Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:46 PM GMT

PDB ID	:	1CFN
Title	:	ANTI-P24 (HIV-1) FAB FRAGMENT CB41 COMPLEXED WITH AN EPITOPE-RELATED PEPTIDE
Authors	:	Keitel, T.; Kramer, A.; Wessner, H.; Scholz, C.; Schneider-Mergener, J.; Hoehne, W.
Deposited on	:	1999-03-19
Resolution	:	2.65 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:

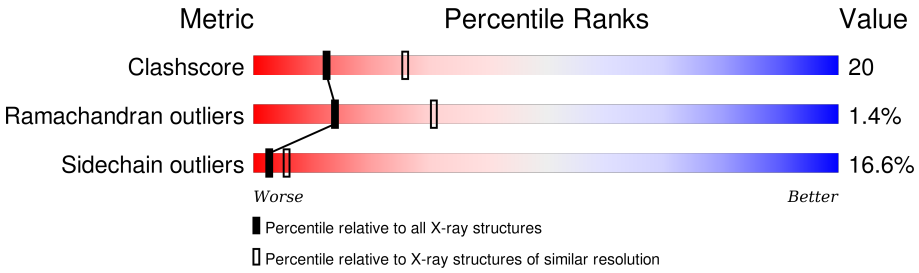
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.65 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	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)

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 <=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	57% 33% 6% •
2	B	213	60% 31% 8% •
3	C	10	40% 40% 20%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NLE	C	10	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3369 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 (BOUND PEPTIDE).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	0	0	0
			71	43	12	16			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total	O	0	0
			10	10		
4	B	13	Total	O	0	0
			13	13		
4	C	2	Total	O	0	0
			2	2		

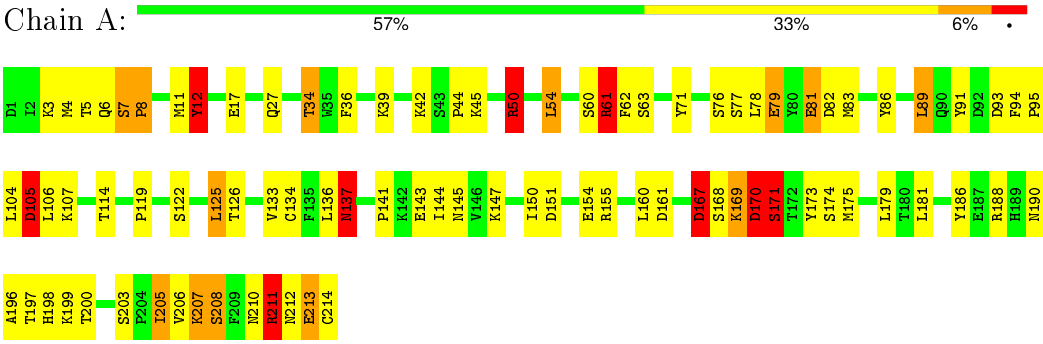
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

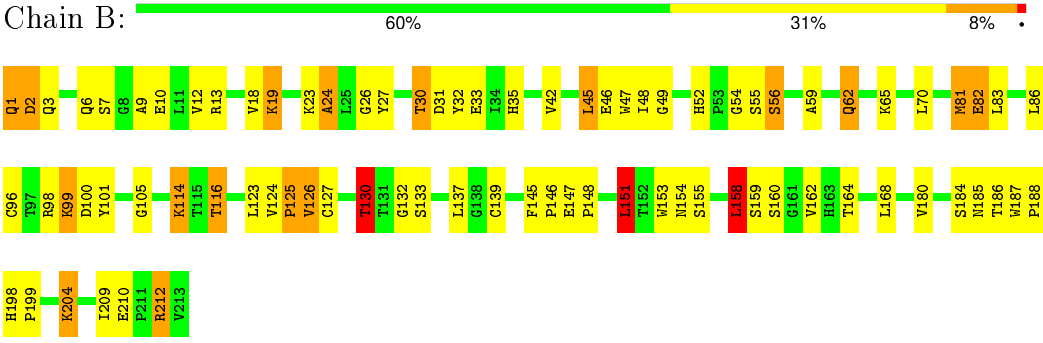
- Molecule 1: PROTEIN (IGG2A KAPPA ANTIBODY CB41 (LIGHT CHAIN))

