



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:25 PM UTC

PDB ID : 1AP2 / pdb_00001ap2
Title : SINGLE CHAIN FV OF C219
Authors : Hoedemaeker, P.J.; Rose, D.R.
Deposited on : 1997-07-23
Resolution : 2.36 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

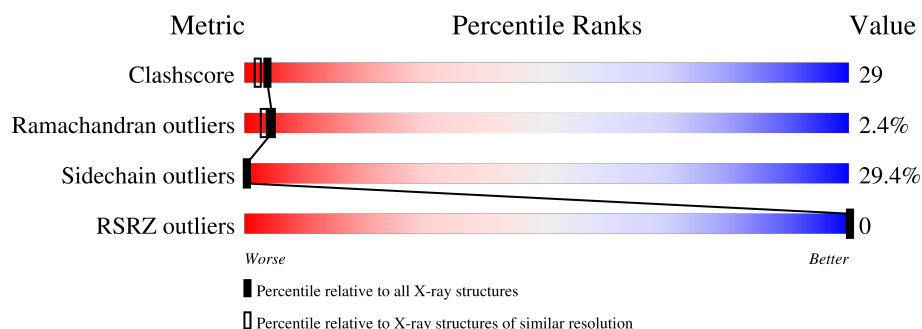
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.36 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))
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	113	49% 36% 14% .
1	C	113	45% 43% 12%
2	B	123	48% 34% 14% ..
2	D	123	28% 51% 20%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3720 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 MONOCLONAL ANTIBODY C219.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	112	Total	C	N	O	S	0	0	0
			859	541	138	176	4			
1	C	113	Total	C	N	O	S	0	0	0
			864	543	139	178	4			

- Molecule 2 is a protein called MONOCLONAL ANTIBODY C219.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	120	Total	C	N	O	S	0	0	0
			939	592	157	187	3			
2	D	123	Total	C	N	O	S	0	0	0
			956	600	160	193	3			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	33	PHE	TYR	conflict	EMBL Z22078
B	56	ASP	GLY	conflict	EMBL Z22078
B	71	ILE	THR	conflict	EMBL Z22078
B	100	GLU	-	insertion	EMBL Z22078
B	101	VAL	-	insertion	EMBL Z22078
B	102	TYR	ASP	conflict	EMBL Z22078
B	103	SER	ASN	conflict	EMBL Z22078
B	106	SER	-	insertion	EMBL Z22078
B	107	PRO	ALA	conflict	EMBL Z22078
B	108	LEU	MET	conflict	EMBL Z22078
B	110	VAL	TYR	conflict	EMBL Z22078
B	113	ALA	GLN	conflict	EMBL Z22078
B	116	THR	SER	conflict	EMBL Z22078
B	120	PRO	SER	conflict	EMBL Z22078
D	33	PHE	TYR	conflict	EMBL Z22078
D	56	ASP	GLY	conflict	EMBL Z22078

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Chain	Residue	Modelled	Actual	Comment	Reference
D	71	ILE	THR	conflict	EMBL Z22078
D	100	GLU	-	insertion	EMBL Z22078
D	101	VAL	-	insertion	EMBL Z22078
D	102	TYR	ASP	conflict	EMBL Z22078
D	103	SER	ASN	conflict	EMBL Z22078
D	106	SER	-	insertion	EMBL Z22078
D	107	PRO	ALA	conflict	EMBL Z22078
D	108	LEU	MET	conflict	EMBL Z22078
D	110	VAL	TYR	conflict	EMBL Z22078
D	113	ALA	GLN	conflict	EMBL Z22078
D	116	THR	SER	conflict	EMBL Z22078
D	120	PRO	SER	conflict	EMBL Z22078

