Full wwPDB X-ray Structure Validation Report ⓘ

Sep 12, 2023 – 09:30 PM EDT

PDB ID	:	4N1H
Title	:	Structure of a single-domain camelid antibody fragment cAb-F11N in complex with the BlaP beta-lactamase from Bacillus licheniformis
Authors	:	Pain, C.; Kerff, F.; Herman, R.; Sauvage, E.; Preumont, S.; Charlier, P.; Dumoulin, M.
Deposited on	:	2013-10-04
Resolution	:	3.00 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:

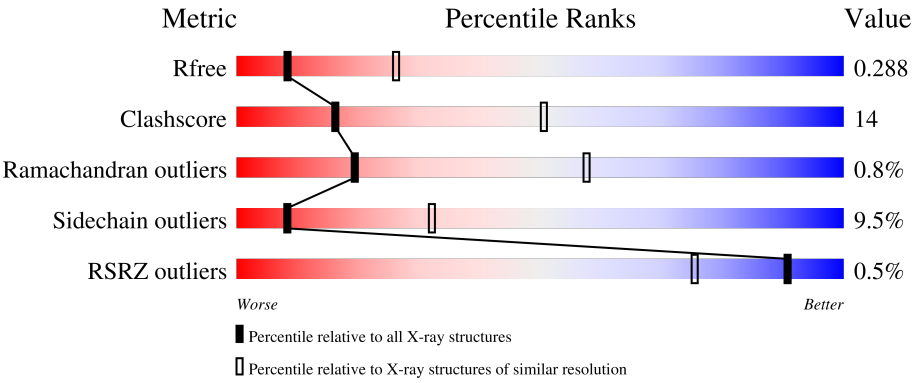
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	273	61% 30% • 6%
1	C	273	59% 31% • 5%
2	B	133	61% 31% • 5%
2	D	133	3% 66% 26% • 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5962 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 Beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			2006	1259	347	397	3			
1	C	258	Total	C	N	O	S	0	0	0
			2014	1263	348	400	3			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	197A	PRO	-	insertion	UNP P00808
A	197B	GLY	-	insertion	UNP P00808
A	296	GLY	-	expression tag	UNP P00808
A	297	PRO	-	expression tag	UNP P00808
A	298	HIS	-	expression tag	UNP P00808
A	299	HIS	-	expression tag	UNP P00808
A	300	HIS	-	expression tag	UNP P00808
A	301	HIS	-	expression tag	UNP P00808
A	302	HIS	-	expression tag	UNP P00808
C	197A	PRO	-	insertion	UNP P00808
C	197B	GLY	-	insertion	UNP P00808
C	296	GLY	-	expression tag	UNP P00808
C	297	PRO	-	expression tag	UNP P00808
C	298	HIS	-	expression tag	UNP P00808
C	299	HIS	-	expression tag	UNP P00808
C	300	HIS	-	expression tag	UNP P00808
C	301	HIS	-	expression tag	UNP P00808
C	302	HIS	-	expression tag	UNP P00808

- Molecule 2 is a protein called Camelid heavy-chain antibody variable fragment cAb-F11N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	126	Total	C	N	O	S	0	0	0
			962	598	168	192	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	126	Total	C	N	O	S	0	0	0
			962	598	168	192	4			

- Molecule 3 is water.

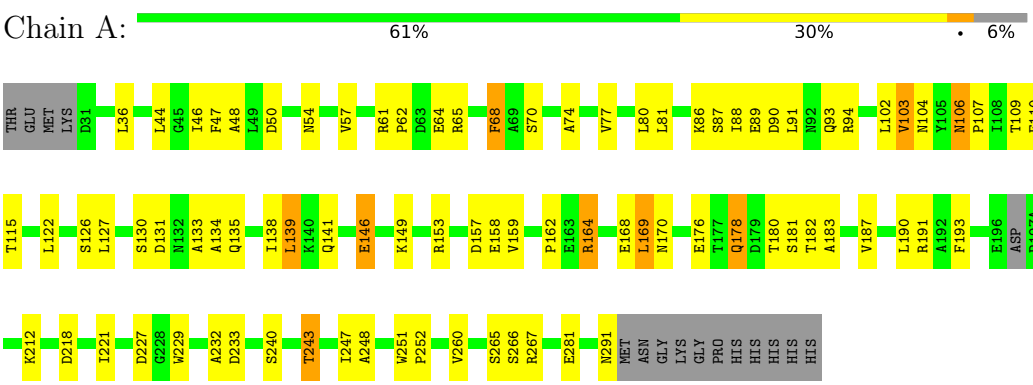
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	8	Total	O	0	0
			8	8		
3	C	10	Total	O	0	0
			10	10		

