



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 06:18 am BST

PDB ID : 4WTZ
Title : Human CEACAM6-CEACAM8 N-domain heterodimer complex
Authors : Kirouac, K.N.; Prive, G.G.
Deposited on : 2014-10-30
Resolution : 2.52 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

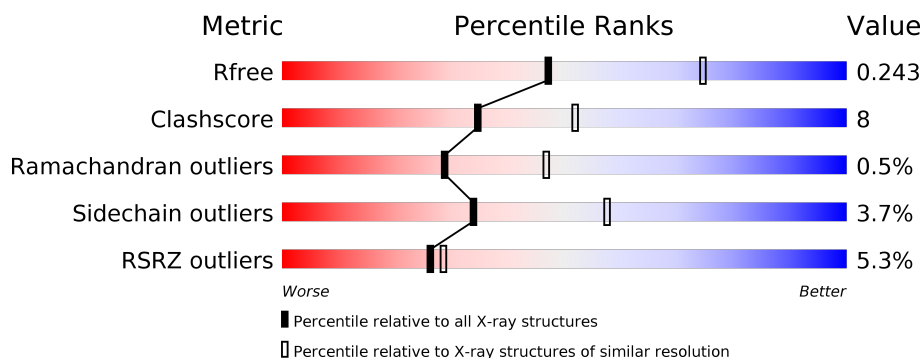
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 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	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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 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	108	<div> <div>90%</div> <div>8%</div> <div>••</div> </div>
1	B	108	<div> <div>%</div> <div>91%</div> <div>6%</div> <div>•</div> </div>
1	C	108	<div> <div>%</div> <div>88%</div> <div>11%</div> <div>•</div> </div>
1	D	108	<div> <div>%</div> <div>84%</div> <div>15%</div> <div>•</div> </div>
1	E	108	<div> <div>4%</div> <div>87%</div> <div>9%</div> <div>•</div> </div>
1	F	108	<div> <div>85%</div> <div>13%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
2	G	109	<div><div></div><div>2%85%13%<div><div></div><div></div><div></div></div></div></div>
2	H	109	<div><div></div><div>92%6%<div><div></div><div></div><div></div></div></div></div>
2	I	109	<div><div></div><div>83%12%<div><div></div><div></div><div></div></div></div></div>
2	J	109	<div><div></div><div>12%74%18%6%<div><div></div><div></div><div></div></div></div></div>
2	K	109	<div><div></div><div>31%59%30%9%<div><div></div><div></div><div></div></div></div></div>
2	L	109	<div><div></div><div>12%83%13%<div><div></div><div></div><div></div></div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10391 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 Carcinoembryonic antigen-related cell adhesion molecule 6.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	108	Total	C	N	O	0	0	0
			843	536	141	166			
1	B	108	Total	C	N	O	0	0	0
			843	536	141	166			
1	C	108	Total	C	N	O	0	0	0
			843	536	141	166			
1	D	108	Total	C	N	O	0	1	0
			851	540	143	168			
1	E	108	Total	C	N	O	0	0	0
			843	536	141	166			
1	F	108	Total	C	N	O	0	0	0
			843	536	141	166			

- Molecule 2 is a protein called Carcinoembryonic antigen-related cell adhesion molecule 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	108	Total	C	N	O	S	0	0	0
			850	532	150	165	3			
2	H	109	Total	C	N	O	S	0	0	0
			855	535	151	166	3			
2	I	109	Total	C	N	O	S	0	1	0
			863	539	153	168	3			
2	J	108	Total	C	N	O	S	0	0	0
			850	532	150	165	3			
2	K	109	Total	C	N	O	S	0	0	0
			855	535	151	166	3			
2	L	109	Total	C	N	O	S	0	0	0
			855	535	151	166	3			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	108	CYS	-	expression tag	UNP Q0Z7S6

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Chain	Residue	Modelled	Actual	Comment	Reference
H	108	CYS	-	expression tag	UNP Q0Z7S6
I	108	CYS	-	expression tag	UNP Q0Z7S6
J	108	CYS	-	expression tag	UNP Q0Z7S6
K	108	CYS	-	expression tag	UNP Q0Z7S6
L	108	CYS	-	expression tag	UNP Q0Z7S6