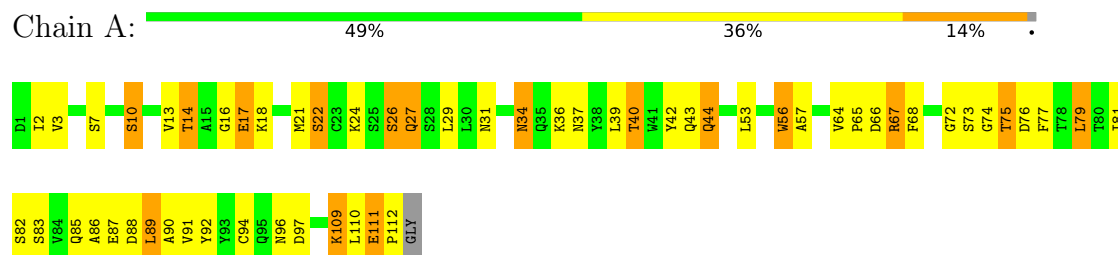
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	28	Total O 28 28	0	0
3	B	19	Total O 19 19	0	0
3	C	29	Total O 29 29	0	0
3	D	26	Total O 26 26	0	0

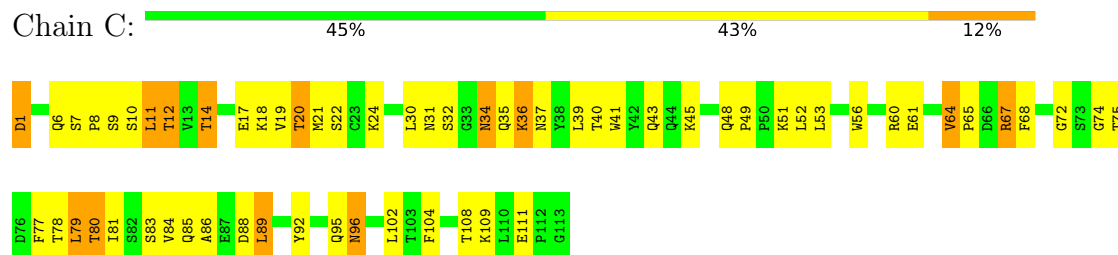
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

