Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 05:35 PM EDT

PDB ID	:	1CFT
Title	:	ANTI-P24 (HIV-1) FAB FRAGMENT CB41 COMPLEXED WITH AN EPITOPE-UNRELATED D-PEPTIDE
Authors	:	Keitel, T.; Kramer, A.; Wessner, H.; Scholz, C.; Schneider-Mergener, J.; Hoehne, W.
Deposited on	:	1999-03-19
Resolution	:	2.80 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 (i) 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 (i)) were used in the production of this report:

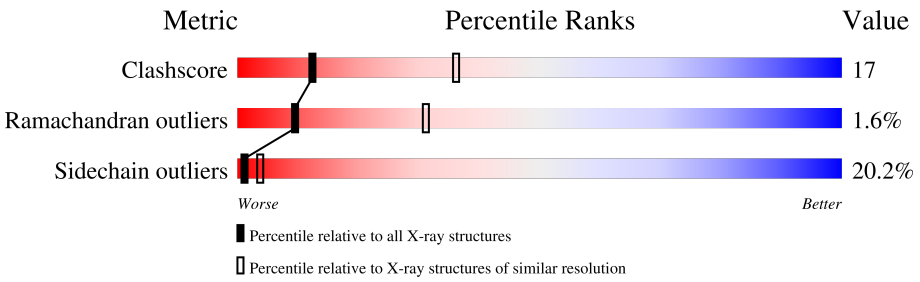
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.80 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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	214	56% 32% 8% •
2	B	213	54% 35% 10%
3	C	5	40% 60%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3314 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
			Total	C	N	O	S			
1	A	214	1678	1052	276	340	10	0	0	0

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	5	37	25	6	6	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	B	3	3	3	0	0
4	C	1	1	1	0	0

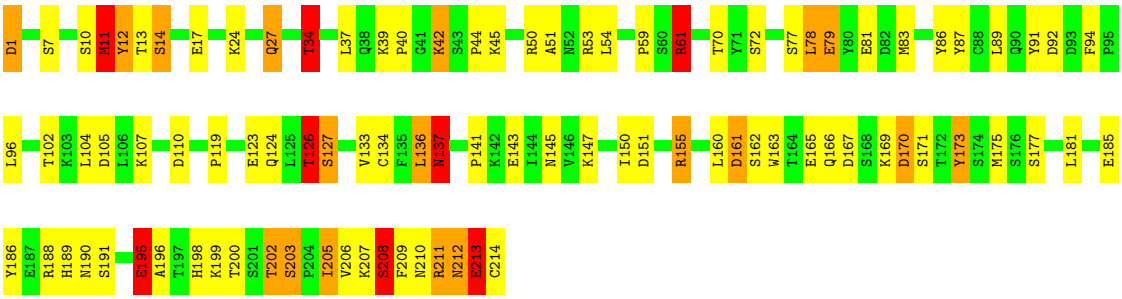
3 Residue-property plots (i)

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. 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.

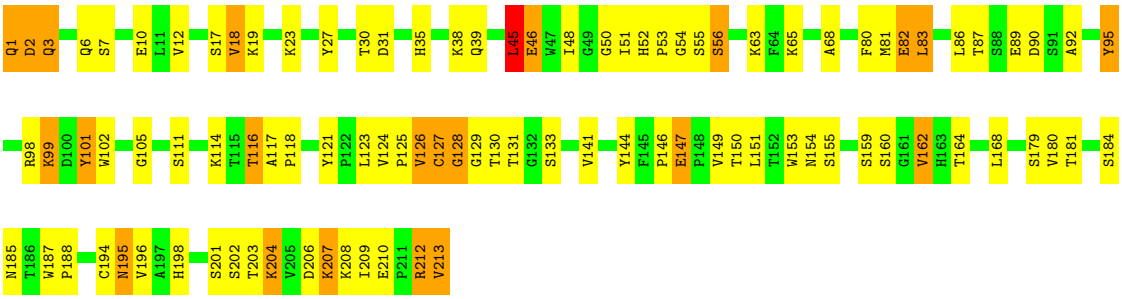
• Molecule 1: PROTEIN (IGG2A KAPPA ANTIBODY CB41 (LIGHT CHAIN))

