Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 11:20 PM EDT

PDB ID	:	7N9U
Title	:	CA-targeting nanobody is a tool for studying HIV-1 capsid lattice interactions
Authors	:	Gerber, E.E.; Digianantonio, K.M.; Tripler, T.N.; Smaga, S.S.; Summers, B.J.; Xiong, Y.
Deposited on	:	2021-06-18
Resolution	:	3.19 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

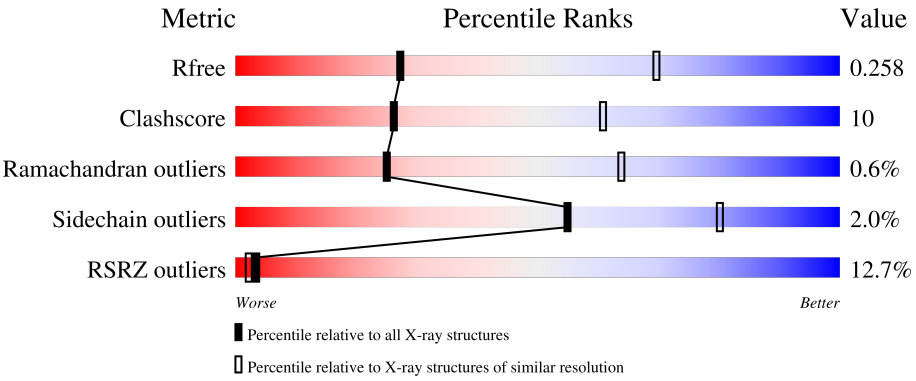
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.19 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 <=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	80% 14%
1	B	223	4% 82% 13%
1	C	223	78% 18%
2	D	118	8% 71% 25%
2	E	118	31% 73% 23%

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Mol	Chain	Length	Quality of chain
2	F	118	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7616 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 Capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	4	0
			1663	1048	290	310	15			
1	B	214	Total	C	N	O	S	0	4	0
			1669	1052	293	309	15			
1	C	219	Total	C	N	O	S	0	4	0
			1680	1058	293	314	15			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	CYS	ALA	conflict	UNP B6DRA0
A	45	CYS	GLU	conflict	UNP B6DRA0
A	184	ALA	TRP	conflict	UNP B6DRA0
A	185	ALA	MET	conflict	UNP B6DRA0
A	223	PRO	-	expression tag	UNP B6DRA0
B	14	CYS	ALA	conflict	UNP B6DRA0
B	45	CYS	GLU	conflict	UNP B6DRA0
B	184	ALA	TRP	conflict	UNP B6DRA0
B	185	ALA	MET	conflict	UNP B6DRA0
B	223	PRO	-	expression tag	UNP B6DRA0
C	14	CYS	ALA	conflict	UNP B6DRA0
C	45	CYS	GLU	conflict	UNP B6DRA0
C	184	ALA	TRP	conflict	UNP B6DRA0
C	185	ALA	MET	conflict	UNP B6DRA0
C	223	PRO	-	expression tag	UNP B6DRA0

- Molecule 2 is a protein called Nanobody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	116	Total	C	N	O	S	0	0	0
			873	547	154	168	4			

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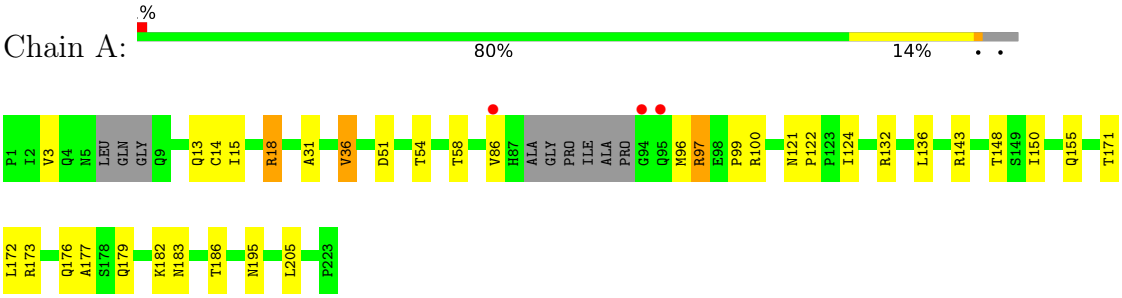
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	116	Total	C	N	O	S	0	0	0
			873	547	154	168	4			
2	F	113	Total	C	N	O	S	0	0	0
			858	538	151	165	4			

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.

