



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 06:44 PM UTC

PDB ID : 1CFS / pdb_00001cfs
Title : ANTI-P24 (HIV-1) FAB FRAGMENT CB41 COMPLEXED WITH AN EPITOPE-UNRELATED PEPTIDE
Authors : Keitel, T.; Kramer, A.; Wessner, H.; Scholz, C.; Schneider-Mergener, J.; Hoehne, W.
Deposited on : 1999-03-19
Resolution : 2.75 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

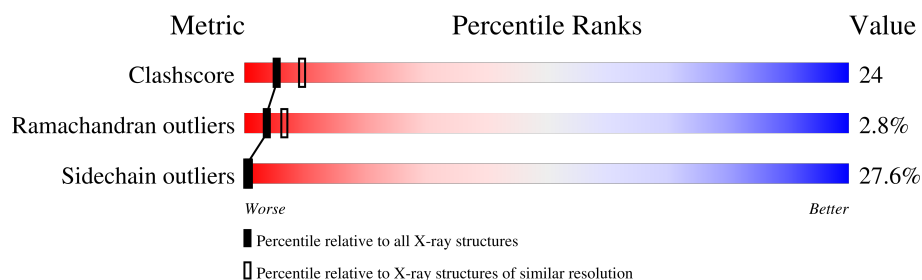
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	214	37% 42% 17% .
2	B	213	40% 35% 22% .
3	C	11	45% 45% 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3388 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 PROTEIN (IGG2A KAPPA ANTIBODY CB41 (LIGHT CHAIN)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1678	1052	276	340	10			

- Molecule 2 is a protein called PROTEIN (IGG2A KAPPA ANTIBODY CB41 (HEAVY CHAIN)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	0	0	0
			1595	1011	263	315	6			

- Molecule 3 is a protein called PROTEIN (ANTIGEN BOUND PEPTIDE).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	11	Total	C	N	O	0	0	0
			87	56	15	16			

- Molecule 4 is water.

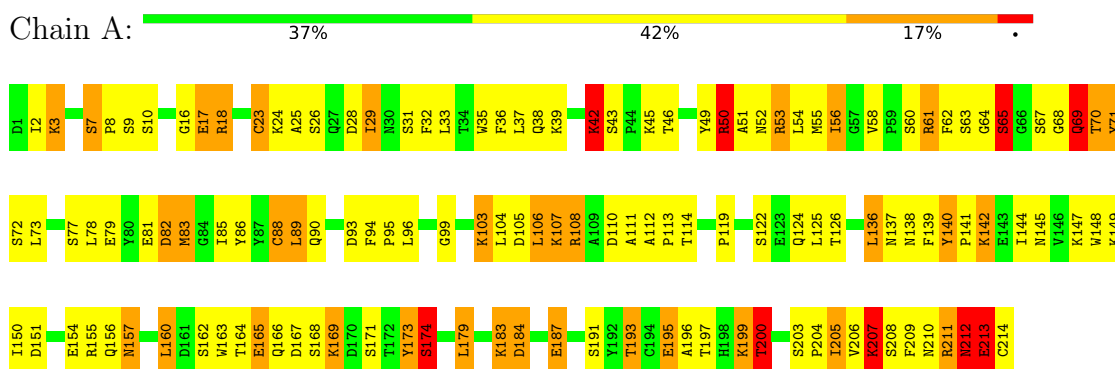
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	11	Total	O	0	0
			11	11		
4	B	14	Total	O	0	0
			14	14		
4	C	3	Total	O	0	0
			3	3		

3 Residue-property plots

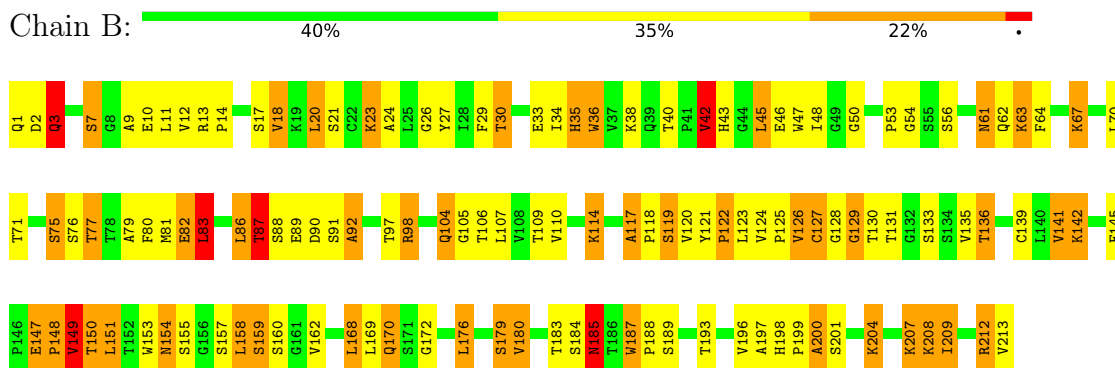
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