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.

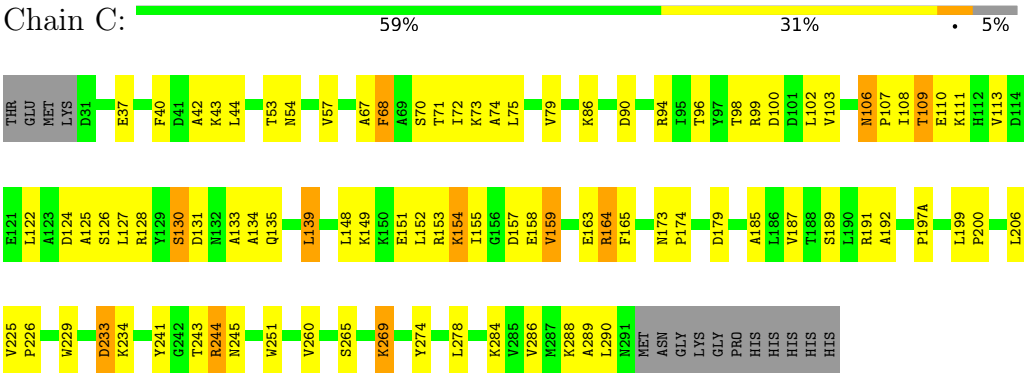
• Molecule 1: Beta-lactamase

Chain A:



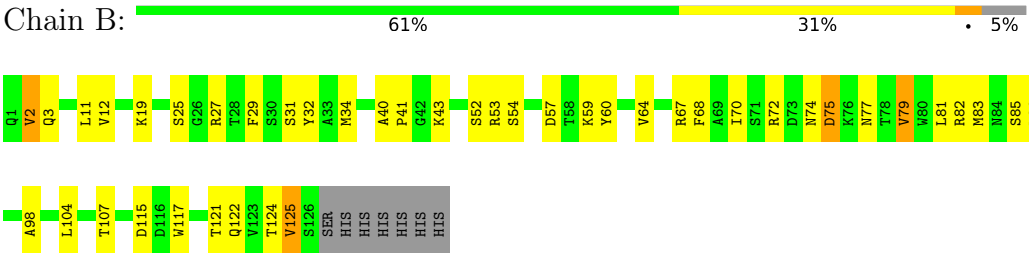
• Molecule 1: Beta-lactamase

Chain C:



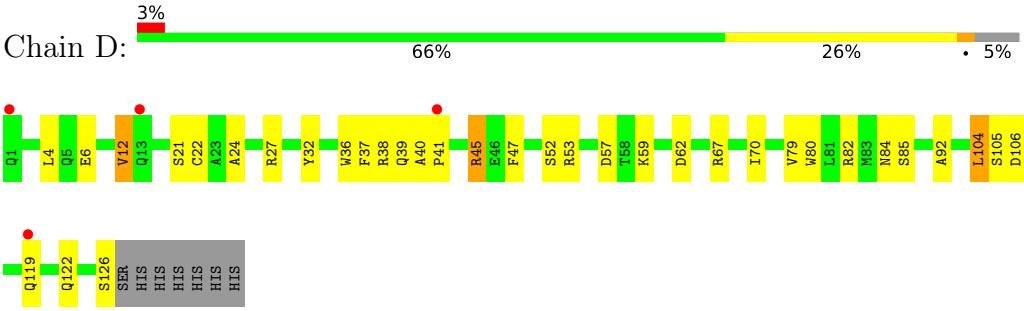
• Molecule 2: Camelid heavy-chain antibody variable fragment cAb-F11N