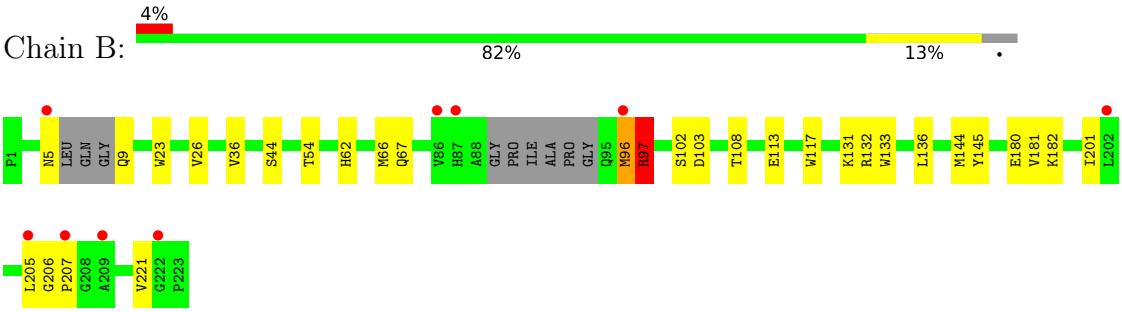
• Molecule 1: Capsid protein

Chain A:



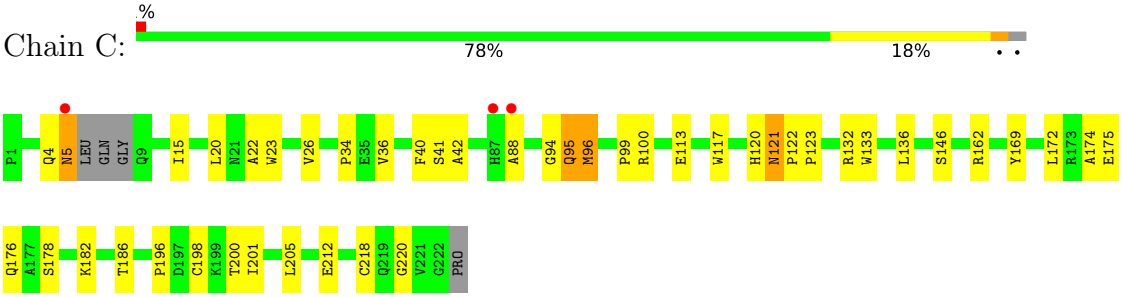
• Molecule 1: Capsid protein

Chain B:



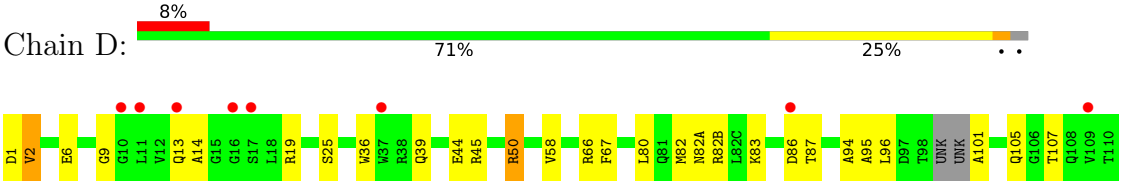
• Molecule 1: Capsid protein

Chain C:



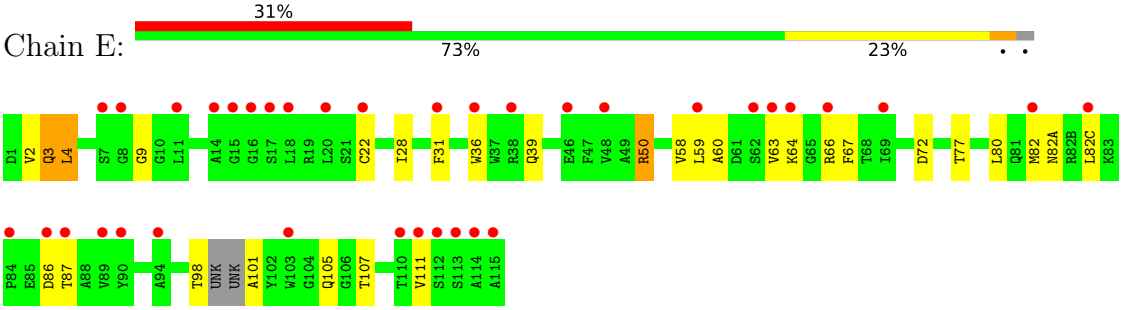
• Molecule 2: Nanobody

Chain D:



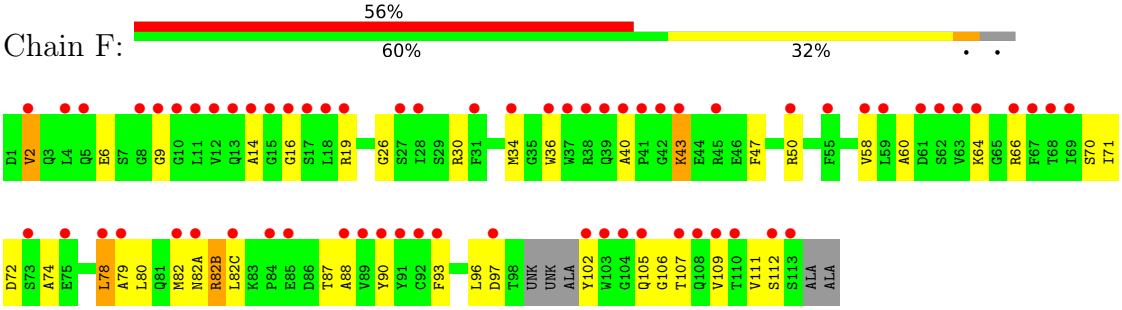
• Molecule 2: Nanobody

Chain E:



• Molecule 2: Nanobody

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	129.70Å 143.57Å 228.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.19 – 3.19 49.19 – 3.19	Depositor EDS
% Data completeness (in resolution range)	91.4 (49.19-3.19) 91.5 (49.19-3.19)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.228 , 0.258 0.228 , 0.258	Depositor DCC
R_{free} test set	1601 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å^2)	106.1	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 98.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7616	wwPDB-VP
Average B, all atoms (Å^2)	155.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.36	0/1702	0.68	0/2311
1	B	0.40	0/1709	0.78	4/2321 (0.2%)
1	C	0.36	0/1721	0.78	2/2341 (0.1%)
2	D	0.52	1/888 (0.1%)	0.93	1/1200 (0.1%)
2	E	0.46	0/889	1.04	4/1203 (0.3%)
2	F	0.53	1/873 (0.1%)	1.08	3/1179 (0.3%)
All	All	0.42	2/7782 (0.0%)	0.85	14/10555 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	VAL	CB-CG2	10.28	1.74	1.52
2	F	2	VAL	CB-CG2	7.46	1.68	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	2	VAL	CG1-CB-CG2	10.58	127.83	110.90
1	C	96	MET	CG-SD-CE	-10.46	83.47	100.20
1	C	96	MET	CB-CG-SD	-10.28	81.56	112.40
2	E	2	VAL	CG1-CB-CG2	9.17	125.58	110.90
2	F	78	LEU	CA-CB-CG	8.74	135.40	115.30
1	B	97	ARG	CB-CG-CD	7.89	132.12	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	43	LYS	N-CA-C	-7.21	91.54	111.00
2	E	3	GLN	CA-CB-CG	6.95	128.69	113.40
2	D	39	GLN	C-N-CA	-6.49	105.48	121.70
2	E	4	LEU	CA-CB-CG	6.47	130.19	115.30
1	B	96	MET	CG-SD-CE	-6.40	89.95	100.20
2	E	39	GLN	C-N-CA	-6.17	106.28	121.70
1	B	96	MET	N-CA-CB	5.66	120.78	110.60
1	B	96	MET	N-CA-C	-5.23	96.87	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	121	ASN	Peptide
1	C	121	ASN	Peptide

