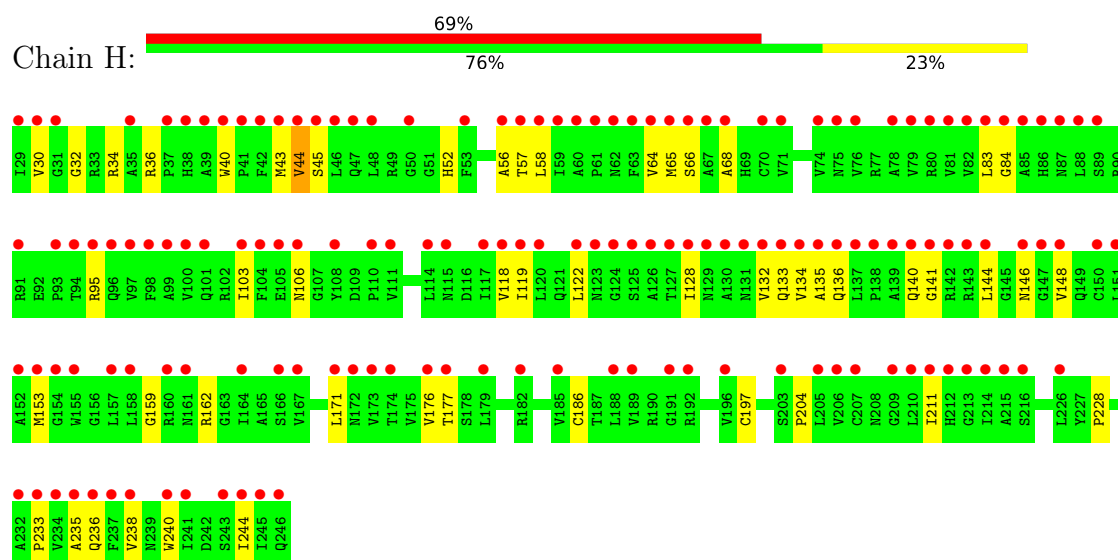
- Molecule 2: Neutrophil elastase



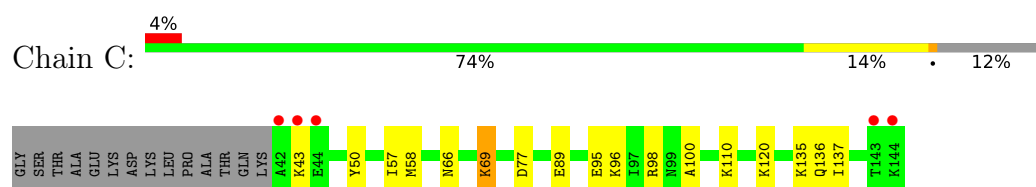
- Molecule 2: Neutrophil elastase



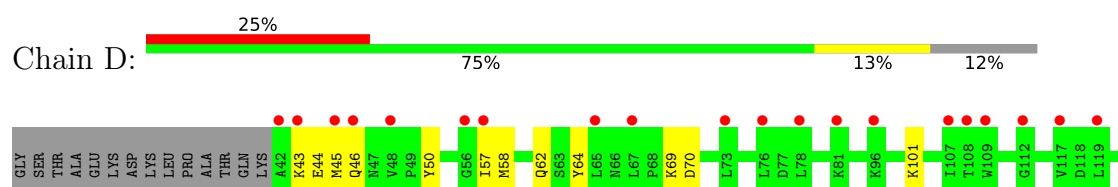
• Molecule 2: Neutrophil elastase

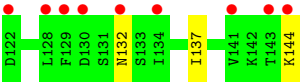


• Molecule 3: MAP domain-containing protein

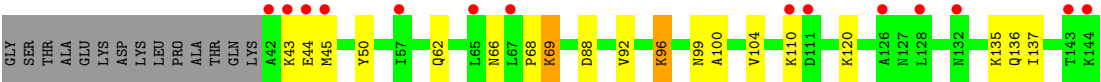


• Molecule 3: MAP domain-containing protein





● Molecule 3: MAP domain-containing protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.15Å 68.43Å 141.90Å 90.00° 102.76° 90.00°	Depositor
Resolution (Å)	46.13 – 1.80 46.13 – 1.80	Depositor EDS
% Data completeness (in resolution range)	89.2 (46.13-1.80) 89.7 (46.13-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 1.79Å)	Xtriage
Refinement program	PHENIX v1.19.2	Depositor
R, R_{free}	0.248 , 0.283 0.248 , 0.283	Depositor DCC
R_{free} test set	1840 reflections (1.23%)	wwPDB-VP
Wilson B-factor (Å ²)	25.4	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.3	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	0.95	EDS
Total number of atoms	13335	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 85.67 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1768e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.25	0/1814	0.48	0/2447
1	F	0.21	0/1814	0.46	0/2447
1	I	0.25	0/1814	0.49	0/2447
2	B	0.17	0/1665	0.40	0/2263
2	E	0.14	0/1665	0.42	0/2263
2	H	0.15	0/1665	0.40	0/2263
3	C	0.23	0/831	0.44	0/1120
3	D	0.19	0/831	0.39	0/1120
3	G	0.21	0/831	0.41	0/1120
All	All	0.20	0/12930	0.44	0/17490