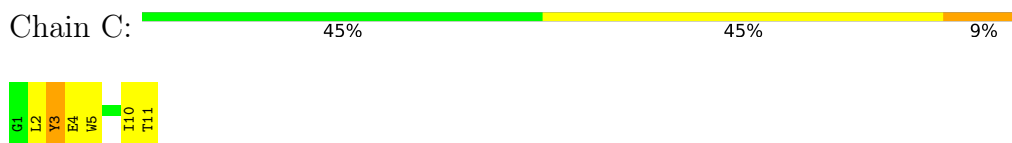
- Molecule 1: PROTEIN (IGG2A KAPPA ANTIBODY CB41 (LIGHT CHAIN))



- Molecule 2: PROTEIN (IGG2A KAPPA ANTIBODY CB41 (HEAVY CHAIN))



- Molecule 3: PROTEIN (ANTIGEN BOUND PEPTIDE)



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	85.32Å 85.32Å 136.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.00 – 2.75	Depositor
% Data completeness (in resolution range)	100.0 (72.00-2.75)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CCP4	Depositor
R, R_{free}	0.232 , 0.332	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3388	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

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	0.80	1/1715 (0.1%)	2.08	66/2321 (2.8%)
2	B	0.83	3/1635 (0.2%)	2.19	83/2233 (3.7%)
3	C	0.91	0/89	2.21	6/118 (5.1%)
All	All	0.81	4/3439 (0.1%)	2.14	155/4672 (3.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	70	THR	CB-OG1	5.77	1.52	1.43
2	B	150	THR	CB-OG1	5.56	1.52	1.43
2	B	131	THR	CB-OG1	5.35	1.52	1.43
2	B	87	THR	CB-OG1	5.28	1.52	1.43