Chain B:



• Molecule 2: Camelid heavy-chain antibody variable fragment cAb-F11N

Chain D:


3%
66%
26%
5%
Q1
L4
Q5
E6
V12
Q13
S21
C22
A23
A24
R27
Y32
W36
F37
R38
Q39
A40
P41
R45
E46
F47
S52
R53
D57
T58
K59
D62
R67
I70
V79
W80
L81
R82
M83
N84
S85
A92
L104
S105
D106
T107
Y108
I109
H112
Q119
Q122
S126
SER
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	59.09Å 89.82Å 75.75Å 90.00° 95.17° 90.00°	Depositor
Resolution (Å)	75.44 – 3.00 48.57 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (75.44-3.00) 99.5 (48.57-3.00)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.40 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.208 , 0.284 0.211 , 0.288	Depositor DCC
R_{free} test set	794 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	47.5	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 37.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	5962	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.63% 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	0.46	1/2036 (0.0%)	0.66	0/2755
1	C	0.46	1/2045 (0.0%)	0.63	0/2770
2	B	0.53	1/981 (0.1%)	0.63	0/1326
2	D	0.55	1/981 (0.1%)	0.62	0/1326
All	All	0.49	4/6043 (0.1%)	0.64	0/8177

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	117	TRP	CD2-CE2	5.24	1.47	1.41
1	A	229	TRP	CD2-CE2	5.16	1.47	1.41
1	C	251	TRP	CD2-CE2	5.01	1.47	1.41
2	D	80	TRP	CD2-CE2	5.00	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2006	0	2022	55	0
1	C	2014	0	2026	65	0
2	B	962	0	918	29	0
2	D	962	0	918	21	0
3	A	8	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	10	0	0	0	0
All	All	5962	0	5884	170	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 (170) 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:D:52:SER:HB2	2:D:57:ASP:HB2	1.30	1.12
1:C:106:ASN:HB3	1:C:109:THR:HG22	1.32	1.09
1:C:109:THR:HG21	1:C:133:ALA:HB3	1.34	1.04
2:B:34:MET:HG2	2:B:79:VAL:HG21	1.45	0.97
2:B:34:MET:HE1	2:B:98:ALA:HB2	1.64	0.79
2:D:36:TRP:HD1	2:D:70:ILE:HD12	1.49	0.77
1:A:44:LEU:HG	1:A:46:ILE:HD11	1.68	0.76
1:C:106:ASN:HB3	1:C:109:THR:CG2	2.15	0.75
1:C:224:GLY:HA2	1:C:284:LYS:HE3	1.69	0.74
2:B:2:VAL:HG21	2:B:32:TYR:CE1	2.23	0.73
2:B:34:MET:CE	2:B:98:ALA:HB2	2.17	0.73
1:C:109:THR:HG21	1:C:133:ALA:CB	2.18	0.70
1:C:244:ARG:HG2	1:C:274:TYR:CG	2.27	0.69
2:B:59:LYS:HB2	2:B:107:THR:HG21	1.75	0.68
