



# Full wwPDB X-ray Structure Validation Report ⓘ

May 5, 2021 – 02:09 pm BST

PDB ID : 6RLO  
Title : Crystal structure of AT1412dm Fab fragment in complex with CD9 large extracellular loop  
Authors : Neviani, V.; Pearce, N.M.; Pos, W.; Schotte, R.; Spits, H.; Gros, P.  
Deposited on : 2019-05-02  
Resolution : 2.20 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](mailto: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.

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

MolProbity : 4.02b-467  
Xtrriage (Phenix) : 1.13  
EDS : 2.18  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.18

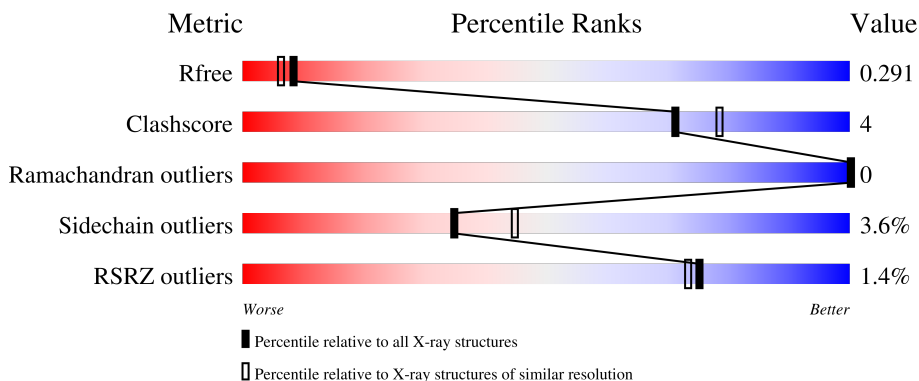
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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.



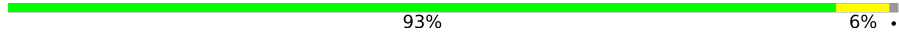
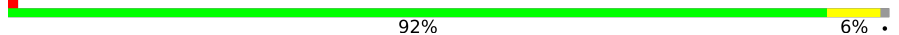


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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  $\geq 3$ , 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	223	 87% 7% • 5%
1	C	223	 87% 7% • 5%
1	E	223	 84% 10% • 5%
1	G	223	 87% 8% • 5%
2	B	220	 90% 9%

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Mol	Chain	Length	Quality of chain
2	D	220	 93% 6%
2	F	220	 92% 6%
2	H	220	 93% 6%
3	I	90	 68% 17% 4% 14%
3	J	90	 69% 17% 4% 13%
3	K	90	 69% 17% 6% 14%
3	L	90	 69% 14% 4% 13%

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 15875 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 AT1412dm Fab Fragment (Heavy Chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	211	Total 1598	C 1023	N 265	O 305	S 5	0	0	0
1	C	211	Total 1598	C 1023	N 265	O 305	S 5	0	0	0
1	E	211	Total 1595	C 1020	N 264	O 306	S 5	0	0	0
1	G	212	Total 1604	C 1026	N 266	O 307	S 5	0	0	0

- Molecule 2 is a protein called AT1412dm Fab Fragment (Light Chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	219	Total 1699	C 1062	N 284	O 348	S 5	0	0	0
2	D	218	Total 1690	C 1057	N 283	O 345	S 5	0	0	0
2	F	217	Total 1686	C 1055	N 282	O 344	S 5	0	0	0
2	H	218	Total 1690	C 1057	N 283	O 345	S 5	0	0	0