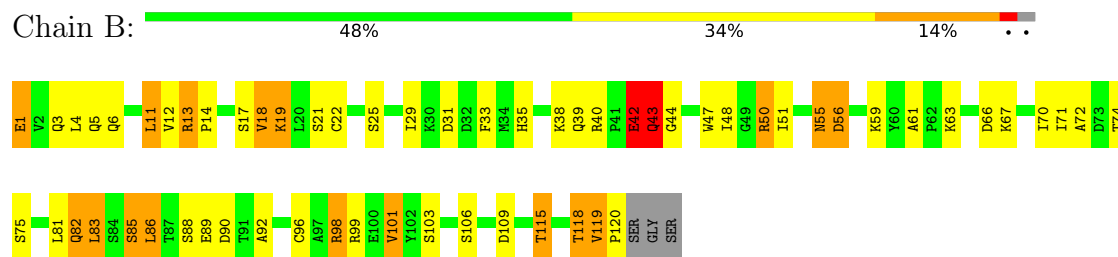
• Molecule 1: MONOCLONAL ANTIBODY C219



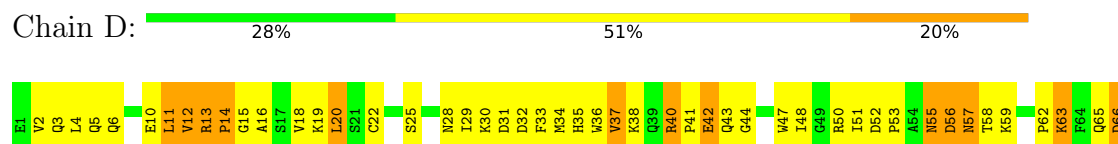
• Molecule 1: MONOCLONAL ANTIBODY C219



• Molecule 2: MONOCLONAL ANTIBODY C219



• Molecule 2: MONOCLONAL ANTIBODY C219



K67	A68	T69	T74	S75	S76	N77	T78	L81	Q82	L83	S84	S85	L86	T87	S88	E89	D90	T91	A92	V93	Y94	Y95	R98	R99	E100	V101	Y102	S103	Y104	Y105	S106	P107	L108	D109	V110	W111	G114	T115	T118	V119	P120	S121	G122	S123
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.04Å 64.35Å 154.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.36 6.00 – 2.38	Depositor EDS
% Data completeness (in resolution range)	78.4 (6.00-2.36) 72.6 (6.00-2.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.39Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.204 , 0.284 0.217 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	14.4	Xtriage
Anisotropy	0.607	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3720	wwPDB-VP
Average B, all atoms (Å ²)	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% 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	A	0.50	1/879 (0.1%)	0.90	1/1197 (0.1%)
1	C	0.41	1/884 (0.1%)	0.84	2/1202 (0.2%)
2	B	0.36	0/961	0.72	1/1310 (0.1%)
2	D	0.39	0/978	0.88	3/1331 (0.2%)
All	All	0.42	2/3702 (0.1%)	0.83	7/5040 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	56	TRP	NE1-CE2	-5.38	1.31	1.37
1	A	56	TRP	NE1-CE2	-5.28	1.31	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	13	ARG	CA-C-N	6.34	127.76	119.84
2	D	13	ARG	C-N-CA	6.34	127.76	119.84
2	B	61	ALA	N-CA-C	-5.63	102.98	110.07
2	D	109	ASP	N-CA-C	5.53	120.08	113.23
1	C	84	VAL	N-CA-C	5.39	116.65	109.37
1	C	64	VAL	N-CA-C	5.27	113.16	108.63
1	A	94	CYS	N-CA-C	-5.10	101.84	109.95

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	859	0	831	50	0
1	C	864	0	834	46	0
2	B	939	0	904	43	0
2	D	956	0	917	73	0
3	A	28	0	0	2	0
3	B	19	0	0	0	0
3	C	29	0	0	3	0
3	D	26	0	0	0	0
All	All	3720	0	3486	204	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 29.