Chain A: 56% 32% 8% •



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

Chain B: 54% 35% 10%



• Molecule 3: PROTEIN (ANTIGEN BOUND PEPTIDE)

Chain C: 40% 60%

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	106.06Å 106.06Å 294.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	65.00 – 2.80	Depositor
% Data completeness (in resolution range)	97.0 (65.00-2.80)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CCP4	Depositor
R, R_{free}	0.237 , 0.328	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3314	wwPDB-VP
Average B, all atoms (Å^2)	57.0	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	0.64	0/1715	1.70	26/2321 (1.1%)
2	B	0.73	1/1635 (0.1%)	1.59	20/2233 (0.9%)
3	C	3.80	6/37 (16.2%)	8.13	26/47 (55.3%)
All	All	0.79	7/3387 (0.2%)	1.83	72/4601 (1.6%)

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	5
2	B	0	6
3	C	0	3
All	All	0	14

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	4	PRO	N-CA	11.85	1.67	1.47
2	B	213	VAL	C-OXT	11.34	1.44	1.23
3	C	3	GLY	N-CA	7.58	1.57	1.46
3	C	1	LEU	C-O	7.23	1.37	1.23
3	C	2	LYS	C-O	7.04	1.36	1.23
3	C	2	LYS	N-CA	6.64	1.59	1.46
3	C	4	PRO	C-O	6.49	1.36	1.23

