



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:22 PM UTC

PDB ID : 6RLO / pdb_00006rlo
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

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:

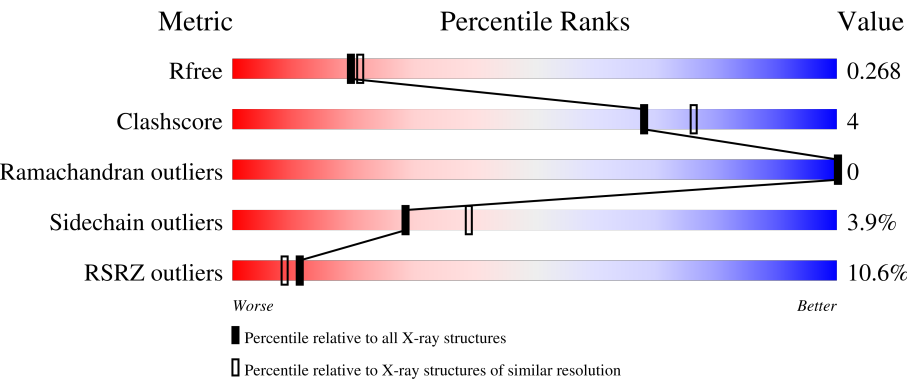
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 ≥ 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	6% 86% 9% 5%
1	C	223	6% 86% 8% 5%
1	E	223	18% 83% 11% 5%
1	G	223	13% 86% 9% 5%
2	B	220	4% 90% 9%

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Mol	Chain	Length	Quality of chain
2	D	220	5% 93% 6%
2	F	220	9% 92% 6%
2	H	220	9% 93% 6%
3	I	90	13% 68% 17% 14%
3	J	90	10% 68% 18% 13%
3	K	90	21% 69% 17% 14%
3	L	90	22% 68% 16% 13%

2 Entry composition

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
1	A	211	Total	C	N	O	S	0	0	0
			1598	1023	265	305	5			
1	C	211	Total	C	N	O	S	0	0	0
			1598	1023	265	305	5			
1	E	211	Total	C	N	O	S	0	0	0
			1595	1020	264	306	5			
1	G	212	Total	C	N	O	S	0	0	0
			1604	1026	266	307	5			

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

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

- Molecule 3 is a protein called CD9 antigen.

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

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 (CCD ID: 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 (CCD ID: K) (formula: K).

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

- Molecule 6 is SODIUM ION (CCD ID: 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 1	Na 1	0	0

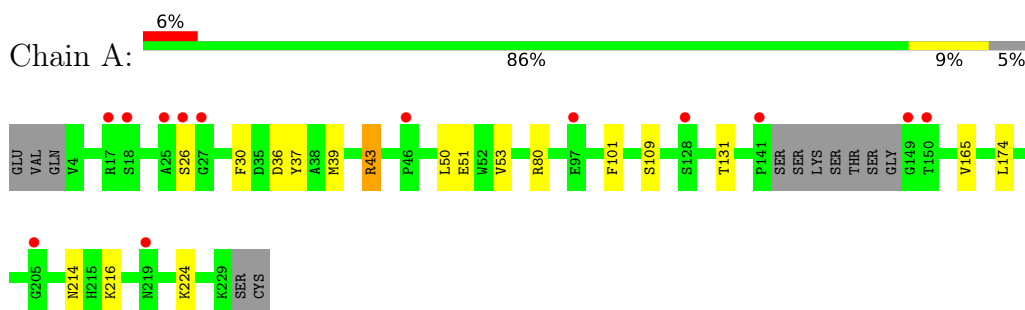
- Molecule 7 is water.

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

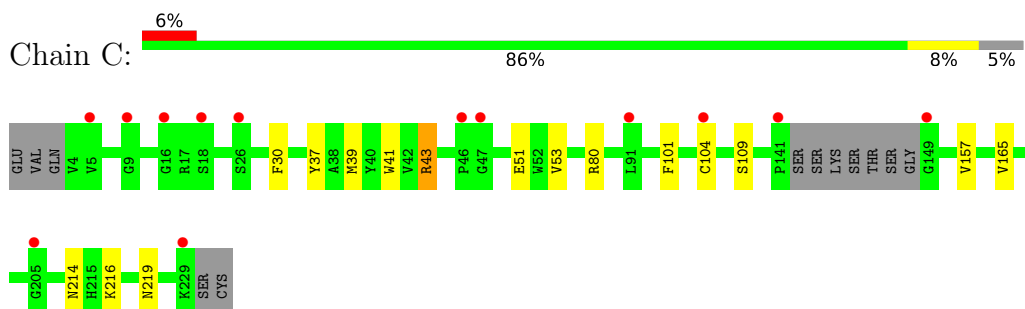
3 Residue-property plots [i](#)

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 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.