All (204) 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:A:3:VAL:H	1:A:26:SER:HB2	1.32	0.94
1:C:31:ASN:HB3	1:C:34:ASN:HD21	1.37	0.88
2:B:38:LYS:HB2	2:B:48:ILE:HD11	1.61	0.83
1:C:1:ASP:HB2	3:C:125:HOH:O	1.83	0.78
2:D:12:VAL:HG23	2:D:119:VAL:HG22	1.65	0.78
1:C:31:ASN:HB3	1:C:34:ASN:ND2	1.99	0.77
2:B:35:HIS:HD2	2:B:47:TRP:HE1	1.33	0.74
1:C:52:LEU:HD21	2:D:107:PRO:HB2	1.68	0.74
2:D:35:HIS:HD2	2:D:47:TRP:HE1	1.36	0.73
2:D:43:GLN:HG2	2:D:44:GLY:H	1.53	0.72
1:A:67:ARG:O	1:A:81:ILE:HA	1.89	0.72
1:C:14:THR:HB	1:C:17:GLU:OE2	1.90	0.72
1:A:10:SER:HB3	1:A:111:GLU:OE2	1.89	0.71
1:C:8:PRO:HG2	1:C:11:LEU:HG	1.73	0.70
2:B:98:ARG:C	2:B:98:ARG:HD3	2.16	0.70
2:D:11:LEU:HD22	2:D:118:THR:HB	1.73	0.70
2:D:35:HIS:CD2	2:D:47:TRP:HE1	2.11	0.69
1:A:44:GLN:O	1:A:90:ALA:HB1	1.94	0.68
1:A:3:VAL:N	1:A:26:SER:HB2	2.05	0.67
2:B:35:HIS:CD2	2:B:47:TRP:HE1	2.13	0.66
2:B:19:LYS:HG3	2:B:82:GLN:HG3	1.76	0.65
1:A:13:VAL:HG23	1:A:17:GLU:CD	2.22	0.65
2:B:88:SER:OG	2:B:120:PRO:HG3	1.96	0.64
1:C:52:LEU:CD2	2:D:107:PRO:HB2	2.27	0.64
2:B:4:LEU:HD23	2:B:22:CYS:SG	2.38	0.64
2:B:42:GLU:O	2:B:43:GLN:HB3	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:THR:O	1:A:17:GLU:HB3	1.97	0.64
1:C:37:ASN:HD21	1:C:74:GLY:HA2	1.62	0.64
2:D:76:SER:HB2	2:D:78:THR:OG1	1.97	0.64
1:A:97:ASP:OD2	2:B:99:ARG:NH2	2.31	0.63
1:A:31:ASN:HB3	1:A:34:ASN:HD21	1.63	0.62
2:B:39:GLN:NE2	2:B:43:GLN:O	2.32	0.62
1:A:34:ASN:HD22	1:A:34:ASN:H	1.46	0.62
1:A:75:THR:HG22	1:A:76:ASP:OD1	2.00	0.61
2:D:40:ARG:HB2	2:D:43:GLN:HB3	1.81	0.61
1:A:44:GLN:C	1:A:90:ALA:HB1	2.24	0.61
1:C:34:ASN:ND2	1:C:36:LYS:HB2	2.16	0.61
1:C:8:PRO:O	1:C:108:THR:HG23	2.01	0.61
2:D:55:ASN:HD22	2:D:57:ASN:HB3	1.66	0.61
2:D:43:GLN:HG2	2:D:44:GLY:N	2.17	0.60
2:D:83:LEU:HB3	2:D:86:LEU:HD11	1.83	0.59
2:B:119:VAL:HB	2:B:120:PRO:CD	2.33	0.59
1:A:85:GLN:NE2	1:A:85:GLN:HA	2.17	0.59
2:D:62:PRO:HB2	2:D:63:LYS:NZ	2.18	0.59
1:C:60:ARG:NE	1:C:68:PHE:O	2.33	0.58
2:D:35:HIS:CD2	2:D:50:ARG:HB3	2.38	0.58
1:C:52:LEU:HD23	2:D:109:ASP:HB3	1.85	0.58
2:D:20:LEU:HD23	2:D:81:LEU:HD13	1.85	0.58
1:A:3:VAL:H	1:A:26:SER:CB	2.11	0.58
2:D:32:ASP:HB3	2:D:34:MET:CE	2.34	0.58
2:D:55:ASN:ND2	2:D:57:ASN:HB3	2.19	0.58
1:C:52:LEU:HG	1:C:61:GLU:HG3	1.85	0.57