- Molecule 3 is a protein called CD9 antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	I	77	Total 617	C 393	N 98	O 122	S 4	0	0	0
3	J	78	Total 625	C 397	N 100	O 124	S 4	0	0	0
3	K	77	Total 617	C 393	N 98	O 122	S 4	0	0	0
3	L	78	Total 625	C 397	N 100	O 124	S 4	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	111	MET	-	initiating methionine	UNP P21926
I	112	GLY	-	expression tag	UNP P21926
I	113	SER	-	expression tag	UNP P21926
I	192	ALA	-	expression tag	UNP P21926
I	193	ALA	-	expression tag	UNP P21926
I	194	ALA	-	expression tag	UNP P21926
I	195	HIS	-	expression tag	UNP P21926
I	196	HIS	-	expression tag	UNP P21926
I	197	HIS	-	expression tag	UNP P21926
I	198	HIS	-	expression tag	UNP P21926
I	199	HIS	-	expression tag	UNP P21926
I	200	HIS	-	expression tag	UNP P21926
J	111	MET	-	initiating methionine	UNP P21926
J	112	GLY	-	expression tag	UNP P21926
J	113	SER	-	expression tag	UNP P21926
J	192	ALA	-	expression tag	UNP P21926
J	193	ALA	-	expression tag	UNP P21926
J	194	ALA	-	expression tag	UNP P21926
J	195	HIS	-	expression tag	UNP P21926
J	196	HIS	-	expression tag	UNP P21926
J	197	HIS	-	expression tag	UNP P21926
J	198	HIS	-	expression tag	UNP P21926
J	199	HIS	-	expression tag	UNP P21926
J	200	HIS	-	expression tag	UNP P21926
K	111	MET	-	initiating methionine	UNP P21926
K	112	GLY	-	expression tag	UNP P21926
K	113	SER	-	expression tag	UNP P21926
K	192	ALA	-	expression tag	UNP P21926
K	193	ALA	-	expression tag	UNP P21926
K	194	ALA	-	expression tag	UNP P21926
K	195	HIS	-	expression tag	UNP P21926
K	196	HIS	-	expression tag	UNP P21926
K	197	HIS	-	expression tag	UNP P21926
K	198	HIS	-	expression tag	UNP P21926
K	199	HIS	-	expression tag	UNP P21926
K	200	HIS	-	expression tag	UNP P21926
L	111	MET	-	initiating methionine	UNP P21926
L	112	GLY	-	expression tag	UNP P21926
L	113	SER	-	expression tag	UNP P21926
L	192	ALA	-	expression tag	UNP P21926
L	193	ALA	-	expression tag	UNP P21926
L	194	ALA	-	expression tag	UNP P21926

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Chain	Residue	Modelled	Actual	Comment	Reference
L	195	HIS	-	expression tag	UNP P21926
L	196	HIS	-	expression tag	UNP P21926
L	197	HIS	-	expression tag	UNP P21926
L	198	HIS	-	expression tag	UNP P21926
L	199	HIS	-	expression tag	UNP P21926
L	200	HIS	-	expression tag	UNP P21926

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Cl 2 2	0	0
4	B	1	Total Cl 1 1	0	0
4	I	1	Total Cl 1 1	0	0
4	C	2	Total Cl 2 2	0	0
4	D	2	Total Cl 2 2	0	0
4	F	1	Total Cl 1 1	0	0
4	G	1	Total Cl 1 1	0	0
4	H	1	Total Cl 1 1	0	0

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total K 1 1	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Na 1 1	0	0
6	C	2	Total Na 2 2	0	0
6	D	3	Total Na 3 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Na	0	0
			1	1		


- Molecule 7 is water.

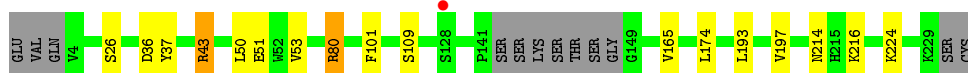
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	17	Total	O	0	0
			17	17		
7	B	44	Total	O	0	0
			44	44		
7	I	4	Total	O	0	0
			4	4		
7	C	13	Total	O	0	0
			13	13		
7	D	37	Total	O	0	0
			37	37		
7	J	6	Total	O	0	0
			6	6		
7	E	12	Total	O	0	0
			12	12		
7	F	34	Total	O	0	0
			34	34		
7	K	4	Total	O	0	0
			4	4		
7	G	17	Total	O	0	0
			17	17		
7	H	22	Total	O	0	0
			22	22		
7	L	2	Total	O	0	0
			2	2		

### 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 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: AT1412dm Fab Fragment (Heavy Chain)

Chain A: 




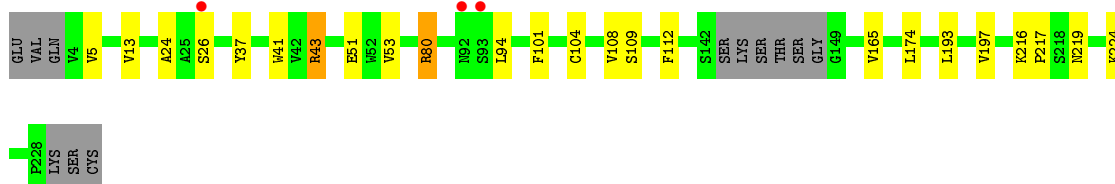
- Molecule 1: AT1412dm Fab Fragment (Heavy Chain)

