



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:16 AM UTC

PDB ID : 5X7V / pdb_00005x7v
Title : Crystal structure of Nucleosome assembly protein S (PfNapS) from Plasmodium falciparum
Authors : Gill, J.; Yogavel, M.; Sharma, A.
Deposited on : 2017-02-27
Resolution : 2.80 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

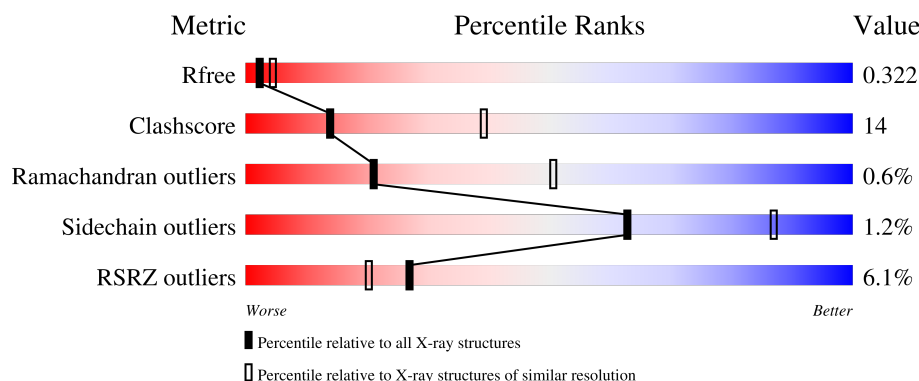
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	193	3% 70% 21% 8%
1	B	193	6% 60% 21% 17%
1	C	193	9% 57% 32% 7%
1	D	193	4% 66% 22% 11%
1	E	193	3% 55% 30% 13%

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Mol	Chain	Length	Quality of chain
1	F	193	8% 61% 23% • 13%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8441 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.

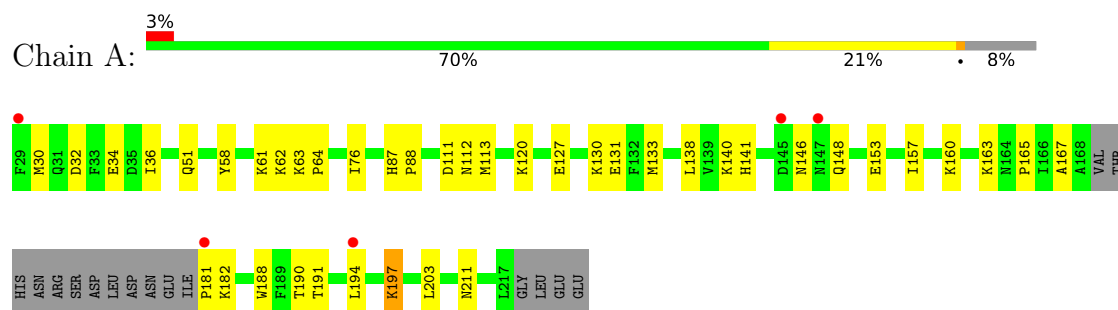
- Molecule 1 is a protein called Nucleosome assembly protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	177	Total	C	N	O	S	0	0	0
			1467	948	242	271	6			
1	B	160	Total	C	N	O	S	0	0	0
			1330	862	219	244	5			
1	C	179	Total	C	N	O	S	0	0	0
			1450	943	240	261	6			
1	D	172	Total	C	N	O	S	0	0	0
			1437	931	238	262	6			
1	E	167	Total	C	N	O	S	0	0	0
			1377	893	226	252	6			
1	F	168	Total	C	N	O	S	0	0	0
			1380	896	228	250	6			

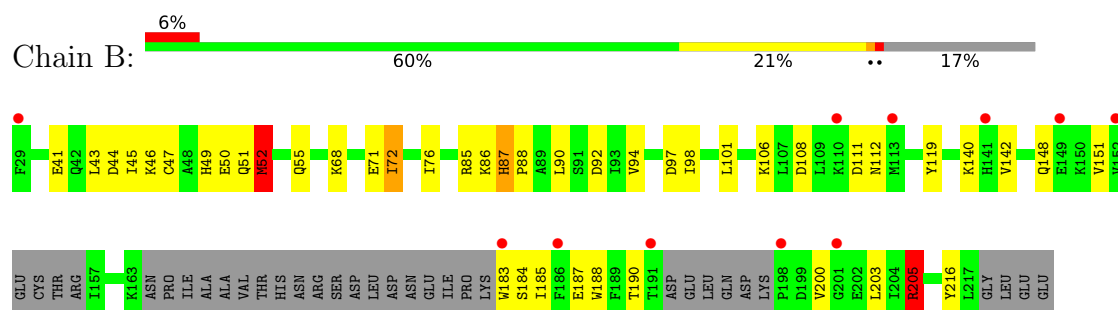
3 Residue-property plots [i](#)

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.