2:D:18:VAL:HG22	2:D:86:LEU:HD21	1.86	0.57
1:A:13:VAL:HG22	1:A:14:THR:N	2.20	0.57
1:C:67:ARG:HG3	1:C:81:ILE:HG23	1.86	0.57
1:A:66:ASP:C	1:A:68:PHE:H	2.12	0.56
2:D:51:ILE:HG12	2:D:52:ASP:N	2.19	0.56
2:D:51:ILE:O	2:D:53:PRO:HD3	2.05	0.56
2:D:12:VAL:HG11	2:D:18:VAL:HG13	1.87	0.56
2:B:13:ARG:HE	2:B:14:PRO:HD2	1.70	0.56
2:D:12:VAL:O	2:D:120:PRO:HD2	2.05	0.56
2:B:119:VAL:O	2:B:120:PRO:C	2.49	0.56
1:C:79:LEU:HD22	1:C:80:THR:H	1.70	0.56
2:D:65:GLN:O	2:D:66:ASP:HB3	2.05	0.56
2:D:101:VAL:HG23	2:D:102:TYR:HD1	1.70	0.56
1:A:18:LYS:HG3	1:A:82:SER:HA	1.88	0.56
2:D:13:ARG:O	2:D:15:GLY:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:52:ASP:O	2:D:56:ASP:N	2.40	0.55
2:D:20:LEU:HD23	2:D:81:LEU:CD1	2.37	0.55
2:B:55:ASN:O	2:B:56:ASP:HB2	2.05	0.55
2:B:35:HIS:HD2	2:B:47:TRP:NE1	2.03	0.55
1:A:13:VAL:HG23	1:A:17:GLU:OE2	2.07	0.55
1:C:60:ARG:HD3	1:C:64:VAL:HG12	1.89	0.54
2:B:86:LEU:HB3	2:B:119:VAL:HG21	1.90	0.54
2:D:42:GLU:H	2:D:42:GLU:CD	2.14	0.54
1:A:24:LYS:NZ	1:A:76:ASP:HB3	2.23	0.54
2:B:33:PHE:CE1	2:B:101:VAL:HG11	2.42	0.54
1:C:37:ASN:ND2	1:C:74:GLY:HA2	2.22	0.54
1:A:43:GLN:HB2	1:A:53:LEU:HD11	1.89	0.54
2:B:1:GLU:HA	2:B:1:GLU:OE1	2.08	0.54
1:A:86:ALA:C	1:A:88:ASP:H	2.16	0.53
2:B:55:ASN:N	2:B:55:ASN:HD22	2.06	0.53
2:D:40:ARG:HE	2:D:41:PRO:HD2	1.73	0.53
2:B:38:LYS:CB	2:B:48:ILE:HD11	2.36	0.53
2:D:38:LYS:HB2	2:D:48:ILE:HD11	1.89	0.53
2:D:28:ASN:HA	2:D:77:ASN:HD21	1.74	0.53
2:B:51:ILE:HD12	2:B:70:ILE:O	2.08	0.53
2:D:65:GLN:C	2:D:67:LYS:H	2.18	0.52
1:C:34:ASN:HD22	1:C:35:GLN:N	2.06	0.52
2:D:13:ARG:HE	2:D:14:PRO:HD2	1.75	0.52
1:C:52:LEU:HD21	2:D:107:PRO:CB	2.37	0.52
2:D:33:PHE:CD1	2:D:101:VAL:HG11	2.45	0.52
2:D:51:ILE:HB	2:D:58:THR:HG22	1.92	0.52
1:A:112:PRO:HB3	3:A:139:HOH:O	2.10	0.51
1:C:43:GLN:HB2	1:C:53:LEU:HD11	1.91	0.51
2:D:86:LEU:HB3	2:D:119:VAL:HG21	1.93	0.51
2:B:4:LEU:HD23	2:B:96:CYS:SG	2.51	0.51
2:B:39:GLN:O	2:B:92:ALA:HB1	2.11	0.51
2:D:93:VAL:HG22	2:D:94:TYR:N	2.26	0.51
1:A:2:ILE:HG12	1:A:27:GLN:CG	2.41	0.51
1:A:34:ASN:HD22	1:A:34:ASN:N	2.06	0.51
1:C:67:ARG:HD2	1:C:88:ASP:OD2	2.11	0.51
2:D:62:PRO:HA	2:D:65:GLN:HG3	1.91	0.51
2:D:38:LYS:CB	2:D:48:ILE:HD11	2.41	0.51
1:A:86:ALA:O	1:A:89:LEU:HD22	2.11	0.50
