



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 06:59 am GMT

PDB ID : 1CFS
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

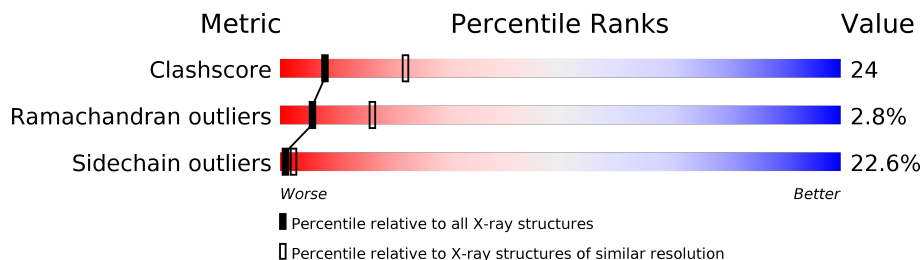
1 Overall quality at a glance

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	112137	4174 (2.80-2.72)
Ramachandran outliers	110173	4103 (2.80-2.72)
Sidechain outliers	110143	4106 (2.80-2.72)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	214	
2	B	213	
3	C	11	

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.

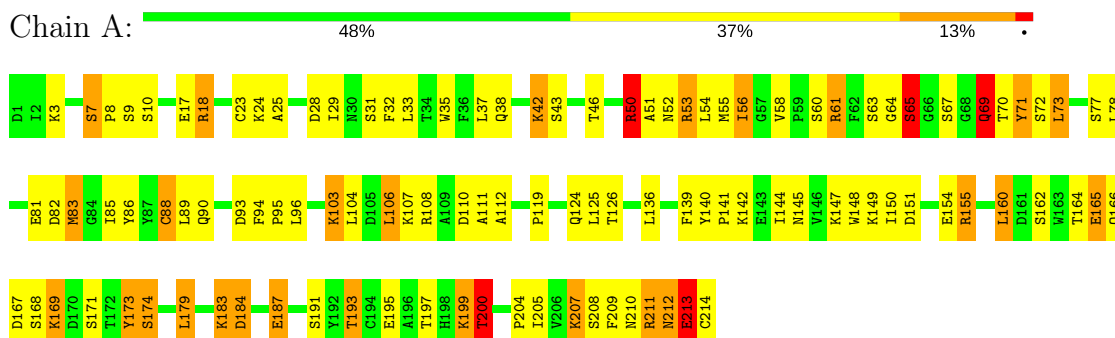
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	11	Total	O	0	0
			11	11		
4	B	14	Total	O	0	0
			14	14		
4	C	3	Total	O	0	0
			3	3		

3 Residue-property plots

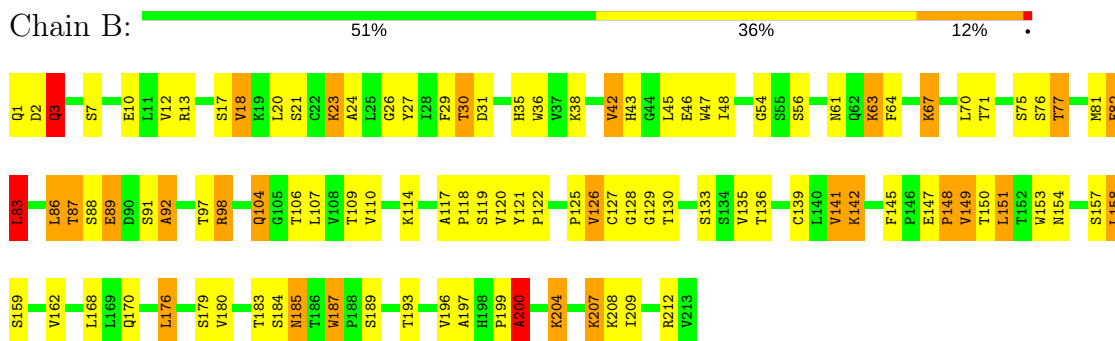
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