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Ni 1 1	0	0
3	A	2	Total Ni 2 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	31	Total O 31 31	0	0
4	B	22	Total O 22 22	0	0
4	C	16	Total O 16 16	0	0
4	D	27	Total O 27 27	0	0
4	E	15	Total O 15 15	0	0
4	F	12	Total O 12 12	0	0
4	G	8	Total O 8 8	0	0
4	H	26	Total O 26 26	0	0
4	I	17	Total O 17 17	0	0
4	J	10	Total O 10 10	0	0
4	K	3	Total O 3 3	0	0
4	L	7	Total O 7 7	0	0

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 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: Carcinoembryonic antigen-related cell adhesion molecule 6

Chain A: 




- Molecule 1: Carcinoembryonic antigen-related cell adhesion molecule 6

Chain B: 




- Molecule 1: Carcinoembryonic antigen-related cell adhesion molecule 6

Chain C: 




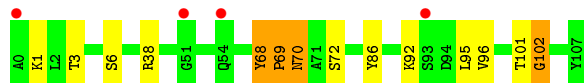
- Molecule 1: Carcinoembryonic antigen-related cell adhesion molecule 6

Chain D: 




- Molecule 1: Carcinoembryonic antigen-related cell adhesion molecule 6

Chain E: 




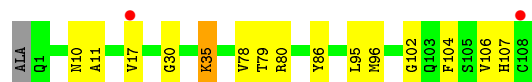
- Molecule 1: Carcinoembryonic antigen-related cell adhesion molecule 6

Chain F:  85% 13% .



- Molecule 2: Carcinoembryonic antigen-related cell adhesion molecule 8

Chain G:  85% 13% ..




- Molecule 2: Carcinoembryonic antigen-related cell adhesion molecule 8

Chain H:  92% 6% ..



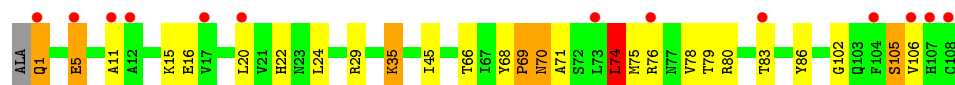
- Molecule 2: Carcinoembryonic antigen-related cell adhesion molecule 8

Chain I:  83% 12% . .



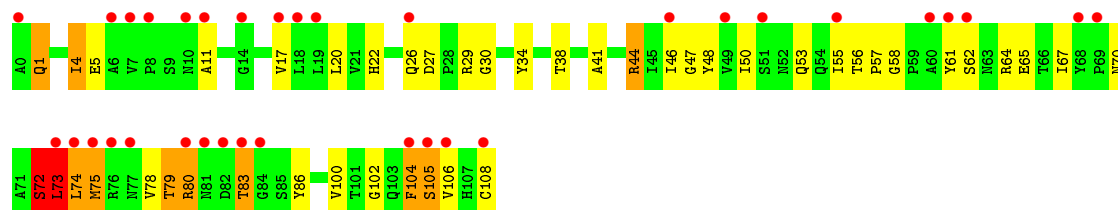
- Molecule 2: Carcinoembryonic antigen-related cell adhesion molecule 8

Chain J:  74% 18% 6% ..




- Molecule 2: Carcinoembryonic antigen-related cell adhesion molecule 8

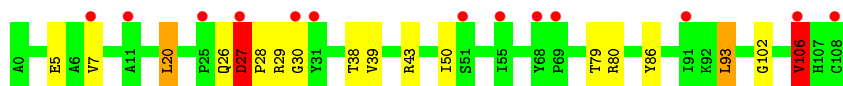
Chain K:  59% 30% 9% .



- Molecule 2: Carcinoembryonic antigen-related cell adhesion molecule 8

Chain L:  83% 13% . .





