



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:25 AM UTC

PDB ID : 8D7K / pdb_00008d7k
Title : Bifunctional Inhibition of Neutrophil Elastase and Cathepsin G by Eap2 from *S. aureus*
Authors : Gido, C.D.; Herdendorf, T.J.; Geisbrecht, B.V.
Deposited on : 2022-06-07
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

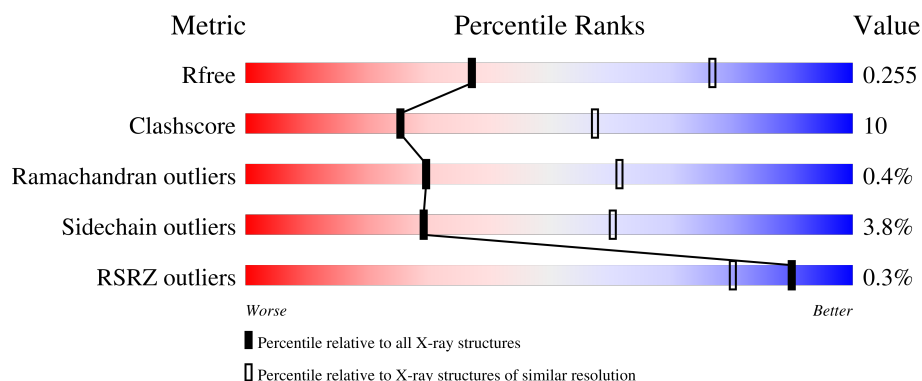
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	C	223	% 74% 25% .
1	F	223	70% 30% .
1	I	223	75% 24%
1	L	223	78% 22% .
2	B	100	% 73% 21% .

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Mol	Chain	Length	Quality of chain
2	E	100	69%26%
2	H	100	% 72%23%
2	K	100	% 70%26%
3	A	218	76%22%
3	D	218	76%23%
3	G	218	77%22%
3	J	218	77%23%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16684 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, C-terminal truncated form.

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

- Molecule 2 is a protein called Extracellular Adherence Protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	97	Total	C	N	O	0	0	0
			756	474	131	151			
2	E	97	Total	C	N	O	0	0	0
			756	474	131	151			
2	H	97	Total	C	N	O	0	0	0
			756	474	131	151			
2	K	97	Total	C	N	O	0	0	0
			756	474	131	151			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	155	GLY	-	expression tag	UNP Q99QS1
B	156	SER	-	expression tag	UNP Q99QS1
B	157	THR	-	expression tag	UNP Q99QS1
E	155	GLY	-	expression tag	UNP Q99QS1
E	156	SER	-	expression tag	UNP Q99QS1
E	157	THR	-	expression tag	UNP Q99QS1
H	155	GLY	-	expression tag	UNP Q99QS1
H	156	SER	-	expression tag	UNP Q99QS1

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Chain	Residue	Modelled	Actual	Comment	Reference
H	157	THR	-	expression tag	UNP Q99QS1
K	155	GLY	-	expression tag	UNP Q99QS1
K	156	SER	-	expression tag	UNP Q99QS1
K	157	THR	-	expression tag	UNP Q99QS1

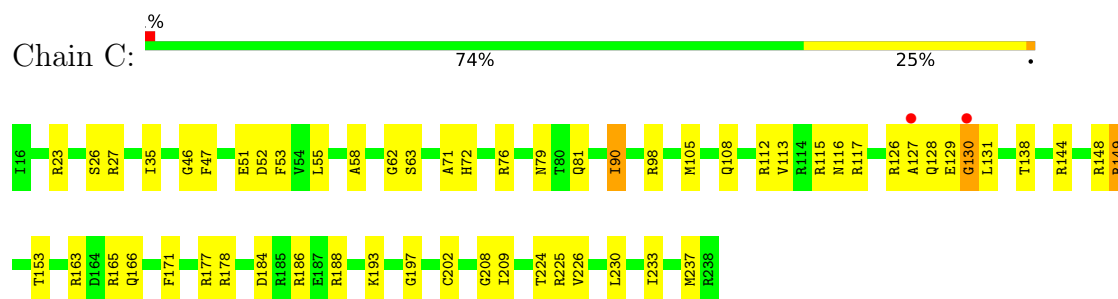
- Molecule 3 is a protein called Neutrophil elastase.

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

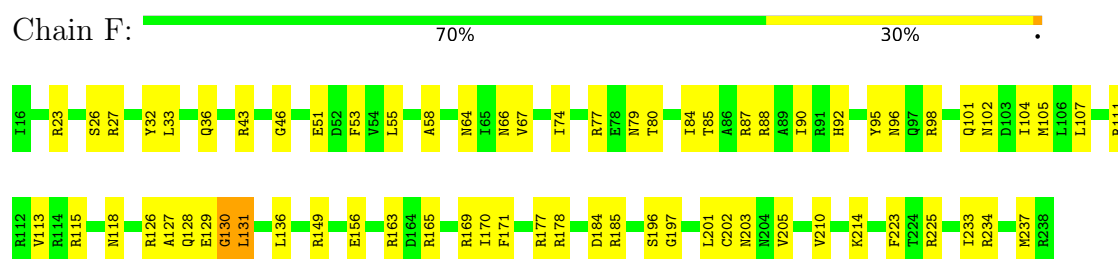
3 Residue-property plots

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.