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	1663	0	1639	24	0
1	B	1669	0	1647	30	0
1	C	1680	0	1640	28	0
2	D	873	0	853	28	0
2	E	873	0	854	23	0
2	F	858	0	838	41	0
All	All	7616	0	7471	157	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 (157) 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:B:207:PRO:HD2	2:F:50:ARG:HH22	1.34	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:ILE:HD13	2:D:95:ALA:HB1	1.56	0.87
2:D:13:GLN:HB2	2:D:114:ALA:HB2	1.60	0.83
2:D:87:THR:HG22	2:D:111:VAL:H	1.44	0.82
2:E:87:THR:HG22	2:E:111:VAL:H	1.44	0.82
2:D:67:PHE:CZ	2:D:82:MET:HE3	2.23	0.72
2:E:67:PHE:CZ	2:E:82:MET:HE3	2.25	0.72
1:B:206:GLY:HA3	2:F:50:ARG:NH2	2.05	0.71
2:E:98:THR:HG22	2:E:101:ALA:H	1.55	0.71
1:B:96:MET:HG2	1:B:97:ARG:O	1.91	0.71
2:F:82:MET:HE1	2:F:109:VAL:HG11	1.74	0.70
2:E:59:LEU:HG	2:E:63:VAL:HG23	1.75	0.69
2:F:36:TRP:CG	2:F:80:LEU:HD12	2.28	0.69
2:F:40:ALA:HB3	2:F:43:LYS:HE3	1.76	0.68
2:E:59:LEU:HD21	2:E:67:PHE:HB2	1.74	0.67
2:E:82(C):LEU:HB3	2:E:111:VAL:HG11	1.77	0.65
1:A:99:PRO:HG2	1:A:124:ILE:HG21	1.79	0.65
2:D:13:GLN:CB	2:D:114:ALA:HB2	2.26	0.64
1:A:183:ASN:HB2	1:A:186:THR:HG23	1.80	0.63
1:C:99:PRO:HG3	1:C:117:TRP:CE2	2.34	0.62
1:C:132:ARG:O	1:C:136:LEU:HG	1.99	0.61
1:A:18:ARG:HD3	1:A:18:ARG:H	1.66	0.61
2:F:66:ARG:HB2	2:F:82(A):ASN:O	2.01	0.60
2:E:36:TRP:CG	2:E:80:LEU:HD12	2.37	0.60
1:B:96:MET:SD	1:B:117:TRP:CE2	2.95	0.60
1:A:132:ARG:O	1:A:136:LEU:HG	2.02	0.59
1:C:146:SER:OG	1:C:175:GLU:HG2	2.02	0.59
1:B:221:VAL:HG22	2:F:97:ASP:H	1.67	0.59
1:A:148:THR:OG1	1:A:171:THR:HG21	2.03	0.59
2:F:40:ALA:HB3	2:F:43:LYS:HB3	1.82	0.59
1:B:144:MET:CE	1:C:212:GLU:HG2	2.32	0.59
1:A:173:ARG:HG3	1:A:179:GLN:HA	1.84	0.59
1:C:96:MET:HE1	1:C:113:GLU:HG2	1.84	0.58
2:D:36:TRP:CG	2:D:80:LEU:HD12	2.39	0.58
2:F:2:VAL:HG11	2:F:102:TYR:CE2	2.39	0.58
1:B:144:MET:HE1	1:C:212:GLU:HG2	1.86	0.57
1:C:96:MET:CE	1:C:113:GLU:HA	2.33	0.57
2:F:19:ARG:NH2	2:F:79:ALA:HB2	2.20	0.57
2:D:13:GLN:HG3	2:D:14:ALA:O	2.05	0.57
2:F:16:GLY:O	2:F:82(C):LEU:HD13	2.05	0.57
1:B:96:MET:HG2	1:B:97:ARG:N	2.20	0.56
1:C:121:ASN:O	1:C:123:PRO:HD3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:PRO:O	1:C:200:THR:HG23	2.06	0.56
1:A:13:GLN:HG2	1:A:13:GLN:O	2.05	0.56
1:A:86:VAL:HG13	1:A:100:ARG:HH12	1.71	0.55
1:A:172:LEU:O	1:A:176:GLN:HB2	2.06	0.55
2:E:28:ILE:HG23	2:E:31:PHE:HD2	1.72	0.55
1:B:132:ARG:O	1:B:136:LEU:HG	2.06	0.55
2:D:94:ALA:O	2:D:101:ALA:HB3	2.07	0.55
1:C:22:ALA:O	1:C:26:VAL:HG23	2.08	0.54