Chain A:



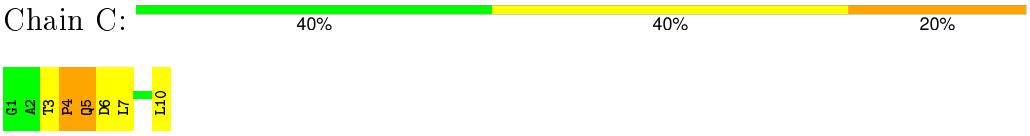
- Molecule 2: PROTEIN (IGG2A-KAPPA ANTIBODY CB41 (HEAVY CHAIN))

Chain B:



- Molecule 3: PROTEIN (BOUND PEPTIDE)

Chain C:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	105.44Å 105.44Å 295.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	90.00 – 2.65	Depositor
% Data completeness (in resolution range)	98.0 (90.00-2.65)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CCP4	Depositor
R, R_{free}	0.277 , 0.325	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3369	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NLE

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	0.88	3/1715 (0.2%)	1.59	24/2321 (1.0%)
2	B	0.67	1/1635 (0.1%)	1.47	17/2233 (0.8%)
3	C	0.96	0/63	1.77	1/86 (1.2%)
All	All	0.79	4/3413 (0.1%)	1.54	42/4640 (0.9%)

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	6
2	B	0	4
All	All	0	10

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	61	ARG	C-N	22.10	1.84	1.34
1	A	171	SER	N-CA	9.93	1.66	1.46
1	A	79	GLU	C-N	6.75	1.49	1.34
2	B	30	THR	CB-OG1	5.54	1.54	1.43

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	11	MET	CA-CB-CG	13.16	135.67	113.30
1	A	105	ASP	CB-CG-OD1	11.76	128.88	118.30
1	A	61	ARG	CA-C-N	-11.03	92.94	117.20
1	A	168	SER	N-CA-CB	8.91	123.87	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	31	ASP	CB-CG-OD2	-8.61	110.56	118.30
1	A	170	ASP	CB-CG-OD2	8.52	125.97	118.30
1	A	167	ASP	C-N-CA	8.21	142.21	121.70
1	A	34	THR	CA-CB-CG2	7.93	123.50	112.40
1	A	50	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	A	171	SER	N-CA-CB	7.69	122.04	110.50
2	B	10	GLU	OE1-CD-OE2	7.64	132.47	123.30
2	B	147	GLU	OE1-CD-OE2	7.59	132.41	123.30
1	A	50	ARG	NE-CZ-NH1	7.58	124.09	120.30
2	B	13	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	A	211	ARG	NE-CZ-NH2	-7.39	116.60	120.30
1	A	105	ASP	CA-CB-CG	7.29	129.43	113.40
2	B	212	ARG	NE-CZ-NH2	7.14	123.87	120.30
2	B	151	LEU	CA-CB-CG	6.42	130.07	115.30
2	B	158	LEU	CA-CB-CG	6.19	129.53	115.30
2	B	81	MET	CG-SD-CE	-6.06	90.50	100.20
1	A	79	GLU	O-C-N	5.97	132.25	122.70
2	B	100	ASP	CB-CG-OD2	-5.83	113.06	118.30
1	A	54	LEU	CA-CB-CG	5.75	128.53	115.30
1	A	71	TYR	CB-CG-CD1	-5.74	117.56	121.00
1	A	168	SER	N-CA-C	-5.69	95.63	111.00
1	A	211	ARG	N-CA-CB	5.69	120.84	110.60
1	A	89	LEU	CA-CB-CG	5.56	128.09	115.30
1	A	102	THR	CA-CB-CG2	-5.55	104.62	112.40
2	B	126	VAL	CA-CB-CG1	5.55	119.23	110.90
2	B	125	PRO	O-C-N	-5.55	113.82	122.70
2	B	9	ALA	CB-CA-C	-5.47	101.90	110.10
1	A	151	ASP	CB-CG-OD1	5.42	123.17	118.30
1	A	61	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	A	61	ARG	NE-CZ-NH2	5.29	122.95	120.30
2	B	100	ASP	CB-CG-OD1	5.27	123.04	118.30
2	B	147	GLU	N-CA-C	-5.26	96.79	111.00
2	B	126	VAL	CA-CB-CG2	5.22	118.72	110.90
3	C	6	ASP	O-C-N	5.18	130.99	122.70
1	A	137	ASN	OD1-CG-ND2	5.18	133.81	121.90
2	B	3	GLN	N-CA-C	5.13	124.85	111.00
2	B	45	LEU	CA-CB-CG	5.12	127.08	115.30
1	A	79	GLU	CA-C-N	-5.07	106.05	117.20