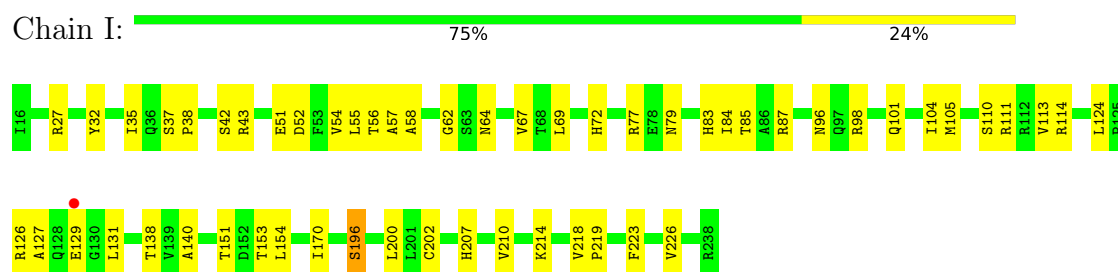
- Molecule 1: Cathepsin G, C-terminal truncated form



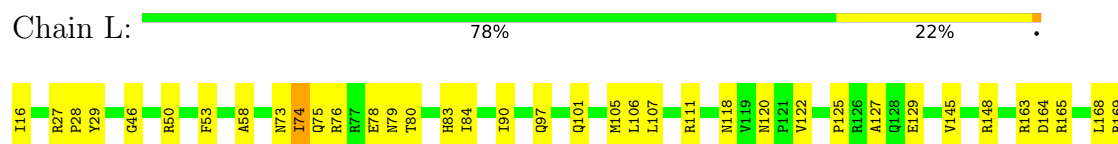
- Molecule 1: Cathepsin G, C-terminal truncated form



- Molecule 1: Cathepsin G, C-terminal truncated form



- Molecule 1: Cathepsin G, C-terminal truncated form





• Molecule 2: Extracellular Adherence Protein



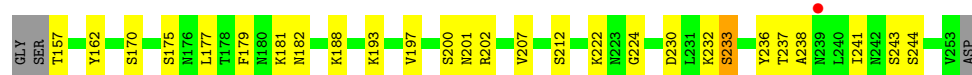
• Molecule 2: Extracellular Adherence Protein



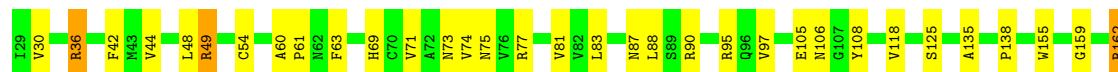
• Molecule 2: Extracellular Adherence Protein



• Molecule 2: Extracellular Adherence Protein

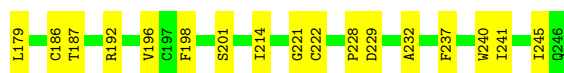


• Molecule 3: Neutrophil elastase

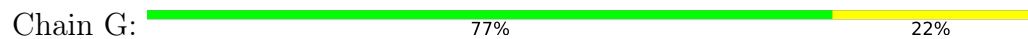


• Molecule 3: Neutrophil elastase

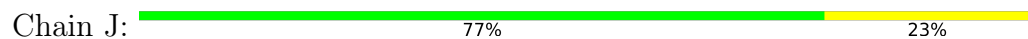




● Molecule 3: Neutrophil elastase



● Molecule 3: Neutrophil elastase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	97.59Å 107.44Å 105.42Å 90.00° 91.52° 90.00°	Depositor
Resolution (Å)	43.83 – 3.10 43.83 – 3.10	Depositor EDS
% Data completeness (in resolution range)	95.9 (43.83-3.10) 95.8 (43.83-3.10)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.15 (at 3.12Å)	Xtriage
Refinement program	PHENIX v1.9.2	Depositor
R, R_{free}	0.184 , 0.258 0.186 , 0.255	Depositor DCC
R_{free} test set	1986 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	51.0	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.020 for -h,-l,-k 0.001 for -h,l,k 0.032 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16684	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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	C	0.41	0/1814	0.66	0/2447
1	F	0.41	0/1814	0.64	0/2447
1	I	0.44	0/1814	0.62	0/2447
1	L	0.35	0/1814	0.62	0/2447
2	B	0.45	0/762	0.68	0/1029
2	E	0.52	0/762	0.73	0/1029
2	H	0.51	0/762	0.70	1/1029 (0.1%)
2	K	0.42	0/762	0.68	0/1029
3	A	0.38	0/1665	0.63	0/2263
3	D	0.44	0/1665	0.67	0/2263
3	G	0.35	0/1665	0.53	0/2263
3	J	0.31	0/1665	0.52	0/2263
All	All	0.41	0/16964	0.63	1/22956 (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	H	239	ASN	N-CA-C	5.52	119.06	110.17

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	C	1780	0	1793	41	0
1	F	1780	0	1793	47	0
1	I	1780	0	1793	36	0
1	L	1780	0	1793	30	0
2	B	756	0	788	17	0
2	E	756	0	788	30	0
2	H	756	0	788	18	0
2	K	756	0	788	19	0
3	A	1635	0	1652	31	0
3	D	1635	0	1652	44	0
3	G	1635	0	1652	32	0
3	J	1635	0	1652	34	0
All	All	16684	0	16932	324	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 10.