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 [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	1780	0	1793	16	0
1	F	1780	0	1793	22	0
1	I	1780	0	1793	12	0
2	B	1635	0	1652	19	0
2	E	1635	0	1652	33	0
2	H	1635	0	1652	35	0
3	C	819	0	836	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	819	0	836	13	0
3	G	819	0	836	15	0
4	A	134	0	0	1	0
4	B	93	0	0	1	0
4	C	65	0	0	0	0
4	D	34	0	0	0	0
4	E	20	0	0	2	0
4	F	85	0	0	1	0
4	G	47	0	0	1	0
4	H	30	0	0	4	0
4	I	125	0	0	4	0
All	All	13335	0	12843	164	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 6.

All (164) 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:45:SER:HG	2:H:52:HIS:HD1	1.11	0.91
3:D:101:LYS:HD3	3:D:144:LYS:HD2	1.67	0.74
2:B:92:GLU:HB2	2:B:95:ARG:HD3	1.72	0.72
2:H:141:GLY:HA2	2:H:235:ALA:HB1	1.71	0.72
1:I:148:ARG:HG3	1:I:149:ARG:HG3	1.71	0.72
2:B:48:LEU:HD21	2:B:79:VAL:HG22	1.73	0.70
2:E:140:GLN:HG2	2:E:238:VAL:HB	1.74	0.70
2:H:44:VAL:HG22	2:H:56:ALA:HB3	1.74	0.69
2:E:30:VAL:HG13	2:E:159:GLY:HA2	1.75	0.69
2:H:34:ARG:H	2:H:34:ARG:HD3	1.56	0.69
2:H:65:MET:HE2	2:H:136:GLN:HE22	1.56	0.69
2:H:84:GLY:HA3	2:H:132:VAL:HG22	1.75	0.68
1:A:148:ARG:HG3	1:A:149:ARG:HG3	1.76	0.66
1:F:21:GLU:HA	1:F:155:ARG:HG2	1.77	0.66
1:I:51:GLU:OE2	1:I:115:ARG:NH1	2.29	0.65
2:H:134:VAL:HG22	2:H:135:ALA:H	1.61	0.65
3:C:110:LYS:HE2	3:C:135:LYS:HD3	1.78	0.64
3:C:95:GLU:HG3	3:C:98:ARG:HH22	1.63	0.64
2:E:65:MET:HE3	2:E:214:ILE:HD11	1.79	0.64
2:H:40:TRP:CG	2:H:153:MET:HE1	2.33	0.63
2:E:44:VAL:HG22	2:E:56:ALA:HB3	1.80	0.63
2:E:140:GLN:HE21	2:E:239:ASN:H	1.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:133:GLN:HG2	2:H:134:VAL:H	1.67	0.60
1:F:214:LYS:NZ	4:F:302:HOH:O	2.29	0.59
3:G:99:ASN:ND2	4:G:203:HOH:O	2.34	0.59
3:C:100:ALA:O	3:C:120:LYS:NZ	2.26	0.59
2:H:204:PRO:HB2	2:H:211:ILE:HD12	1.84	0.59
2:B:180:CYS:SG	4:B:374:HOH:O	2.57	0.59
1:I:214:LYS:NZ	4:I:302:HOH:O	2.26	0.58
2:E:29:ILE:HB	2:E:157:LEU:O	2.04	0.57
2:E:60:ALA:HB3	2:E:63:PHE:HB2	1.86	0.57
2:B:129:ASN:O	2:B:133:GLN:NE2	2.36	0.57
1:I:78:GLU:HB2	1:I:81:GLN:HG3	1.87	0.57
3:G:45:MET:HB3	3:G:69:LYS:HB2	1.86	0.57
2:B:102:ARG:HD2	2:B:104:PHE:CZ	2.40	0.56
2:E:38:HIS:ND1	4:E:301:HOH:O	2.32	0.56
2:H:36:ARG:NH1	4:H:302:HOH:O	2.38	0.56
3:G:44:GLU:HA	3:G:68:PRO:HA	1.87	0.56
2:B:182:ARG:CZ	2:B:182:ARG:H	2.19	0.56
2:E:74:VAL:HG12	2:E:76:VAL:H	1.70	0.56
2:B:29:ILE:HG21	2:B:200:ASP:OD2	2.05	0.55
3:G:44:GLU:HB3	3:G:66:ASN:HB3	1.87	0.55
2:E:101:GLN:HE21	2:E:123:ASN:HA	1.71	0.55
3:D:58:MET:HE3	1:F:193:LYS:HE3	1.88	0.55
2:E:33:ARG:NH1	2:E:172:ASN:OD1	2.29	0.55
2:E:63:PHE:HE2	2:E:244:ILE:HG22	1.71	0.55
2:H:58:LEU:HD13	2:H:83:LEU:HD21	1.88	0.55
3:C:43:LYS:HA	3:C:69:LYS:HD2	1.88	0.55
2:H:65:MET:HE2	2:H:136:GLN:NE2	2.21	0.55
2:E:58:LEU:HD13	2:E:83:LEU:HD21	1.89	0.55