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	12	TYR	Mainchain
1	A	125	LEU	Mainchain
1	A	167	ASP	Peptide
1	A	170	ASP	Peptide
1	A	188	ARG	Mainchain
1	A	8	PRO	Mainchain
2	B	164	THR	Mainchain
2	B	204	LYS	Mainchain
2	B	24	ALA	Mainchain
2	B	89	GLU	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	1624	64	0
2	B	1595	0	1576	66	0
3	C	71	0	70	14	0
4	A	10	0	0	0	0
4	B	13	0	0	0	0
4	C	2	0	0	0	0
All	All	3369	0	3270	129	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 20.

All (129) 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:61:ARG:C	1:A:62:PHE:N	1.84	1.28
2:B:124:VAL:CG1	2:B:125:PRO:HD2	1.84	1.06
3:C:3:THR:O	3:C:5:GLN:N	1.94	1.00
2:B:162:VAL:HG22	2:B:180:VAL:HG12	1.40	0.99
1:A:79:GLU:HB3	1:A:81:GLU:OE1	1.65	0.96
1:A:210:ASN:HB2	1:A:214:CYS:HA	1.45	0.96
2:B:124:VAL:HG12	2:B:125:PRO:HD2	1.49	0.93
1:A:79:GLU:CB	1:A:81:GLU:OE1	2.17	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:VAL:HG13	2:B:125:PRO:HD2	1.53	0.90
2:B:30:THR:HG23	2:B:54:GLY:HA2	1.52	0.89
2:B:59:ALA:HB3	3:C:10:NLE:HE2	1.61	0.82
1:A:79:GLU:HB3	1:A:81:GLU:CD	1.99	0.81
1:A:61:ARG:NH1	1:A:82:ASP:OD2	2.15	0.79
1:A:61:ARG:CA	1:A:62:PHE:N	2.46	0.78
2:B:30:THR:HG23	2:B:54:GLY:CA	2.16	0.74
2:B:155:SER:H	2:B:195:ASN:HD21	1.32	0.74
1:A:190:ASN:HD21	1:A:212:ASN:H	1.35	0.74
2:B:12:VAL:HG21	2:B:86:LEU:HD13	1.69	0.74
2:B:155:SER:H	2:B:195:ASN:ND2	1.86	0.73
1:A:210:ASN:HB2	1:A:214:CYS:CA	2.18	0.73
2:B:124:VAL:HG12	2:B:125:PRO:CD	2.17	0.73
1:A:79:GLU:HB3	1:A:81:GLU:OE2	1.89	0.72
2:B:19:LYS:HD2	2:B:82:GLU:HG3	1.71	0.72
3:C:5:GLN:C	3:C:7:LEU:H	1.92	0.72
2:B:1:GLN:HA	2:B:101:TYR:OH	1.91	0.71
2:B:2:ASP:HB2	2:B:26:GLY:HA3	1.71	0.71
2:B:35:HIS:HD2	2:B:47:TRP:HE1	1.38	0.71
1:A:119:PRO:HD3	2:B:126:VAL:HG12	1.73	0.70
1:A:61:ARG:HH12	1:A:79:GLU:HB2	1.56	0.70
2:B:59:ALA:CB	3:C:10:NLE:HE2	2.22	0.69
1:A:196:ALA:HB3	1:A:205:ILE:HG23	1.74	0.68
1:A:210:ASN:CB	1:A:214:CYS:HA	2.23	0.68
2:B:6:GLN:HE22	2:B:95:TYR:HA	1.58	0.67
1:A:119:PRO:HB2	2:B:212:ARG:NH1	2.10	0.66
2:B:1:GLN:N	2:B:27:TYR:HB3	2.11	0.66
1:A:81:GLU:CD	1:A:81:GLU:H	1.97	0.66