All (324) 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:E:239:ASN:HD22	3:D:69:HIS:CD2	1.64	1.14
2:E:239:ASN:ND2	3:D:69:HIS:CD2	2.40	0.89
2:E:239:ASN:ND2	3:D:69:HIS:HD2	1.72	0.87
3:G:144:LEU:HD22	3:G:148:VAL:HG11	1.56	0.85
2:E:239:ASN:HD22	3:D:69:HIS:HD2	0.87	0.84
1:C:130:GLY:HA3	1:C:225:ARG:HH11	1.42	0.83
1:C:149:ARG:HH11	2:E:225:THR:HG22	1.44	0.82
2:H:239:ASN:OD1	2:H:240:LEU:N	2.18	0.76
3:A:90:ARG:O	3:A:95:ARG:NH1	2.20	0.75
1:C:165:ARG:HH22	1:F:185:ARG:HH21	1.35	0.74
3:G:87:ASN:O	3:G:95:ARG:NH2	2.22	0.72
1:C:127:ALA:HA	1:C:230:LEU:HD13	1.73	0.71
2:B:226:LYS:HD3	1:F:149:ARG:HH12	1.58	0.69
3:G:106:ASN:HB2	3:G:240:TRP:CE2	2.29	0.68
3:A:105:GLU:HG2	3:A:118:VAL:HG23	1.76	0.68
3:A:75:ASN:HD21	3:A:77:ARG:HD2	1.59	0.67
3:G:31:GLY:O	3:G:192:ARG:NH2	2.28	0.67
1:L:50:ARG:HH22	1:L:238:ARG:HB2	1.60	0.66
1:L:27:ARG:NH1	1:L:29:TYR:OH	2.27	0.66
1:I:98:ARG:HH22	2:H:208:ASP:CG	2.04	0.66
3:D:161:ASN:OD1	1:I:111:ARG:NH1	2.30	0.65
2:H:239:ASN:OD1	2:H:240:LEU:O	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:ARG:HH22	3:D:105:GLU:H	1.45	0.65
3:D:109:ASP:OD2	3:D:112:ASN:ND2	2.24	0.64
1:I:129:GLU:HG2	1:I:207:HIS:NE2	2.12	0.63
1:C:130:GLY:HA3	1:C:225:ARG:NH1	2.13	0.63
2:E:188:LYS:HE2	3:D:221:GLY:HA2	1.80	0.63
1:F:27:ARG:NE	1:F:156:GLU:OE1	2.22	0.63
1:L:125:PRO:O	1:L:230:LEU:HD11	1.98	0.63
2:B:162:TYR:CZ	2:B:175:SER:HB3	2.33	0.63
1:C:47:PHE:CZ	1:C:55:LEU:HD23	2.35	0.62
2:K:162:TYR:CZ	2:K:175:SER:HB3	2.34	0.62
3:D:66:SER:OG	3:D:67:ALA:N	2.30	0.62
2:E:188:LYS:HE3	3:D:198:PHE:HE2	1.65	0.62
3:A:186:CYS:HB3	3:A:228:PRO:HB2	1.82	0.61
2:K:188:LYS:HE2	3:J:221:GLY:HA2	1.83	0.61
2:H:227:LYS:HG2	2:H:229:ILE:HD11	1.83	0.61
3:J:174:THR:HG21	3:J:190:ARG:HH22	1.66	0.61
1:F:165:ARG:O	1:F:169:ARG:HG3	2.01	0.60
3:A:185:VAL:HG23	3:A:233:PRO:HB3	1.84	0.60
1:L:58:ALA:HA	1:L:105:MET:HB2	1.84	0.60
3:A:204:PRO:HB2	3:A:211:ILE:HD12	1.84	0.60
2:B:212:SER:O	2:B:232:LYS:HE3	2.02	0.59
3:J:186:CYS:HB3	3:J:228:PRO:HB2	1.83	0.59
1:F:92:HIS:HB2	1:F:104:ILE:HG23	1.84	0.59
3:J:37:PRO:HA	3:J:86:HIS:CD2	2.37	0.59
1:C:163:ARG:CG	1:C:165:ARG:HG2	2.32	0.59
2:B:226:LYS:HD3	1:F:149:ARG:NH1	2.18	0.58
2:K:230:ASP:HB3	2:K:233:SER:HB3	1.84	0.58
3:G:186:CYS:HB3	3:G:228:PRO:HB2	1.85	0.58
2:H:226:LYS:HD3	1:L:148:ARG:HH22	1.68	0.58
3:J:33:ARG:NH2	3:J:172:ASN:OD1	2.34	0.58
1:C:149:ARG:NH1	2:E:225:THR:HG22	2.17	0.57
1:I:124:LEU:HD22	1:I:226:VAL:HG11	1.86	0.57
3:D:160:ARG:HG2	3:D:222:CYS:HB2	1.86	0.57
2:B:239:ASN:OD1	3:A:54:CYS:SG	2.62	0.57
3:J:66:SER:OG	3:J:67:ALA:N	2.37	0.57
2:E:164:ILE:HD11	2:E:197:VAL:HG23	1.87	0.57
3:J:185:VAL:HG23	3:J:233:PRO:HB3	1.86	0.56
2:K:182:ASN:HD21	3:J:49:ARG:HD2	1.71	0.56
3:G:44:VAL:HB	3:G:56:ALA:HB3	1.85	0.56
2:E:162:TYR:CZ	2:E:175:SER:HB3	2.40	0.55
2:K:193:LYS:O	2:K:197:VAL:HG22	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:30:VAL:HG22	3:D:159:GLY:HA2	1.88	0.54
3:G:42:PHE:CG	3:G:135:ALA:HB2	2.42	0.54
1:L:16:ILE:O	1:L:145:VAL:HA	2.07	0.54
1:I:52:ASP:OD1	1:I:52:ASP:N	2.34	0.54
1:F:203:ASN:O	1:F:205:VAL:HG23	2.08	0.54
1:I:32:TYR:OH	1:I:43:ARG:NE	2.39	0.54
3:G:189:VAL:HG11	3:G:194:ALA:HB3	1.90	0.54
3:A:30:VAL:HG22	3:A:159:GLY:HA2	1.89	0.54
1:F:171:PHE:HD1	2:E:169:THR:HG22	1.72	0.54
1:L:165:ARG:NH1	1:L:169:ARG:HH22	2.06	0.54
1:L:208:GLY:HA2	1:L:224:THR:O	2.08	0.54
2:H:227:LYS:HG2	2:H:229:ILE:CD1	2.38	0.53
1:C:163:ARG:HG2	1:C:165:ARG:HG2	1.90	0.53
1:F:163:ARG:HG3	1:F:165:ARG:H	1.74	0.53
2:H:212:SER:O	2:H:232:LYS:HE3	2.08	0.53
1:F:87:ARG:HE	1:F:88:ARG:HH12	1.57	0.53
3:D:90:ARG:O	3:D:95:ARG:NH2	2.42	0.53
2:H:197:VAL:O	2:H:201:ASN:HB2	2.09	0.53
2:E:212:SER:O	2:E:232:LYS:HE3	2.09	0.53
1:F:127:ALA:HB1	1:F:128:GLN:HG2	1.90	0.53
1:I:98:ARG:NH2	2:H:208:ASP:OD1	2.41	0.53