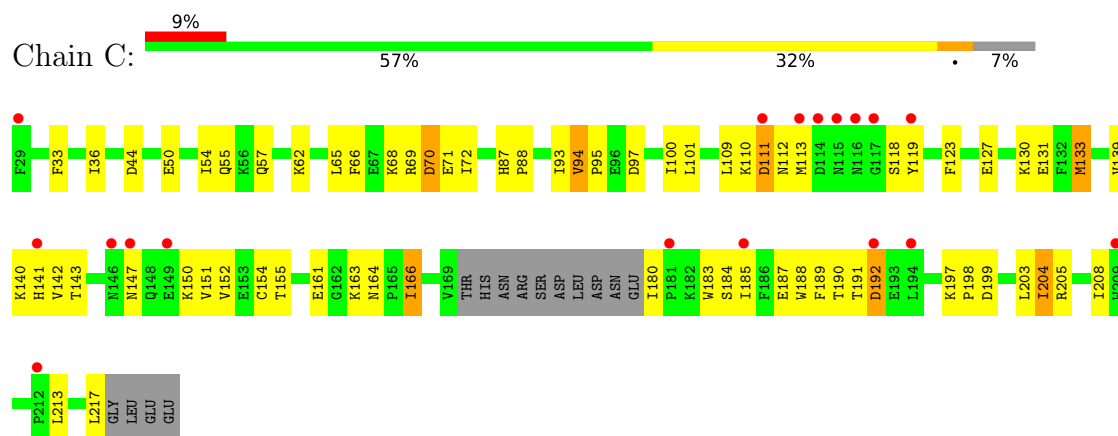
• Molecule 1: Nucleosome assembly protein



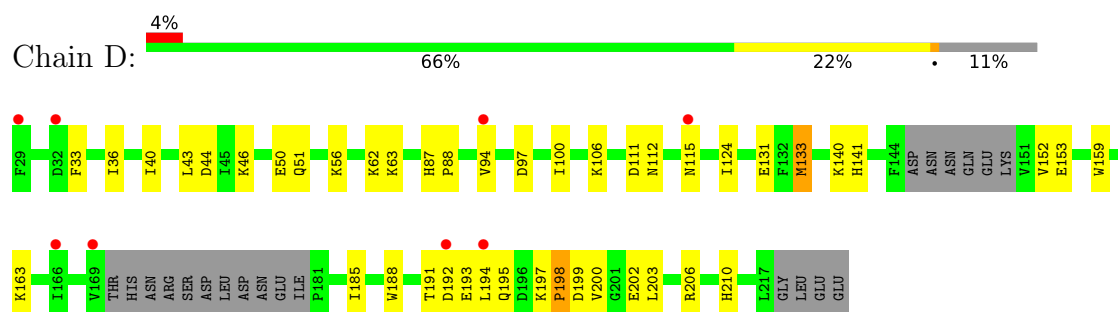
• Molecule 1: Nucleosome assembly protein



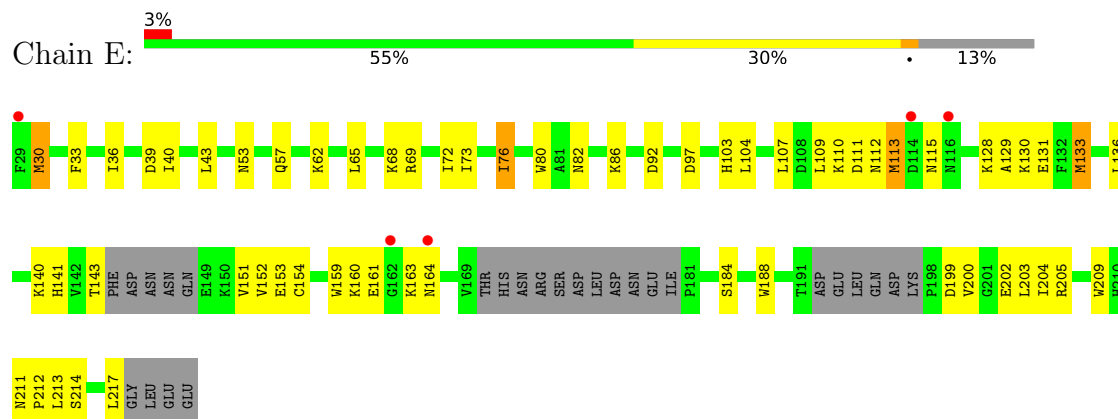
• Molecule 1: Nucleosome assembly protein



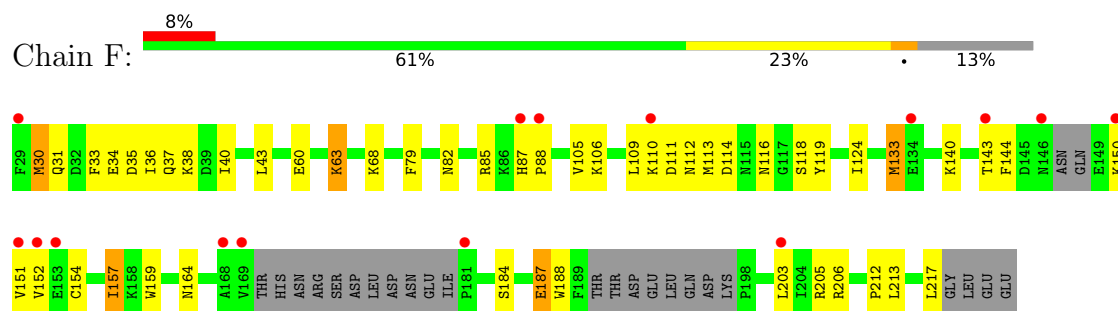
• Molecule 1: Nucleosome assembly protein