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	109.15Å 113.58Å 123.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	83.49 – 2.52 83.49 – 2.52	Depositor EDS
% Data completeness (in resolution range)	99.9 (83.49-2.52) 99.9 (83.49-2.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.205 , 0.234 0.211 , 0.243	Depositor DCC
R_{free} test set	1998 reflections (3.82%)	wwPDB-VP
Wilson B-factor (Å ²)	52.6	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10391	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.36 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.7668e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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: NI

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	0.92	1/861 (0.1%)	0.91	2/1173 (0.2%)
1	B	0.95	1/861 (0.1%)	0.92	1/1173 (0.1%)
1	C	0.89	2/861 (0.2%)	0.86	2/1173 (0.2%)
1	D	0.97	1/869 (0.1%)	0.86	2/1184 (0.2%)
1	E	0.90	1/861 (0.1%)	0.96	5/1173 (0.4%)
1	F	0.91	2/861 (0.2%)	0.96	5/1173 (0.4%)
2	G	0.79	0/866	0.92	1/1180 (0.1%)
2	H	0.90	2/871 (0.2%)	0.95	3/1187 (0.3%)
2	I	0.88	1/879 (0.1%)	1.05	8/1198 (0.7%)
2	J	0.80	1/866 (0.1%)	1.08	5/1180 (0.4%)
2	K	0.84	0/871	1.29	10/1187 (0.8%)
2	L	0.72	0/871	0.99	4/1187 (0.3%)
All	All	0.87	12/10398 (0.1%)	0.99	48/14168 (0.3%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	102	GLY	N-CA	-8.80	1.32	1.46
1	C	102	GLY	N-CA	-8.06	1.33	1.46
2	I	13	GLU	CG-CD	7.97	1.64	1.51
2	H	13	GLU	CG-CD	7.50	1.63	1.51
2	H	13	GLU	CD-OE1	7.49	1.33	1.25
1	B	102	GLY	N-CA	-6.80	1.35	1.46
1	A	102	GLY	N-CA	-6.78	1.35	1.46
1	F	102	GLY	N-CA	-6.73	1.35	1.46
1	C	16	GLU	CD-OE1	6.09	1.32	1.25
1	E	102	GLY	N-CA	-5.83	1.37	1.46
1	F	68	TYR	CE1-CZ	5.34	1.45	1.38
2	J	76	ARG	CD-NE	5.20	1.55	1.46

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	44	ARG	NE-CZ-NH1	10.65	125.62	120.30
2	K	75	MET	CG-SD-CE	-9.48	85.04	100.20
2	J	74	LEU	CB-CG-CD1	9.05	126.39	111.00
2	I	13	GLU	OE1-CD-OE2	-8.12	113.56	123.30
2	K	64	ARG	NE-CZ-NH1	8.11	124.36	120.30
2	I	29	ARG	NE-CZ-NH1	7.79	124.19	120.30
2	I	76	ARG	NE-CZ-NH1	7.74	124.17	120.30
2	K	29	ARG	N-CA-C	-7.57	90.58	111.00
1	F	68	TYR	CB-CG-CD1	7.34	125.41	121.00
2	J	76	ARG	NE-CZ-NH1	7.27	123.94	120.30
2	K	73	LEU	N-CA-C	6.92	129.67	111.00
1	F	68	TYR	CB-CG-CD2	-6.89	116.86	121.00
2	K	44	ARG	NE-CZ-NH2	-6.88	116.86	120.30
2	H	13	GLU	OE1-CD-OE2	-6.72	115.23	123.30
2	K	50	ILE	CG1-CB-CG2	-6.42	97.27	111.40
1	C	101	THR	CA-C-N	6.38	128.96	116.20
2	K	72	SER	N-CA-C	6.35	128.15	111.00
2	L	50	ILE	CG1-CB-CG2	-6.35	97.44	111.40
2	I	29	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	E	69	PRO	N-CA-C	-6.21	95.96	112.10
1	D	101	THR	CA-C-N	6.14	128.48	116.20
2	J	29	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	E	101	THR	CA-C-N	6.09	128.39	116.20
1	B	101	THR	CA-C-N	6.06	128.32	116.20
2	K	64	ARG	NE-CZ-NH2	-5.97	117.32	120.30
2	K	80	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	F	68	TYR	CA-CB-CG	5.92	124.66	113.40
2	H	106	VAL	CA-CB-CG1	5.80	119.60	110.90
1	F	101	THR	CA-C-N	5.74	127.69	116.20
1	A	101	THR	CA-C-N	5.69	127.59	116.20
2	L	93	LEU	CA-CB-CG	5.60	128.17	115.30
2	L	106	VAL	CA-CB-CG1	5.54	119.20	110.90
2	J	74	LEU	CB-CG-CD2	-5.45	101.74	111.00
2	I	76	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	E	68	TYR	CB-CG-CD1	5.41	124.25	121.00
2	I	106	VAL	CA-CB-CG1	5.35	118.93	110.90
2	I	15	LYS	CD-CE-NZ	5.35	124.00	111.70
1	C	64	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	A	27	ASN	N-CA-CB	-5.32	101.02	110.60
1	E	68	TYR	CB-CG-CD2	-5.23	117.86	121.00
2	J	1	GLN	CA-CB-CG	5.20	124.84	113.40
1	E	68	TYR	CA-CB-CG	5.15	123.19	113.40
1	D	101	THR	O-C-N	-5.12	114.49	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	35	LYS	CA-CB-CG	5.08	124.59	113.40
2	L	27	ASP	C-N-CD	5.05	139.00	128.40
2	I	91	ILE	CG1-CB-CG2	-5.03	100.33	111.40
2	H	103	GLN	CB-CA-C	-5.01	100.38	110.40
1	F	53	GLN	O-C-N	5.00	130.71	122.70