1:F:23:ARG:O	1:F:26:SER:OG	2.22	0.52
1:I:27:ARG:NH2	1:I:138:THR:HG21	2.24	0.52
3:G:69:HIS:HB3	3:G:108:TYR:OH	2.09	0.52
1:C:165:ARG:NH2	1:F:185:ARG:HH21	2.06	0.52
2:E:162:TYR:CE2	2:E:175:SER:HB3	2.44	0.52
3:A:106:ASN:HB2	3:A:240:TRP:CE2	2.43	0.52
1:I:55:LEU:HD11	1:I:104:ILE:HD11	1.91	0.52
3:D:192:ARG:NH1	1:I:114:ARG:HH21	2.07	0.52
1:L:125:PRO:HB2	1:L:129:GLU:HB3	1.92	0.51
3:D:137:LEU:HD21	3:D:241:ILE:HG21	1.92	0.51
2:E:188:LYS:HE3	3:D:198:PHE:CE2	2.43	0.51
2:K:222:LYS:NZ	2:K:244:SER:O	2.36	0.51
1:F:87:ARG:HE	1:F:88:ARG:NH1	2.07	0.51
2:E:215:ALA:HB1	2:E:231:LEU:HD12	1.93	0.51
2:K:212:SER:O	2:K:232:LYS:HE3	2.11	0.51
1:C:163:ARG:HG3	1:C:165:ARG:H	1.74	0.51
3:G:108:TYR:CE2	3:G:110:PRO:HB3	2.45	0.51
1:L:74:ILE:HD12	1:L:75:GLN:HG2	1.91	0.51
3:A:71:VAL:HA	3:A:74:VAL:HG22	1.92	0.51
1:I:58:ALA:HA	1:I:105:MET:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:182:ASN:HD21	3:J:49:ARG:HB3	1.76	0.51
2:K:157:THR:OG1	2:K:181:LYS:HB2	2.11	0.51
3:D:106:ASN:HB2	3:D:240:TRP:CE2	2.46	0.50
3:J:180:CYS:SG	3:J:181:ARG:N	2.80	0.50
2:E:183:GLN:O	2:E:243:SER:OG	2.23	0.50
3:D:161:ASN:HB3	1:I:85:THR:HG23	1.94	0.50
3:J:174:THR:HG21	3:J:190:ARG:NH2	2.27	0.50
3:D:67:ALA:O	3:D:70:CYS:HB2	2.12	0.50
3:J:106:ASN:HB2	3:J:240:TRP:CE2	2.47	0.50
3:D:237:PHE:O	3:D:241:ILE:HG13	2.12	0.49
1:C:72:HIS:O	1:C:153:THR:HA	2.11	0.49
3:D:34:ARG:NH1	1:I:79:ASN:HA	2.27	0.49
1:C:144:ARG:NH2	1:C:148:ARG:O	2.45	0.49
1:F:66:ASN:OD1	1:F:85:THR:HG22	2.13	0.49
1:I:196:SER:HA	1:I:210:VAL:HG12	1.94	0.49
3:J:138:PRO:HA	3:J:210:LEU:HD13	1.94	0.49
1:C:27:ARG:NH2	1:C:138:THR:HG21	2.27	0.49
1:C:165:ARG:HH12	1:F:185:ARG:NH2	2.11	0.49
1:C:177:ARG:HH12	1:C:178:ARG:HE	1.61	0.49
2:B:188:LYS:HE2	3:A:221:GLY:HA2	1.94	0.49
3:G:94:THR:HB	3:G:131:ASN:ND2	2.28	0.49
1:F:58:ALA:HA	1:F:105:MET:HB2	1.95	0.49
1:F:98:ARG:HH22	2:E:208:ASP:CG	2.21	0.49
1:L:80:THR:HB	1:L:118:ASN:HD22	1.77	0.48
1:L:127:ALA:HA	1:L:230:LEU:HD12	1.95	0.48
1:C:165:ARG:HG3	1:C:166:GLN:N	2.27	0.48
1:C:171:PHE:HD1	2:B:169:THR:HG22	1.78	0.48
1:F:170:ILE:CG2	1:F:214:LYS:HE2	2.43	0.48
1:I:56:THR:OG1	1:I:57:ALA:N	2.46	0.48
2:H:239:ASN:OD1	2:H:239:ASN:C	2.57	0.48
1:L:105:MET:HE3	1:L:107:LEU:HD21	1.96	0.48
3:J:44:VAL:HB	3:J:56:ALA:HB3	1.96	0.48
1:I:42:SER:HA	2:H:174:LEU:O	2.14	0.48
1:L:212:TYR:HB2	2:K:170:SER:O	2.14	0.48
2:H:162:TYR:CZ	2:H:175:SER:HB3	2.49	0.47
3:J:42:PHE:CG	3:J:135:ALA:HB2	2.49	0.47
3:G:70:CYS:SG	3:G:201:SER:HB3	2.54	0.47
3:J:35:ALA:O	3:J:86:HIS:NE2	2.44	0.47
1:F:115:ARG:HE	1:F:115:ARG:HB3	1.45	0.47
1:C:51:GLU:HG2	1:C:115:ARG:HD2	1.96	0.47
1:C:98:ARG:H	1:C:98:ARG:HG3	1.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:44:VAL:HG22	3:A:83:LEU:HD23	1.96	0.47
3:A:87:ASN:HA	3:A:166:SER:O	2.14	0.47
1:F:33:LEU:HD22	1:F:67:VAL:HG22	1.96	0.47
3:G:156:GLY:N	3:G:200:ASP:OD1	2.44	0.47
3:J:30:VAL:HG13	3:J:159:GLY:HA2	1.96	0.47
3:J:58:LEU:HD12	3:J:64:VAL:HG12	1.97	0.47
2:B:207:VAL:O	2:B:211:LEU:HG	2.15	0.47
2:B:237:THR:HG22	2:B:239:ASN:H	1.78	0.47
2:E:237:THR:HG22	3:D:69:HIS:CE1	2.49	0.47
1:I:96:ASN:HB3	1:I:101:GLN:HB3	1.97	0.47
1:I:98:ARG:NH1	2:H:203:GLY:O	2.48	0.47
2:K:177:LEU:HD22	2:K:193:LYS:HD3	1.97	0.47
1:F:55:LEU:HD12	1:F:105:MET:O	2.14	0.47
2:E:188:LYS:HE2	3:D:221:GLY:CA	2.45	0.47
2:E:238:ALA:HB3	3:D:201:SER:OG	2.14	0.47
1:F:233:ILE:HG22	1:F:237:MET:HE2	1.97	0.47
1:I:140:ALA:HB1	1:I:154:LEU:HD11	1.96	0.47
1:L:97:GLN:NE2	2:K:200:SER:O	2.45	0.47
3:D:88:LEU:HG	3:D:155:TRP:CD1	2.50	0.47
3:G:69:HIS:C	3:G:69:HIS:CD2	2.93	0.47
3:D:42:PHE:CG	3:D:135:ALA:HB2	2.49	0.47
3:G:184:ASN:HA	3:G:233:PRO:HD3	1.97	0.47
1:F:177:ARG:HH21	1:F:178:ARG:HH21	1.63	0.46
1:C:76:ARG:NH2	3:D:105:GLU:H	2.10	0.46