• Molecule 1: Nucleosome assembly protein



• Molecule 1: Nucleosome assembly protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	95.79Å 114.90Å 139.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.24 – 2.80 29.24 – 2.80	Depositor EDS
% Data completeness (in resolution range)	89.1 (29.24-2.80) 91.1 (29.24-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.82 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.243 , 0.312 0.263 , 0.322	Depositor DCC
R_{free} test set	1752 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	14.3	Xtriage
Anisotropy	2.267	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8441	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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	0.65	0/1502	0.96	6/2026 (0.3%)
1	B	0.75	0/1361	1.01	7/1834 (0.4%)
1	C	0.79	1/1485 (0.1%)	1.03	7/2007 (0.3%)
1	D	0.76	1/1471 (0.1%)	1.05	6/1983 (0.3%)
1	E	0.70	0/1409	1.02	6/1900 (0.3%)
1	F	0.74	0/1412	1.09	7/1903 (0.4%)
All	All	0.73	2/8640 (0.0%)	1.03	39/11653 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	94	VAL	CA-C	-6.31	1.47	1.52
1	D	100	ILE	CA-CB	-5.93	1.48	1.54

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	63	LYS	CA-C-N	-10.22	109.32	119.64
1	F	63	LYS	C-N-CA	-10.22	109.32	119.64
1	F	114	ASP	N-CA-C	-8.02	102.54	111.28
1	C	147	ASN	N-CA-C	7.84	119.45	111.07
1	B	94	VAL	CA-C-N	7.31	128.98	119.84
1	B	94	VAL	C-N-CA	7.31	128.98	119.84
1	C	113	MET	N-CA-C	7.11	118.68	111.07
1	B	205	ARG	N-CA-C	7.04	119.98	111.82
1	F	87	HIS	CA-C-N	-6.92	111.72	120.23
1	F	87	HIS	C-N-CA	-6.92	111.72	120.23
1	C	133	MET	N-CA-C	6.82	118.15	108.74
1	F	116	ASN	N-CA-C	6.72	120.51	111.24
1	B	148	GLN	N-CA-C	6.69	119.59	109.95
1	A	197	LYS	CA-C-N	6.54	128.02	119.84
1	A	197	LYS	C-N-CA	6.54	128.02	119.84
1	A	76	ILE	CA-C-N	6.17	127.55	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	76	ILE	C-N-CA	6.17	127.55	119.84
1	E	133	MET	N-CA-C	6.00	117.97	108.79
1	B	87	HIS	N-CA-C	-5.94	102.17	109.65
1	E	76	ILE	CA-C-N	5.90	127.21	119.84
1	E	76	ILE	C-N-CA	5.90	127.21	119.84
1	D	198	PRO	N-CA-C	5.83	121.52	113.65
1	D	191	THR	N-CA-C	-5.71	106.19	114.12
1	E	30	MET	N-CA-C	-5.66	104.73	111.69
1	A	211	ASN	CA-C-N	5.61	125.23	119.56
1	A	211	ASN	C-N-CA	5.61	125.23	119.56
1	E	164	ASN	CA-C-N	5.60	125.27	119.56
1	E	164	ASN	C-N-CA	5.60	125.27	119.56
1	C	204	ILE	N-CA-C	5.59	115.73	110.30
1	C	94	VAL	N-CA-CB	5.53	115.69	109.99
1	C	161	GLU	N-CA-C	5.48	117.96	111.33
1	D	133	MET	N-CA-C	5.40	117.05	108.79
1	B	72	ILE	CB-CA-C	-5.33	104.86	112.22
1	F	157	ILE	CB-CA-C	-5.29	103.53	110.98
1	D	152	VAL	N-CA-C	5.19	115.33	107.75
1	C	192	ASP	N-CA-C	5.17	121.81	110.80
1	D	63	LYS	CA-C-N	-5.15	114.77	119.82
1	D	63	LYS	C-N-CA	-5.15	114.77	119.82
1	B	52	MET	N-CA-C	-5.04	105.43	111.03

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	1467	0	1440	34	0
1	B	1330	0	1287	45	0
1	C	1450	0	1419	63	0
1	D	1437	0	1426	34	0
1	E	1377	0	1356	43	0
1	F	1380	0	1347	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8441	0	8275	240	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 14.