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	843	0	826	10	0
1	B	843	0	826	6	0
1	C	843	0	826	8	0
1	D	851	0	831	8	2
1	E	843	0	826	11	0
1	F	843	0	826	10	0
2	G	850	0	843	15	0
2	H	855	0	848	8	0
2	I	863	0	853	12	1
2	J	850	0	843	19	2
2	K	855	0	848	67	0
2	L	855	0	848	10	1
3	A	2	0	0	0	0
3	B	1	0	0	0	0
4	A	31	0	0	0	0
4	B	22	0	0	0	0
4	C	16	0	0	0	0
4	D	27	0	0	0	0
4	E	15	0	0	0	0
4	F	12	0	0	0	0
4	G	8	0	0	0	0
4	H	26	0	0	0	0
4	I	17	0	0	0	0
4	J	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	3	0	0	0	0
4	L	7	0	0	0	0
All	All	10391	0	10044	168	3

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 8.

All (168) 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:J:69:PRO:O	2:J:71:ALA:N	1.73	1.20
2:K:58:GLY:O	2:K:61:TYR:HD2	1.24	1.19
2:K:70:ASN:OD1	2:K:72:SER:OG	1.69	1.10
2:K:58:GLY:O	2:K:61:TYR:CD2	2.05	1.08
1:F:26:GLN:O	1:F:27:ASN:ND2	1.88	1.07
2:K:5:GLU:OE2	2:K:20:LEU:HD22	1.56	1.06
2:K:17:VAL:HG11	2:K:104:PHE:CZ	1.91	1.05
2:I:3:THR:HG22	2:I:22:HIS:HB2	1.41	1.01
2:K:83:THR:HG22	2:K:105:SER:HA	1.43	0.99
2:K:46:ILE:CG1	2:K:67:ILE:HD11	1.93	0.97
2:K:67:ILE:N	2:K:67:ILE:HD12	1.79	0.95
1:E:68:TYR:HB3	1:E:69:PRO:HD2	1.52	0.92
2:K:4:ILE:HD13	2:K:4:ILE:H	1.35	0.91
2:K:44:ARG:HH22	2:K:56:THR:HG23	1.34	0.91
2:K:46:ILE:HG12	2:K:67:ILE:CD1	2.03	0.89
2:K:46:ILE:HG12	2:K:67:ILE:HD11	1.53	0.88
2:K:46:ILE:CD1	2:K:67:ILE:HD11	2.06	0.86
2:K:67:ILE:HD12	2:K:67:ILE:H	1.40	0.84
2:K:5:GLU:OE2	2:K:20:LEU:CD2	2.27	0.81
2:K:17:VAL:CG1	2:K:104:PHE:CZ	2.64	0.80
2:K:17:VAL:HG11	2:K:104:PHE:CE1	2.17	0.80
2:J:69:PRO:C	2:J:71:ALA:H	1.85	0.80
2:K:46:ILE:HD13	2:K:67:ILE:HD11	1.67	0.75
1:F:38:ARG:HD2	2:K:38:THR:HG21	1.68	0.74
2:J:86:TYR:O	2:J:102:GLY:HA3	1.88	0.74