2:E:82(C):LEU:HD23	2:E:111:VAL:CG2	2.37	0.54
2:D:80:LEU:HD22	2:D:82:MET:HG2	1.90	0.54
1:B:102:SER:OG	1:B:108:THR:OG1	2.11	0.54
2:D:82(B):ARG:N	2:D:82(B):ARG:HD2	2.22	0.54
1:B:5:ASN:OD1	1:B:9:GLN:N	2.41	0.53
2:F:26:GLY:HA3	2:F:30:ARG:HH22	1.73	0.53
2:F:82(C):LEU:HB3	2:F:111:VAL:HG11	1.89	0.53
2:F:71:ILE:HA	2:F:78:LEU:HB2	1.89	0.53
1:B:181:VAL:HG12	1:B:182:LYS:HG2	1.91	0.52
1:C:172:LEU:O	1:C:176:GLN:HB2	2.10	0.52
1:A:155:GLN:CD	1:A:195:ASN:HD22	2.13	0.52
2:E:60:ALA:O	2:E:64:LYS:HG3	2.09	0.52
1:A:143:ARG:HG3	1:A:177:ALA:HB2	1.91	0.52
1:B:205:LEU:O	2:F:50:ARG:CZ	2.58	0.52
1:B:96:MET:HE1	1:B:113:GLU:HB3	1.92	0.52
1:C:220:GLY:HA3	2:D:96:LEU:O	2.09	0.52
2:F:105:GLN:H	2:F:105:GLN:CD	2.14	0.51
2:F:36:TRP:NE1	2:F:80:LEU:HB2	2.26	0.51
2:F:60:ALA:O	2:F:64:LYS:HG3	2.11	0.51
2:E:4:LEU:HG	2:E:22:CYS:SG	2.51	0.51
2:D:44:GLU:OE1	2:D:45:ARG:HB2	2.11	0.51
2:F:14:ALA:N	2:F:112:SER:O	2.44	0.50
2:D:2:VAL:HA	2:D:25:SER:OG	2.10	0.50
2:D:82(A):ASN:HB3	2:D:82(B):ARG:HD2	1.94	0.50
1:B:96:MET:SD	1:B:117:TRP:NE1	2.84	0.50
2:F:80:LEU:HD22	2:F:82:MET:HG2	1.93	0.50
2:F:70:SER:O	2:F:78:LEU:HB2	2.12	0.49
1:A:3:VAL:HG11	1:A:13:GLN:OE1	2.12	0.49
1:C:4:GLN:O	1:C:5:ASN:C	2.51	0.49
1:B:133:TRP:O	1:B:136:LEU:HB2	2.12	0.49
1:B:207:PRO:HD2	2:F:50:ARG:NH2	2.16	0.48
1:C:94:GLY:O	1:C:95:GLN:CB	2.61	0.48
2:D:66:ARG:NH1	2:D:83:LYS:HE3	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:SER:OG	1:B:131:LYS:HE2	2.12	0.48
2:F:87:THR:HA	2:F:109:VAL:O	2.14	0.48
1:B:206:GLY:HA3	2:F:50:ARG:HH22	1.76	0.48
2:E:59:LEU:HD23	2:E:64:LYS:HA	1.96	0.48
2:F:50:ARG:CG	2:F:58:VAL:HB	2.43	0.48
2:E:80:LEU:HD22	2:E:82:MET:HG2	1.96	0.47
1:B:103:ASP:HB3	1:B:117:TRP:CH2	2.49	0.47
1:B:180:GLU:O	1:B:180:GLU:HG2	2.15	0.47
2:E:50:ARG:HG2	2:E:58:VAL:HB	1.96	0.47
2:E:82(C):LEU:HD23	2:E:111:VAL:HG21	1.95	0.47
2:F:40:ALA:O	2:F:43:LYS:O	2.33	0.47
1:B:96:MET:CE	1:B:113:GLU:HB3	2.44	0.47
2:D:105:GLN:CD	2:D:105:GLN:H	2.18	0.47
2:F:2:VAL:HG11	2:F:102:TYR:CD2	2.50	0.46
1:C:133:TRP:O	1:C:136:LEU:HB2	2.15	0.46
2:F:72:ASP:OD1	2:F:74:ALA:HB3	2.16	0.46
2:D:6:GLU:OE1	2:D:6:GLU:N	2.47	0.46
2:F:82(C):LEU:HD23	2:F:111:VAL:HG22	1.98	0.46
1:C:120:HIS:HB3	1:C:122:PRO:O	2.16	0.46
2:E:105:GLN:H	2:E:105:GLN:CD	2.18	0.46
2:E:66:ARG:HB2	2:E:82(A):ASN:O	2.16	0.45
2:E:9:GLY:H	2:E:107:THR:HG21	1.82	0.45
1:A:150:ILE:HG12	1:A:172:LEU:HD13	1.99	0.45
2:D:13:GLN:HA	2:D:112:SER:O	2.16	0.45
1:B:180:GLU:O	1:B:181:VAL:HG23	2.17	0.45