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	4	PRO	CB-CA-C	18.25	157.63	112.00
3	C	2	LYS	CA-C-N	16.03	148.25	116.20
3	C	4	PRO	CA-N-CD	-14.93	90.60	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	61	ARG	NE-CZ-NH2	14.74	127.67	120.30
3	C	2	LYS	CB-CA-C	14.64	139.67	110.40
3	C	4	PRO	N-CA-CB	-14.15	86.32	103.30
3	C	4	PRO	N-CA-C	-13.01	78.27	112.10
1	A	61	ARG	NE-CZ-NH1	-12.92	113.84	120.30
3	C	3	GLY	CA-C-O	12.88	143.78	120.60
3	C	1	LEU	CA-C-O	-12.26	94.36	120.10
3	C	5	LEU	CB-CG-CD1	12.14	131.65	111.00
3	C	4	PRO	CA-C-N	-11.57	91.74	117.20
3	C	2	LYS	CA-C-O	-10.96	97.08	120.10
1	A	53	ARG	NE-CZ-NH2	10.81	125.71	120.30
1	A	211	ARG	NE-CZ-NH2	-10.48	115.06	120.30
1	A	137	ASN	CB-CA-C	10.17	130.73	110.40
3	C	3	GLY	N-CA-C	-9.86	88.46	113.10
3	C	5	LEU	N-CA-C	-9.70	84.82	111.00
2	B	147	GLU	CA-C-O	-9.67	99.79	120.10
3	C	4	PRO	CA-C-O	9.51	143.02	120.20
3	C	4	PRO	O-C-N	-9.50	107.49	122.70
1	A	170	ASP	CB-CG-OD1	8.91	126.32	118.30
3	C	4	PRO	CA-CB-CG	-8.89	87.10	104.00
2	B	212	ARG	CD-NE-CZ	8.73	135.83	123.60
2	B	89	GLU	OE1-CD-OE2	8.52	133.53	123.30
1	A	161	ASP	CB-CG-OD2	8.44	125.89	118.30
1	A	211	ARG	NE-CZ-NH1	8.32	124.46	120.30
3	C	1	LEU	CA-C-N	8.15	135.13	117.20
2	B	3	GLN	CA-CB-CG	7.73	130.41	113.40
2	B	3	GLN	N-CA-CB	-7.54	97.02	110.60
2	B	212	ARG	NE-CZ-NH1	-7.32	116.64	120.30
1	A	211	ARG	N-CA-CB	7.20	123.55	110.60
3	C	1	LEU	N-CA-CB	7.00	124.39	110.40
1	A	11	MET	CA-CB-CG	6.99	125.17	113.30
3	C	3	GLY	C-N-CD	6.92	142.93	128.40
2	B	179	SER	N-CA-CB	-6.88	100.17	110.50
3	C	5	LEU	CB-CG-CD2	-6.49	99.97	111.00
2	B	147	GLU	O-C-N	6.40	133.26	121.10
2	B	38	LYS	CA-CB-CG	6.38	127.43	113.40
3	C	3	GLY	CA-C-N	-6.26	99.56	117.10
2	B	213	VAL	CA-CB-CG1	6.24	120.26	110.90
1	A	212	ASN	C-N-CA	6.16	137.09	121.70
3	C	5	LEU	CA-C-O	-6.14	107.21	120.10
1	A	208	SER	CB-CA-C	-6.10	98.51	110.10
2	B	46	GLU	CA-CB-CG	6.04	126.70	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1	LEU	CA-CB-CG	6.01	129.12	115.30
1	A	53	ARG	NE-CZ-NH1	-5.95	117.33	120.30
3	C	4	PRO	C-N-CA	5.94	136.54	121.70
2	B	31	ASP	CB-CG-OD1	5.93	123.64	118.30
1	A	155	ARG	NE-CZ-NH2	-5.93	117.34	120.30
1	A	34	THR	CA-CB-CG2	5.87	120.61	112.40
2	B	63	LYS	CA-CB-CG	5.69	125.93	113.40
2	B	45	LEU	CA-CB-CG	5.61	128.21	115.30
1	A	127	SER	N-CA-CB	5.59	118.89	110.50
3	C	1	LEU	C-N-CA	-5.48	108.00	121.70
1	A	213	GLU	OE1-CD-OE2	-5.45	116.76	123.30
2	B	90	ASP	CB-CG-OD2	5.44	123.20	118.30
2	B	128	GLY	N-CA-C	-5.43	99.53	113.10
2	B	89	GLU	CA-CB-CG	-5.42	101.47	113.40
1	A	102	THR	CA-CB-OG1	5.42	120.38	109.00
1	A	195	GLU	CA-CB-CG	5.41	125.29	113.40
1	A	12	TYR	CB-CA-C	5.33	121.06	110.40
2	B	126	VAL	CA-CB-CG2	5.31	118.86	110.90
1	A	1	ASP	CB-CG-OD1	5.27	123.04	118.30
1	A	173	TYR	CA-CB-CG	5.25	123.38	113.40
1	A	167	ASP	CB-CG-OD1	-5.22	113.60	118.30
1	A	136	LEU	C-N-CA	-5.22	108.64	121.70
1	A	126	THR	CA-CB-CG2	5.17	119.64	112.40
2	B	65	LYS	C-N-CA	5.16	133.13	122.30
1	A	213	GLU	CB-CG-CD	5.13	128.06	114.20
2	B	141	VAL	CA-CB-CG1	5.10	118.56	110.90
3	C	2	LYS	O-C-N	-5.02	114.66	123.20

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	150	ILE	Mainchain
1	A	208	SER	Mainchain
1	A	27	GLN	Mainchain
1	A	34	THR	Mainchain
1	A	87	TYR	Mainchain
2	B	101	TYR	Mainchain
2	B	128	GLY	Mainchain
2	B	162	VAL	Mainchain
2	B	164	THR	Mainchain
2	B	181	THR	Mainchain

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Mol	Chain	Res	Type	Group
2	B	95	TYR	Mainchain
3	C	1	LEU	Mainchain,Peptide
3	C	4	PRO	Mainchain

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	1678	0	1625	54	0
2	B	1595	0	1576	59	0
3	C	37	0	47	7	0
4	B	3	0	0	0	0
4	C	1	0	0	0	0
All	All	3314	0	3248	111	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 17.