All (240) 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:F:133:MET:CE	1:F:159:TRP:CZ3	2.18	1.26
1:F:133:MET:HE3	1:F:159:TRP:HZ3	1.20	1.06
1:F:133:MET:HE3	1:F:159:TRP:CZ3	1.93	1.02
1:F:133:MET:CE	1:F:159:TRP:HZ3	1.64	0.97
1:E:30:MET:CE	1:F:217:LEU:HD21	1.96	0.95
1:A:51:GLN:O	1:B:51:GLN:NE2	2.01	0.93
1:E:30:MET:HE2	1:F:217:LEU:HD21	1.50	0.91
1:F:133:MET:HE2	1:F:159:TRP:CZ3	2.06	0.88
1:C:150:LYS:O	1:C:151:VAL:HG23	1.81	0.81
1:C:164:ASN:OD1	1:C:166:ILE:HG13	1.81	0.81
1:B:87:HIS:HD2	1:B:88:PRO:HD2	1.46	0.79
1:C:69:ARG:O	1:C:71:GLU:N	2.16	0.78
1:B:90:LEU:CD2	1:B:183:TRP:HH2	1.97	0.77
1:C:101:LEU:HD11	1:C:185:ILE:CD1	2.16	0.76
1:C:164:ASN:OD1	1:C:166:ILE:CG1	2.34	0.75
1:F:36:ILE:O	1:F:40:ILE:HD12	1.87	0.73
1:C:101:LEU:HD11	1:C:185:ILE:HD12	1.69	0.73
1:F:133:MET:HE1	1:F:159:TRP:CZ3	2.23	0.73
1:F:206:ARG:O	1:F:206:ARG:HG2	1.88	0.72
1:C:154:CYS:SG	1:C:190:THR:N	2.62	0.72
1:D:87:HIS:HD2	1:D:88:PRO:HD2	1.55	0.72
1:D:195:GLN:HG3	1:D:195:GLN:O	1.90	0.72
1:C:150:LYS:O	1:C:151:VAL:CG2	2.38	0.71
1:F:34:GLU:O	1:F:38:LYS:HG2	1.90	0.71
1:A:181:PRO:O	1:A:182:LYS:HG3	1.91	0.70
1:D:87:HIS:HE1	1:D:203:LEU:HD22	1.56	0.70
1:A:194:LEU:HD22	1:A:197:LYS:HD2	1.74	0.69
1:A:188:TRP:HD1	1:A:194:LEU:HD11	1.58	0.69
1:E:141:HIS:HB3	1:E:153:GLU:HB2	1.75	0.68
1:E:110:LYS:HG3	1:E:113:MET:HG3	1.75	0.68
1:E:103:HIS:CE1	1:E:128:LYS:HD2	2.29	0.68
1:B:140:LYS:HG2	1:B:188:TRP:CH2	2.29	0.68
1:C:69:ARG:O	1:C:70:ASP:C	2.35	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:HIS:HD2	1:C:88:PRO:HD2	1.58	0.68
1:C:139:VAL:HG22	1:C:155:THR:OG1	1.94	0.67
1:E:211:ASN:ND2	1:E:214:SER:OG	2.27	0.67
1:C:180:ILE:HD12	1:C:180:ILE:O	1.95	0.67
1:B:52:MET:O	1:B:55:GLN:N	2.28	0.67
1:B:97:ASP:OD2	1:B:185:ILE:N	2.26	0.66
1:C:213:LEU:HD22	1:D:33:PHE:HB3	1.78	0.65
1:B:119:TYR:CE2	1:B:205:ARG:HD3	2.32	0.65
1:E:217:LEU:HD21	1:F:30:MET:HE3	1.78	0.65
1:B:46:LYS:O	1:B:47:CYS:C	2.39	0.64
1:C:142:VAL:HG22	1:C:152:VAL:HG22	1.80	0.64
1:A:141:HIS:HB3	1:A:153:GLU:HB2	1.81	0.63
1:A:188:TRP:CD1	1:A:194:LEU:HD11	2.33	0.63
1:D:133:MET:HE2	1:D:159:TRP:CZ3	2.34	0.63
1:E:133:MET:HE2	1:E:159:TRP:CZ3	2.33	0.63
1:A:61:LYS:HB3	1:B:43:LEU:HD21	1.80	0.62
1:F:109:LEU:O	1:F:111:ASP:N	2.32	0.62
1:A:32:ASP:HB3	1:B:72:ILE:CD1	2.30	0.61
1:F:159:TRP:NE1	1:F:164:ASN:OD1	2.34	0.61
1:B:87:HIS:CD2	1:B:88:PRO:HD2	2.32	0.61
1:C:44:ASP:OD1	1:D:62:LYS:NZ	2.26	0.61
1:F:88:PRO:HG2	1:F:203:LEU:HD22	1.82	0.61
1:C:111:ASP:OD1	1:C:111:ASP:N	2.24	0.61
1:A:32:ASP:HB3	1:B:72:ILE:HD11	1.83	0.60
1:A:32:ASP:O	1:A:36:ILE:HG12	2.01	0.60
1:B:183:TRP:HZ3	1:B:185:ILE:HA	1.67	0.59
1:C:62:LYS:NZ	1:D:44:ASP:OD1	2.30	0.59
1:C:150:LYS:C	1:C:151:VAL:HG23	2.25	0.59