3:G:58:LEU:HD23	3:G:133:GLN:O	2.15	0.46
3:G:185:VAL:HG23	3:G:233:PRO:HB3	1.96	0.46
3:J:64:VAL:CG2	3:J:120:LEU:HB2	2.45	0.46
1:C:46:GLY:HA2	1:C:197:GLY:O	2.15	0.46
3:A:69:HIS:HB3	3:A:108:TYR:OH	2.14	0.46
3:D:214:ILE:HB	3:D:232:ALA:HB3	1.96	0.46
3:J:42:PHE:CD2	3:J:135:ALA:HB2	2.51	0.46
1:F:87:ARG:HG3	1:F:88:ARG:HG3	1.96	0.46
1:I:87:ARG:HB2	1:I:110:SER:HA	1.98	0.46
1:L:122:VAL:HG21	1:L:201:LEU:CD2	2.45	0.46
1:L:203:ASN:O	1:L:205:VAL:HG23	2.16	0.46
1:C:149:ARG:HG3	2:E:223:ASN:O	2.15	0.46
3:D:178:SER:O	3:D:179:LEU:HB2	2.15	0.46
3:G:106:ASN:OD1	1:L:76:ARG:NH2	2.49	0.46
3:G:205:LEU:HB2	3:G:231:PHE:CE2	2.51	0.46
3:D:186:CYS:HB3	3:D:228:PRO:HB2	1.97	0.46
1:I:131:LEU:HD12	1:I:131:LEU:HA	1.71	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:ASP:HB3	1:C:112:ARG:HG2	1.98	0.46
1:C:209:ILE:HG13	1:C:226:VAL:HG22	1.98	0.46
2:E:209:LEU:O	2:E:232:LYS:HE2	2.16	0.46
1:L:212:TYR:O	1:L:221:GLU:HB2	2.16	0.46
2:B:202:ARG:HD2	2:B:202:ARG:HA	1.68	0.45
1:I:84:ILE:HD12	1:I:113:VAL:HG12	1.97	0.45
3:G:71:VAL:HA	3:G:74:VAL:HG22	1.98	0.45
1:L:83:HIS:O	1:L:111:ARG:NH1	2.48	0.45
3:G:68:ALA:HA	3:G:118:VAL:HB	1.98	0.45
3:A:235:ALA:HA	3:A:238:VAL:HG23	1.98	0.45
3:J:115:ASN:HA	3:J:237:PHE:CZ	2.51	0.45
3:A:87:ASN:HB3	3:A:90:ARG:HD3	1.97	0.45
1:I:218:VAL:HA	1:I:219:PRO:HD3	1.85	0.45
1:L:28:PRO:HG2	1:L:120:ASN:OD1	2.16	0.45
2:B:206:ASP:O	2:B:210:ARG:HG3	2.17	0.45
3:A:60:ALA:HB3	3:A:63:PHE:HB2	1.99	0.45
1:I:170:ILE:CG2	1:I:214:LYS:HE2	2.47	0.45
1:C:23:ARG:HG2	1:C:26:SER:HB3	1.99	0.45
1:C:127:ALA:HB1	1:C:128:GLN:HG2	1.99	0.45
1:F:53:PHE:CG	1:F:237:MET:HG2	2.53	0.44
1:F:55:LEU:HD11	1:F:104:ILE:HG13	1.98	0.44
1:F:32:TYR:OH	1:F:43:ARG:NE	2.50	0.44
1:F:84:ILE:HD12	1:F:113:VAL:HG12	1.99	0.44
1:F:129:GLU:OE1	1:F:129:GLU:HA	2.16	0.44
1:I:42:SER:HB3	2:H:173:ILE:HD11	1.97	0.44
3:G:104:PHE:HB2	3:G:244:ILE:HD13	1.99	0.44
1:L:46:GLY:HA2	1:L:197:GLY:O	2.17	0.44
1:I:170:ILE:HG22	1:I:214:LYS:HE2	1.99	0.44
1:F:80:THR:HB	1:F:118:ASN:HD22	1.83	0.44
3:J:45:SER:HB2	3:J:155:TRP:CZ3	2.52	0.44
3:J:144:LEU:HD22	3:J:148:VAL:HG11	1.98	0.44
1:F:46:GLY:HA2	1:F:197:GLY:O	2.17	0.44
2:K:197:VAL:O	2:K:201:ASN:HB2	2.17	0.44
2:E:164:ILE:HD13	2:E:164:ILE:HG21	1.77	0.44
2:K:202:ARG:HA	2:K:202:ARG:HD2	1.85	0.44
1:C:116:ASN:HB2	1:C:117:ARG:H	1.64	0.44
1:C:163:ARG:HG3	1:C:165:ARG:HG2	1.98	0.44
3:D:102:ARG:HB3	3:D:121:GLN:HB3	2.00	0.44
1:I:54:VAL:HG21	1:I:67:VAL:HG11	2.00	0.44
3:A:186:CYS:HA	3:A:229:ASP:O	2.18	0.43
1:F:36:GLN:HB3	1:F:64:ASN:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:186:CYS:HA	3:D:229:ASP:O	2.18	0.43
1:C:35:ILE:HG23	1:C:62:GLY:HA3	1.99	0.43
3:G:171:LEU:HD21	3:G:189:VAL:HG21	1.99	0.43
3:J:64:VAL:HG22	3:J:120:LEU:HB2	1.99	0.43
1:C:53:PHE:CE1	1:C:108:GLN:HB2	2.54	0.43
1:C:130:GLY:CA	1:C:225:ARG:HH11	2.20	0.43
3:A:189:VAL:HG12	3:A:192:ARG:HB2	1.99	0.43
1:C:58:ALA:HA	1:C:105:MET:HB2	2.00	0.43
1:C:144:ARG:N	1:C:193:LYS:O	2.49	0.43
1:C:208:GLY:HA2	1:C:224:THR:O	2.18	0.43
3:A:184:ASN:HA	3:A:233:PRO:HD3	2.01	0.43
3:J:30:VAL:HG23	3:J:197:CYS:HB2	2.00	0.43
3:J:140:GLN:HB2	3:J:238:VAL:HB	2.00	0.43
2:K:188:LYS:HE3	3:J:198:PHE:CE2	2.54	0.43
3:D:63:PHE:CG	3:D:245:ILE:HG22	2.54	0.43
2:B:183:GLN:O	2:B:243:SER:OG	2.35	0.43
3:D:44:VAL:HB	3:D:56:ALA:HB3	2.00	0.43
1:I:126:ARG:O	1:I:127:ALA:C	2.62	0.43
1:L:50:ARG:NH2	1:L:238:ARG:HD3	2.34	0.43
3:G:240:TRP:CE2	3:G:244:ILE:HD11	2.54	0.43
3:J:219:ARG:C	3:J:221:GLY:H	2.27	0.43
1:C:233:ILE:HG22	1:C:237:MET:HE2	2.00	0.43
1:F:234:ARG:HD3	1:F:234:ARG:HA	1.89	0.43
3:G:43:MET:HE2	3:G:154:GLY:HA2	2.01	0.43
3:G:186:CYS:HA	3:G:229:ASP:O	2.18	0.43
2:K:238:ALA:HB3	3:J:201:SER:OG	2.19	0.43
1:F:171:PHE:CD1	2:E:169:THR:HG22	2.51	0.42
2:H:205:THR:O	2:H:208:ASP:HB2	2.19	0.42