All (155) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	187	TRP	CA-C-O	-14.91	99.73	120.16
1	A	64	GLY	CA-C-N	12.19	144.83	121.54
1	A	64	GLY	C-N-CA	12.19	144.83	121.54
2	B	3	GLN	N-CA-C	11.72	125.82	109.18
1	A	52	ASN	CA-C-O	-9.91	108.54	119.34
2	B	86	LEU	CA-C-O	9.28	131.56	121.16
2	B	185	ASN	CA-CB-CG	9.22	121.82	112.60
2	B	212	ARG	N-CA-C	9.10	123.32	107.49
2	B	98	ARG	CA-C-O	8.86	130.40	119.95
2	B	77	THR	CA-CB-OG1	8.76	122.74	109.60
2	B	209	ILE	N-CA-CB	8.59	122.15	111.41
1	A	64	GLY	CA-C-O	8.52	135.39	120.57
1	A	69	GLN	CA-CB-CG	8.43	130.97	114.10
2	B	9	ALA	CA-C-O	8.27	130.28	121.19
2	B	14	PRO	CB-CA-C	8.20	121.69	111.12
2	B	61	ASN	CA-CB-CG	-7.97	104.63	112.60
1	A	71	TYR	CA-C-O	-7.64	112.50	121.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	11	THR	CA-CB-OG1	7.58	120.98	109.60
1	A	29	ILE	CA-C-O	7.54	127.68	120.14
1	A	61	ARG	CA-CB-CG	7.53	129.16	114.10
3	C	10	ILE	CA-C-O	7.42	128.26	120.25
1	A	62	PHE	CA-CB-CG	-7.41	106.39	113.80
2	B	71	THR	O-C-N	-7.35	112.87	122.94
1	A	68	GLY	CA-C-N	-7.33	110.56	121.99
1	A	68	GLY	C-N-CA	-7.33	110.56	121.99
2	B	123	LEU	CA-C-O	7.28	129.00	120.70
1	A	137	ASN	N-CA-C	7.26	121.87	110.32
1	A	200	THR	CA-CB-CG2	7.23	122.79	110.50
1	A	93	ASP	CA-CB-CG	7.18	119.78	112.60
1	A	88	CYS	O-C-N	7.18	132.53	123.19
2	B	141	VAL	CA-CB-CG1	7.17	122.59	110.40
2	B	198	HIS	CA-CB-CG	7.04	120.84	113.80
2	B	80	PHE	CA-C-O	7.01	128.14	120.71
2	B	187	TRP	O-C-N	7.00	129.37	121.32
1	A	200	THR	CB-CA-C	6.90	116.66	109.83
2	B	82	GLU	CA-CB-CG	6.89	127.88	114.10
2	B	179	SER	N-CA-C	6.89	119.64	108.34
1	A	205	ILE	CB-CA-C	6.83	120.94	110.96
1	A	26	SER	CA-CB-OG	6.77	124.65	111.10
1	A	138	ASN	N-CA-C	6.77	120.73	111.39
2	B	75	SER	CA-C-O	-6.72	113.77	120.82
2	B	98	ARG	O-C-N	-6.70	114.02	122.26
2	B	18	VAL	CA-CB-CG1	6.59	121.61	110.40
1	A	61	ARG	NE-CZ-NH2	6.58	125.12	119.20
2	B	180	VAL	N-CA-CB	6.57	120.19	111.25
2	B	36	TRP	CA-C-N	6.55	132.04	122.94
2	B	36	TRP	C-N-CA	6.55	132.04	122.94
2	B	50	GLY	CA-C-O	6.53	127.25	121.57
1	A	93	ASP	CA-C-O	-6.53	114.46	121.45
2	B	90	ASP	CA-CB-CG	-6.51	106.09	112.60
1	A	39	LYS	CB-CA-C	6.50	118.77	109.08
1	A	88	CYS	CA-C-O	-6.44	113.83	121.11
1	A	61	ARG	NE-CZ-NH1	-6.42	115.08	121.50
2	B	63	LYS	CA-CB-CG	6.42	126.94	114.10
1	A	108	ARG	N-CA-C	6.35	117.50	108.74
2	B	98	ARG	CA-C-N	6.30	133.57	121.54
2	B	98	ARG	C-N-CA	6.30	133.57	121.54
2	B	105	GLY	CA-C-O	6.29	127.18	121.77
2	B	142	LYS	CA-CB-CG	6.28	126.65	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	98	ARG	NE-CZ-NH2	-6.26	113.57	119.20
1	A	69	GLN	CB-CA-C	6.22	120.45	109.75
2	B	98	ARG	CD-NE-CZ	6.21	133.10	124.40
1	A	17	GLU	CA-C-N	6.20	131.23	121.99
1	A	17	GLU	C-N-CA	6.20	131.23	121.99
1	A	113	PRO	N-CA-C	6.08	121.05	111.38
2	B	129	GLY	CA-C-N	6.08	133.15	121.54
2	B	129	GLY	C-N-CA	6.08	133.15	121.54
1	A	50	ARG	CA-CB-CG	6.03	126.16	114.10
1	A	3	LYS	CB-CA-C	6.03	119.30	109.90
2	B	124	VAL	N-CA-CB	-5.96	103.85	109.99
2	B	35	HIS	N-CA-CB	5.95	121.25	111.08
1	A	79	GLU	CA-C-N	5.89	128.49	120.54
1	A	79	GLU	C-N-CA	5.89	128.49	120.54
2	B	154	ASN	CA-CB-CG	5.88	118.48	112.60
1	A	137	ASN	CA-C-N	5.87	130.69	122.36
1	A	137	ASN	C-N-CA	5.87	130.69	122.36
1	A	163	TRP	CA-C-O	5.86	127.79	121.16