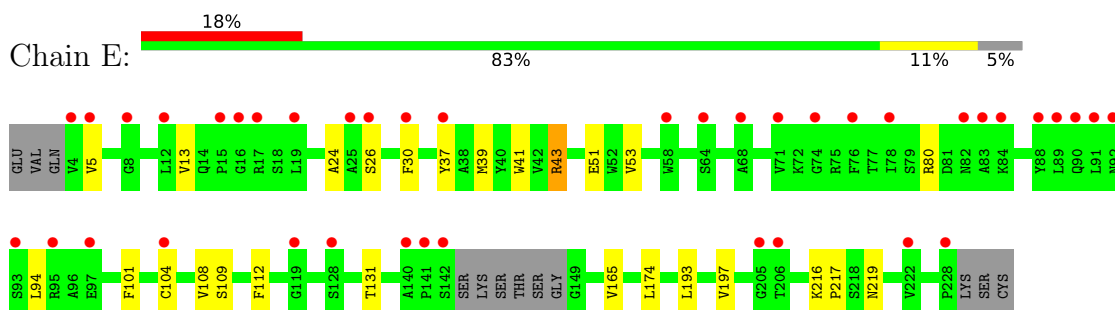
- Molecule 1: AT1412dm Fab Fragment (Heavy Chain)



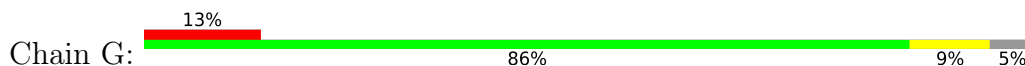
- Molecule 1: AT1412dm Fab Fragment (Heavy Chain)

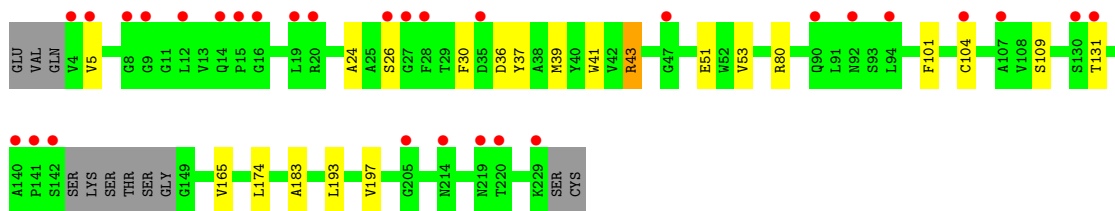


- Molecule 1: AT1412dm Fab Fragment (Heavy Chain)

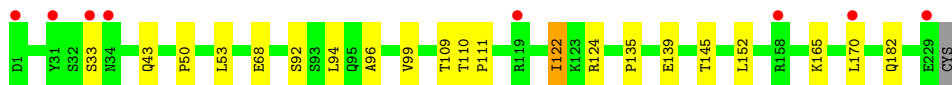
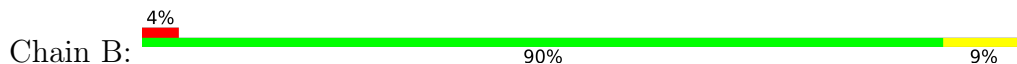


- Molecule 1: AT1412dm Fab Fragment (Heavy Chain)

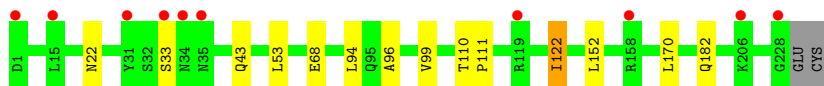




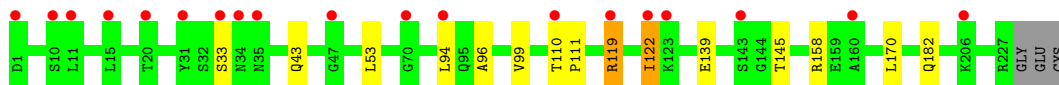
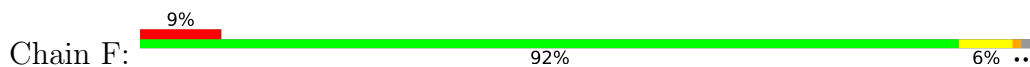
• Molecule 2: AT1412dm Fab Fragment (Light Chain)