2:B:48:LEU:HD23	2:B:53:PHE:CE1	2.42	0.54
2:B:210:LEU:HB2	2:B:212:HIS:CE1	2.42	0.54
3:D:46:GLN:HB2	3:D:69:LYS:HG2	1.89	0.54
1:I:94:GLN:NE2	4:I:303:HOH:O	2.30	0.54
1:F:126:ARG:HH21	1:F:129:GLU:HG3	1.72	0.54
2:E:129:ASN:O	2:E:133:GLN:NE2	2.41	0.54
2:E:36:ARG:NH1	4:E:303:HOH:O	2.41	0.52
2:E:140:GLN:HG3	2:E:239:ASN:CG	2.35	0.52
2:H:43:MET:HE3	2:H:153:MET:HE2	1.92	0.52
1:A:170:ILE:HD11	1:A:220:PRO:HG2	1.91	0.52
2:E:29:ILE:HG12	2:E:200:ASP:OD2	2.09	0.52
3:C:110:LYS:HD3	3:C:135:LYS:HB2	1.92	0.52
1:F:80:THR:HB	1:F:118:ASN:HD22	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:55:LEU:HD11	1:F:104:ILE:HD11	1.91	0.50
2:B:52:HIS:HE1	2:B:199:GLY:O	1.95	0.50
3:D:57:ILE:HG22	1:F:171:PHE:HD1	1.75	0.50
1:F:136:LEU:HD21	1:I:77:ARG:HH12	1.76	0.50
2:B:233:PRO:HB2	2:B:236:GLN:HG3	1.94	0.50
2:E:68:ALA:HA	2:E:118:VAL:HB	1.93	0.50
2:E:29:ILE:HG23	2:E:169:GLN:HG3	1.94	0.49
2:H:68:ALA:HA	2:H:118:VAL:HB	1.94	0.49
2:H:144:LEU:HD22	2:H:148:VAL:HG21	1.93	0.49
2:E:64:VAL:HG12	2:E:120:LEU:HB2	1.93	0.49
3:G:62:GLN:NE2	1:I:144:ARG:HH11	2.10	0.49
3:C:50:TYR:HA	3:C:137:ILE:O	2.12	0.49
3:D:69:LYS:HD3	3:D:132:ASN:HD21	1.76	0.49
2:B:144:LEU:HD23	2:B:148:VAL:HG11	1.95	0.48
3:G:44:GLU:CB	3:G:66:ASN:HB3	2.43	0.48
1:F:16:ILE:HG13	1:F:195:ASP:OD1	2.13	0.48
3:D:43:LYS:NZ	3:D:70:ASP:OD2	2.48	0.47
2:E:49:ARG:HG2	2:E:49:ARG:O	2.13	0.47
1:F:125:PRO:HB3	1:F:129:GLU:HB2	1.95	0.47
2:H:58:LEU:HD23	2:H:134:VAL:HA	1.96	0.47
2:B:56:ALA:HB1	2:B:64:VAL:HG13	1.96	0.47
1:F:127:ALA:O	1:F:128:GLN:HB2	2.15	0.46
1:F:157:VAL:HG21	1:F:189:LYS:HB3	1.97	0.46
2:E:140:GLN:HE21	2:E:239:ASN:HB2	1.80	0.46
2:H:186:CYS:HB3	2:H:228:PRO:HB2	1.97	0.46
1:F:20:ARG:HB3	1:I:111:ARG:HH21	1.81	0.46
3:G:110:LYS:HE2	3:G:135:LYS:HD2	1.98	0.46
3:D:64:TYR:HB2	1:F:41:GLN:HG3	1.98	0.46
2:H:146:ASN:ND2	2:H:176:VAL:HA	2.31	0.46
2:E:186:CYS:HB3	2:E:228:PRO:HB2	1.98	0.46
1:F:58:ALA:HA	1:F:105:MET:HB2	1.98	0.46
2:B:59:ILE:HD13	2:B:65:MET:HB2	1.97	0.45
3:G:45:MET:HB3	3:G:69:LYS:CB	2.45	0.45
3:G:50:TYR:HA	3:G:137:ILE:O	2.16	0.45
1:I:75:GLN:NE2	4:I:307:HOH:O	2.48	0.45
1:F:131:LEU:HD23	1:F:131:LEU:HA	1.78	0.45
3:D:50:TYR:HA	3:D:137:ILE:O	2.16	0.45
2:H:140:GLN:HA	2:H:238:VAL:HG11	1.98	0.45
1:F:210:VAL:HG22	1:F:223:PHE:CE2	2.52	0.45
3:G:62:GLN:HE22	1:I:144:ARG:HH11	1.63	0.45
1:A:131:LEU:HD12	1:A:131:LEU:HA	1.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:SER:HA	3:C:58:MET:HE2	2.00	0.44
3:C:43:LYS:HD2	3:C:69:LYS:HD2	1.99	0.44
2:E:160:ARG:O	2:E:161:ASN:HB2	2.17	0.44
1:A:163:ARG:HG3	3:G:88:ASP:HB2	1.99	0.44
3:D:62:GLN:NE2	1:F:144:ARG:HH11	2.15	0.44
3:C:50:TYR:OH	3:C:89:GLU:OE2	2.33	0.44
1:F:52:ASP:OD1	1:F:52:ASP:N	2.49	0.44
2:H:57:THR:HG21	2:H:204:PRO:HB3	1.99	0.44
1:I:165:ARG:HA	1:I:168:LEU:HD12	1.99	0.44
3:D:43:LYS:O	3:D:69:LYS:HB2	2.17	0.44