Chain C: 




- Molecule 1: AT1412dm Fab Fragment (Heavy Chain)

Chain E: 




- Molecule 1: AT1412dm Fab Fragment (Heavy Chain)

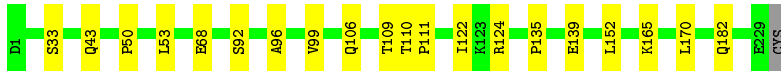
Chain G: 



- Molecule 2: AT1412dm Fab Fragment (Light Chain)

Chain B: 

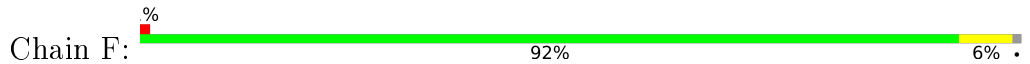




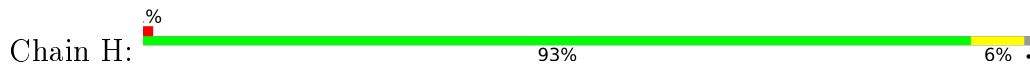
- Molecule 2: AT1412dm Fab Fragment (Light Chain)



- Molecule 2: AT1412dm Fab Fragment (Light Chain)



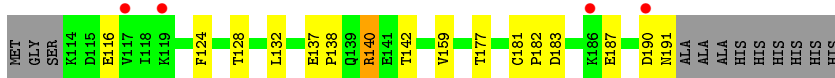
- Molecule 2: AT1412dm Fab Fragment (Light Chain)



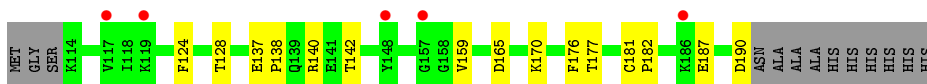
- Molecule 3: CD9 antigen



- Molecule 3: CD9 antigen



- Molecule 3: CD9 antigen



- Molecule 3: CD9 antigen

Chain L:  4% 69% 14% 13%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.78Å 89.86Å 91.53Å 71.12° 89.59° 85.96°	Depositor
Resolution (Å)	84.80 – 2.20 84.80 – 2.20	Depositor EDS
% Data completeness (in resolution range)	92.6 (84.80-2.20) 92.6 (84.80-2.20)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 2.20Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.254 , 0.287 0.259 , 0.291	Depositor DCC
$R_{free}$ test set	5338 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.7	Xtrriage
Anisotropy	0.651	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 28.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.000 for -h,l,k	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	15875	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.81% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, CL, NA

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	0.63	0/1641	0.78	0/2237
1	C	0.64	0/1641	0.78	0/2237
1	E	0.64	0/1638	0.78	0/2234
1	G	0.64	0/1647	0.79	0/2245
2	B	0.65	0/1736	0.79	0/2359
2	D	0.65	0/1727	0.79	0/2347
2	F	0.64	0/1723	0.79	0/2342
2	H	0.64	0/1727	0.78	0/2347
3	I	0.66	0/627	0.74	0/843
3	J	0.67	0/635	0.74	0/854
3	K	0.66	0/627	0.74	0/843
3	L	0.66	0/635	0.75	0/854
All	All	0.65	0/16004	0.78	0/21742

There are no bond length outliers.

There are no bond angle outliers.

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	1598	0	1555	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1598	0	1555	10	0
1	E	1595	0	1547	18	0
1	G	1604	0	1560	15	0
2	B	1699	0	1640	13	0
2	D	1690	0	1635	7	0
2	F	1686	0	1632	5	0
2	H	1690	0	1635	5	0
3	I	617	0	612	7	0
3	J	625	0	618	6	0
3	K	617	0	612	6	0
3	L	625	0	618	9	0
4	A	2	0	0	1	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	1	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	1	0
5	B	1	0	0	0	0
6	B	1	0	0	0	0
6	C	2	0	0	0	0
6	D	3	0	0	0	0
6	F	1	0	0	0	0
7	A	17	0	0	0	0
7	B	44	0	0	2	0
7	C	13	0	0	0	0
7	D	37	0	0	0	0
7	E	12	0	0	0	0
7	F	34	0	0	0	0
7	G	17	0	0	1	0
7	H	22	0	0	0	0
7	I	4	0	0	0	0
7	J	6	0	0	1	0
7	K	4	0	0	0	0
7	L	2	0	0	0	0
All	All	15875	0	15219	108	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 4.