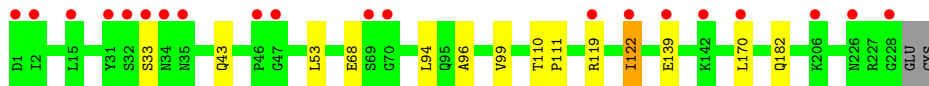
• Molecule 2: AT1412dm Fab Fragment (Light Chain)



• Molecule 2: AT1412dm Fab Fragment (Light Chain)



• Molecule 2: AT1412dm Fab Fragment (Light Chain)



• Molecule 3: CD9 antigen



• Molecule 3: CD9 antigen

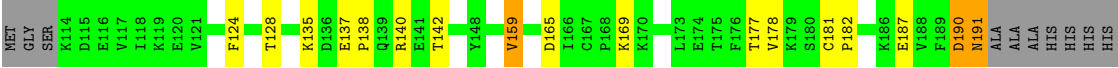




● Molecule 3: CD9 antigen



● Molecule 3: CD9 antigen



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.254 , 0.287 (Not available) , 0.268	Depositor DCC
R_{free} test set	5340 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	23.7	Xtriage
Anisotropy	0.651	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 23.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	15875	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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	0.96	0/1641	1.24	0/2237
1	C	0.98	0/1641	1.24	0/2237
1	E	0.97	0/1638	1.24	0/2234
1	G	0.98	0/1647	1.24	0/2245
2	B	0.98	0/1736	1.26	0/2359
2	D	0.98	0/1727	1.27	0/2347
2	F	0.98	0/1723	1.26	0/2342
2	H	0.98	0/1727	1.26	0/2347
3	I	1.00	0/627	1.51	0/843
3	J	1.00	0/635	1.50	0/854
3	K	1.01	0/627	1.50	0/843
3	L	1.02	0/635	1.51	0/854
All	All	0.98	0/16004	1.30	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 [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	1598	0	1555	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1598	0	1555	11	0
1	E	1595	0	1547	19	0
1	G	1604	0	1560	16	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	112	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 (112) 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
2:F:110:THR:HA	2:F:111:PRO:C	2.28	0.59
1:A:165:VAL:HG23	1:A:193:LEU:HD21	1.84	0.58
2:H:110:THR:HA	2:H:111:PRO:C	2.27	0.58
1:E:165:VAL:HG23	1:E:193:LEU:HD21	1.85	0.57
2:B:110:THR:HA	2:B:111:PRO:C	2.30	0.57
1:G:165:VAL:HG23	1:G:193:LEU:HD21	1.86	0.57
2:D:110:THR:HA	2:D:111:PRO:C	2.31	0.56
1:G:36:ASP:OD1	3:L:169:LYS:HE2	2.07	0.55
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
1:G:37:TYR:O	1:G:80:ARG:NH2	2.37	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: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
1:G:30:PHE:CE1	1:G:39:MET:HE3	2.47	0.50
2:H:43:GLN:HB2	2:H:53:LEU:HD11	1.95	0.49
1:A:30:PHE:CE1	1:A:39:MET:HE3	2.47	0.49
1:C:30:PHE:CE1	1:C:39:MET:HE3	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:30:PHE:CE1	1:E:39:MET:HE3	2.48	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
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
1:E:193:LEU:HD12	1:E:193:LEU:C	2.40	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:A:193:LEU:HD12	1:A:193:LEU:C	2.40	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
1:G:193:LEU:C	1:G:193:LEU:HD12	2.40	0.46
1:C:193:LEU:C	1:C:193:LEU:HD12	2.41	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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: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
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 ⓘ

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	207/223 (93%)	205 (99%)	2 (1%)	0	100	100
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 ⓘ