2:D:52:SER:CB	2:D:57:ASP:HB2	2.18	0.68
2:B:54:SER:HB3	2:B:104:LEU:HG	1.76	0.68
1:A:146:GLU:OE2	1:A:146:GLU:HA	1.94	0.67
1:A:86:LYS:HD2	1:A:90:ASP:HB3	1.75	0.67
2:D:36:TRP:CD1	2:D:70:ILE:HD12	2.29	0.66
1:C:71:THR:CG2	1:C:245:ASN:HB3	2.27	0.65
1:A:178:GLN:HE21	1:A:178:GLN:H	1.45	0.65
2:B:72:ARG:NH2	2:B:74:ASN:OD1	2.29	0.65
1:A:47:PHE:HD2	1:A:187:VAL:HG21	1.60	0.64
1:A:240:SER:O	1:A:243:THR:OG1	2.16	0.64
2:D:59:LYS:HD3	2:D:107:THR:HG21	1.79	0.64
2:B:52:SER:HB3	2:B:57:ASP:HB2	1.81	0.63
1:C:131:ASP:HB3	1:C:134:ALA:HB3	1.80	0.63
1:A:48:ALA:HB3	1:A:57:VAL:HB	1.82	0.62
2:B:2:VAL:HG21	2:B:32:TYR:HE1	1.63	0.61
1:C:102:LEU:HD21	1:C:110:GLU:HA	1.82	0.60
1:C:192:ALA:HA	1:C:197(A):PRO:HD2	1.81	0.60
1:A:159:VAL:HG11	1:A:182:THR:HG23	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:39:GLN:HB2	2:D:45:ARG:HG2	1.83	0.60
1:C:288:LYS:C	1:C:290:LEU:H	2.05	0.60
1:C:110:GLU:HG3	1:C:111:LYS:HG3	1.83	0.60
1:C:111:LYS:HB2	1:C:111:LYS:NZ	2.17	0.59
1:A:243:THR:HG23	1:A:266:SER:HB3	1.85	0.59
1:C:71:THR:HG21	1:C:245:ASN:HB3	1.85	0.59
1:A:190:LEU:HD22	1:A:247:ILE:HD12	1.85	0.59
1:A:193:PHE:O	1:A:199:LEU:HD12	2.04	0.58
1:C:106:ASN:CB	1:C:109:THR:HG22	2.22	0.57
1:C:74:ALA:HA	1:C:127:LEU:HD21	1.85	0.57
1:C:159:VAL:HG22	1:C:185:ALA:CB	2.34	0.57
1:C:139:LEU:HD13	1:C:165:PHE:CD1	2.38	0.57
2:D:40:ALA:HB1	2:D:41:PRO:HD2	1.87	0.56
1:A:77:VAL:O	1:A:81:LEU:HG	2.06	0.56
1:A:80:LEU:HD13	1:A:138:ILE:HG23	1.88	0.56
1:A:153:ARG:HD3	1:A:157:ASP:O	2.05	0.55
2:B:93:VAL:HG22	2:B:122:GLN:HE22	1.72	0.55
2:D:38:ARG:HB2	2:D:92:ALA:HB3	1.88	0.54
1:A:122:LEU:HD22	1:A:134:ALA:HA	1.89	0.54
1:C:98:THR:HG22	1:C:99:ARG:N	2.23	0.54
1:C:173:ASN:HB3	1:C:174:PRO:HD2	1.90	0.54
1:A:111:LYS:HB2	1:A:112:HIS:CD2	2.42	0.54
1:C:128:ARG:HD2	1:C:213:ARG:O	2.08	0.54
1:C:241:TYR:HA	1:C:269:LYS:O	2.08	0.53
1:A:221:ILE:HD13	1:A:248:ALA:HB3	1.90	0.53
2:B:83:MET:HB3	2:B:86:LEU:HD21	1.89	0.53
2:B:40:ALA:HB3	2:B:43:LYS:HB2	1.88	0.53
1:C:159:VAL:HG22	1:C:185:ALA:HB2	1.91	0.53
2:B:19:LYS:HA	2:B:81:LEU:O	2.09	0.53
2:B:31:SER:C	2:B:53:ARG:HD2	2.29	0.52
2:B:52:SER:CB	2:B:57:ASP:HB2	2.39	0.52
2:B:77:ASN:HD22	2:B:77:ASN:N	2.07	0.52
2:B:59:LYS:CB	2:B:107:THR:HG21	2.40	0.52
1:C:74:ALA:HA	1:C:127:LEU:CD2	2.40	0.51
1:C:98:THR:HG22	1:C:100:ASP:H	1.75	0.51
1:A:47:PHE:HD2	1:A:187:VAL:CG2	2.22	0.51