1:C:21:MET:O	1:C:78:THR:HA	2.11	0.50
1:C:34:ASN:HD22	1:C:34:ASN:C	2.20	0.50
1:A:97:ASP:CG	2:B:99:ARG:HH22	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:55:ASN:N	2:B:55:ASN:ND2	2.60	0.50
2:D:98:ARG:HD2	2:D:98:ARG:C	2.37	0.50
1:A:39:LEU:HD13	1:A:39:LEU:C	2.36	0.50
1:A:91:VAL:HG22	1:A:109:LYS:HD2	1.93	0.50
1:A:34:ASN:H	1:A:34:ASN:ND2	2.10	0.49
1:A:22:SER:OG	1:A:24:LYS:HE3	2.12	0.49
2:D:103:SER:O	2:D:104:TYR:C	2.55	0.49
2:B:109:ASP:OD1	2:B:109:ASP:N	2.42	0.49
1:C:49:PRO:HB3	2:D:95:TYR:CE1	2.48	0.49
2:D:120:PRO:O	2:D:121:SER:HB3	2.13	0.49
2:D:14:PRO:O	2:D:86:LEU:O	2.31	0.49
2:D:40:ARG:NH1	2:D:89:GLU:HA	2.27	0.49
2:D:93:VAL:CG2	2:D:94:TYR:N	2.76	0.48
2:D:4:LEU:HD22	2:D:22:CYS:SG	2.53	0.48
1:A:13:VAL:HG22	1:A:14:THR:H	1.78	0.48
2:D:40:ARG:HB2	2:D:43:GLN:CB	2.43	0.48
1:C:72:GLY:HA3	1:C:77:PHE:HA	1.94	0.48
2:D:101:VAL:HG23	2:D:102:TYR:CD1	2.49	0.48
2:B:55:ASN:HD22	2:B:55:ASN:H	1.61	0.48
2:D:33:PHE:CG	2:D:101:VAL:HG11	2.48	0.48
1:A:40:THR:HG21	3:A:119:HOH:O	2.12	0.47
2:B:86:LEU:HD12	2:B:90:ASP:CB	2.44	0.47
1:C:20:THR:HG22	1:C:78:THR:CG2	2.44	0.47
2:B:119:VAL:HB	2:B:120:PRO:HD3	1.97	0.47
2:B:50:ARG:HG3	2:B:59:LYS:HB3	1.95	0.47
1:C:79:LEU:HD22	1:C:80:THR:N	2.30	0.47
2:D:91:THR:HG23	2:D:118:THR:HA	1.95	0.47
2:B:103:SER:HA	2:D:100:GLU:OE1	2.14	0.47
2:D:13:ARG:NE	2:D:14:PRO:HD2	2.29	0.47
2:D:40:ARG:HA	2:D:92:ALA:CB	2.46	0.46
2:D:84:SER:O	2:D:85:SER:C	2.58	0.46
2:B:18:VAL:HG12	2:B:83:LEU:HB2	1.97	0.46
1:A:65:PRO:HG2	1:A:68:PHE:CD2	2.50	0.46
1:A:75:THR:HG22	1:A:76:ASP:CG	2.41	0.46
2:B:43:GLN:HE21	2:B:44:GLY:H	1.64	0.46
1:A:91:VAL:CG2	1:A:109:LYS:HD2	2.45	0.46
2:B:43:GLN:NE2	2:B:44:GLY:H	2.14	0.46
2:D:93:VAL:HG23	2:D:115:THR:O	2.16	0.46
1:C:67:ARG:CZ	1:C:85:GLN:HG3	2.46	0.45
1:A:16:GLY:O	1:A:83:SER:HA	2.16	0.45
2:B:29:ILE:C	2:B:31:ASP:H	2.23	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:PRO:HG2	1:C:11:LEU:CG	2.43	0.45
2:B:55:ASN:O	2:B:56:ASP:CB	2.64	0.45
1:A:66:ASP:C	1:A:68:PHE:N	2.71	0.45
1:A:34:ASN:N	1:A:34:ASN:ND2	2.63	0.45
1:C:12:THR:HA	1:C:111:GLU:O	2.17	0.45
1:C:67:ARG:HH11	1:C:88:ASP:CG	2.24	0.45
1:C:21:MET:HG2	3:C:114:HOH:O	2.16	0.45
2:D:29:ILE:H	2:D:77:ASN:HD21	1.65	0.45
1:A:85:GLN:O	1:A:88:ASP:HB2	2.17	0.45