1:A:79:GLU:HB2	1:A:81:GLU:OE1	1.95	0.66
3:C:7:LEU:HG	3:C:7:LEU:O	1.97	0.65
2:B:124:VAL:CG1	2:B:125:PRO:CD	2.69	0.65
1:A:119:PRO:HB2	2:B:212:ARG:HH12	1.62	0.65
1:A:137:ASN:C	1:A:137:ASN:HD22	1.98	0.65
1:A:210:ASN:HD22	1:A:214:CYS:HA	1.62	0.65
2:B:12:VAL:HG11	2:B:18:VAL:CG1	2.30	0.62
2:B:30:THR:HG22	2:B:30:THR:O	2.01	0.61
2:B:55:SER:O	2:B:56:SER:HB2	2.00	0.61
1:A:3:LYS:HD2	1:A:4:MET:N	2.19	0.58
1:A:94:PHE:CZ	3:C:10:NLE:HD3	2.39	0.58
2:B:35:HIS:CD2	2:B:47:TRP:HE1	2.22	0.57
1:A:167:ASP:O	1:A:171:SER:N	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:GLN:H3	2:B:27:TYR:HB3	1.69	0.57
1:A:186:TYR:CZ	1:A:211:ARG:HD2	2.41	0.56
1:A:50:ARG:HG3	1:A:50:ARG:O	2.06	0.56
3:C:3:THR:OG1	3:C:5:GLN:HB2	2.06	0.55
2:B:124:VAL:HB	2:B:212:ARG:HE	1.71	0.55
1:A:79:GLU:O	1:A:82:ASP:HB2	2.05	0.55
2:B:52:HIS:HB2	3:C:10:NLE:HB2	1.88	0.55
1:A:91:TYR:O	3:C:7:LEU:HD23	2.07	0.55
1:A:150:ILE:HD11	1:A:179:LEU:HD21	1.89	0.54
2:B:124:VAL:HG22	2:B:209:ILE:HG23	1.90	0.53
2:B:114:LYS:O	2:B:116:THR:HG22	2.07	0.53
2:B:35:HIS:HD2	2:B:47:TRP:NE1	2.06	0.53
1:A:210:ASN:ND2	1:A:214:CYS:HA	2.25	0.52
2:B:30:THR:CG2	2:B:30:THR:O	2.58	0.52
3:C:3:THR:HB	3:C:4:PRO:HD2	1.92	0.51
1:A:190:ASN:ND2	1:A:212:ASN:H	2.04	0.51
1:A:211:ARG:C	1:A:213:GLU:H	2.13	0.51
2:B:137:LEU:HG	2:B:209:ILE:HG21	1.92	0.51
1:A:122:SER:O	1:A:126:THR:HG23	2.11	0.51
1:A:210:ASN:HB2	1:A:214:CYS:N	2.26	0.50
1:A:206:VAL:O	1:A:207:LYS:HD2	2.12	0.50
2:B:125:PRO:HG3	2:B:187:TRP:CZ3	2.48	0.49
2:B:98:ARG:O	2:B:99:LYS:HB2	2.12	0.49
2:B:187:TRP:CG	2:B:188:PRO:HA	2.48	0.49
2:B:48:ILE:HG21	2:B:81:MET:CE	2.42	0.48
1:A:83:MET:HE1	1:A:106:LEU:HD21	1.94	0.48
2:B:12:VAL:HG21	2:B:86:LEU:CD1	2.41	0.48
1:A:137:ASN:HB2	1:A:174:SER:OG	2.13	0.48
1:A:195:GLU:HG2	1:A:206:VAL:HG22	1.95	0.48
1:A:141:PRO:O	1:A:198:HIS:HE1	1.97	0.48
2:B:59:ALA:HB3	3:C:10:NLE:CE	2.37	0.48
1:A:94:PHE:HZ	3:C:10:NLE:HD3	1.76	0.48
1:A:3:LYS:NZ	1:A:5:THR:OG1	2.45	0.47
2:B:151:LEU:HD23	2:B:196:VAL:HG22	1.95	0.47
1:A:61:ARG:HG2	1:A:76:SER:OG	2.15	0.47
1:A:161:ASP:O	2:B:168:LEU:HD11	2.14	0.47