2:H:57:THR:OG1	2:H:65:MET:HG2	2.18	0.44
2:B:219:ARG:HD3	2:B:227:TYR:CD1	2.53	0.44
1:A:29:TYR:OH	1:A:201:LEU:HD22	2.18	0.43
3:D:44:GLU:HG3	3:D:45:MET:HG2	1.99	0.43
1:A:84:ILE:HG21	1:A:109:LEU:HB3	2.00	0.43
2:B:179:LEU:HD23	2:B:179:LEU:HA	1.82	0.43
1:A:144:ARG:HA	1:A:150:GLY:HA2	2.00	0.43
2:H:30:VAL:HG23	2:H:197:CYS:HB2	1.99	0.43
2:B:45:SER:OG	2:B:52:HIS:HD2	2.01	0.43
2:E:140:GLN:NE2	2:E:239:ASN:H	2.13	0.43
3:G:100:ALA:O	3:G:120:LYS:NZ	2.38	0.43
2:H:56:ALA:HB2	2:H:66:SER:HB2	2.00	0.43
1:A:58:ALA:HA	1:A:105:MET:HB2	2.00	0.43
3:C:136:GLN:HG3	3:C:137:ILE:N	2.33	0.43
2:H:32:GLY:HA2	2:H:171:LEU:HD13	2.01	0.43
2:H:122:LEU:HB2	4:H:312:HOH:O	2.19	0.43
1:A:35:ILE:CG2	1:A:62:GLY:HA3	2.49	0.43
1:A:148:ARG:NH1	4:A:308:HOH:O	2.49	0.43
1:F:32:TYR:CZ	1:F:74:ILE:HD13	2.53	0.43
2:H:103:ILE:HA	2:H:119:ILE:O	2.18	0.43
2:E:44:VAL:HG21	2:E:64:VAL:HG21	2.01	0.42
3:G:92:VAL:HA	3:G:96:LYS:HZ3	1.84	0.42
2:H:233:PRO:HB2	2:H:236:GLN:HG3	2.00	0.42
2:H:132:VAL:HG12	4:H:309:HOH:O	2.19	0.42
2:E:85:ALA:HB2	2:E:95:ARG:HD2	2.01	0.42
2:H:159:GLY:O	2:H:162:ARG:HG2	2.20	0.42
1:A:39:ALA:HA	3:C:66:ASN:HB2	2.01	0.42
2:E:139:ALA:HB3	2:E:142:ARG:NH2	2.34	0.42
3:G:136:GLN:HG3	3:G:137:ILE:N	2.34	0.42
3:D:58:MET:HE2	1:F:215:SER:HA	2.02	0.41
3:D:57:ILE:O	3:D:57:ILE:HG13	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:57:THR:OG1	2:E:65:MET:HG2	2.20	0.41
2:H:106:ASN:HB2	2:H:240:TRP:CE2	2.55	0.41
1:I:66:ASN:ND2	4:I:310:HOH:O	2.53	0.41
2:B:160:ARG:NH1	3:C:77:ASP:OD1	2.53	0.41
1:A:165:ARG:HA	1:A:168:LEU:HD12	2.01	0.41
2:E:106:ASN:HB2	2:E:240:TRP:CE2	2.55	0.41
1:A:74:ILE:H	1:A:74:ILE:HG13	1.68	0.41
1:A:200:LEU:HB2	1:A:223:PHE:CD2	2.56	0.41
2:H:146:ASN:HD22	2:H:177:THR:H	1.69	0.41
1:A:129:GLU:HG2	1:A:207:HIS:HE1	1.86	0.41
2:E:33:ARG:O	2:E:34:ARG:HB2	2.21	0.41
2:H:240:TRP:O	2:H:244:ILE:HG12	2.21	0.41
2:B:41:PRO:HG2	2:B:133:GLN:HB2	2.02	0.40
2:H:36:ARG:HE	2:H:36:ARG:HA	1.86	0.40
1:F:16:ILE:HD12	1:F:155:ARG:HB2	2.04	0.40
2:E:142:ARG:HG2	2:E:212:HIS:HE1	1.86	0.40
2:E:173:VAL:HB	2:E:187:THR:HB	2.03	0.40
3:G:110:LYS:HD3	3:G:135:LYS:HB2	2.04	0.40
2:H:95:ARG:NH1	4:H:306:HOH:O	2.55	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	221/223 (99%)	216 (98%)	5 (2%)	0	100	100
1	F	221/223 (99%)	213 (96%)	7 (3%)	1 (0%)	24	14
1	I	221/223 (99%)	213 (96%)	8 (4%)	0	100	100
2	B	216/218 (99%)	209 (97%)	7 (3%)	0	100	100
2	E	216/218 (99%)	198 (92%)	16 (7%)	2 (1%)	14	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	216/218 (99%)	203 (94%)	13 (6%)	0	100	100
3	C	101/117 (86%)	99 (98%)	2 (2%)	0	100	100
3	D	101/117 (86%)	99 (98%)	2 (2%)	0	100	100
3	G	101/117 (86%)	101 (100%)	0	0	100	100
All	All	1614/1674 (96%)	1551 (96%)	60 (4%)	3 (0%)	43	31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	34	ARG
2	E	161	ASN
1	F	128	GLN