1:A:176:GLU:HB3	1:A:178:GLN:HE22	1.76	0.51
2:D:67:ARG:HG2	2:D:84:ASN:O	2.11	0.51
1:C:214:ASN:ND2	1:C:233:ASP:OD2	2.45	0.50
2:D:38:ARG:HB2	2:D:92:ALA:CB	2.41	0.50
1:A:107:PRO:HD2	1:A:131:ASP:OD2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:MET:HG2	2:B:79:VAL:CG2	2.30	0.50
2:D:27:ARG:HB3	2:D:32:TYR:HE2	1.77	0.50
1:A:74:ALA:HA	1:A:127:LEU:CD2	2.42	0.50
2:B:3:GLN:HB2	2:B:25:SER:HB3	1.93	0.49
1:C:37:GLU:HG2	1:C:42:ALA:O	2.11	0.49
1:C:86:LYS:HB3	1:C:90:ASP:HB2	1.94	0.49
1:A:64:GLU:HG3	3:A:407:HOH:O	2.12	0.49
1:C:243:THR:HA	1:C:265:SER:O	2.12	0.49
1:C:107:PRO:O	1:C:111:LYS:HE3	2.12	0.49
1:A:178:GLN:HE21	1:A:178:GLN:N	2.11	0.49
1:C:53:THR:O	1:C:54:ASN:HB2	2.12	0.49
2:D:59:LYS:HB2	2:D:107:THR:HG21	1.94	0.49
1:C:86:LYS:HB3	1:C:90:ASP:CB	2.43	0.48
1:C:94:ARG:HD3	1:C:115:THR:O	2.13	0.48
2:B:75:ASP:OD2	2:B:75:ASP:N	2.47	0.48
1:C:122:LEU:HD22	1:C:134:ALA:HA	1.94	0.48
1:C:131:ASP:HB3	1:C:134:ALA:CB	2.43	0.48
2:B:29:PHE:HZ	2:B:79:VAL:HG22	1.79	0.47
1:A:64:GLU:CG	3:A:407:HOH:O	2.62	0.47
1:C:109:THR:HB	1:C:131:ASP:OD1	2.15	0.47
1:C:70:SER:HB3	1:C:73:LYS:HD2	1.96	0.47
2:D:27:ARG:HB3	2:D:32:TYR:CE2	2.50	0.46
1:A:111:LYS:HB2	1:A:112:HIS:HD2	1.81	0.46
1:A:126:SER:O	1:A:130:SER:HA	2.15	0.46
1:C:73:LYS:HB2	1:C:234:LYS:HE2	1.97	0.46
1:C:75:LEU:HD13	1:C:152:LEU:HD21	1.96	0.46
2:B:93:VAL:HG22	2:B:122:GLN:NE2	2.31	0.46
1:C:187:VAL:O	1:C:191:ARG:HB2	2.16	0.45
1:A:62:PRO:HA	1:A:183:ALA:HB3	1.99	0.45
1:A:106:ASN:O	1:A:110:GLU:HG2	2.17	0.45
1:C:151:GLU:HA	1:C:154:LYS:HG2	1.99	0.44
1:A:44:LEU:O	1:A:61:ARG:HD2	2.18	0.44
1:C:37:GLU:OE2	1:C:43:LYS:HA	2.16	0.44
1:C:79:VAL:HG21	1:C:148:LEU:HD12	1.99	0.44
2:D:22:CYS:HB3	2:D:79:VAL:HG12	1.98	0.44
1:A:94:ARG:HH11	1:A:115:THR:HG22	1.82	0.44
1:A:176:GLU:HB3	1:A:178:GLN:NE2	2.33	0.44
1:C:199:LEU:HD23	1:C:200:PRO:HD2	1.99	0.44
2:B:12:VAL:O	2:B:125:VAL:HA	2.17	0.44
1:A:50:ASP:O	1:A:54:ASN:HA	2.18	0.43
1:A:65:ARG:HD3	1:A:180:THR:OG1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:LYS:HG3	1:A:162:PRO:HD2	1.99	0.43
1:A:74:ALA:HA	1:A:127:LEU:HD21	2.00	0.43
1:A:102:LEU:HD21	1:A:110:GLU:HA	1.99	0.43
2:B:64:VAL:HB	2:B:68:PHE:CG	2.54	0.43
1:A:164:ARG:HG2	1:A:168:GLU:CG	2.49	0.43
1:C:226:PRO:O	1:C:229:TRP:HB2	2.17	0.43
1:A:164:ARG:HG2	1:A:168:GLU:HG2	2.01	0.43
1:C:111:LYS:HB2	1:C:111:LYS:HZ3	1.82	0.43