All (111) 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:210:ASN:HD22	1:A:214:CYS:HA	1.37	0.88
1:A:196:ALA:HB3	1:A:205:ILE:HG23	1.54	0.88
3:C:3:GLY:O	3:C:4:PRO:HB2	1.74	0.88
2:B:162:VAL:HG22	2:B:180:VAL:HG12	1.55	0.87
2:B:155:SER:H	2:B:195:ASN:ND2	1.77	0.82
1:A:190:ASN:HD21	1:A:212:ASN:H	1.30	0.79
1:A:119:PRO:HD3	2:B:126:VAL:HG12	1.67	0.77
2:B:48:ILE:HG21	2:B:81:MET:HE2	1.66	0.74
1:A:210:ASN:HB2	1:A:214:CYS:HA	1.70	0.74
3:C:4:PRO:HD3	3:C:5:LEU:OXT	1.88	0.73
3:C:3:GLY:O	3:C:4:PRO:CB	2.34	0.73
2:B:155:SER:H	2:B:195:ASN:HD21	1.36	0.71
1:A:210:ASN:ND2	1:A:214:CYS:HA	2.05	0.70
2:B:12:VAL:HG21	2:B:86:LEU:HD13	1.75	0.69
2:B:30:THR:HG23	2:B:54:GLY:HA2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:GLN:HE22	2:B:95:TYR:HA	1.59	0.68
1:A:137:ASN:C	1:A:137:ASN:HD22	1.98	0.66
2:B:124:VAL:HG22	2:B:209:ILE:HG22	1.77	0.66
1:A:61:ARG:NH1	1:A:79:GLU:HB2	2.10	0.66
2:B:12:VAL:HG11	2:B:18:VAL:HG23	1.77	0.66
1:A:161:ASP:O	2:B:168:LEU:HD11	1.96	0.65
2:B:48:ILE:HG21	2:B:81:MET:CE	2.26	0.64
1:A:190:ASN:ND2	1:A:212:ASN:H	1.94	0.64
2:B:124:VAL:HG22	2:B:209:ILE:CG2	2.31	0.61
1:A:133:VAL:HG21	2:B:123:LEU:HD21	1.83	0.61
2:B:151:LEU:HD23	2:B:196:VAL:HG22	1.81	0.61
1:A:186:TYR:CE2	1:A:211:ARG:HD2	2.36	0.61
2:B:1:GLN:N	2:B:27:TYR:HB3	2.15	0.61
2:B:208:LYS:NZ	2:B:210:GLU:HG2	2.16	0.60
1:A:83:MET:HE1	1:A:104:LEU:HB3	1.83	0.60
1:A:94:PHE:CE2	3:C:5:LEU:HB3	2.37	0.59
1:A:59:PRO:HG2	1:A:61:ARG:HH21	1.68	0.59
1:A:209:PHE:HA	1:A:214:CYS:SG	2.44	0.57
1:A:210:ASN:HB2	1:A:214:CYS:CA	2.35	0.57
2:B:98:ARG:O	2:B:99:LYS:HB2	2.03	0.57
1:A:195:GLU:HB3	1:A:206:VAL:HG12	1.88	0.56
2:B:124:VAL:CG1	2:B:125:PRO:HD2	2.35	0.56
2:B:124:VAL:HG21	2:B:210:GLU:O	2.05	0.56
1:A:136:LEU:HD21	1:A:196:ALA:HB2	1.87	0.56
1:A:79:GLU:HB3	1:A:81:GLU:OE1	2.05	0.56
1:A:124:GLN:HG3	2:B:121:TYR:CE2	2.41	0.56
2:B:208:LYS:HZ1	2:B:210:GLU:HG2	1.72	0.55
1:A:78:LEU:HD11	1:A:83:MET:HE3	1.89	0.54
2:B:1:GLN:HA	2:B:101:TYR:OH	2.06	0.54
1:A:39:LYS:O	1:A:42:LYS:HB2	2.07	0.54
1:A:105:ASP:OD2	1:A:173:TYR:OH	2.23	0.54
1:A:81:GLU:H	1:A:81:GLU:CD	2.11	0.53
3:C:4:PRO:O	3:C:5:LEU:HD23	2.08	0.53
1:A:170:ASP:O	1:A:171:SER:HB2	2.08	0.53
1:A:210:ASN:HB2	1:A:214:CYS:N	2.24	0.53
2:B:198:HIS:HD2	2:B:201:SER:OG	1.92	0.53
1:A:24:LYS:HD2	1:A:70:THR:HG23	1.91	0.52
2:B:212:ARG:O	2:B:213:VAL:HB	2.09	0.52
1:A:11:MET:HG3	1:A:13:THR:HG23	1.90	0.52
2:B:124:VAL:HG13	2:B:125:PRO:HD2	1.92	0.52
2:B:114:LYS:O	2:B:116:THR:HG22	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:GLN:HB2	2:B:45:LEU:HD12	1.93	0.51