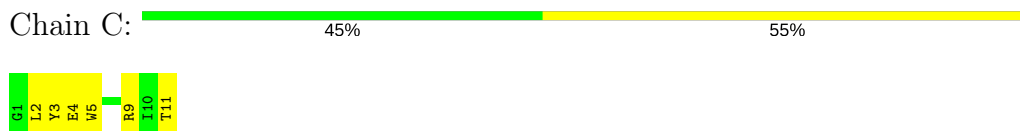
• Molecule 1: PROTEIN (IGG2A KAPPA ANTIBODY CB41 (LIGHT CHAIN))



• 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 ⓘ

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	0.62	0/1715	1.58	18/2321 (0.8%)
2	B	0.65	0/1635	1.69	23/2233 (1.0%)
3	C	0.78	0/89	1.85	2/118 (1.7%)
All	All	0.64	0/3439	1.64	43/4672 (0.9%)

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	98	ARG	NE-CZ-NH2	-13.46	113.57	120.30
1	A	61	ARG	NE-CZ-NH1	-10.44	115.08	120.30
2	B	187	TRP	CA-C-O	-9.70	99.73	120.10
1	A	61	ARG	NE-CZ-NH2	9.64	125.12	120.30
1	A	64	GLY	C-N-CA	9.25	144.83	121.70
1	A	64	GLY	CA-C-O	8.21	135.39	120.60
2	B	31	ASP	CB-CG-OD1	8.08	125.57	118.30
1	A	69	GLN	CA-CB-CG	7.98	130.97	113.40
2	B	141	VAL	CA-CB-CG1	7.79	122.59	110.90
2	B	98	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	A	200	THR	CA-CB-CG2	7.42	122.79	112.40
1	A	61	ARG	CA-CB-CG	7.17	129.16	113.40
2	B	18	VAL	CA-CB-CG1	7.14	121.61	110.90
2	B	31	ASP	CB-CG-OD2	-7.11	111.90	118.30
2	B	98	ARG	CD-NE-CZ	6.79	133.10	123.60
2	B	82	GLU	CA-CB-CG	6.58	127.88	113.40
2	B	77	THR	CA-CB-OG1	6.54	122.74	109.00
3	C	9	ARG	NE-CZ-NH1	-6.48	117.06	120.30
2	B	89	GLU	OE1-CD-OE2	6.26	130.81	123.30
1	A	73	LEU	CA-CB-CG	6.23	129.62	115.30
2	B	63	LYS	CA-CB-CG	6.16	126.94	113.40
2	B	71	THR	O-C-N	-6.14	112.87	122.70
1	A	88	CYS	O-C-N	6.14	132.53	122.70
1	A	93	ASP	CB-CG-OD1	6.11	123.80	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	142	LYS	CA-CB-CG	6.02	126.65	113.40
1	A	81	GLU	OE1-CD-OE2	-5.94	116.17	123.30
2	B	35	HIS	N-CA-CB	5.91	121.25	110.60
2	B	83	LEU	CB-CG-CD1	5.91	121.04	111.00
1	A	155	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	50	ARG	CA-CB-CG	5.80	126.16	113.40
3	C	11	THR	CA-CB-OG1	5.70	120.98	109.00
2	B	18	VAL	CA-CB-CG2	5.68	119.42	110.90
1	A	160	LEU	CA-CB-CG	5.60	128.17	115.30
2	B	67	LYS	CA-CB-CG	5.53	125.56	113.40
1	A	52	ASN	CA-C-O	-5.50	108.54	120.10
2	B	3	GLN	N-CA-C	5.49	125.82	111.00
2	B	86	LEU	CA-C-O	5.46	131.56	120.10
2	B	98	ARG	O-C-N	-5.42	114.02	122.70
1	A	184	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	71	TYR	CB-CG-CD2	-5.08	117.95	121.00
2	B	200	ALA	N-CA-CB	5.08	117.21	110.10
2	B	128	GLY	N-CA-C	-5.08	100.41	113.10
1	A	69	GLN	CB-CA-C	5.02	120.45	110.40