2	B	136	THR	CA-CB-OG1	5.86	118.38	109.60
2	B	40	THR	CA-C-O	5.85	125.88	119.91
1	A	64	GLY	O-C-N	-5.85	115.10	122.70
2	B	53	PRO	CB-CA-C	5.81	121.28	112.21
2	B	201	SER	N-CA-C	-5.79	106.08	114.12
2	B	50	GLY	O-C-N	-5.76	118.30	123.37
1	A	200	THR	CA-C-O	5.74	123.89	119.18
2	B	67	LYS	CA-CB-CG	5.73	125.56	114.10
1	A	122	SER	CA-C-N	5.71	129.38	120.82
1	A	122	SER	C-N-CA	5.71	129.38	120.82
2	B	45	LEU	CA-C-O	5.69	127.18	120.69
2	B	71	THR	CA-CB-OG1	5.68	118.12	109.60
2	B	71	THR	CA-C-O	5.67	128.15	121.58
2	B	117	ALA	N-CA-CB	5.66	116.31	109.74
2	B	180	VAL	CA-C-O	5.66	126.47	120.48
2	B	79	ALA	CA-C-O	-5.63	114.18	120.54
2	B	170	GLN	OE1-CD-NE2	5.62	128.22	122.60
1	A	105	ASP	CA-CB-CG	5.61	118.21	112.60
2	B	208	LYS	CA-C-O	-5.59	114.38	120.81
2	B	33	GLU	CA-C-N	-5.56	116.29	123.19
2	B	33	GLU	C-N-CA	-5.56	116.29	123.19
2	B	105	GLY	O-C-N	-5.56	117.97	122.64
1	A	108	ARG	CA-C-O	5.55	127.25	121.36
2	B	129	GLY	N-CA-C	5.55	119.21	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	16	GLY	CA-C-O	5.54	124.38	119.56
2	B	40	THR	CB-CA-C	-5.50	100.92	109.55
2	B	155	SER	N-CA-C	5.49	118.77	111.30
2	B	160	SER	N-CA-C	-5.49	107.24	114.04
2	B	34	ILE	N-CA-CB	5.47	118.69	111.25
1	A	42	LYS	N-CA-C	5.45	117.96	109.52
1	A	206	VAL	N-CA-C	5.44	115.73	108.11
1	A	39	LYS	N-CA-C	-5.44	102.92	109.72
1	A	82	ASP	CA-CB-CG	-5.41	107.19	112.60
1	A	207	LYS	N-CA-C	-5.40	101.54	109.81
2	B	128	GLY	N-CA-C	-5.39	100.41	113.18
3	C	10	ILE	CA-C-N	5.38	131.39	121.70
3	C	10	ILE	C-N-CA	5.38	131.39	121.70
2	B	114	LYS	CA-C-N	-5.38	113.06	121.02
2	B	114	LYS	C-N-CA	-5.38	113.06	121.02
3	C	3	TYR	CA-C-N	5.38	128.03	120.28
3	C	3	TYR	C-N-CA	5.38	128.03	120.28
1	A	49	TYR	CA-C-N	5.37	131.79	121.54
1	A	49	TYR	C-N-CA	5.37	131.79	121.54
1	A	157	ASN	CA-CB-CG	-5.36	107.24	112.60
2	B	83	LEU	CA-C-N	-5.35	113.47	123.05
2	B	83	LEU	C-N-CA	-5.35	113.47	123.05
1	A	174	SER	CA-CB-OG	-5.35	100.40	111.10
2	B	212	ARG	CB-CA-C	-5.33	104.11	110.94
1	A	195	GLU	N-CA-C	5.32	117.63	109.07
2	B	18	VAL	CA-CB-CG2	5.31	119.42	110.40
1	A	23	CYS	CA-C-N	-5.29	115.53	122.99
1	A	23	CYS	C-N-CA	-5.29	115.53	122.99
1	A	81	GLU	CB-CG-CD	5.28	121.57	112.60
2	B	20	LEU	CA-C-N	5.27	130.57	122.93
2	B	20	LEU	C-N-CA	5.27	130.57	122.93
1	A	99	GLY	N-CA-C	-5.26	104.38	112.85
1	A	212	ASN	CA-CB-CG	5.25	117.85	112.60
2	B	67	LYS	N-CA-CB	-5.24	103.93	110.90
2	B	7	SER	CA-C-O	-5.24	115.79	121.87
1	A	140	TYR	O-C-N	5.23	127.33	121.32
1	A	3	LYS	N-CA-C	-5.23	102.31	110.10
1	A	136	LEU	CA-C-O	-5.20	115.14	121.58
2	B	61	ASN	OD1-CG-ND2	5.19	127.79	122.60
1	A	36	PHE	CA-CB-CG	5.17	118.97	113.80
2	B	75	SER	N-CA-CB	5.15	117.47	110.01
2	B	127	CYS	CA-C-O	5.15	127.16	121.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	122	PRO	CA-C-O	-5.15	115.72	121.23
2	B	188	PRO	CA-N-CD	-5.14	104.81	112.00
2	B	213	VAL	N-CA-CB	5.13	120.23	111.50
2	B	20	LEU	O-C-N	-5.13	117.21	123.16
1	A	196	ALA	N-CA-C	5.13	116.75	108.34
2	B	172	GLY	N-CA-C	-5.09	108.64	114.69
2	B	119	SER	CA-C-N	-5.07	116.03	122.37
2	B	119	SER	C-N-CA	-5.07	116.03	122.37
1	A	82	ASP	N-CA-C	5.06	119.21	113.19
1	A	184	ASP	CA-CB-CG	5.05	117.65	112.60
1	A	113	PRO	CB-CA-C	-5.04	104.38	110.98
2	B	150	THR	CA-C-O	-5.03	114.95	120.43