2:B:130:THR:HG22	2:B:131:THR:H	1.76	0.51
2:B:153:TRP:O	2:B:154:ASN:HB2	2.10	0.51
2:B:39:GLN:O	2:B:92:ALA:HB1	2.11	0.51
1:A:190:ASN:O	1:A:210:ASN:HA	2.11	0.50
2:B:35:HIS:ND1	2:B:50:GLY:HA3	2.27	0.50
2:B:55:SER:O	2:B:56:SER:CB	2.59	0.49
3:C:4:PRO:O	3:C:5:LEU:HB2	2.12	0.49
2:B:55:SER:O	2:B:56:SER:HB2	2.12	0.49
1:A:210:ASN:HB2	1:A:214:CYS:H	1.78	0.49
1:A:210:ASN:CB	1:A:214:CYS:HA	2.38	0.49
2:B:151:LEU:CD2	2:B:196:VAL:HG22	2.43	0.49
1:A:155:ARG:NH2	1:A:185:GLU:OE2	2.45	0.49
2:B:204:LYS:HE3	2:B:206:ASP:OD2	2.12	0.49
1:A:78:LEU:HD11	1:A:83:MET:CE	2.43	0.48
2:B:118:PRO:HB3	2:B:144:TYR:HB3	1.95	0.48
2:B:1:GLN:H3	2:B:27:TYR:HB3	1.78	0.48
1:A:186:TYR:CZ	1:A:211:ARG:HD2	2.49	0.47
1:A:151:ASP:OD2	1:A:189:HIS:HB3	2.15	0.47
1:A:37:LEU:HD21	1:A:39:LYS:HD2	1.96	0.47
1:A:91:TYR:HA	1:A:96:LEU:HD22	1.96	0.47
2:B:187:TRP:CG	2:B:188:PRO:HA	2.50	0.46
2:B:162:VAL:HG22	2:B:180:VAL:CG1	2.38	0.46
2:B:6:GLN:NE2	2:B:105:GLY:H	2.12	0.46
2:B:51:ILE:O	2:B:53:PRO:HD3	2.16	0.46
1:A:110:ASP:OD1	1:A:141:PRO:HD3	2.16	0.46
1:A:83:MET:CE	1:A:104:LEU:HB3	2.46	0.45
1:A:119:PRO:CD	2:B:126:VAL:HG12	2.41	0.45
1:A:105:ASP:HB3	1:A:166:GLN:OE1	2.17	0.45
1:A:126:THR:HG22	1:A:126:THR:O	2.17	0.45
1:A:202:THR:OG1	1:A:203:SER:N	2.44	0.45
2:B:98:ARG:O	2:B:99:LYS:CB	2.65	0.45
1:A:198:HIS:HD2	1:A:200:THR:OG1	2.00	0.44
2:B:117:ALA:CB	2:B:203:THR:HG21	2.47	0.44
1:A:50:ARG:O	1:A:51:ALA:HB3	2.18	0.44
1:A:96:LEU:HD11	2:B:35:HIS:CD2	2.53	0.44
1:A:213:GLU:O	1:A:214:CYS:OXT	2.35	0.43
2:B:68:ALA:HA	2:B:82:GLU:O	2.17	0.43
2:B:126:VAL:HG23	2:B:127:CYS:O	2.18	0.43
2:B:204:LYS:HB3	2:B:204:LYS:HE2	1.88	0.43
2:B:213:VAL:O	2:B:213:VAL:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:30:THR:HG23	2:B:54:GLY:CA	2.46	0.43
1:A:185:GLU:HA	1:A:188:ARG:HD3	2.02	0.42
1:A:44:PRO:HG2	2:B:102:TRP:CD2	2.54	0.42
2:B:83:LEU:HB3	2:B:86:LEU:HD21	2.00	0.42
2:B:18:VAL:HB	2:B:86:LEU:HD11	2.02	0.42
2:B:195:ASN:OD1	2:B:206:ASP:OD1	2.37	0.42
2:B:146:PRO:O	2:B:198:HIS:HE1	2.02	0.41
1:A:175:MET:HE3	1:A:175:MET:HB2	1.92	0.41
2:B:52:HIS:HB3	2:B:55:SER:OG	2.21	0.41
2:B:130:THR:HG22	2:B:131:THR:N	2.35	0.41
1:A:92:ASP:O	3:C:2:LYS:HE2	2.21	0.40
1:A:14:SER:O	1:A:17:GLU:HB3	2.21	0.40
2:B:207:LYS:HD3	2:B:207:LYS:HA	1.88	0.40
1:A:37:LEU:HD13	1:A:86:TYR:CE1	2.56	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%)	197 (93%)	12 (6%)	3 (1%)	11	34
2	B	211/213 (99%)	195 (92%)	13 (6%)	3 (1%)	11	34
3	C	3/5 (60%)	0	2 (67%)	1 (33%)	0	0
All	All	426/432 (99%)	392 (92%)	27 (6%)	7 (2%)	9	31