1:C:96:MET:HE3	1:C:113:GLU:HA	1.98	0.45
2:D:66:ARG:HB2	2:D:82(A):ASN:O	2.16	0.45
2:F:40:ALA:CB	2:F:43:LYS:HE3	2.46	0.45
1:B:23:TRP:O	1:B:26:VAL:HG12	2.17	0.45
2:D:9:GLY:HA3	2:D:107:THR:HG22	1.99	0.45
2:F:82(B):ARG:HA	2:F:82(B):ARG:HD2	1.70	0.45
1:B:207:PRO:CD	2:F:50:ARG:HH22	2.19	0.45
1:C:34:PRO:HG3	1:C:174:ALA:HB2	1.99	0.45
1:B:62:HIS:O	1:B:66[A]:MET:HG2	2.17	0.44
2:E:72:ASP:HB3	2:E:77:THR:HG22	1.99	0.44
2:F:80:LEU:CD2	2:F:82:MET:HG2	2.48	0.44
2:E:87:THR:HG22	2:E:111:VAL:N	2.23	0.44
2:F:34:MET:HA	2:F:93:PHE:O	2.18	0.44
2:F:47:PHE:CZ	2:F:50:ARG:NE	2.79	0.44
2:D:44:GLU:OE1	2:D:45:ARG:N	2.51	0.43
2:F:6:GLU:OE1	2:F:6:GLU:N	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:LEU:O	2:E:50:ARG:HD3	2.19	0.43
1:C:205:LEU:O	2:D:50:ARG:HD3	2.19	0.43
1:B:54:THR:HG21	1:C:42:ALA:HB2	2.00	0.43
1:A:172:LEU:HD12	1:A:172:LEU:HA	1.84	0.43
2:E:82(C):LEU:HD23	2:E:111:VAL:HG22	2.01	0.43
2:F:43:LYS:NZ	2:F:88:ALA:HB2	2.34	0.42
1:A:173:ARG:CZ	1:A:179:GLN:HG3	2.49	0.42
2:F:90:TYR:O	2:F:106:GLY:HA2	2.18	0.42
1:A:96:MET:O	1:A:97:ARG:HG2	2.18	0.42
1:A:86:VAL:HG13	1:A:100:ARG:NH1	2.34	0.42
1:B:201:ILE:CD1	1:B:221:VAL:HG21	2.50	0.42
2:F:30:ARG:HG2	2:F:96:LEU:HD22	2.00	0.42
1:C:176:GLN:C	1:C:178:SER:N	2.72	0.42
2:E:28:ILE:HG22	2:E:28:ILE:O	2.19	0.42
2:D:96:LEU:HD12	2:D:96:LEU:HA	1.86	0.42
1:A:31:ALA:O	1:A:36[B]:VAL:HG21	2.20	0.41
1:A:54:THR:O	1:A:58:THR:HG23	2.20	0.41
1:A:155:GLN:NE2	1:A:195:ASN:HD22	2.17	0.41
1:B:145:TYR:CZ	1:C:162:ARG:HD3	2.55	0.41
1:C:23:TRP:CZ3	1:C:40:PHE:HB2	2.55	0.41
2:F:9:GLY:HA3	2:F:107:THR:HG22	2.02	0.41
2:D:66:ARG:HH12	2:D:83:LYS:HE3	1.85	0.41
2:D:9:GLY:H	2:D:107:THR:HG21	1.85	0.41
2:F:82(C):LEU:HB3	2:F:111:VAL:CG1	2.51	0.41
1:C:201:ILE:CD1	2:D:95:ALA:HB1	2.39	0.41
1:A:15:ILE:HD11	1:A:51:ASP:HA	2.02	0.41
1:B:67:GLN:HG3	1:C:169:TYR:CD1	2.55	0.41
1:A:100:ARG:HA	1:A:100:ARG:HD2	1.71	0.41
1:C:15:ILE:HG12	1:C:20:LEU:HG	2.03	0.40
2:D:1:ASP:O	2:D:2:VAL:HG13	2.21	0.40
1:A:182:LYS:O	1:A:182:LYS:HG3	2.22	0.40
1:C:182:LYS:O	1:C:186:THR:HG23	2.21	0.40
2:D:50:ARG:HG2	2:D:58:VAL:HB	2.04	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	212/223 (95%)	206 (97%)	3 (1%)	3 (1%)	11 46
1	B	212/223 (95%)	209 (99%)	3 (1%)	0	100 100
1	C	219/223 (98%)	212 (97%)	5 (2%)	2 (1%)	17 56
2	D	112/118 (95%)	107 (96%)	5 (4%)	0	100 100
2	E	114/118 (97%)	110 (96%)	3 (3%)	1 (1%)	17 56
2	F	109/118 (92%)	107 (98%)	2 (2%)	0	100 100
All	All	978/1023 (96%)	951 (97%)	21 (2%)	6 (1%)	25 64