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%)	188 (99%)	2 (1%)	65	60
1	F	190/190 (100%)	189 (100%)	1 (0%)	81	80
1	I	190/190 (100%)	187 (98%)	3 (2%)	55	47
2	B	172/172 (100%)	164 (95%)	8 (5%)	23	11
2	E	172/172 (100%)	167 (97%)	5 (3%)	37	25
2	H	172/172 (100%)	169 (98%)	3 (2%)	53	45
3	C	92/103 (89%)	89 (97%)	3 (3%)	33	21
3	D	92/103 (89%)	92 (100%)	0	100	100
3	G	92/103 (89%)	88 (96%)	4 (4%)	26	13
All	All	1362/1395 (98%)	1333 (98%)	29 (2%)	47	36

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	VAL
1	A	188	ARG
2	B	48	LEU
2	B	64	VAL
2	B	83	LEU
2	B	91	ARG
2	B	105	GLU
2	B	182	ARG
2	B	186	CYS
2	B	190	ARG
3	C	57	ILE
3	C	69	LYS
3	C	96	LYS
2	E	36	ARG
2	E	44	VAL
2	E	48	LEU
2	E	64	VAL
2	E	226	LEU
1	F	204	ASN
3	G	43	LYS
3	G	69	LYS
3	G	96	LYS
3	G	104	VAL
2	H	44	VAL
2	H	64	VAL
2	H	128	ILE
1	I	77	ARG
1	I	188	ARG
1	I	238	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	158	GLN
2	B	52	HIS
2	B	106	ASN
2	B	169	GLN
2	B	236	GLN
2	B	246	GLN
3	D	62	GLN
2	E	106	ASN
2	E	131	ASN

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Mol	Chain	Res	Type
2	E	140	GLN
2	E	236	GLN
1	F	36	GLN
1	F	118	ASN
3	G	47	ASN
3	G	62	GLN
2	H	112	ASN
2	H	136	GLN
2	H	146	ASN
2	H	161	ASN
1	I	120	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	223/223 (100%)	0.22	6 (2%) 56 56	16, 28, 50, 88	0
1	F	223/223 (100%)	1.13	43 (19%) 3 2	21, 39, 73, 99	0
1	I	223/223 (100%)	0.36	8 (3%) 46 46	15, 29, 54, 87	0
2	B	218/218 (100%)	1.08	30 (13%) 6 5	26, 41, 68, 93	0
2	E	218/218 (100%)	2.30	128 (58%) 0 0	61, 78, 103, 137	0
2	H	218/218 (100%)	2.95	150 (68%) 0 0	45, 80, 116, 134	0
3	C	103/117 (88%)	0.72	5 (4%) 35 33	19, 31, 67, 124	0
3	D	103/117 (88%)	1.69	29 (28%) 1 1	26, 48, 79, 109	0
3	G	103/117 (88%)	1.00	14 (13%) 7 5	19, 40, 77, 105	0
All	All	1632/1674 (97%)	1.29	413 (25%) 1 1	15, 43, 99, 137	0