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%)	37	51
1	C	175/186 (94%)	172 (98%)	3 (2%)	53	69
1	E	175/186 (94%)	170 (97%)	5 (3%)	37	51
1	G	176/186 (95%)	172 (98%)	4 (2%)	44	59
2	B	195/196 (100%)	189 (97%)	6 (3%)	35	48
2	D	194/196 (99%)	190 (98%)	4 (2%)	47	63
2	F	194/196 (99%)	186 (96%)	8 (4%)	27	37
2	H	194/196 (99%)	188 (97%)	6 (3%)	35	48
3	I	70/79 (89%)	65 (93%)	5 (7%)	13	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	J	71/79 (90%)	63 (89%)	8 (11%)	5	5
3	K	70/79 (89%)	64 (91%)	6 (9%)	10	10
3	L	71/79 (90%)	63 (89%)	8 (11%)	5	5
All	All	1760/1844 (95%)	1692 (96%)	68 (4%)	28	39

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	SER
1	A	43	ARG
1	A	109	SER
1	A	131	THR
1	A	224	LYS
2	B	33	SER
2	B	68	GLU
2	B	94	LEU
2	B	122	ILE
2	B	139	GLU
2	B	145	THR
3	I	140	ARG
3	I	142	THR
3	I	161	GLN
3	I	177	THR
3	I	178	VAL
1	C	43	ARG
1	C	109	SER
1	C	219	ASN
2	D	33	SER
2	D	68	GLU
2	D	94	LEU
2	D	122	ILE
3	J	116	GLU
3	J	140	ARG
3	J	142	THR
3	J	159	VAL
3	J	177	THR
3	J	178	VAL
3	J	190	ASP
3	J	191	ASN
1	E	26	SER
1	E	43	ARG

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Mol	Chain	Res	Type
1	E	109	SER
1	E	131	THR
1	E	219	ASN
2	F	33	SER
2	F	94	LEU
2	F	119	ARG
2	F	122	ILE
2	F	139	GLU
2	F	145	THR
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	178	VAL
3	K	187	GLU
1	G	26	SER
1	G	43	ARG
1	G	109	SER
1	G	131	THR
2	H	33	SER
2	H	68	GLU
2	H	94	LEU
2	H	119	ARG
2	H	122	ILE
2	H	139	GLU
3	L	140	ARG
3	L	142	THR
3	L	159	VAL
3	L	177	THR
3	L	178	VAL
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 (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	GLN
1	A	179	HIS
1	A	214	ASN

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Mol	Chain	Res	Type
2	B	215	GLN
2	D	163	GLN
3	J	191	ASN
1	E	207	GLN
1	E	214	ASN
2	F	35	ASN
2	F	48	GLN
3	K	161	GLN
1	G	59	ASN
1	G	85	ASN
1	G	207	GLN
1	G	214	ASN
1	G	219	ASN
2	H	22	ASN
2	H	35	ASN
3	L	161	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 oligosaccharides 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

6.1 Protein, DNA and RNA chains

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, 95th 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 ²)	Q < 0.9
1	A	211/223 (94%)	0.83	14 (6%)	24 21	15, 30, 44, 54	0
1	C	211/223 (94%)	0.88	13 (6%)	26 23	17, 30, 44, 59	0
1	E	211/223 (94%)	1.37	40 (18%)	3 2	23, 36, 53, 63	0
1	G	212/223 (95%)	1.15	30 (14%)	6 4	21, 34, 49, 63	0
2	B	219/220 (99%)	0.57	8 (3%)	45 42	18, 25, 42, 59	0
2	D	218/220 (99%)	0.62	10 (4%)	37 34	17, 26, 41, 53	0
2	F	217/220 (98%)	0.85	19 (8%)	15 13	20, 30, 48, 64	0
2	H	218/220 (99%)	0.87	20 (9%)	14 12	20, 31, 45, 57	0
3	I	77/90 (85%)	1.11	12 (15%)	5 4	23, 34, 49, 54	0
3	J	78/90 (86%)	1.14	9 (11%)	9 7	22, 35, 56, 60	0
3	K	77/90 (85%)	1.35	19 (24%)	2 1	24, 35, 53, 64	0
3	L	78/90 (86%)	1.31	20 (25%)	1 1	23, 35, 55, 61	0
All	All	2027/2132 (95%)	0.94	214 (10%)	11 8	15, 31, 49, 64	0