All (108) 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)
2:B:109:THR:HG21	7:B:438:HOH:O	1.74	0.87
1:A:43:ARG:HG2	1:A:53:VAL:CG2	2.17	0.73
1:G:43:ARG:HG2	1:G:53:VAL:CG2	2.17	0.73
1:C:43:ARG:HG2	1:C:53:VAL:CG2	2.18	0.73
1:E:43:ARG:HG2	1:E:53:VAL:CG2	2.18	0.73
1:G:5:VAL:HG22	1:G:24:ALA:HB3	1.72	0.71
1:E:5:VAL:HG22	1:E:24:ALA:HB3	1.75	0.69
3:I:124:PHE:O	3:I:128:THR:HG23	1.95	0.67
3:J:124:PHE:O	3:J:128:THR:HG23	1.96	0.66
3:L:124:PHE:O	3:L:128:THR:HG23	1.96	0.65
3:K:124:PHE:O	3:K:128:THR:HG23	1.97	0.65
3:K:170:LYS:HG3	3:K:176:PHE:CZ	2.33	0.64
1:A:165:VAL:HG23	1:A:193:LEU:HD21	1.84	0.58
1:E:165:VAL:HG23	1:E:193:LEU:HD21	1.85	0.57
1:G:165:VAL:HG23	1:G:193:LEU:HD21	1.86	0.57
1:G:36:ASP:OD1	3:L:169:LYS:HE2	2.07	0.55
2:F:110:THR:HA	2:F:111:PRO:C	2.28	0.54
3:I:183:ASP:O	3:I:187:GLU:HG2	2.08	0.54
3:J:183:ASP:O	3:J:187:GLU:HG2	2.08	0.54
1:C:37:TYR:O	1:C:80:ARG:NH2	2.37	0.53
2:H:110:THR:HA	2:H:111:PRO:C	2.27	0.53
1:G:37:TYR:O	1:G:80:ARG:NH2	2.37	0.52
2:B:110:THR:HA	2:B:111:PRO:C	2.30	0.52
2:F:99:VAL:HG21	2:F:182:GLN:HB3	1.92	0.52
1:E:108:VAL:HG23	1:E:112:PHE:H	1.75	0.52
1:E:37:TYR:O	1:E:80:ARG:NH2	2.37	0.51
2:H:99:VAL:HG21	2:H:182:GLN:HB3	1.92	0.51
1:A:37:TYR:O	1:A:80:ARG:NH2	2.37	0.51
2:B:43:GLN:HB2	2:B:53:LEU:HD11	1.93	0.51
2:B:124:ARG:HB2	7:B:426:HOH:O	2.09	0.51
2:D:110:THR:HA	2:D:111:PRO:C	2.31	0.51
2:B:165:LYS:HE3	2:B:170:LEU:HD11	1.92	0.51
2:D:43:GLN:HB2	2:D:53:LEU:HD11	1.92	0.51
3:I:174:GLU:HG2	4:I:301:CL:CL	2.48	0.50
2:B:99:VAL:HG21	2:B:182:GLN:HB3	1.92	0.50
2:H:43:GLN:HB2	2:H:53:LEU:HD11	1.95	0.49
2:F:119:ARG:CZ	2:F:119:ARG:HB2	2.40	0.49
1:A:36:ASP:OD1	3:I:169:LYS:HE2	2.13	0.48
2:D:99:VAL:HG21	2:D:182:GLN:HB3	1.94	0.48
3:I:137:GLU:N	3:I:138:PRO:CD	2.76	0.48
3:L:137:GLU:N	3:L:138:PRO:CD	2.76	0.48
1:E:174:LEU:HD21	1:E:197:VAL:HG21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:LEU:HD21	1:A:197:VAL:HG21	1.95	0.48
2:B:92:SER:HB2	3:L:135:LYS:HG3	1.96	0.48
2:F:43:GLN:HB2	2:F:53:LEU:HD11	1.95	0.48
3:K:137:GLU:N	3:K:138:PRO:CD	2.76	0.48
1:C:174:LEU:HD21	1:C:197:VAL:HG21	1.95	0.47
2:D:22:ASN:ND2	4:D:302:CL:CL	2.76	0.47
1:G:174:LEU:HD21	1:G:197:VAL:HG21	1.96	0.47
3:J:137:GLU:N	3:J:138:PRO:CD	2.77	0.47
1:E:108:VAL:HG22	1:E:112:PHE:HB3	1.97	0.47
2:D:170:LEU:H	2:D:170:LEU:HD22	1.81	0.46
1:G:41:TRP:CH2	1:G:104:CYS:SG	3.09	0.46
1:G:43:ARG:HG2	1:G:53:VAL:HG21	1.95	0.46
1:E:41:TRP:CH2	1:E:104:CYS:SG	3.09	0.46
7:G:414:HOH:O	3:L:159:VAL:HG13	2.16	0.45
2:B:170:LEU:HD22	2:B:170:LEU:H	1.82	0.45
1:C:41:TRP:CH2	1:C:104:CYS:SG	3.10	0.45
2:B:165:LYS:HE3	2:B:170:LEU:CD1	2.47	0.44
1:G:37:TYR:OH	3:L:165:ASP:HB3	2.16	0.44
1:E:108:VAL:HG23	1:E:112:PHE:N	2.32	0.44
1:A:43:ARG:HG2	1:A:53:VAL:HG21	1.97	0.44
1:E:43:ARG:HA	1:E:101:PHE:O	2.18	0.44
1:C:43:ARG:HA	1:C:101:PHE:O	2.18	0.44
1:A:43:ARG:HA	1:A:101:PHE:O	2.18	0.43
1:E:43:ARG:HD2	1:E:51:GLU:OE1	2.18	0.43
1:G:43:ARG:HD2	1:G:51:GLU:OE1	2.18	0.43
1:A:43:ARG:HD2	1:A:51:GLU:OE1	2.18	0.43
1:A:50:LEU:HD11	2:B:50:PRO:HG3	2.01	0.43