1:L:53:PHE:CD1	1:L:106:LEU:HD22	2.54	0.42
2:K:179:PHE:CZ	2:K:193:LYS:HD2	2.54	0.42
1:F:210:VAL:HG22	1:F:223:PHE:CE2	2.54	0.42
2:E:193:LYS:O	2:E:196:SER:HB3	2.19	0.42
2:E:198:LEU:HB3	2:E:204:ILE:HB	2.02	0.42
3:D:161:ASN:ND2	3:D:161:ASN:H	2.18	0.42
1:F:95:TYR:HA	1:F:102:ASN:HB2	2.00	0.42
1:F:177:ARG:NH2	1:F:178:ARG:HH21	2.18	0.42
3:D:87:ASN:OD1	3:D:89:SER:OG	2.22	0.42
3:A:42:PHE:CG	3:A:135:ALA:HB2	2.55	0.42
1:F:105:MET:HE3	1:F:107:LEU:HD21	2.02	0.42
1:L:163:ARG:NH1	1:L:164:ASP:HB2	2.35	0.42
3:J:153:MET:O	3:J:203:SER:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:69:HIS:CD2	3:D:69:HIS:C	2.97	0.42
3:G:214:ILE:HB	3:G:232:ALA:HB3	2.01	0.42
3:A:36:ARG:HD2	3:A:36:ARG:HA	1.78	0.42
1:I:35:ILE:HG23	1:I:62:GLY:HA3	2.02	0.42
3:A:88:LEU:HD12	3:A:164:ILE:HD12	2.02	0.42
2:E:241:ILE:HD13	2:E:241:ILE:HG21	1.70	0.42
3:J:245:ILE:O	3:J:246:GLN:HB2	2.19	0.42
2:B:190:LEU:HD12	2:B:190:LEU:HA	1.82	0.42
3:A:88:LEU:HG	3:A:155:TRP:CD1	2.55	0.42
1:I:200:LEU:HB2	1:I:223:PHE:CE2	2.55	0.42
3:A:81:VAL:O	3:A:97:VAL:HA	2.20	0.41
1:F:136:LEU:HD23	1:F:136:LEU:HA	1.81	0.41
2:E:237:THR:HG21	3:D:69:HIS:CG	2.56	0.41
3:D:158:LEU:HD11	3:D:165:ALA:HA	2.01	0.41
3:J:152:ALA:O	3:J:170:GLU:HA	2.20	0.41
1:F:111:ARG:HD3	3:G:162:ARG:HH12	1.85	0.41
1:L:165:ARG:HA	1:L:168:LEU:HD12	2.02	0.41
2:B:188:LYS:CE	3:A:221:GLY:HA2	2.49	0.41
1:F:53:PHE:CD2	1:F:237:MET:HG2	2.55	0.41
1:F:130:GLY:HA2	1:F:225:ARG:HD3	2.02	0.41
1:L:73:ASN:N	1:L:78:GLU:OE2	2.36	0.41
1:C:71:ALA:HB2	1:C:81:GLN:HG2	2.01	0.41
2:H:169:THR:HG1	2:H:202:ARG:HH22	1.68	0.41
2:B:221:PHE:CD1	3:A:73:ASN:HB3	2.55	0.41
3:A:48:LEU:O	3:A:49:ARG:C	2.64	0.41
1:F:87:ARG:HH21	1:F:88:ARG:HH22	1.68	0.41
1:I:51:GLU:OE1	1:I:51:GLU:N	2.39	0.41
1:L:84:ILE:HG23	1:L:111:ARG:HG2	2.03	0.41
1:C:129:GLU:OE1	1:C:129:GLU:HA	2.21	0.41
3:A:138:PRO:HB3	3:A:212:HIS:NE2	2.35	0.41
2:E:239:ASN:OD1	2:E:239:ASN:O	2.39	0.41
1:F:111:ARG:NH1	3:G:162:ARG:NH1	2.69	0.41
1:F:196:SER:HA	1:F:210:VAL:HG12	2.02	0.41
2:E:188:LYS:CE	3:D:222:CYS:H	2.34	0.41
1:I:37:SER:HB3	1:I:38:PRO:HD2	2.02	0.41
1:I:151:THR:OG1	1:I:153:THR:O	2.34	0.41
2:H:226:LYS:CD	1:L:148:ARG:HH22	2.34	0.41
2:K:222:LYS:C	2:K:224:GLY:H	2.29	0.41
2:K:182:ASN:ND2	3:J:49:ARG:HB3	2.35	0.41
3:D:157:LEU:HG	3:D:163:GLY:HA2	2.03	0.40
3:D:162:ARG:NH1	1:I:83:HIS:CG	2.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:174:THR:O	3:D:187:THR:HA	2.22	0.40
2:B:182:ASN:OD1	3:A:49:ARG:HB3	2.20	0.40
1:F:96:ASN:HB3	1:F:101:GLN:HB3	2.03	0.40
3:D:34:ARG:HH12	1:I:79:ASN:HA	1.85	0.40
3:G:36:ARG:HD2	3:G:36:ARG:HA	1.92	0.40
1:C:90:ILE:C	1:C:105:MET:HG3	2.47	0.40
3:A:61:PRO:O	3:A:125:SER:HA	2.22	0.40
1:I:72:HIS:O	1:I:153:THR:HA	2.21	0.40
3:G:105:GLU:HG2	3:G:118:VAL:HG23	2.02	0.40
3:J:106:ASN:HD22	3:J:237:PHE:HD1	1.69	0.40
1:C:131:LEU:HD12	1:C:131:LEU:HA	1.78	0.40
2:B:162:TYR:CD2	2:B:177:LEU:HG	2.57	0.40
2:H:164:ILE:HG22	2:H:166:VAL:HG23	2.03	0.40
3:G:45:SER:HB2	3:G:155:TRP:CZ3	2.57	0.40
1:L:101:GLN:HG3	1:L:178:ARG:HH11	1.87	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	C	221/223 (99%)	213 (96%)	7 (3%)	1 (0%)	24	57
1	F	221/223 (99%)	205 (93%)	14 (6%)	2 (1%)	14	44
1	I	221/223 (99%)	214 (97%)	7 (3%)	0	100	100
1	L	221/223 (99%)	212 (96%)	9 (4%)	0	100	100
2	B	95/100 (95%)	92 (97%)	3 (3%)	0	100	100
2	E	95/100 (95%)	93 (98%)	2 (2%)	0	100	100
2	H	95/100 (95%)	91 (96%)	4 (4%)	0	100	100
2	K	95/100 (95%)	91 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	216/218 (99%)	197 (91%)	17 (8%)	2 (1%)	14	44
3	D	216/218 (99%)	197 (91%)	17 (8%)	2 (1%)	14	44
3	G	216/218 (99%)	199 (92%)	16 (7%)	1 (0%)	24	57
3	J	216/218 (99%)	201 (93%)	14 (6%)	1 (0%)	24	57
All	All	2128/2164 (98%)	2005 (94%)	114 (5%)	9 (0%)	30	61