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	1678	0	1625	83	0
2	B	1595	0	1576	79	0
3	C	87	0	83	4	0
4	A	11	0	0	5	0
4	B	14	0	0	4	0
4	C	3	0	0	2	0
All	All	3388	0	3284	161	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 24.

All (161) 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:150:ILE:HD12	1:A:155:ARG:NH1	1.73	1.04
1:A:150:ILE:CD1	1:A:155:ARG:NH1	2.22	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:LEU:HB3	2:B:168:LEU:HD13	1.45	0.94
1:A:199:LYS:O	1:A:200:THR:HG22	1.69	0.92
1:A:56:ILE:H	1:A:56:ILE:HD12	1.33	0.92
1:A:85:ILE:HG12	1:A:103:LYS:HG3	1.52	0.90
2:B:48:ILE:HD13	2:B:81:MET:HE1	1.58	0.85
1:A:65:SER:HB3	1:A:71:TYR:HB3	1.57	0.85
1:A:150:ILE:HD12	1:A:155:ARG:CZ	2.09	0.82
1:A:150:ILE:HD13	1:A:155:ARG:NH1	1.96	0.79
2:B:126:VAL:HG23	2:B:129:GLY:HA3	1.62	0.78
2:B:48:ILE:HG21	2:B:81:MET:CE	2.14	0.77
2:B:150:THR:HG23	2:B:150:THR:O	1.83	0.77
1:A:65:SER:HA	1:A:72:SER:H	1.50	0.76
2:B:87:THR:CG2	2:B:89:GLU:H	2.03	0.71
2:B:104:GLN:H	2:B:104:GLN:NE2	1.88	0.71
2:B:162:VAL:HG22	2:B:180:VAL:HG22	1.70	0.70
2:B:141:VAL:HB	2:B:176:LEU:HD23	1.74	0.69
1:A:125:LEU:HB3	1:A:183:LYS:HE3	1.74	0.68
2:B:185:ASN:HD22	2:B:185:ASN:N	1.91	0.68
2:B:104:GLN:H	2:B:104:GLN:HE21	1.40	0.68
1:A:54:LEU:HD22	1:A:58:VAL:CG1	2.24	0.67
1:A:25:ALA:O	1:A:69:GLN:HG3	1.95	0.67
1:A:65:SER:HB3	1:A:71:TYR:CB	2.26	0.66
2:B:12:VAL:HG11	2:B:18:VAL:HG12	1.78	0.66
1:A:54:LEU:HD22	1:A:58:VAL:HG11	1.78	0.66
2:B:97:THR:HG23	4:B:217:HOH:O	1.94	0.66
2:B:38:LYS:HB2	2:B:48:ILE:HD11	1.79	0.64
1:A:150:ILE:HD11	1:A:179:LEU:HD11	1.80	0.64
1:A:150:ILE:HD13	1:A:155:ARG:HH12	1.63	0.64
1:A:50:ARG:O	1:A:51:ALA:HB3	1.98	0.63
2:B:87:THR:HG23	2:B:88:SER:N	2.13	0.63
1:A:108:ARG:NH2	1:A:111:ALA:HB2	2.14	0.62
1:A:183:LYS:O	1:A:187:GLU:HG3	2.00	0.62
2:B:1:GLN:HA	2:B:26:GLY:O	2.00	0.62
2:B:87:THR:CG2	2:B:89:GLU:HG3	2.29	0.62
2:B:120:VAL:HG22	2:B:141:VAL:HG22	1.83	0.60
2:B:120:VAL:O	2:B:207:LYS:HD3	2.02	0.60
1:A:167:ASP:HB2	4:A:217:HOH:O	2.01	0.60
2:B:154:ASN:HB2	2:B:158:LEU:HB3	1.84	0.59
1:A:210:ASN:HB3	1:A:212:ASN:OD1	2.04	0.58
2:B:118:PRO:CB	2:B:141:VAL:HG13	2.32	0.58
1:A:199:LYS:O	1:A:200:THR:CG2	2.47	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:159:SER:HA	2:B:162:VAL:HG23	1.84	0.58
1:A:37:LEU:HD13	1:A:86:TYR:CZ	2.39	0.57
1:A:56:ILE:H	1:A:56:ILE:CD1	2.04	0.57
1:A:61:ARG:NH1	1:A:82:ASP:OD2	2.39	0.56
2:B:147:GLU:HB3	2:B:148:PRO:HA	1.85	0.56
1:A:212:ASN:O	1:A:213:GLU:HB2	2.05	0.56
1:A:160:LEU:HD13	2:B:168:LEU:HB3	1.87	0.56
2:B:117:ALA:HB1	2:B:118:PRO:HD2	1.88	0.56
1:A:37:LEU:HD13	1:A:86:TYR:CE1	2.42	0.55
2:B:135:VAL:HG23	2:B:184:SER:HA	1.89	0.55
2:B:150:THR:O	2:B:150:THR:CG2	2.54	0.55
2:B:162:VAL:HG22	2:B:180:VAL:CG2	2.37	0.54
3:C:2:LEU:HD22	3:C:5:TRP:NE1	2.22	0.54
1:A:199:LYS:O	1:A:200:THR:HB	2.07	0.54
2:B:12:VAL:HG11	2:B:18:VAL:CG1	2.38	0.54
2:B:87:THR:HG23	2:B:89:GLU:H	1.71	0.54
1:A:139:PHE:CE2	1:A:174:SER:HA	2.43	0.53
2:B:48:ILE:HG21	2:B:81:MET:HE3	1.88	0.53
2:B:153:TRP:HB3	2:B:158:LEU:HD13	1.88	0.53
2:B:12:VAL:O	2:B:110:VAL:HA	2.08	0.53
1:A:42:LYS:NZ	1:A:43:SER:O	2.43	0.52
1:A:65:SER:N	1:A:72:SER:O	2.42	0.52
2:B:118:PRO:HB3	2:B:141:VAL:HG13	1.92	0.52
2:B:199:PRO:O	2:B:200:ALA:CB	2.57	0.52
2:B:20:LEU:HD22	2:B:106:THR:HG21	1.92	0.51
2:B:87:THR:HG22	2:B:89:GLU:H	1.73	0.51
2:B:7:SER:HB3	2:B:21:SER:HB2	1.93	0.51
1:A:94:PHE:HA	1:A:95:PRO:C	2.34	0.51
1:A:50:ARG:O	1:A:50:ARG:HG3	2.10	0.51
2:B:122:PRO:HD3	2:B:207:LYS:HG2	1.93	0.51
2:B:12:VAL:HG21	2:B:86:LEU:CD1	2.41	0.50
2:B:127:CYS:HB3	4:B:224:HOH:O	2.11	0.50
2:B:147:GLU:CB	2:B:148:PRO:HA	2.40	0.50
1:A:193:THR:HG22	1:A:208:SER:HB3	1.93	0.50
1:A:32:PHE:O	1:A:90:GLN:HA	2.13	0.49
2:B:125:PRO:O	2:B:126:VAL:C	2.56	0.49