3:J:140:ARG:HB3	7:J:304:HOH:O	2.18	0.43
2:F:96:ALA:HA	2:F:122:ILE:HD12	2.00	0.43
1:E:13:VAL:HG11	1:E:94:LEU:HD13	2.01	0.42
1:G:43:ARG:HA	1:G:101:PHE:O	2.19	0.42
1:C:43:ARG:HG2	1:C:53:VAL:HG22	1.99	0.42
3:L:190:ASP:O	3:L:191:ASN:HB3	2.18	0.42
3:I:181:CYS:N	3:I:182:PRO:CD	2.82	0.42
3:J:181:CYS:N	3:J:182:PRO:CD	2.83	0.42
1:E:193:LEU:HD12	1:E:193:LEU:C	2.40	0.42
2:H:96:ALA:HA	2:H:122:ILE:HD12	2.01	0.42
2:D:96:ALA:HA	2:D:122:ILE:HD12	2.01	0.42
1:E:165:VAL:CG2	1:E:193:LEU:HD21	2.48	0.42
3:K:181:CYS:N	3:K:182:PRO:CD	2.83	0.42
3:L:181:CYS:N	3:L:182:PRO:CD	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:96:ALA:HA	2:B:122:ILE:HD12	2.01	0.41
1:C:157:VAL:HG11	1:C:165:VAL:HG11	2.02	0.41
2:H:170:LEU:H	2:H:170:LEU:HD22	1.84	0.41
1:A:165:VAL:CG2	1:A:193:LEU:HD21	2.49	0.41
1:A:193:LEU:HD12	1:A:193:LEU:C	2.40	0.41
1:C:43:ARG:HD2	1:C:51:GLU:OE1	2.19	0.41
1:E:108:VAL:HG23	1:E:108:VAL:O	2.21	0.41
2:B:152:LEU:N	2:B:152:LEU:HD12	2.35	0.41
1:G:183:ALA:HA	1:G:193:LEU:HB3	2.02	0.41
3:L:124:PHE:CZ	3:L:128:THR:HG21	2.55	0.41
1:A:43:ARG:HG2	1:A:53:VAL:HG22	2.00	0.41
1:E:216:LYS:HB2	1:E:217:PRO:HD3	2.03	0.41
1:G:193:LEU:C	1:G:193:LEU:HD12	2.40	0.41
1:A:214:ASN:ND2	1:A:216:LYS:HE2	2.36	0.41
1:C:214:ASN:ND2	1:C:216:LYS:HE3	2.36	0.41
3:K:124:PHE:CZ	3:K:128:THR:HG21	2.56	0.41
1:G:165:VAL:CG2	1:G:193:LEU:HD21	2.49	0.41
1:C:193:LEU:C	1:C:193:LEU:HD12	2.41	0.41
4:A:302:CL:CL	2:B:135:PRO:O	2.75	0.40
3:I:132:LEU:HD11	3:I:140:ARG:NH1	2.37	0.40
3:J:132:LEU:HD11	3:J:140:ARG:NH1	2.36	0.40
2:D:152:LEU:HD12	2:D:152:LEU:N	2.36	0.40
1:G:5:VAL:CG2	1:G:24:ALA:HB3	2.48	0.40
1:E:37:TYR:OH	3:K:165:ASP:HB3	2.20	0.40
1:E:43:ARG:HG2	1:E:53:VAL:HG21	1.97	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	207/223 (93%)	205 (99%)	2 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	207/223 (93%)	204 (99%)	3 (1%)	0	100	100
1	E	207/223 (93%)	205 (99%)	2 (1%)	0	100	100
1	G	208/223 (93%)	205 (99%)	3 (1%)	0	100	100
2	B	217/220 (99%)	209 (96%)	8 (4%)	0	100	100
2	D	216/220 (98%)	207 (96%)	9 (4%)	0	100	100
2	F	215/220 (98%)	207 (96%)	8 (4%)	0	100	100
2	H	216/220 (98%)	208 (96%)	8 (4%)	0	100	100
3	I	75/90 (83%)	73 (97%)	2 (3%)	0	100	100
3	J	76/90 (84%)	72 (95%)	4 (5%)	0	100	100
3	K	75/90 (83%)	73 (97%)	2 (3%)	0	100	100
3	L	76/90 (84%)	72 (95%)	4 (5%)	0	100	100
All	All	1995/2132 (94%)	1940 (97%)	55 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	175/186 (94%)	170 (97%)	5 (3%)	42	54
1	C	175/186 (94%)	171 (98%)	4 (2%)	50	63
1	E	175/186 (94%)	169 (97%)	6 (3%)	37	47
1	G	176/186 (95%)	171 (97%)	5 (3%)	43	56
2	B	195/196 (100%)	191 (98%)	4 (2%)	53	67
2	D	194/196 (99%)	191 (98%)	3 (2%)	65	78
2	F	194/196 (99%)	188 (97%)	6 (3%)	40	51
2	H	194/196 (99%)	189 (97%)	5 (3%)	46	58
3	I	70/79 (89%)	65 (93%)	5 (7%)	14	16
3	J	71/79 (90%)	64 (90%)	7 (10%)	8	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	K	70/79 (89%)	64 (91%)	6 (9%)	10	10
3	L	71/79 (90%)	64 (90%)	7 (10%)	8	7
All	All	1760/1844 (95%)	1697 (96%)	63 (4%)	35	45