1:C:95:GLN:HG3	1:C:104:PHE:CE2	2.52	0.45
2:D:2:VAL:HA	2:D:25:SER:O	2.17	0.45
2:D:37:VAL:HG11	2:D:111:TRP:CH2	2.52	0.45
2:D:36:TRP:O	2:D:48:ILE:HB	2.17	0.44
1:A:79:LEU:HD23	1:A:79:LEU:HA	1.82	0.44
1:C:6:GLN:HA	1:C:22:SER:O	2.17	0.44
1:A:111:GLU:CB	1:A:112:PRO:HD2	2.47	0.44
2:B:6:GLN:NE2	2:B:115:THR:HG22	2.32	0.44
2:D:32:ASP:OD2	2:D:98:ARG:HD3	2.18	0.44
2:D:63:LYS:HD2	2:D:63:LYS:N	2.32	0.44
2:D:35:HIS:HD2	2:D:47:TRP:NE1	2.10	0.44
1:C:43:GLN:HG3	1:C:92:TYR:CE2	2.53	0.44
2:D:40:ARG:HH12	2:D:89:GLU:HA	1.83	0.44
2:D:51:ILE:HD11	2:D:56:ASP:HA	2.00	0.43
2:D:40:ARG:HB3	2:D:42:GLU:OE2	2.18	0.43
1:A:42:TYR:O	1:A:92:TYR:HA	2.17	0.43
2:B:40:ARG:C	2:B:42:GLU:N	2.77	0.43
2:D:36:TRP:CE2	2:D:81:LEU:HB2	2.53	0.43
1:C:43:GLN:HB2	1:C:53:LEU:CD1	2.49	0.42
2:D:6:GLN:OE1	2:D:114:GLY:N	2.48	0.42
1:A:14:THR:HG22	1:A:17:GLU:OE1	2.19	0.42
1:A:37:ASN:O	1:A:56:TRP:HA	2.18	0.42
1:A:39:LEU:HD13	1:A:40:THR:N	2.34	0.42
1:A:72:GLY:HA3	1:A:77:PHE:HA	2.00	0.42
1:C:89:LEU:HD13	1:C:89:LEU:HA	1.83	0.42
2:D:20:LEU:N	2:D:20:LEU:HD13	2.34	0.42
2:B:119:VAL:CB	2:B:120:PRO:CD	2.96	0.42
1:A:21:MET:HE2	1:A:110:LEU:HD21	2.02	0.41
2:B:88:SER:HA	2:B:120:PRO:HD3	2.02	0.41
1:C:67:ARG:NH1	1:C:88:ASP:OD1	2.53	0.41
2:D:40:ARG:HA	2:D:92:ALA:HB2	2.01	0.41
1:C:21:MET:N	1:C:79:LEU:O	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:VAL:HA	1:C:65:PRO:HD3	1.90	0.41
1:C:86:ALA:O	1:C:89:LEU:HD23	2.20	0.41
2:B:11:LEU:HA	2:B:118:THR:O	2.20	0.41
2:B:42:GLU:O	2:B:43:GLN:CB	2.67	0.41
1:C:1:ASP:CB	3:C:125:HOH:O	2.55	0.41
1:C:41:TRP:CZ2	1:C:79:LEU:HB2	2.54	0.41
1:A:36:LYS:HD2	1:A:56:TRP:CE3	2.56	0.41
1:C:20:THR:HG22	1:C:78:THR:HG21	2.03	0.41
1:C:96:ASN:O	1:C:96:ASN:CG	2.62	0.41
1:C:8:PRO:HG2	1:C:11:LEU:CD1	2.50	0.41
2:D:62:PRO:HB2	2:D:63:LYS:HZ2	1.83	0.40
1:A:17:GLU:HG3	1:A:18:LYS:N	2.36	0.40
1:A:66:ASP:O	1:A:68:PHE:N	2.55	0.40
2:B:71:ILE:HG22	2:B:72:ALA:N	2.36	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	110/113 (97%)	99 (90%)	8 (7%)	3 (3%)	4	2
1	C	111/113 (98%)	100 (90%)	11 (10%)	0	100	100
2	B	118/123 (96%)	101 (86%)	13 (11%)	4 (3%)	3	1
2	D	121/123 (98%)	105 (87%)	12 (10%)	4 (3%)	3	1
All	All	460/472 (98%)	405 (88%)	44 (10%)	11 (2%)	4	3