All (214) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	142	SER	4.3
3	K	119	LYS	4.2
2	H	33	SER	4.1
3	K	117	VAL	4.0
1	A	141	PRO	4.0
3	J	117	VAL	4.0
1	E	92	ASN	3.9
3	K	186	LYS	3.9
2	F	34	ASN	3.8
1	E	5	VAL	3.8
3	J	186	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
3	K	148	TYR	3.7
1	E	76	PHE	3.6
2	B	229	GLU	3.6
2	H	34	ASN	3.6
3	L	119	LYS	3.6
1	E	93	SER	3.6
2	H	228	GLY	3.5
1	C	46	PRO	3.4
1	E	83	ALA	3.4
1	G	142	SER	3.4
2	H	35	ASN	3.4
1	E	4	VAL	3.4
1	E	16	GLY	3.4
3	I	119	LYS	3.4
3	K	178	VAL	3.3
1	E	74	GLY	3.3
1	E	26	SER	3.3
1	A	25	ALA	3.2
3	J	119	LYS	3.2
3	L	186	LYS	3.2
1	E	25	ALA	3.2
1	E	58	TRP	3.2
1	G	104	CYS	3.1
2	F	1	ASP	3.1
3	I	190	ASP	3.1
1	E	84	LYS	3.1
1	G	26	SER	3.1
2	F	143	SER	3.1
1	A	205	GLY	3.1
1	G	16	GLY	3.1
1	E	71	VAL	3.1
1	E	19	LEU	3.1
3	L	178	VAL	3.0
1	G	5	VAL	3.0
3	K	177	THR	3.0
1	G	229	LYS	3.0
1	A	26	SER	3.0
3	L	191	ASN	3.0
2	H	1	ASP	2.9
1	C	141	PRO	2.9
1	C	104	CYS	2.9
1	G	47	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
3	K	188	VAL	2.9
1	G	9	GLY	2.8
1	E	91	LEU	2.8
3	L	170	LYS	2.8
2	F	70	GLY	2.8
2	F	123	LYS	2.8
1	C	47	GLY	2.8
3	L	189	PHE	2.8
3	L	115	ASP	2.8
1	G	4	VAL	2.8
2	B	33	SER	2.7
1	E	89	LEU	2.7
2	D	158	ARG	2.7
3	I	117	VAL	2.7
1	A	18	SER	2.7
2	H	46	PRO	2.7
3	I	173	LEU	2.7
1	E	141	PRO	2.7
2	H	32	SER	2.7
3	L	114	LYS	2.7
2	F	31	TYR	2.7
1	A	128	SER	2.7
1	C	18	SER	2.7
3	I	178	VAL	2.6
1	A	201	SER	2.6
1	C	91	LEU	2.6
1	C	229	LYS	2.6
1	E	97	GLU	2.6
1	A	27	GLY	2.6
3	L	188	VAL	2.6
2	F	33	SER	2.6
3	L	173	LEU	2.6
2	F	119	ARG	2.6
2	B	34	ASN	2.6
1	G	27	GLY	2.6
1	E	37	TYR	2.6
2	H	69	SER	2.6
1	G	219	ASN	2.5
2	B	1	ASP	2.5
3	J	189	PHE	2.5
1	C	5	VAL	2.5
2	H	31	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
3	L	174	GLU	2.5
3	I	156	ALA	2.5
1	G	90	GLN	2.5
2	F	15	LEU	2.5
3	J	156	ALA	2.5
3	K	172	VAL	2.5
3	L	117	VAL	2.5
2	B	31	TYR	2.5
2	D	34	ASN	2.5
2	H	119	ARG	2.4
2	F	122	ILE	2.4
3	K	157	GLY	2.4
1	E	30	PHE	2.4
3	L	148	TYR	2.4
3	J	191	ASN	2.4
3	K	174	GLU	2.4
2	H	142	LYS	2.4
1	E	222	VAL	2.4
3	I	148	TYR	2.4
1	C	16	GLY	2.4
1	G	220	THR	2.4
3	I	186	LYS	2.4
3	K	185	ILE	2.4
2	F	11	LEU	2.4
2	F	35	ASN	2.3
1	E	15	PRO	2.3
1	G	8	GLY	2.3
1	E	64	SER	2.3
1	E	128	SER	2.3
1	A	219	ASN	2.3
2	D	1	ASP	2.3
1	G	141	PRO	2.3
1	E	205	GLY	2.3
1	G	140	ALA	2.3
1	E	90	GLN	2.3
2	H	15	LEU	2.3
1	G	92	ASN	2.3
2	H	206	LYS	2.3