All (413) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	136	GLN	12.5
2	H	59	ILE	8.9
2	H	81	VAL	7.6
3	G	42	ALA	7.2
2	H	76	VAL	7.0
2	H	134	VAL	6.4
2	H	132	VAL	6.0
2	H	135	ALA	6.0
1	F	20	ARG	6.0
2	H	46	LEU	5.9
2	E	63	PHE	5.8
2	H	100	VAL	5.8
2	H	98	PHE	5.8
2	H	57	THR	5.7
2	H	117	ILE	5.7

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Mol	Chain	Res	Type	RSRZ
2	H	82	VAL	5.7
2	E	82	VAL	5.6
2	H	88	LEU	5.6
1	F	16	ILE	5.5
2	E	29	ILE	5.5
2	H	152	ALA	5.5
3	C	42	ALA	5.5
3	G	43	LYS	5.4
2	H	83	LEU	5.4
2	H	85	ALA	5.4
2	H	234	VAL	5.3
2	H	214	ILE	5.3
3	D	143	THR	5.3
2	H	137	LEU	5.1
2	H	128	ILE	5.0
2	E	164	ILE	4.9
2	H	139	ALA	4.9
2	H	65	MET	4.8
2	H	171	LEU	4.7
1	F	17	ILE	4.7
2	H	74	VAL	4.6
2	H	97	VAL	4.6
3	D	43	LYS	4.6
2	H	148	VAL	4.5
2	H	40	TRP	4.5
2	H	118	VAL	4.5
2	E	117	ILE	4.5
3	D	112	GLY	4.5
3	D	42	ALA	4.5
2	H	122	LEU	4.5
2	H	130	ALA	4.4
2	H	58	LEU	4.4
1	I	238	ARG	4.4
2	E	30	VAL	4.3
2	E	137	LEU	4.3
1	F	130	GLY	4.3
2	H	124	GLY	4.3
2	H	205	LEU	4.3
2	E	100	VAL	4.3
2	H	140	GLN	4.3
2	B	50	GLY	4.3
2	E	48	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
2	H	63	PHE	4.2
2	H	141	GLY	4.2
2	H	93	PRO	4.2
2	E	76	VAL	4.2
1	A	127	ALA	4.2
2	H	103	ILE	4.2
2	H	42	PHE	4.1
2	H	44	VAL	4.1
2	H	241	ILE	4.1
2	H	41	PRO	4.1
2	H	114	LEU	4.1
2	H	138	PRO	4.1
2	H	45	SER	4.0
2	H	64	VAL	4.0
2	E	245	ILE	4.0
2	H	210	LEU	3.9
2	H	99	ALA	3.9
2	H	119	ILE	3.9
2	E	83	LEU	3.9
2	H	48	LEU	3.9
2	H	120	LEU	3.9
3	G	44	GLU	3.9
3	C	43	LYS	3.9
2	E	97	VAL	3.9
2	H	71	VAL	3.9
2	H	123	ASN	3.8
2	E	159	GLY	3.8
2	E	71	VAL	3.8
2	E	74	VAL	3.8
2	H	245	ILE	3.8
2	E	85	ALA	3.8
2	B	29	ILE	3.8
2	H	126	ALA	3.7
2	H	95	ARG	3.7
1	F	19	GLY	3.7
2	E	158	LEU	3.7
2	H	151	LEU	3.7
2	E	89	SER	3.7
2	B	245	ILE	3.7
3	G	143	THR	3.7
3	D	144	LYS	3.6
2	H	238	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
2	E	144	LEU	3.6
2	E	80	ARG	3.6
2	E	189	VAL	3.6
2	H	240	TRP	3.6
2	B	246	GLN	3.6
2	H	211	ILE	3.6
2	E	118	VAL	3.6
2	H	80	ARG	3.6
2	E	130	ALA	3.5
3	D	56	GLY	3.5
2	H	153	MET	3.5
2	E	214	ILE	3.5
2	H	244	ILE	3.5
2	H	226	LEU	3.5
2	B	180	CYS	3.5
2	H	196	VAL	3.5
2	E	120	LEU	3.5
2	E	132	VAL	3.4
2	H	212	HIS	3.4
2	E	135	ALA	3.4
2	H	129	ASN	3.4
3	D	45	MET	3.4
2	B	111	VAL	3.4
2	E	60	ALA	3.4
1	F	29	TYR	3.3
2	E	103	ILE	3.3
2	H	39	ALA	3.3
2	H	68	ALA	3.3
2	E	98	PHE	3.3
2	E	183	SER	3.3
2	H	79	VAL	3.3
2	H	213	GLY	3.3
2	B	60	ALA	3.3
2	E	160	ARG	3.3
2	B	159	GLY	3.3
2	E	31	GLY	3.3
2	E	235	ALA	3.2
2	H	127	THR	3.2
2	B	93	PRO	3.2
2	E	241	ILE	3.2
2	H	60	ALA	3.2
2	H	150	CYS	3.2