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	CYS
1	A	97	ARG
1	C	88	ALA
2	E	3	GLN
1	C	95	GLN
1	A	122	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	177/188 (94%)	174 (98%)	3 (2%)	60 83
1	B	178/188 (95%)	175 (98%)	3 (2%)	60 83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	175/188 (93%)	168 (96%)	7 (4%)	31 66
2	D	89/89 (100%)	86 (97%)	3 (3%)	37 70
2	E	89/89 (100%)	87 (98%)	2 (2%)	52 79
2	F	89/89 (100%)	88 (99%)	1 (1%)	73 88
All	All	797/831 (96%)	778 (98%)	19 (2%)	55 77

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	A	36[A]	VAL
1	A	36[B]	VAL
1	B	36[A]	VAL
1	B	36[B]	VAL
1	B	97	ARG
1	C	5	ASN
1	C	36[A]	VAL
1	C	36[B]	VAL
1	C	41	SER
1	C	100	ARG
1	C	198	CYS
1	C	218	CYS
2	D	19	ARG
2	D	50	ARG
2	D	86	ASP
2	E	50	ARG
2	E	86	ASP
2	F	82(B)	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	ASN
1	C	5	ASN
2	F	3	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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, 95^{th} 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	214/223 (95%)	0.17	3 (1%) 75 63	67, 111, 190, 274	0
1	B	214/223 (95%)	0.23	9 (4%) 36 23	73, 116, 226, 330	0
1	C	219/223 (98%)	0.08	3 (1%) 75 63	68, 110, 184, 273	1 (0%)
2	D	116/118 (98%)	0.56	9 (7%) 13 7	104, 153, 231, 270	0
2	E	116/118 (98%)	1.36	36 (31%) 0 0	128, 223, 282, 334	0
2	F	113/118 (95%)	2.68	66 (58%) 0 0	199, 282, 360, 396	0
All	All	992/1023 (96%)	0.63	126 (12%) 3 2	67, 132, 289, 396	1 (0%)