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	213	GLU
3	C	4	PRO
2	B	99	LYS

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Mol	Chain	Res	Type
1	A	126	THR
2	B	2	ASP
2	B	129	GLY
1	A	202	THR

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	193/193 (100%)	152 (79%)	41 (21%)	1 3
2	B	180/180 (100%)	148 (82%)	32 (18%)	2 5
3	C	4/4 (100%)	1 (25%)	3 (75%)	0 0
All	All	377/377 (100%)	301 (80%)	76 (20%)	1 4

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ASP
1	A	7	SER
1	A	10	SER
1	A	11	MET
1	A	12	TYR
1	A	14	SER
1	A	27	GLN
1	A	34	THR
1	A	40	PRO
1	A	42	LYS
1	A	45	LYS
1	A	54	LEU
1	A	61	ARG
1	A	72	SER
1	A	77	SER
1	A	78	LEU
1	A	79	GLU
1	A	89	LEU

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Mol	Chain	Res	Type
1	A	107	LYS
1	A	123	GLU
1	A	127	SER
1	A	134	CYS
1	A	137	ASN
1	A	143	GLU
1	A	145	ASN
1	A	147	LYS
1	A	160	LEU
1	A	162	SER
1	A	163	TRP
1	A	165	GLU
1	A	169	LYS
1	A	177	SER
1	A	181	LEU
1	A	191	SER
1	A	195	GLU
1	A	199	LYS
1	A	203	SER
1	A	205	ILE
1	A	207	LYS
1	A	208	SER
1	A	213	GLU
2	B	1	GLN
2	B	2	ASP
2	B	3	GLN
2	B	7	SER
2	B	10	GLU
2	B	17	SER
2	B	18	VAL
2	B	19	LYS
2	B	23	LYS
2	B	45	LEU
2	B	46	GLU
2	B	56	SER
2	B	80	PHE
2	B	82	GLU
2	B	83	LEU
2	B	87	THR
2	B	111	SER
2	B	116	THR
2	B	127	CYS

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Mol	Chain	Res	Type
2	B	133	SER
2	B	147	GLU
2	B	149	VAL
2	B	150	THR
2	B	159	SER
2	B	160	SER
2	B	184	SER
2	B	185	ASN
2	B	194	CYS
2	B	195	ASN
2	B	202	SER
2	B	204	LYS
2	B	207	LYS
3	C	1	LEU
3	C	4	PRO
3	C	5	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	38	GLN
1	A	137	ASN
1	A	190	ASN
1	A	198	HIS
1	A	210	ASN
2	B	3	GLN
2	B	5	GLN
2	B	6	GLN
2	B	39	GLN
2	B	62	GLN
2	B	195	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 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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.