1:A:61:ARG:N	1:A:62:PHE:N	2.63	0.47
2:B:30:THR:CG2	2:B:54:GLY:HA2	2.35	0.46
1:A:169:LYS:HG2	1:A:169:LYS:H	1.51	0.46
1:A:91:TYR:HA	1:A:96:LEU:HD22	1.98	0.46
1:A:93:ASP:OD1	1:A:94:PHE:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:55:SER:O	2:B:56:SER:CB	2.64	0.45
1:A:136:LEU:HD12	1:A:136:LEU:N	2.32	0.45
2:B:126:VAL:HG23	2:B:127:CYS:O	2.16	0.45
2:B:62:GLN:NE2	2:B:65:LYS:HE3	2.32	0.45
1:A:12:TYR:HD2	1:A:105:ASP:OD1	2.00	0.45
1:A:61:ARG:HB2	1:A:61:ARG:HE	1.36	0.45
1:A:125:LEU:HD23	1:A:125:LEU:HA	1.82	0.45
1:A:133:VAL:HG21	2:B:123:LEU:HD21	1.98	0.44
2:B:6:GLN:NE2	2:B:105:GLY:H	2.15	0.44
2:B:48:ILE:HG21	2:B:81:MET:HE2	1.98	0.44
1:A:95:PRO:HA	2:B:47:TRP:CZ3	2.53	0.44
1:A:7:SER:HA	1:A:8:PRO:C	2.37	0.44
2:B:145:PHE:HA	2:B:146:PRO:HA	1.73	0.44
1:A:193:THR:OG1	1:A:208:SER:HB3	2.17	0.43
2:B:33:GLU:OE2	3:C:10:NLE:HB3	2.18	0.43
2:B:24:ALA:HB1	2:B:27:TYR:CE1	2.54	0.43
2:B:153:TRP:O	2:B:154:ASN:HB2	2.18	0.43
2:B:6:GLN:NE2	2:B:96:CYS:H	2.16	0.42
1:A:61:ARG:HD2	1:A:77:SER:O	2.18	0.42
1:A:61:ARG:NH1	1:A:79:GLU:HB2	2.28	0.42
2:B:123:LEU:HD12	2:B:123:LEU:N	2.35	0.42
1:A:36:PHE:CD2	1:A:44:PRO:HB3	2.54	0.42
2:B:32:TYR:CZ	3:C:4:PRO:HD3	2.54	0.42
2:B:198:HIS:HA	2:B:199:PRO:HD2	1.83	0.42
2:B:47:TRP:CZ2	2:B:49:GLY:HA2	2.55	0.42
1:A:190:ASN:O	1:A:210:ASN:HA	2.20	0.41
1:A:105:ASP:OD2	1:A:173:TYR:OH	2.32	0.41
2:B:70:LEU:HD21	2:B:81:MET:HE3	2.03	0.41
2:B:162:VAL:HG22	2:B:180:VAL:CG1	2.29	0.41
2:B:1:GLN:H2	2:B:27:TYR:HB3	1.84	0.41
1:A:198:HIS:HD2	1:A:200:THR:OG1	2.04	0.41
2:B:139:CYS:HB2	2:B:153:TRP:CH2	2.56	0.41
1:A:79:GLU:O	1:A:82:ASP:CB	2.69	0.40
2:B:124:VAL:HG21	2:B:210:GLU:O	2.21	0.40
1:A:144:ILE:HG13	1:A:197:THR:O	2.21	0.40
2:B:154:ASN:ND2	2:B:158:LEU:HD22	2.36	0.40
1:A:12:TYR:CD1	1:A:12:TYR:N	2.90	0.40
2:B:130:THR:HG23	2:B:132:GLY:H	1.86	0.40
1:A:6:GLN:NE2	1:A:86:TYR:O	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	202 (95%)	10 (5%)	0	100 100
2	B	211/213 (99%)	194 (92%)	12 (6%)	5 (2%)	7 16
3	C	8/10 (80%)	6 (75%)	1 (12%)	1 (12%)	0 0
All	All	431/437 (99%)	402 (93%)	23 (5%)	6 (1%)	14 31