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	31	PHE	10.8
2	F	15	GLY	10.6
2	F	69	ILE	10.4
2	F	16	GLY	9.2
2	F	62	SER	7.5
2	F	82(C)	LEU	7.0
2	F	10	GLY	6.2
2	F	34	MET	6.1
2	F	28	ILE	6.0
2	F	63	VAL	5.4
2	E	8	GLY	5.4
2	E	90	TYR	4.9
2	F	78	LEU	4.9
2	E	7	SER	4.7
2	E	87	THR	4.6
2	F	90	TYR	4.4
2	F	59	LEU	4.4
2	F	17	SER	4.4
2	F	41	PRO	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	95	GLN	4.3
2	F	82	MET	4.2
2	F	89	VAL	4.2
1	A	94	GLY	4.2
2	E	114	ALA	4.2
2	F	113	SER	4.2
2	E	86	ASP	4.2
2	F	67	PHE	4.0
2	F	104	GLY	3.9
2	F	68	THR	3.9
2	E	115	ALA	3.9
2	F	14	ALA	3.9
2	F	8	GLY	3.9
2	E	18	LEU	3.8
2	F	92	CYS	3.8
2	F	2	VAL	3.7
2	E	38	ARG	3.7
2	D	11	LEU	3.7
2	F	91	TYR	3.6
2	F	82(A)	ASN	3.5
1	A	86	VAL	3.4
2	F	64	LYS	3.4
2	E	69	ILE	3.4
2	D	111	VAL	3.3
2	E	17	SER	3.3
2	F	112	SER	3.2
2	F	109	VAL	3.2
2	D	13	GLN	3.2
2	E	82	MET	3.2
2	F	85	GLU	3.1
2	E	11	LEU	3.1
2	E	59	LEU	3.1
2	F	102	TYR	3.1
2	F	110	THR	3.1
1	B	222	GLY	3.1
2	F	13	GLN	3.0
2	F	42	GLY	3.0
1	B	87	HIS	3.0
2	F	40	ALA	2.9
1	C	88	ALA	2.9
2	E	22	CYS	2.9
2	E	14	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
2	E	84	PRO	2.9
2	F	18	LEU	2.8
2	E	16	GLY	2.8
2	F	9	GLY	2.8
2	F	107	THR	2.8
2	E	62	SER	2.8
2	E	63	VAL	2.8
2	F	105	GLN	2.7
2	F	66	ARG	2.7
2	E	66	ARG	2.7
2	F	97	ASP	2.7
2	E	15	GLY	2.7
2	D	37	TRP	2.7
2	E	113	SER	2.6
2	F	93	PHE	2.6
2	E	82(C)	LEU	2.6
2	F	108	GLN	2.6
2	E	110	THR	2.6
2	F	19	ARG	2.6
2	E	36	TRP	2.5
2	F	103	TRP	2.5
1	B	209	ALA	2.5
1	B	86	VAL	2.5
2	F	37	TRP	2.5
2	F	55	PHE	2.5
2	E	112	SER	2.5
2	F	27	SER	2.5
2	D	17	SER	2.5
2	F	79	ALA	2.4
2	F	58	VAL	2.4
2	E	94	ALA	2.4
2	E	89	VAL	2.4
2	F	50	ARG	2.4
2	E	48	VAL	2.4
1	C	5	ASN	2.4
2	F	4	LEU	2.4
1	B	205	LEU	2.3
2	F	36	TRP	2.3
1	C	87	HIS	2.3
2	F	73	SER	2.3
2	D	10	GLY	2.3
2	F	38	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
2	E	31	PHE	2.3
2	E	20	LEU	2.3
1	B	5	ASN	2.3
2	D	86	ASP	2.2
2	E	64	LYS	2.2
2	E	111	VAL	2.2
2	E	46	GLU	2.2
2	F	88	ALA	2.2
2	F	39	GLN	2.2
2	F	45	ARG	2.2
2	F	11	LEU	2.2
1	B	202	LEU	2.2
2	F	61	ASP	2.2
2	F	75	GLU	2.1
1	B	207	PRO	2.1
2	F	43	LYS	2.1
2	D	16	GLY	2.1
2	D	109	VAL	2.1
2	F	12	VAL	2.1
2	E	103	TRP	2.0
2	F	84	PRO	2.0
2	F	5	GLN	2.0
1	B	96	MET	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.