1:F:140:LYS:HG2	1:F:188:TRP:CH2	2.38	0.59
1:A:133:MET:HE3	1:A:157:ILE:HG23	1.84	0.58
1:A:127:GLU:OE2	1:A:130:LYS:NZ	2.36	0.58
1:A:62:LYS:NZ	1:B:44:ASP:OD1	2.31	0.58
1:F:143:THR:O	1:F:150:LYS:HA	2.04	0.58
1:E:39:ASP:O	1:E:43:LEU:HD23	2.04	0.58
1:E:68:LYS:HB3	1:F:36:ILE:HD11	1.85	0.58
1:C:69:ARG:C	1:C:71:GLU:N	2.61	0.57
1:A:133:MET:HE1	1:A:138:LEU:HD11	1.87	0.57
1:F:152:VAL:HG13	1:F:152:VAL:O	2.04	0.57
1:F:159:TRP:CD1	1:F:164:ASN:OD1	2.57	0.57
1:C:100:ILE:CG2	1:C:133:MET:HE2	2.34	0.57
1:C:87:HIS:HE1	1:C:203:LEU:HD22	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:ILE:HD13	1:C:185:ILE:HD11	1.86	0.57
1:C:187:GLU:OE1	1:C:197:LYS:HE2	2.04	0.57
1:E:30:MET:HE1	1:F:217:LEU:HD21	1.81	0.56
1:E:199:ASP:HB3	1:E:202:GLU:HB2	1.87	0.56
1:F:109:LEU:CD2	1:F:205:ARG:HA	2.35	0.56
1:F:144:PHE:CE1	1:F:150:LYS:HB2	2.41	0.56
1:F:109:LEU:HD22	1:F:205:ARG:HA	1.87	0.55
1:F:144:PHE:CE1	1:F:150:LYS:CB	2.89	0.55
1:B:119:TYR:CD2	1:B:205:ARG:HD2	2.42	0.55
1:A:181:PRO:O	1:A:182:LYS:CG	2.54	0.55
1:C:164:ASN:OD1	1:C:166:ILE:HG12	2.05	0.55
1:F:184:SER:O	1:F:187:GLU:HB2	2.06	0.55
1:C:54:ILE:HD13	1:C:57:GLN:NE2	2.23	0.54
1:D:106:LYS:HD2	1:D:124:ILE:HD12	1.89	0.54
1:E:111:ASP:OD1	1:E:112:ASN:N	2.39	0.54
1:A:61:LYS:O	1:A:64:PRO:HD2	2.06	0.54
1:E:200:VAL:O	1:E:204:ILE:HD12	2.07	0.54
1:C:131:GLU:O	1:C:163:LYS:HG3	2.09	0.53
1:E:131:GLU:OE2	1:E:163:LYS:NZ	2.42	0.53
1:F:112:ASN:OD1	1:F:113:MET:N	2.41	0.53
1:E:140:LYS:HD3	1:E:188:TRP:CH2	2.43	0.53
1:B:183:TRP:HE3	1:B:184:SER:O	1.91	0.53
1:C:87:HIS:CD2	1:C:88:PRO:HD2	2.42	0.53
1:B:90:LEU:HD22	1:B:183:TRP:HH2	1.73	0.53
1:C:50:GLU:O	1:C:54:ILE:HG12	2.08	0.53
1:E:213:LEU:HB2	1:F:33:PHE:CE2	2.43	0.53
1:D:111:ASP:OD1	1:D:112:ASN:N	2.42	0.52
1:D:140:LYS:HD3	1:D:188:TRP:CZ2	2.45	0.52
1:B:90:LEU:CD2	1:B:183:TRP:CH2	2.85	0.52
1:B:142:VAL:HG22	1:B:151:VAL:HG23	1.90	0.52
1:B:119:TYR:CD2	1:B:205:ARG:CD	2.93	0.52
1:A:111:ASP:OD1	1:A:112:ASN:N	2.42	0.52
1:C:127:GLU:O	1:C:130:LYS:HG3	2.10	0.52
1:C:69:ARG:C	1:C:71:GLU:H	2.18	0.52
1:A:131:GLU:HG2	1:A:163:LYS:HE3	1.92	0.51
1:B:87:HIS:HE1	1:B:203:LEU:HD22	1.75	0.51
1:E:107:LEU:O	1:E:209:TRP:HZ3	1.92	0.51
1:F:106:LYS:HB3	1:F:124:ILE:HB	1.92	0.51
1:B:119:TYR:CE2	1:B:205:ARG:CD	2.94	0.51
1:A:30:MET:O	1:A:34:GLU:HG3	2.10	0.50
1:B:90:LEU:HD23	1:B:183:TRP:CH2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:GLN:HG2	1:D:51:GLN:HE22	1.77	0.50
1:B:183:TRP:HZ3	1:B:185:ILE:HD12	1.77	0.50
1:F:206:ARG:O	1:F:206:ARG:CG	2.58	0.50
1:A:120:LYS:HG3	1:A:141:HIS:HB2	1.93	0.50
1:A:146:ASN:C	1:A:148:GLN:H	2.20	0.49
1:E:202:GLU:OE1	1:E:205:ARG:NH2	2.44	0.49
1:F:79:PHE:HZ	1:F:212:PRO:HB2	1.77	0.49
1:B:111:ASP:OD1	1:B:112:ASN:N	2.41	0.49