2:B:168:LEU:HG	4:B:219:HOH:O	2.11	0.49
2:B:23:LYS:HE3	2:B:76:SER:O	2.12	0.49
2:B:30:THR:HB	2:B:54:GLY:HA2	1.95	0.48
1:A:160:LEU:HD13	2:B:168:LEU:HD13	1.96	0.48
1:A:166:GLN:HB2	1:A:173:TYR:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:LYS:HG3	1:A:173:TYR:CD2	2.49	0.47
1:A:65:SER:CB	1:A:71:TYR:HB3	2.38	0.47
1:A:199:LYS:O	1:A:200:THR:CB	2.63	0.47
2:B:104:GLN:HE21	2:B:104:GLN:N	2.09	0.47
1:A:29:ILE:HD13	1:A:90:GLN:HB3	1.97	0.47
1:A:151:ASP:HA	1:A:191:SER:OG	2.15	0.47
2:B:119:SER:HB3	2:B:121:TYR:CZ	2.50	0.47
2:B:153:TRP:O	2:B:154:ASN:HB2	2.14	0.46
1:A:136:LEU:HD23	1:A:144:ILE:HD11	1.97	0.46
1:A:67:SER:HA	1:A:71:TYR:CE1	2.51	0.46
2:B:197:ALA:HB2	2:B:204:LYS:HG3	1.98	0.46
1:A:83:MET:HB2	1:A:83:MET:HE2	1.57	0.45
1:A:7:SER:HA	1:A:8:PRO:C	2.40	0.45
2:B:127:CYS:CB	4:B:224:HOH:O	2.64	0.45
1:A:148:TRP:O	1:A:154:GLU:HA	2.16	0.45
2:B:141:VAL:HB	2:B:176:LEU:CD2	2.43	0.45
1:A:86:TYR:HE2	1:A:104:LEU:HD22	1.81	0.45
3:C:2:LEU:HD22	3:C:5:TRP:CD1	2.52	0.45
2:B:87:THR:HG21	2:B:89:GLU:HG3	1.96	0.45
3:C:3:TYR:HB3	4:C:28:HOH:O	2.15	0.45
1:A:110:ASP:OD1	1:A:141:PRO:HD3	2.17	0.45
2:B:42:VAL:HG12	2:B:43:HIS:CG	2.52	0.45
2:B:91:SER:O	2:B:92:ALA:HB2	2.17	0.44
1:A:150:ILE:O	1:A:151:ASP:C	2.60	0.44
2:B:139:CYS:HB2	2:B:153:TRP:CZ2	2.52	0.44
1:A:112:ALA:HB2	4:A:218:HOH:O	2.17	0.44
2:B:151:LEU:C	2:B:151:LEU:HD12	2.43	0.44
3:C:4:GLU:HG3	4:C:28:HOH:O	2.18	0.44
2:B:118:PRO:HB2	2:B:141:VAL:HG13	1.98	0.43
1:A:42:LYS:HE2	1:A:43:SER:H	1.82	0.43
1:A:89:LEU:HD21	1:A:96:LEU:HB3	2.00	0.43
1:A:200:THR:CG2	4:A:218:HOH:O	2.65	0.43
1:A:139:PHE:CZ	1:A:144:ILE:HG21	2.53	0.43
1:A:193:THR:CG2	1:A:208:SER:HB3	2.48	0.43
2:B:159:SER:HA	2:B:162:VAL:CG2	2.47	0.43
2:B:24:ALA:HB1	2:B:27:TYR:OH	2.18	0.43
2:B:153:TRP:CD1	2:B:180:VAL:HG23	2.54	0.43
1:A:46:THR:HG22	1:A:55:MET:HG3	2.01	0.43
1:A:65:SER:CA	1:A:72:SER:H	2.26	0.43
2:B:83:LEU:HB3	2:B:86:LEU:HD21	2.01	0.43
2:B:149:VAL:HG11	2:B:176:LEU:HD22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:PHE:HB3	1:A:95:PRO:HA	2.01	0.42
1:A:106:LEU:HD22	1:A:106:LEU:HA	1.93	0.42
1:A:200:THR:HG23	4:A:218:HOH:O	2.19	0.42
1:A:207:LYS:HA	1:A:207:LYS:HD3	1.80	0.42
2:B:36:TRP:CD1	2:B:70:LEU:HD22	2.54	0.42
1:A:61:ARG:NH2	4:A:223:HOH:O	2.51	0.42
1:A:136:LEU:O	1:A:174:SER:OG	2.38	0.42
2:B:48:ILE:HA	2:B:64:PHE:CD2	2.55	0.42
1:A:53:ARG:HH11	1:A:53:ARG:HD2	1.75	0.42
1:A:119:PRO:HB3	1:A:209:PHE:CE2	2.55	0.42
1:A:83:MET:SD	1:A:106:LEU:HD23	2.60	0.41
2:B:46:GLU:HG2	2:B:63:LYS:NZ	2.35	0.41
2:B:153:TRP:HZ3	2:B:209:ILE:HD13	1.84	0.41
1:A:54:LEU:CD2	1:A:58:VAL:HG11	2.48	0.41
1:A:167:ASP:OD2	1:A:169:LYS:HB2	2.19	0.41
2:B:29:PHE:CD2	2:B:77:THR:HA	2.55	0.41
2:B:126:VAL:CG2	2:B:129:GLY:HA3	2.41	0.41
1:A:17:GLU:HG3	1:A:18:ARG:N	2.35	0.41
1:A:125:LEU:O	1:A:183:LYS:NZ	2.53	0.41
1:A:165:GLU:H	1:A:165:GLU:HG2	1.63	0.41
1:A:107:LYS:HA	1:A:140:TYR:OH	2.20	0.41
2:B:47:TRP:HE3	2:B:61:ASN:HD22	1.69	0.41
1:A:160:LEU:HD13	2:B:168:LEU:CB	2.48	0.41
2:B:153:TRP:CZ3	2:B:209:ILE:HD13	2.56	0.41
1:A:50:ARG:O	1:A:51:ALA:CB	2.65	0.41
2:B:151:LEU:HB2	2:B:196:VAL:HG22	2.02	0.41
2:B:185:ASN:HD22	2:B:185:ASN:H	1.63	0.41
1:A:124:GLN:HB2	2:B:121:TYR:CE2	2.57	0.41
2:B:153:TRP:HB3	2:B:158:LEU:CD1	2.50	0.40
1:A:35:TRP:CZ3	1:A:88:CYS:HB3	2.57	0.40
1:A:199:LYS:HG3	1:A:200:THR:HB	2.02	0.40
2:B:2:ASP:HB3	2:B:3:GLN:HG3	2.03	0.40
1:A:85:ILE:HG12	1:A:103:LYS:CG	2.38	0.40
1:A:187:GLU:HG2	1:A:211:ARG:HH21	1.87	0.40
1:A:145:ASN:HB2	1:A:197:THR:OG1	2.22	0.40
2:B:120:VAL:HG21	2:B:196:VAL:HB	2.03	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	212/214 (99%)	193 (91%)	16 (8%)	3 (1%)	9	17
2	B	211/213 (99%)	185 (88%)	17 (8%)	9 (4%)	2	3
3	C	9/11 (82%)	8 (89%)	1 (11%)	0	100	100
All	All	432/438 (99%)	386 (89%)	34 (8%)	12 (3%)	4	6