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	42	GLU

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Mol	Chain	Res	Type
2	B	43	GLN
2	D	14	PRO
1	A	74	GLY
2	D	120	PRO
2	D	88	SER
1	A	67	ARG
2	B	85	SER
2	D	16	ALA
2	B	119	VAL
1	A	57	ALA

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	98/98 (100%)	78 (80%)	20 (20%)	1	1
1	C	98/98 (100%)	69 (70%)	29 (30%)	0	0
2	B	102/104 (98%)	70 (69%)	32 (31%)	0	0
2	D	104/104 (100%)	67 (64%)	37 (36%)	0	0
All	All	402/404 (100%)	284 (71%)	118 (29%)	0	0

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	10	SER
1	A	14	THR
1	A	17	GLU
1	A	22	SER
1	A	26	SER
1	A	27	GLN
1	A	29	LEU
1	A	34	ASN
1	A	40	THR
1	A	44	GLN

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Mol	Chain	Res	Type
1	A	64	VAL
1	A	73	SER
1	A	75	THR
1	A	79	LEU
1	A	87	GLU
1	A	89	LEU
1	A	96	ASN
1	A	109	LYS
1	A	111	GLU
2	B	1	GLU
2	B	3	GLN
2	B	5	GLN
2	B	11	LEU
2	B	12	VAL
2	B	13	ARG
2	B	17	SER
2	B	18	VAL
2	B	19	LYS
2	B	21	SER
2	B	25	SER
2	B	42	GLU
2	B	43	GLN
2	B	50	ARG
2	B	55	ASN
2	B	56	ASP
2	B	63	LYS
2	B	66	ASP
2	B	67	LYS
2	B	74	THR
2	B	75	SER
2	B	81	LEU
2	B	82	GLN
2	B	83	LEU
2	B	85	SER
2	B	86	LEU
2	B	89	GLU
2	B	98	ARG
2	B	101	VAL
2	B	106	SER
2	B	115	THR
2	B	118	THR
1	C	1	ASP

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Mol	Chain	Res	Type
1	C	7	SER
1	C	9	SER
1	C	10	SER
1	C	11	LEU
1	C	12	THR
1	C	14	THR
1	C	18	LYS
1	C	19	VAL
1	C	20	THR
1	C	24	LYS
1	C	30	LEU
1	C	32	SER
1	C	34	ASN
1	C	36	LYS
1	C	39	LEU
1	C	40	THR
1	C	45	LYS
1	C	48	GLN
1	C	51	LYS
1	C	67	ARG
1	C	75	THR
1	C	79	LEU
1	C	80	THR
1	C	83	SER
1	C	89	LEU
1	C	96	ASN
1	C	102	LEU
1	C	109	LYS
2	D	3	GLN
2	D	5	GLN
2	D	10	GLU
2	D	11	LEU
2	D	12	VAL
2	D	19	LYS
2	D	20	LEU
2	D	30	LYS
2	D	31	ASP
2	D	37	VAL
2	D	40	ARG
2	D	42	GLU
2	D	55	ASN
2	D	56	ASP

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Mol	Chain	Res	Type
2	D	57	ASN
2	D	59	LYS
2	D	63	LYS
2	D	66	ASP
2	D	67	LYS
2	D	69	THR
2	D	74	THR
2	D	75	SER
2	D	76	SER
2	D	77	ASN
2	D	78	THR
2	D	81	LEU
2	D	82	GLN
2	D	83	LEU
2	D	86	LEU
2	D	87	THR
2	D	88	SER
2	D	89	GLU
2	D	93	VAL
2	D	106	SER
2	D	108	LEU
2	D	110	VAL
2	D	123	SER

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	34	ASN
1	A	35	GLN
1	A	43	GLN
1	A	85	GLN
2	B	3	GLN
2	B	5	GLN
2	B	35	HIS
2	B	43	GLN
2	B	55	ASN
1	C	27	GLN
1	C	34	ASN
1	C	35	GLN
1	C	37	ASN
2	D	35	HIS
2	D	43	GLN

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Mol	Chain	Res	Type
2	D	55	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 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	A	112/113 (99%)	-1.48	0 100 100	2, 7, 20, 25	0
1	C	113/113 (100%)	-1.47	0 100 100	2, 6, 19, 35	0
2	B	120/123 (97%)	-1.41	0 100 100	2, 7, 24, 34	0
2	D	123/123 (100%)	-1.38	0 100 100	2, 9, 33, 44	0
All	All	468/472 (99%)	-1.43	0 100 100	2, 7, 24, 44	0

There are no RSRZ outliers to report.

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.