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

Mol	Chain	Res	Type
1	A	26	SER
1	A	43	ARG
1	A	80	ARG
1	A	109	SER
1	A	224	LYS
2	B	33	SER
2	B	68	GLU
2	B	106	GLN
2	B	139	GLU
3	I	140	ARG
3	I	142	THR
3	I	161	GLN
3	I	177	THR
3	I	190	ASP
1	C	43	ARG
1	C	80	ARG
1	C	109	SER
1	C	219	ASN
2	D	33	SER
2	D	68	GLU
2	D	106	GLN
3	J	116	GLU
3	J	140	ARG
3	J	142	THR
3	J	159	VAL
3	J	177	THR
3	J	190	ASP
3	J	191	ASN
1	E	26	SER
1	E	43	ARG
1	E	80	ARG
1	E	109	SER
1	E	219	ASN
1	E	224	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	F	33	SER
2	F	106	GLN
2	F	119	ARG
2	F	139	GLU
2	F	158	ARG
2	F	170	LEU
3	K	140	ARG
3	K	142	THR
3	K	159	VAL
3	K	177	THR
3	K	187	GLU
3	K	190	ASP
1	G	26	SER
1	G	43	ARG
1	G	80	ARG
1	G	85	ASN
1	G	109	SER
2	H	33	SER
2	H	68	GLU
2	H	106	GLN
2	H	119	ARG
2	H	139	GLU
3	L	140	ARG
3	L	142	THR
3	L	159	VAL
3	L	177	THR
3	L	187	GLU
3	L	190	ASP
3	L	191	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	215	GLN
3	J	191	ASN
2	F	22	ASN
2	F	48	GLN
1	G	85	ASN
3	L	122	GLN