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	SER
1	A	213	GLU
2	B	149	VAL
2	B	187	TRP
2	B	200	ALA
2	B	126	VAL
2	B	30	THR
1	A	204	PRO
2	B	92	ALA
2	B	145	PHE
2	B	42	VAL
2	B	148	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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	193/193 (100%)	132 (68%)	61 (32%)	0	0
2	B	180/180 (100%)	136 (76%)	44 (24%)	1	1
3	C	7/7 (100%)	7 (100%)	0	100	100
All	All	380/380 (100%)	275 (72%)	105 (28%)	0	1

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	3	LYS
1	A	7	SER
1	A	9	SER
1	A	10	SER
1	A	18	ARG
1	A	23	CYS
1	A	24	LYS
1	A	28	ASP
1	A	31	SER
1	A	33	LEU
1	A	38	GLN
1	A	42	LYS
1	A	45	LYS
1	A	50	ARG
1	A	53	ARG
1	A	56	ILE
1	A	60	SER
1	A	63	SER
1	A	65	SER
1	A	69	GLN
1	A	70	THR
1	A	73	LEU
1	A	77	SER
1	A	78	LEU
1	A	83	MET
1	A	89	LEU
1	A	103	LYS
1	A	106	LEU
1	A	107	LYS
1	A	114	THR