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Mol	Chain	Res	Type	RSRZ
2	H	207	CYS	3.2
1	F	39	ALA	3.2
1	I	127	ALA	3.2
1	F	151	THR	3.2
2	H	31	GLY	3.2
2	E	57	THR	3.1
2	E	161	ASN	3.1
2	H	101	GLN	3.1
2	E	58	LEU	3.1
2	E	64	VAL	3.1
2	E	81	VAL	3.1
2	E	185	VAL	3.1
2	H	164	ILE	3.1
2	H	30	VAL	3.1
1	F	73	ASN	3.1
2	H	215	ALA	3.1
2	H	189	VAL	3.1
2	E	50	GLY	3.1
2	H	147	GLY	3.1
2	H	176	VAL	3.0
2	E	240	TRP	3.0
3	G	45	MET	3.0
2	H	75	ASN	3.0
1	F	153	THR	3.0
3	D	73	LEU	3.0
2	H	115	ASN	3.0
2	B	63	PHE	3.0
2	E	231	PHE	3.0
1	F	24	PRO	3.0
2	E	179	LEU	2.9
2	H	66	SER	2.9
2	B	191	GLY	2.9
2	E	163	GLY	2.9
2	H	106	ASN	2.9
1	F	74	ILE	2.9
2	H	89	SER	2.9
1	F	149	ARG	2.9
2	H	173	VAL	2.9
2	H	94	THR	2.9
2	H	174	THR	2.9
2	B	161	ASN	2.9
2	H	56	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
2	H	243	SER	2.9
1	F	28	PRO	2.9
1	F	72	HIS	2.9
2	H	192	ARG	2.9
2	B	243	SER	2.9
2	E	45	SER	2.9
2	E	229	ASP	2.9
2	B	83	LEU	2.9
2	E	210	LEU	2.9
2	E	51	GLY	2.9
2	H	154	GLY	2.9
2	E	79	VAL	2.8
2	E	173	VAL	2.8
2	E	175	VAL	2.8
2	E	218	VAL	2.8
2	H	155	TRP	2.8
2	E	59	ILE	2.8
1	F	150	GLY	2.8
2	H	191	GLY	2.8
2	E	246	GLN	2.8
2	H	133	GLN	2.8
1	F	76	ARG	2.8
1	I	126	ARG	2.8
1	F	127	ALA	2.8
2	H	37	PRO	2.8
2	H	206	VAL	2.8
2	H	108	TYR	2.8
2	E	126	ALA	2.8
2	H	237	PHE	2.8
2	H	131	ASN	2.8
1	I	51	GLU	2.8
2	H	105	GLU	2.8
3	D	67	LEU	2.8
1	F	84	ILE	2.8
3	D	108	THR	2.8
2	E	61	PRO	2.8
2	H	35	ALA	2.7
2	E	119	ILE	2.7
2	E	142	ARG	2.7
3	D	141	VAL	2.7
2	E	99	ALA	2.7
2	E	230	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	130	GLY	2.7
1	F	154	LEU	2.7
2	E	182	ARG	2.7
2	H	38	HIS	2.7
2	E	53	PHE	2.7
2	E	104	PHE	2.7
2	E	237	PHE	2.7
2	E	114	LEU	2.7
3	D	65	LEU	2.7
2	B	241	ILE	2.7
2	B	100	VAL	2.7
2	E	206	VAL	2.7
2	E	139	ALA	2.6
2	E	141	GLY	2.6
2	E	145	GLY	2.6
2	E	101	GLN	2.6
2	H	177	THR	2.6
2	H	216	SER	2.6
2	E	226	LEU	2.6
2	H	87	ASN	2.6
2	H	144	LEU	2.6
2	H	161	ASN	2.6
2	E	134	VAL	2.6
2	H	142	ARG	2.6
2	E	186	CYS	2.6
3	G	110	LYS	2.6
2	E	75	ASN	2.6
2	H	172	ASN	2.6
2	H	61	PRO	2.6
2	B	179	LEU	2.6
2	E	46	LEU	2.6
2	H	96	GLN	2.6
2	H	67	ALA	2.6
2	H	167	VAL	2.6
3	C	143	THR	2.6
2	E	93	PRO	2.6
2	H	47	GLN	2.6
2	H	29	ILE	2.6
3	C	44	GLU	2.6
3	D	107	ILE	2.6
2	E	111	VAL	2.6
2	H	78	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	H	235	ALA	2.6
2	E	138	PRO	2.5
3	D	134	ILE	2.5
1	F	71	ALA	2.5
2	E	223	ALA	2.5
2	H	146	ASN	2.5
2	H	185	VAL	2.5
2	E	127	THR	2.5
2	H	182	ARG	2.5
1	F	131	LEU	2.5
2	E	209	GLY	2.5