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	161	ASN
1	C	130	GLY
1	F	130	GLY
3	A	162	ARG
1	F	131	LEU
3	G	162	ARG
3	J	146	ASN
3	D	146	ASN
3	A	191	GLY

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	C	190/190 (100%)	180 (95%)	10 (5%)	20	51
1	F	190/190 (100%)	180 (95%)	10 (5%)	20	51
1	I	190/190 (100%)	185 (97%)	5 (3%)	40	68
1	L	190/190 (100%)	184 (97%)	6 (3%)	34	64
2	B	90/92 (98%)	83 (92%)	7 (8%)	11	38
2	E	90/92 (98%)	84 (93%)	6 (7%)	15	43
2	H	90/92 (98%)	84 (93%)	6 (7%)	15	43
2	K	90/92 (98%)	84 (93%)	6 (7%)	15	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	172/172 (100%)	167 (97%)	5 (3%)	37	66
3	D	172/172 (100%)	168 (98%)	4 (2%)	44	70
3	G	172/172 (100%)	169 (98%)	3 (2%)	53	74
3	J	172/172 (100%)	171 (99%)	1 (1%)	78	83
All	All	1808/1816 (100%)	1739 (96%)	69 (4%)	29	60

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	63	SER
1	C	79	ASN
1	C	90	ILE
1	C	113	VAL
1	C	126	ARG
1	C	149	ARG
1	C	184	ASP
1	C	186	ARG
1	C	188	ARG
1	C	202	CYS
2	B	207	VAL
2	B	227	LYS
2	B	232	LYS
2	B	233	SER
2	B	236	TYR
2	B	237	THR
2	B	241	ILE
3	A	36	ARG
3	A	49	ARG
3	A	162	ARG
3	A	164	ILE
3	A	188	LEU
1	F	51	GLU
1	F	74	ILE
1	F	77	ARG
1	F	79	ASN
1	F	90	ILE
1	F	126	ARG
1	F	131	LEU
1	F	184	ASP
1	F	201	LEU
1	F	202	CYS