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Mol	Chain	Res	Type
1	A	126	THR
1	A	142	LYS
1	A	147	LYS
1	A	149	LYS
1	A	156	GLN
1	A	157	ASN
1	A	160	LEU
1	A	162	SER
1	A	164	THR
1	A	165	GLU
1	A	168	SER
1	A	169	LYS
1	A	171	SER
1	A	173	TYR
1	A	174	SER
1	A	179	LEU
1	A	183	LYS
1	A	184	ASP
1	A	187	GLU
1	A	193	THR
1	A	195	GLU
1	A	199	LYS
1	A	200	THR
1	A	203	SER
1	A	205	ILE
1	A	207	LYS
1	A	211	ARG
1	A	212	ASN
1	A	213	GLU
1	A	214	CYS
2	B	3	GLN
2	B	10	GLU
2	B	11	LEU
2	B	13	ARG
2	B	17	SER
2	B	23	LYS
2	B	35	HIS
2	B	42	VAL
2	B	45	LEU
2	B	56	SER
2	B	62	GLN
2	B	67	LYS

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Mol	Chain	Res	Type
2	B	75	SER
2	B	82	GLU
2	B	83	LEU
2	B	87	THR
2	B	98	ARG
2	B	104	GLN
2	B	107	LEU
2	B	109	THR
2	B	114	LYS
2	B	130	THR
2	B	133	SER
2	B	136	THR
2	B	142	LYS
2	B	147	GLU
2	B	149	VAL
2	B	151	LEU
2	B	157	SER
2	B	158	LEU
2	B	159	SER
2	B	168	LEU
2	B	169	LEU
2	B	170	GLN
2	B	176	LEU
2	B	179	SER
2	B	183	THR
2	B	185	ASN
2	B	189	SER
2	B	193	THR
2	B	204	LYS
2	B	207	LYS
2	B	208	LYS
2	B	212	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	38	GLN
2	B	5	GLN
2	B	39	GLN
2	B	104	GLN
2	B	170	GLN

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Mol	Chain	Res	Type
2	B	185	ASN
2	B	198	HIS

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.