1:B:46:LYS:O	1:B:49:HIS:N	2.44	0.49
1:C:87:HIS:CE1	1:C:203:LEU:HD13	2.48	0.49
1:C:199:ASP:O	1:C:203:LEU:HG	2.12	0.49
1:F:140:LYS:HE3	1:F:154:CYS:HB2	1.94	0.49
1:E:130:LYS:HG3	1:E:136:LEU:HD11	1.94	0.48
1:D:192:ASP:C	1:D:192:ASP:OD1	2.56	0.48
1:E:103:HIS:HE1	1:E:128:LYS:HD2	1.77	0.48
1:F:105:VAL:HG12	1:F:124:ILE:O	2.12	0.48
1:E:160:LYS:O	1:E:161:GLU:C	2.55	0.48
1:D:202:GLU:OE1	1:D:206:ARG:NE	2.47	0.48
1:F:43:LEU:HA	1:F:43:LEU:HD23	1.60	0.48
1:C:140:LYS:HD3	1:C:188:TRP:CH2	2.49	0.48
1:F:144:PHE:CE1	1:F:150:LYS:HB3	2.49	0.48
1:D:194:LEU:O	1:D:194:LEU:HG	2.13	0.47
1:B:142:VAL:HG22	1:B:151:VAL:CG2	2.45	0.47
1:D:185:ILE:HG13	1:D:200:VAL:HG11	1.95	0.47
1:C:140:LYS:HD3	1:C:188:TRP:CZ2	2.50	0.47
1:C:164:ASN:CG	1:C:166:ILE:HG13	2.39	0.47
1:E:82:ASN:O	1:E:86:LYS:HD2	2.15	0.47
1:C:213:LEU:HG	1:C:217:LEU:HD23	1.96	0.47
1:D:140:LYS:HD3	1:D:188:TRP:CH2	2.50	0.47
1:C:183:TRP:CZ2	1:C:198:PRO:HG2	2.50	0.47
1:F:82:ASN:OD1	1:F:85:ARG:NH1	2.48	0.47
1:D:188:TRP:CG	1:D:200:VAL:HG22	2.50	0.46
1:B:183:TRP:CZ3	1:B:185:ILE:HA	2.48	0.46
1:E:141:HIS:ND1	1:E:153:GLU:OE1	2.48	0.46
1:C:68:LYS:HB3	1:D:36:ILE:HD13	1.97	0.46
1:E:129:ALA:HB3	1:E:136:LEU:HD22	1.98	0.46
1:D:87:HIS:CD2	1:D:88:PRO:HD2	2.44	0.46
1:D:141:HIS:HB3	1:D:153:GLU:HB2	1.98	0.46
1:E:80:TRP:HB3	1:E:104:LEU:HD23	1.97	0.46
1:F:68:LYS:HD2	1:F:68:LYS:HA	1.79	0.46
1:C:123:PHE:CD1	1:C:189:PHE:HZ	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:LYS:HB3	1:D:198:PRO:HD2	1.98	0.46
1:C:112:ASN:N	1:C:118:SER:O	2.49	0.46
1:C:213:LEU:HG	1:C:217:LEU:CD2	2.46	0.45
1:A:32:ASP:CB	1:B:72:ILE:HD13	2.46	0.45
1:A:87:HIS:ND1	1:A:88:PRO:HD2	2.30	0.45
1:C:100:ILE:HG21	1:C:133:MET:HE2	1.96	0.45
1:A:63:LYS:HB2	1:A:64:PRO:HD3	1.97	0.45
1:E:211:ASN:HA	1:F:37:GLN:NE2	2.31	0.45
1:C:101:LEU:CD1	1:C:185:ILE:HD12	2.43	0.45
1:C:110:LYS:O	1:C:119:TYR:HA	2.17	0.45
1:C:69:ARG:O	1:C:72:ILE:N	2.50	0.45
1:E:72:ILE:O	1:E:76:ILE:HD12	2.16	0.45
1:B:43:LEU:HD12	1:B:43:LEU:HA	1.82	0.45
1:D:193:GLU:OE1	1:D:193:GLU:N	2.50	0.45
1:E:212:PRO:HG2	1:F:33:PHE:HZ	1.81	0.45
1:F:203:LEU:C	1:F:203:LEU:HD12	2.41	0.45
1:D:94:VAL:O	1:D:97:ASP:HB2	2.17	0.45
1:B:106:LYS:HE2	1:B:108:ASP:OD2	2.17	0.44
1:C:44:ASP:OD2	1:D:210:HIS:NE2	2.50	0.44
1:B:76:ILE:O	1:B:76:ILE:HG22	2.18	0.44
1:C:213:LEU:HD13	1:D:33:PHE:CG	2.53	0.44
1:D:197:LYS:HB3	1:D:198:PRO:CD	2.48	0.44
1:E:62:LYS:HA	1:E:65:LEU:HD23	1.97	0.44
1:B:45:ILE:O	1:B:46:LYS:C	2.54	0.44
1:C:33:PHE:O	1:C:36:ILE:HG22	2.18	0.44
1:C:139:VAL:CG2	1:C:155:THR:OG1	2.62	0.44
1:E:97:ASP:OD1	1:E:184:SER:OG	2.34	0.44
1:E:211:ASN:OD1	1:F:37:GLN:NE2	2.46	0.44
1:A:87:HIS:HE2	1:A:203:LEU:HD22	1.83	0.44
1:E:36:ILE:O	1:E:40:ILE:HG12	2.18	0.44
1:F:119:TYR:CD1	1:F:205:ARG:HD3	2.53	0.44