3	J	138	PRO	2.3
1	C	149	GLY	2.3
2	F	47	GLY	2.3
2	H	70	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
3	I	187	GLU	2.3
3	K	175	THR	2.3
1	G	130	SER	2.3
2	F	206	LYS	2.3
3	L	179	LYS	2.3
3	I	188	VAL	2.3
1	G	35	ASP	2.2
1	A	46	PRO	2.2
1	A	149	GLY	2.2
1	G	107	ALA	2.2
3	L	118	ILE	2.2
3	K	189	PHE	2.2
3	L	190	ASP	2.2
1	A	97	GLU	2.2
3	K	170	LYS	2.2
1	G	131	THR	2.2
2	F	20	THR	2.2
3	L	166	ILE	2.2
1	E	12	LEU	2.2
1	G	19	LEU	2.2
1	G	94	LEU	2.2
1	G	28	PHE	2.2
1	G	214	ASN	2.2
2	B	158	ARG	2.2
3	K	171	ASP	2.2
1	E	119	GLY	2.2
1	E	140	ALA	2.2
2	D	15	LEU	2.2
2	D	35	ASN	2.2
2	D	228	GLY	2.2
2	H	47	GLY	2.2
3	K	128	THR	2.2
1	E	17	ARG	2.1
2	D	31	TYR	2.1
2	B	170	LEU	2.1
3	K	173	LEU	2.1
3	K	114	LYS	2.1
3	J	182	PRO	2.1
1	G	14	GLN	2.1
1	C	205	GLY	2.1
1	E	8	GLY	2.1
1	E	104	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	206	LYS	2.1
1	A	150	THR	2.1
1	G	205	GLY	2.1
1	A	17	ARG	2.1
1	E	95	ARG	2.1
2	F	110	THR	2.1
3	K	142	THR	2.1
1	E	68	ALA	2.1
2	F	160	ALA	2.1
3	I	116	GLU	2.1
2	H	170	LEU	2.1
1	E	78	ILE	2.1
2	H	2	ILE	2.1
2	H	122	ILE	2.1
1	E	88	TYR	2.1
1	E	228	PRO	2.1
3	J	188	VAL	2.1
3	L	121	VAL	2.1
3	L	176	PHE	2.1
2	B	119	ARG	2.1
2	D	33	SER	2.0
2	H	139	GLU	2.0
1	E	82	ASN	2.0
2	F	94	LEU	2.0
2	H	226	ASN	2.0
1	G	15	PRO	2.0
1	C	9	GLY	2.0
1	C	26	SER	2.0
1	E	206	THR	2.0
2	F	10	SER	2.0
1	G	12	LEU	2.0
1	G	20	ARG	2.0
2	D	119	ARG	2.0
3	L	168	PRO	2.0
3	I	126	LYS	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th 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($\text{\AA}^2$)	Q<0.9
6	NA	F	302	1/1	0.86	0.09	29,29,29,29	0
6	NA	C	303	1/1	0.87	0.14	32,32,32,32	0
6	NA	D	304	1/1	0.89	0.11	39,39,39,39	0
4	CL	I	301	1/1	0.92	0.10	42,42,42,42	0
4	CL	A	302	1/1	0.92	0.11	40,40,40,40	0
4	CL	C	302	1/1	0.93	0.22	43,43,43,43	0
6	NA	C	304	1/1	0.93	0.10	32,32,32,32	0
6	NA	D	305	1/1	0.94	0.16	33,33,33,33	0
6	NA	B	303	1/1	0.95	0.12	30,30,30,30	0
4	CL	F	301	1/1	0.95	0.09	30,30,30,30	0
6	NA	D	303	1/1	0.96	0.05	28,28,28,28	0
4	CL	D	302	1/1	0.96	0.16	42,42,42,42	0
4	CL	H	301	1/1	0.96	0.20	44,44,44,44	0
5	K	B	302	1/1	0.96	0.23	44,44,44,44	0
4	CL	B	301	1/1	0.97	0.22	42,42,42,42	0
4	CL	D	301	1/1	0.97	0.25	44,44,44,44	0
4	CL	G	301	1/1	0.97	0.06	32,32,32,32	0
4	CL	C	301	1/1	0.98	0.04	34,34,34,34	0
4	CL	A	301	1/1	0.99	0.03	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.