1:A:36:LEU:HD21	1:A:281:GLU:HB3	2.01	0.43
1:A:103:VAL:HG23	1:A:104:ASN:H	1.84	0.43
2:B:77:ASN:HD22	2:B:77:ASN:H	1.65	0.42
1:A:68:PHE:HD2	1:A:181:SER:HB2	1.84	0.42
1:C:40:PHE:CG	1:C:278:LEU:HB2	2.54	0.42
1:A:243:THR:HA	1:A:265:SER:O	2.18	0.42
2:D:4:LEU:HD23	2:D:24:ALA:HB2	2.01	0.42
2:D:53:ARG:NH2	2:D:104:LEU:HD12	2.34	0.42
1:C:99:ARG:HA	1:C:102:LEU:HD13	2.00	0.42
1:A:87:SER:O	1:A:91:LEU:HG	2.20	0.42
1:A:187:VAL:HB	1:A:260:VAL:HG12	2.01	0.42
1:C:187:VAL:HG13	1:C:260:VAL:HG12	2.01	0.42
2:D:22:CYS:HB3	2:D:79:VAL:CG1	2.49	0.42
1:A:87:SER:O	1:A:90:ASP:HB2	2.19	0.42
1:A:208:ILE:HG22	1:A:212:LYS:HD2	2.01	0.41
1:A:221:ILE:HD13	1:A:248:ALA:CB	2.50	0.41
1:C:288:LYS:C	1:C:290:LEU:N	2.73	0.41
1:A:212:LYS:HA	1:A:232:ALA:HA	2.02	0.41
1:A:169:LEU:HD12	1:A:170:ASN:N	2.34	0.41
2:B:60:TYR:CE1	2:B:70:ILE:HG22	2.55	0.41
1:C:70:SER:C	1:C:72:ILE:N	2.74	0.41
1:C:57:VAL:HG11	1:C:286:VAL:HG22	2.01	0.41
1:C:67:ALA:O	1:C:245:ASN:ND2	2.54	0.41
1:C:149:LYS:HE2	1:C:153:ARG:NH2	2.35	0.41
1:C:43:LYS:O	1:C:265:SER:HA	2.21	0.41
2:D:37:PHE:CD1	2:D:47:PHE:HA	2.54	0.41
1:A:135:GLN:O	1:A:139:LEU:HB2	2.21	0.41
1:A:251:TRP:HA	1:A:252:PRO:HD2	1.98	0.41
1:C:126:SER:O	1:C:130:SER:HA	2.21	0.41
2:D:6:GLU:HA	2:D:21:SER:O	2.21	0.41
1:A:88:ILE:HA	1:A:91:LEU:HD12	2.02	0.41
2:B:83:MET:CB	2:B:86:LEU:HD21	2.51	0.41
1:C:157:ASP:HB2	1:C:189:SER:OG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:THR:HG21	1:A:133:ALA:CB	2.51	0.40
1:C:108:ILE:HG21	1:C:125:ALA:HB2	2.03	0.40
1:C:135:GLN:O	1:C:139:LEU:HB2	2.21	0.40
2:D:12:VAL:O	2:D:126:SER:N	2.54	0.40
2:B:72:ARG:HD3	2:B:74:ASN:OD1	2.20	0.40
1:C:68:PHE:CD1	1:C:72:ILE:HB	2.56	0.40
1:C:120:LYS:HE3	1:C:206:LEU:HD21	2.02	0.40
1:A:94:ARG:NH1	1:A:115:THR:HG22	2.36	0.40
1:C:37:GLU:HG3	1:C:44:LEU:HG	2.04	0.40
1:C:151:GLU:O	1:C:155:ILE:HG12	2.22	0.40
1:C:244:ARG:HG2	1:C:274:TYR:CB	2.52	0.40
2:D:47:PHE:CD2	2:D:109:ILE:HG23	2.56	0.40
1:A:208:ILE:O	1:A:212:LYS:HB2	2.22	0.40
2:B:32:TYR:O	2:B:53:ARG:HA	2.22	0.40
1:C:164:ARG:NE	1:C:179:ASP:OD2	2.44	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	253/273 (93%)	241 (95%)	11 (4%)	1 (0%)	34	72
1	C	256/273 (94%)	241 (94%)	13 (5%)	2 (1%)	19	57
2	B	124/133 (93%)	114 (92%)	9 (7%)	1 (1%)	19	57
2	D	124/133 (93%)	110 (89%)	12 (10%)	2 (2%)	9	40
All	All	757/812 (93%)	706 (93%)	45 (6%)	6 (1%)	19	57