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	1624	81	0
2	B	1595	0	1576	78	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	3283	158	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 (158) 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
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
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:104:GLN:NE2	2:B:104:GLN:H	1.88	0.71
2:B:87:THR:CG2	2:B:89:GLU:H	2.03	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:HE21	2:B:104:GLN:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:212:ASN:O	1:A:213:GLU:HB2	2.05	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: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:CG2	2:B:150:THR:O	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: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:48:ILE:HG21	2:B:81:MET:HE3	1.89	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
1:A:50:ARG:O	1:A:50:ARG:HG3	2.10	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
2:B:122:PRO:HD3	2:B:207:LYS:HG2	1.93	0.51
2:B:127:CYS:HB3	4:B:224:HOH:O	2.11	0.50
2:B:12:VAL:HG21	2:B:86:LEU:CD1	2.41	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: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:166:GLN:HB2	1:A:173:TYR:CE2	2.48	0.48
1:A:160:LEU:HD13	2:B:168:LEU:HD13	1.96	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:151:ASP:HA	1:A:191:SER:OG	2.15	0.47
1:A:29:ILE:HD13	1:A:90:GLN:HB3	1.97	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:94:PHE:HA	1:A:95:PRO:C	2.34	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
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
2:B:125:PRO:O	2:B:126:VAL:C	2.56	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
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:200:THR:CG2	4:A:218:HOH:O	2.65	0.43
1:A:89:LEU:HD21	1:A:96:LEU:HB3	2.00	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:153:TRP:CD1	2:B:180:VAL:HG23	2.54	0.43
2:B:24:ALA:HB1	2:B:27:TYR:OH	2.18	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:THR:HG23	4:A:218:HOH:O	2.19	0.42
1:A:207:LYS:HD3	1:A:207:LYS:HA	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:119:PRO:HB3	1:A:209:PHE:CE2	2.55	0.42
1:A:53:ARG:HH11	1:A:53:ARG:HD2	1.75	0.42
1:A:83:MET:SD	1:A:106:LEU:HD23	2.60	0.41
2:B:153:TRP:HZ3	2:B:209:ILE:HD13	1.84	0.41
2:B:46:GLU:HG2	2:B:63:LYS:NZ	2.35	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:165:GLU:H	1:A:165:GLU:HG2	1.63	0.41
1:A:125:LEU:O	1:A:183:LYS:NZ	2.53	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
2:B:48:ILE:HD13	2:B:81:MET:CE	2.51	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:199:LYS:HG3	1:A:200:THR:HB	2.02	0.40
1:A:35:TRP:CZ3	1:A:88:CYS:HB3	2.57	0.40
1:A:7:SER:HA	1:A:8:PRO:C	2.40	0.40
2:B:2:ASP:HB3	2:B:3:GLN:HG3	2.03	0.40
1:A:187:GLU:HG2	1:A:211:ARG:HH21	1.87	0.40
1:A:85:ILE:HG12	1:A:103:LYS:CG	2.38	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%)	13	35
2	B	211/213 (99%)	185 (88%)	17 (8%)	9 (4%)	3	8
3	C	9/11 (82%)	8 (89%)	1 (11%)	0	100	100
All	All	432/438 (99%)	386 (89%)	34 (8%)	12 (3%)	6	16

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%)	142 (74%)	51 (26%)	0 1
2	B	180/180 (100%)	145 (81%)	35 (19%)	1 4
3	C	7/7 (100%)	7 (100%)	0	100 100
All	All	380/380 (100%)	294 (77%)	86 (23%)	1 2

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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	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	103	LYS
1	A	106	LEU
1	A	126	THR
1	A	147	LYS
1	A	149	LYS
1	A	162	SER
1	A	164	THR

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Mol	Chain	Res	Type
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	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	13	ARG
2	B	17	SER
2	B	23	LYS
2	B	45	LEU
2	B	56	SER
2	B	67	LYS
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	151	LEU

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Mol	Chain	Res	Type
2	B	157	SER
2	B	158	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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	38	GLN
1	A	190	ASN
1	A	198	HIS
2	B	1	GLN
2	B	5	GLN
2	B	39	GLN
2	B	104	GLN
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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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.