1:A:190:THR:OG1	1:A:191:THR:N	2.51	0.43
1:D:56:LYS:NZ	1:D:115:ASN:OD1	2.36	0.43
1:C:150:LYS:C	1:C:151:VAL:CG2	2.90	0.43
1:D:46:LYS:O	1:D:50:GLU:HG3	2.18	0.43
1:D:87:HIS:CE1	1:D:203:LEU:HD22	2.45	0.43
1:F:35:ASP:O	1:F:38:LYS:HB2	2.17	0.43
1:F:133:MET:CE	1:F:159:TRP:CH2	2.90	0.43
1:C:65:LEU:HD23	1:C:65:LEU:HA	1.82	0.43
1:B:200:VAL:HA	1:B:203:LEU:HD12	2.01	0.43
1:C:62:LYS:HG3	1:D:43:LEU:CD2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:LEU:HD22	1:C:205:ARG:HA	2.01	0.43
1:A:130:LYS:O	1:A:160:LYS:NZ	2.46	0.42
1:E:33:PHE:CG	1:F:213:LEU:HD13	2.54	0.42
1:B:142:VAL:HA	1:B:151:VAL:HG23	2.01	0.42
1:A:188:TRP:HD1	1:A:194:LEU:CD1	2.29	0.42
1:E:199:ASP:O	1:E:203:LEU:HG	2.19	0.42
1:F:140:LYS:HG2	1:F:188:TRP:CZ2	2.54	0.42
1:C:204:ILE:HA	1:C:208:ILE:HB	2.00	0.42
1:C:183:TRP:CH2	1:C:198:PRO:HG2	2.55	0.42
1:E:143:THR:HB	1:E:151:VAL:HG12	2.01	0.42
1:B:90:LEU:C	1:B:92:ASP:H	2.28	0.42
1:A:165:PRO:C	1:A:167:ALA:H	2.26	0.42
1:C:97:ASP:OD2	1:C:184:SER:HA	2.19	0.42
1:C:55:GLN:HG2	1:D:51:GLN:NE2	2.35	0.42
1:B:86:LYS:HE2	1:B:216:TYR:O	2.20	0.42
1:C:191:THR:O	1:C:191:THR:HG22	2.20	0.42
1:B:101:LEU:HD23	1:B:101:LEU:HA	1.84	0.41
1:C:141:HIS:CE1	1:C:143:THR:HG22	2.55	0.41
1:A:165:PRO:C	1:A:167:ALA:N	2.77	0.41
1:B:68:LYS:O	1:B:72:ILE:HG13	2.21	0.41
1:C:139:VAL:H	1:C:155:THR:HG1	1.66	0.41
1:E:69:ARG:O	1:E:73:ILE:HG13	2.20	0.41
1:A:32:ASP:HB3	1:B:72:ILE:HD13	2.03	0.41
1:A:140:LYS:HD3	1:A:188:TRP:CZ2	2.56	0.41
1:B:187:GLU:O	1:B:190:THR:HG23	2.21	0.41
1:F:150:LYS:O	1:F:150:LYS:HG2	2.21	0.41
1:A:58:TYR:OH	1:B:50:GLU:OE2	2.35	0.41
1:B:85:ARG:HD3	1:B:98:ILE:HD12	2.03	0.41
1:B:90:LEU:HD22	1:B:185:ILE:HD13	2.02	0.41
1:C:66:PHE:CE1	1:D:40:ILE:HD13	2.56	0.41
1:D:131:GLU:O	1:D:163:LYS:HG3	2.20	0.41
1:E:53:ASN:O	1:E:57:GLN:HG3	2.21	0.41
1:E:115:ASN:HD22	1:E:115:ASN:HA	1.60	0.41
1:E:213:LEU:HB2	1:F:33:PHE:CD2	2.56	0.41
1:F:118:SER:HB3	1:F:143:THR:HA	2.03	0.41
1:D:185:ILE:HD13	1:D:185:ILE:HG21	1.88	0.41
1:E:109:LEU:HD23	1:E:209:TRP:CD1	2.56	0.41
1:A:113:MET:HE3	1:A:113:MET:HB2	1.86	0.40
1:E:92:ASP:OD1	1:E:92:ASP:N	2.52	0.40
1:E:152:VAL:HG12	1:E:153:GLU:N	2.36	0.40
1:B:41:GLU:O	1:B:44:ASP:HB2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:60:GLU:O	1:F:63:LYS:HG2	2.21	0.40
1:C:94:VAL:HA	1:C:95:PRO:HD3	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	173/193 (90%)	163 (94%)	10 (6%)	0	100	100
1	B	152/193 (79%)	136 (90%)	16 (10%)	0	100	100
1	C	175/193 (91%)	156 (89%)	17 (10%)	2 (1%)	11	36
1	D	166/193 (86%)	156 (94%)	9 (5%)	1 (1%)	21	51
1	E	159/193 (82%)	147 (92%)	11 (7%)	1 (1%)	21	51
1	F	160/193 (83%)	151 (94%)	7 (4%)	2 (1%)	9	31
All	All	985/1158 (85%)	909 (92%)	70 (7%)	6 (1%)	21	51