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	45	ARG
1	A	103	VAL
1	C	289	ALA
2	D	112	HIS
1	C	103	VAL
2	B	41	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	216/230 (94%)	196 (91%)	20 (9%)	9 33
1	C	217/230 (94%)	199 (92%)	18 (8%)	11 39
2	B	99/106 (93%)	86 (87%)	13 (13%)	4 18
2	D	99/106 (93%)	90 (91%)	9 (9%)	9 34
All	All	631/672 (94%)	571 (90%)	60 (10%)	8 32

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	PHE
1	A	70	SER
1	A	89	GLU
1	A	93	GLN
1	A	106	ASN
1	A	114	ASP
1	A	139	LEU
1	A	141	GLN
1	A	146	GLU
1	A	158	GLU
1	A	164	ARG
1	A	169	LEU
1	A	178	GLN
1	A	191	ARG
1	A	218	ASP
1	A	227	ASP

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Mol	Chain	Res	Type
1	A	233	ASP
1	A	243	THR
1	A	267	ARG
1	A	291	ASN
2	B	2	VAL
2	B	11	LEU
2	B	27	ARG
2	B	67	ARG
2	B	75	ASP
2	B	79	VAL
2	B	82	ARG
2	B	85	SER
2	B	95	TYR
2	B	115	ASP
2	B	121	THR
2	B	124	THR
2	B	125	VAL
1	C	68	PHE
1	C	96	THR
1	C	106	ASN
1	C	109	THR
1	C	113	VAL
1	C	118	THR
1	C	124	ASP
1	C	130	SER
1	C	139	LEU
1	C	154	LYS
1	C	158	GLU
1	C	159	VAL
1	C	163	GLU
1	C	164	ARG
1	C	225	VAL
1	C	233	ASP
1	C	244	ARG
1	C	269	LYS
2	D	12	VAL
2	D	62	ASP
2	D	82	ARG
2	D	85	SER
2	D	104	LEU
2	D	105	SER
2	D	106	ASP

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Mol	Chain	Res	Type
2	D	119	GLN
2	D	122	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	HIS
1	A	141	GLN
1	A	178	GLN
2	B	39	GLN
2	B	77	ASN
2	B	112	HIS
2	B	122	GLN
1	C	54	ASN
1	C	83	GLN
1	C	170	ASN
2	D	77	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 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	257/273 (94%)	-0.42	0	100	100	21, 38, 62, 75	0
1	C	258/273 (94%)	-0.46	0	100	100	21, 38, 64, 76	0
2	B	126/133 (94%)	-0.02	0	100	100	31, 49, 82, 110	0
2	D	126/133 (94%)	0.05	4 (3%)	47	20	35, 50, 80, 94	0
All	All	767/812 (94%)	-0.29	4 (0%)	91	75	21, 42, 71, 110	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	41	PRO	2.9
2	D	1	GLN	2.3
2	D	13	GLN	2.1
2	D	119	GLN	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.