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Mol	Chain	Res	Type
2	E	219	VAL
2	E	229	ILE
2	E	233	SER
2	E	236	TYR
2	E	237	THR
2	E	241	ILE
3	D	77	ARG
3	D	161	ASN
3	D	162	ARG
3	D	196	VAL
1	I	64	ASN
1	I	69	LEU
1	I	77	ARG
1	I	196	SER
1	I	202	CYS
2	H	206	ASP
2	H	207	VAL
2	H	229	ILE
2	H	236	TYR
2	H	237	THR
2	H	241	ILE
3	G	36	ARG
3	G	181	ARG
3	G	196	VAL
1	L	74	ILE
1	L	79	ASN
1	L	90	ILE
1	L	184	ASP
1	L	201	LEU
1	L	202	CYS
2	K	207	VAL
2	K	233	SER
2	K	236	TYR
2	K	237	THR
2	K	241	ILE
2	K	243	SER
3	J	192	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	36	GLN

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Mol	Chain	Res	Type
1	C	97	GLN
2	B	176	ASN
2	B	220	ASN
3	A	75	ASN
3	A	121	GLN
1	F	25	HIS
1	F	64	ASN
1	F	166	GLN
2	E	176	ASN
2	E	220	ASN
2	E	239	ASN
2	E	250	ASN
3	D	38	HIS
3	D	73	ASN
3	D	101	GLN
3	D	133	GLN
3	D	212	HIS
3	D	236	GLN
1	I	101	GLN
1	I	120	ASN
2	H	220	ASN
2	H	250	ASN
3	G	75	ASN
1	L	118	ASN
2	K	159	GLN
2	K	182	ASN
2	K	183	GLN
3	J	115	ASN
3	J	121	GLN
3	J	169	GLN

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 [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 [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	C	223/223 (100%)	-0.36	2 (0%) 81 63	19, 43, 75, 93	0
1	F	223/223 (100%)	-0.42	0 100 100	17, 39, 64, 80	0
1	I	223/223 (100%)	-0.53	1 (0%) 88 76	18, 35, 61, 68	0
1	L	223/223 (100%)	-0.35	0 100 100	24, 49, 71, 82	0
2	B	97/100 (97%)	-0.42	1 (1%) 79 61	23, 34, 54, 57	0
2	E	97/100 (97%)	-0.51	0 100 100	15, 29, 45, 52	0
2	H	97/100 (97%)	-0.53	1 (1%) 79 61	14, 29, 44, 58	0
2	K	97/100 (97%)	-0.32	1 (1%) 79 61	27, 43, 68, 83	0
3	A	218/218 (100%)	-0.44	0 100 100	22, 46, 65, 91	0
3	D	218/218 (100%)	-0.58	0 100 100	20, 35, 58, 82	0
3	G	218/218 (100%)	-0.16	0 100 100	33, 57, 85, 97	0
3	J	218/218 (100%)	-0.08	0 100 100	27, 72, 97, 108	0
All	All	2152/2164 (99%)	-0.38	6 (0%) 90 80	14, 43, 79, 108	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	239	ASN	3.6
2	K	239	ASN	3.5
1	C	127	ALA	3.4
2	B	239	ASN	3.2
1	I	129	GLU	2.3
1	C	130	GLY	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.