### 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](#)

Of 19 ligands modelled in this entry, 19 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	211/223 (94%)	0.21	1 (0%) 91 90	15, 30, 44, 54	0
1	C	211/223 (94%)	0.28	2 (0%) 84 83	17, 30, 44, 59	0
1	E	211/223 (94%)	0.43	3 (1%) 75 73	23, 36, 53, 63	0
1	G	212/223 (95%)	0.32	1 (0%) 91 90	21, 34, 49, 63	0
2	B	219/220 (99%)	0.09	0 100 100	18, 25, 42, 59	0
2	D	218/220 (99%)	0.15	0 100 100	17, 26, 41, 53	0
2	F	217/220 (98%)	0.23	3 (1%) 75 73	20, 30, 48, 64	0
2	H	218/220 (99%)	0.19	2 (0%) 84 83	20, 31, 45, 57	0
3	I	77/90 (85%)	0.50	4 (5%) 27 26	23, 34, 49, 54	0
3	J	78/90 (86%)	0.52	4 (5%) 28 26	22, 35, 56, 60	0
3	K	77/90 (85%)	0.54	5 (6%) 18 17	24, 35, 53, 64	0
3	L	78/90 (86%)	0.53	4 (5%) 28 26	23, 35, 55, 61	0
All	All	2027/2132 (95%)	0.28	29 (1%) 75 73	15, 31, 49, 64	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	93	SER	3.5
3	K	186	LYS	3.5
3	K	119	LYS	3.3
1	C	47	GLY	3.2
3	J	186	LYS	3.1
3	J	119	LYS	3.0
3	L	186	LYS	2.9
3	L	119	LYS	2.8
2	F	34	ASN	2.7
2	F	143	SER	2.7
3	J	117	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
3	I	186	LYS	2.5
3	K	157	GLY	2.4
3	L	117	VAL	2.4
3	K	148	TYR	2.4
3	K	117	VAL	2.4
1	E	92	ASN	2.4
1	G	26	SER	2.4
2	H	33	SER	2.3
1	C	46	PRO	2.2
1	E	26	SER	2.2
2	F	1	ASP	2.1
3	I	119	LYS	2.1
3	I	190	ASP	2.1
3	J	190	ASP	2.1
3	I	184	ALA	2.1
2	H	46	PRO	2.1
1	A	128	SER	2.1
3	L	115	ASP	2.0

## 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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	NA	D	304	1/1	0.82	0.12	39,39,39,39	0
6	NA	F	302	1/1	0.84	0.12	29,29,29,29	0
6	NA	D	305	1/1	0.90	0.19	33,33,33,33	0
6	NA	C	304	1/1	0.91	0.09	32,32,32,32	0
4	CL	A	302	1/1	0.93	0.06	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CL	I	301	1/1	0.93	0.08	42,42,42,42	0
6	NA	B	303	1/1	0.94	0.12	30,30,30,30	0
4	CL	H	301	1/1	0.95	0.21	44,44,44,44	0
4	CL	B	301	1/1	0.95	0.19	42,42,42,42	0
4	CL	C	302	1/1	0.95	0.23	43,43,43,43	0
4	CL	F	301	1/1	0.96	0.07	30,30,30,30	0
4	CL	G	301	1/1	0.97	0.08	32,32,32,32	0
6	NA	C	303	1/1	0.97	0.27	32,32,32,32	0
4	CL	D	302	1/1	0.98	0.09	42,42,42,42	0
6	NA	D	303	1/1	0.98	0.10	28,28,28,28	0
5	K	B	302	1/1	0.98	0.16	44,44,44,44	0
4	CL	C	301	1/1	0.98	0.12	34,34,34,34	0
4	CL	D	301	1/1	0.98	0.20	44,44,44,44	0
4	CL	A	301	1/1	0.99	0.12	27,27,27,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.