1	F	116	ASN	2.5
2	H	86	HIS	2.5
2	B	82	VAL	2.5
1	F	137	CYS	2.5
3	G	65	LEU	2.5
2	H	91	ARG	2.5
2	E	52	HIS	2.5
1	F	119	VAL	2.5
3	C	144	LYS	2.5
3	D	96	LYS	2.5
2	E	199	GLY	2.4
2	H	62	ASN	2.4
2	E	66	SER	2.4
2	H	84	GLY	2.4
2	E	194	ALA	2.4
2	E	196	VAL	2.4
2	E	122	LEU	2.4
2	E	42	PHE	2.4
2	E	198	PHE	2.4
1	A	39	ALA	2.4
2	E	67	ALA	2.4
2	B	106	ASN	2.4
2	H	125	SER	2.4
2	H	203	SER	2.4
3	D	81	LYS	2.4
3	G	144	LYS	2.4
2	E	197	CYS	2.4
3	G	67	LEU	2.3
2	H	53	PHE	2.3
2	E	56	ALA	2.3
2	E	244	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
2	E	124	GLY	2.3
2	H	179	LEU	2.3
2	H	104	PHE	2.3
2	E	68	ALA	2.3
2	B	61	PRO	2.3
2	H	160	ARG	2.3
1	F	152	ASP	2.3
3	D	48	VAL	2.3
2	E	88	LEU	2.3
2	E	155	TRP	2.3
2	E	128	ILE	2.3
2	E	154	GLY	2.3
2	H	50	GLY	2.3
2	E	243	SER	2.3
1	F	195	ASP	2.3
3	D	130	ASP	2.3
2	E	234	VAL	2.3
3	D	78	LEU	2.3
2	E	35	ALA	2.2
2	E	191	GLY	2.2
2	E	227	TYR	2.2
1	A	170	ILE	2.2
1	I	170	ILE	2.2
2	B	59	ILE	2.2
1	A	128	GLN	2.2
1	F	128	GLN	2.2
2	B	81	VAL	2.2
2	E	148	VAL	2.2
2	B	91	ARG	2.2
1	F	136	LEU	2.2
2	E	157	LEU	2.2
3	D	128	LEU	2.2
1	F	70	GLY	2.2
2	E	166	SER	2.2
1	F	142	TRP	2.2
2	B	240	TRP	2.2
1	F	233	ILE	2.2
2	B	103	ILE	2.2
1	F	79	ASN	2.2
2	E	123	ASN	2.2
1	F	113	VAL	2.2
2	H	246	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	206	ALA	2.2
2	E	39	ALA	2.2
2	H	232	ALA	2.2
1	A	29	TYR	2.2
1	F	158	GLN	2.2
3	G	111	ASP	2.2
1	F	22	SER	2.2
1	I	130	GLY	2.2
2	H	188	LEU	2.2
3	G	128	LEU	2.2
1	I	123	ALA	2.2
3	G	126	ALA	2.2
1	F	126	ARG	2.2
2	B	160	ARG	2.2
2	B	190	ARG	2.2
2	H	43	MET	2.1
2	E	211	ILE	2.1
2	E	47	GLN	2.1
3	D	109	TRP	2.1
3	D	122	ASP	2.1
1	F	139	VAL	2.1
2	B	89	SER	2.1
1	F	23	ARG	2.1
2	H	157	LEU	2.1
2	E	165	ALA	2.1
3	G	132	ASN	2.1
2	E	33	ARG	2.1
2	E	44	VAL	2.1
2	E	84	GLY	2.1
2	H	209	GLY	2.1
2	E	86	HIS	2.1
2	E	207	CYS	2.1
2	E	212	HIS	2.1
2	H	110	PRO	2.1
2	H	158	LEU	2.1
3	D	129	PHE	2.1
3	G	57	ILE	2.1
1	F	26	SER	2.1
1	I	114	ARG	2.1
2	H	143	ARG	2.1
1	F	147	MET	2.1
2	E	129	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	176	VAL	2.1
3	D	117	VAL	2.1
2	H	233	PRO	2.1
3	D	76	LEU	2.1
3	D	119	LEU	2.1
2	H	166	SER	2.0
3	D	57	ILE	2.0
3	D	46	GLN	2.0
3	D	132	ASN	2.0
2	H	111	VAL	2.0
2	B	226	LEU	2.0
2	E	40	TRP	2.0
2	H	70	CYS	2.0
1	F	148	ARG	2.0
2	E	34	ARG	2.0
2	B	42	PHE	2.0
2	E	136	GLN	2.0
2	H	236	GLN	2.0
2	E	91	ARG	2.0
2	E	162	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 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.