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	2	ASP
2	B	99	LYS
2	B	130	THR
3	C	4	PRO
2	B	186	THR
2	B	42	VAL

5.3.2 Protein sidechains

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%)	153 (79%)	40 (21%)	1 3
2	B	180/180 (100%)	158 (88%)	22 (12%)	6 12
3	C	7/7 (100%)	6 (86%)	1 (14%)	4 8
All	All	380/380 (100%)	317 (83%)	63 (17%)	3 6

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	12	TYR
1	A	17	GLU
1	A	27	GLN
1	A	34	THR
1	A	39	LYS
1	A	42	LYS
1	A	45	LYS
1	A	50	ARG
1	A	54	LEU
1	A	60	SER
1	A	61	ARG
1	A	63	SER
1	A	78	LEU
1	A	81	GLU
1	A	89	LEU
1	A	104	LEU
1	A	105	ASP
1	A	107	LYS
1	A	114	THR
1	A	134	CYS
1	A	137	ASN
1	A	143	GLU
1	A	145	ASN
1	A	147	LYS
1	A	154	GLU
1	A	155	ARG
1	A	160	LEU
1	A	169	LYS
1	A	170	ASP
1	A	171	SER
1	A	175	MET
1	A	181	LEU
1	A	199	LYS
1	A	203	SER
1	A	205	ILE
1	A	207	LYS
1	A	208	SER
1	A	211	ARG
1	A	213	GLU
2	B	1	GLN
2	B	7	SER

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Mol	Chain	Res	Type
2	B	19	LYS
2	B	23	LYS
2	B	45	LEU
2	B	46	GLU
2	B	56	SER
2	B	62	GLN
2	B	82	GLU
2	B	83	LEU
2	B	114	LYS
2	B	116	THR
2	B	130	THR
2	B	133	SER
2	B	148	PRO
2	B	151	LEU
2	B	158	LEU
2	B	159	SER
2	B	160	SER
2	B	184	SER
2	B	185	ASN
2	B	204	LYS
3	C	5	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) 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
2	B	5	GLN
2	B	6	GLN
2	B	35	HIS
2	B	39	GLN
2	B	195	ASN
2	B	198	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NLE	C	10	3	6,7,8	1.62	1 (16%)	5,7,9	1.49	1 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NLE	C	10	3	-	0/4/6/8	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	10	NLE	CB-CA	3.70	1.57	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	10	NLE	CG-CB-CA	2.34	123.98	114.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	10	NLE	7	0

5.5 Carbohydrates

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.