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	110	LYS
1	C	70	ASP
1	C	192	ASP
1	D	199	ASP
1	E	154	CYS
1	F	151	VAL

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	159/181 (88%)	159 (100%)	0	100	100
1	B	143/181 (79%)	140 (98%)	3 (2%)	47	79
1	C	153/181 (84%)	151 (99%)	2 (1%)	61	86
1	D	158/181 (87%)	158 (100%)	0	100	100
1	E	150/181 (83%)	149 (99%)	1 (1%)	76	91
1	F	147/181 (81%)	142 (97%)	5 (3%)	32	68
All	All	910/1086 (84%)	899 (99%)	11 (1%)	63	87

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	52	MET
1	B	71	GLU
1	B	205	ARG
1	C	111	ASP
1	C	166	ILE
1	E	113	MET
1	F	30	MET
1	F	31	GLN
1	F	133	MET
1	F	157	ILE
1	F	187	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	146	ASN
1	B	53	ASN
1	B	82	ASN
1	B	87	HIS
1	B	103	HIS

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Mol	Chain	Res	Type
1	C	57	GLN
1	C	87	HIS
1	C	141	HIS
1	D	87	HIS
1	E	51	GLN
1	E	102	ASN
1	E	103	HIS
1	E	115	ASN
1	E	211	ASN
1	F	37	GLN
1	F	211	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	177/193 (91%)	0.27	5 (2%) 55 45	50, 57, 76, 85	0
1	B	160/193 (82%)	0.62	11 (6%) 23 16	53, 65, 86, 104	0
1	C	179/193 (92%)	0.65	18 (10%) 12 9	52, 62, 84, 95	0
1	D	172/193 (89%)	0.46	8 (4%) 36 29	50, 59, 73, 88	0
1	E	167/193 (86%)	0.42	5 (2%) 52 42	54, 65, 82, 100	0
1	F	168/193 (87%)	0.59	15 (8%) 15 11	52, 64, 84, 94	0
All	All	1023/1158 (88%)	0.50	62 (6%) 27 20	50, 62, 82, 104	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	147	ASN	4.4
1	C	114	ASP	4.3
1	C	116	ASN	3.9
1	F	151	VAL	3.8
1	D	29	PHE	3.5
1	F	88	PRO	3.5
1	C	29	PHE	3.4
1	C	192	ASP	3.3
1	B	29	PHE	3.3
1	A	147	ASN	3.2
1	E	162	GLY	3.2
1	D	32	ASP	3.1
1	C	117	GLY	3.1
1	B	186	PHE	3.0
1	F	87	HIS	2.9
1	A	145	ASP	2.9
1	F	181	PRO	2.9
1	F	134	GLU	2.8
1	F	110	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	152	VAL	2.8
1	B	113	MET	2.8
1	C	209	TRP	2.7
1	C	113	MET	2.7
1	B	191	THR	2.7
1	A	194	LEU	2.7
1	B	149	GLU	2.6
1	B	152	VAL	2.6
1	A	29	PHE	2.6
1	F	153	GLU	2.6
1	F	203	LEU	2.6
1	B	198	PRO	2.6
1	D	169	VAL	2.6
1	C	146	ASN	2.6
1	C	185	ILE	2.5
1	A	181	PRO	2.5
1	F	29	PHE	2.5
1	E	164	ASN	2.5
1	F	146	ASN	2.5
1	B	183	TRP	2.4
1	C	149	GLU	2.4
1	D	94	VAL	2.4
1	C	111	ASP	2.4
1	D	192	ASP	2.4
1	B	141	HIS	2.3
1	C	212	PRO	2.3
1	C	119	TYR	2.3
1	F	143	THR	2.3
1	C	194	LEU	2.2
1	D	194	LEU	2.2
1	D	166	ILE	2.2
1	F	169	VAL	2.2
1	F	168	ALA	2.2
1	E	114	ASP	2.2
1	E	29	PHE	2.2
1	B	110	LYS	2.2
1	B	201	GLY	2.1
1	C	141	HIS	2.1
1	C	115	ASN	2.1
1	C	181	PRO	2.0
1	D	115	ASN	2.0
1	E	116	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	150	LYS	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.