2:K:86:TYR:O	2:K:102:GLY:HA3	1.87	0.73
2:I:86:TYR:O	2:I:102:GLY:HA3	1.89	0.73
2:K:80:ARG:O	2:K:83:THR:OG1	2.06	0.73
2:K:83:THR:CG2	2:K:105:SER:HA	2.18	0.73
2:G:86:TYR:O	2:G:102:GLY:HA3	1.88	0.71
2:H:86:TYR:O	2:H:102:GLY:HA3	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:86:TYR:O	2:L:102:GLY:HA3	1.89	0.71
2:L:7:VAL:HG21	2:L:20:LEU:HD12	1.71	0.71
2:K:79:THR:O	2:K:106:VAL:HG11	1.91	0.71
2:I:3:THR:CG2	2:I:22:HIS:HB2	2.20	0.70
2:J:79:THR:O	2:J:106:VAL:HG11	1.91	0.70
1:D:92:LYS:HE2	1:D:96:VAL:O	1.91	0.69
2:G:79:THR:O	2:G:106:VAL:HG11	1.92	0.68
1:E:92:LYS:HE2	1:E:96:VAL:O	1.93	0.68
1:A:92:LYS:HE2	1:A:96:VAL:O	1.94	0.68
2:L:80:ARG:HA	2:L:106:VAL:HG12	1.75	0.67
1:B:92:LYS:HE2	1:B:96:VAL:O	1.94	0.66
1:F:92:LYS:HE2	1:F:96:VAL:O	1.94	0.66
2:G:80:ARG:HA	2:G:106:VAL:CG1	2.25	0.66
1:C:92:LYS:HE2	1:C:96:VAL:O	1.95	0.66
2:K:4:ILE:CD1	2:K:4:ILE:H	2.08	0.65
1:F:86:TYR:O	1:F:102:GLY:HA3	1.98	0.64
1:F:26:GLN:C	1:F:27:ASN:HD22	2.00	0.64
2:I:80:ARG:O	2:I:83:THR:HG23	1.97	0.63
1:C:86:TYR:O	1:C:102:GLY:HA3	1.99	0.63
2:H:80:ARG:O	2:H:83:THR:HG23	1.99	0.63
1:B:86:TYR:O	1:B:102:GLY:HA3	2.00	0.62
2:L:26:GLN:O	2:L:27:ASP:HB2	2.00	0.62
2:K:74:LEU:HD12	2:K:75:MET:N	2.14	0.62
1:D:86:TYR:O	1:D:102:GLY:HA3	2.00	0.62
1:A:86:TYR:O	1:A:102:GLY:HA3	1.99	0.61
1:B:26:GLN:O	1:B:27:ASN:HB2	2.00	0.61
2:K:11:ALA:HB3	2:K:104:PHE:HZ	1.65	0.61
2:K:5:GLU:CD	2:K:20:LEU:HD22	2.20	0.61
2:K:83:THR:HG22	2:K:105:SER:CA	2.26	0.61
1:A:26:GLN:CD	1:A:26:GLN:H	2.05	0.61
1:E:68:TYR:HB3	1:E:69:PRO:CD	2.29	0.60
1:E:1:LYS:O	1:E:3:THR:HG23	2.01	0.60
1:E:86:TYR:O	1:E:102:GLY:HA3	2.02	0.60
2:H:80:ARG:HA	2:H:106:VAL:HG12	1.82	0.60
2:K:4:ILE:HG13	2:K:102:GLY:HA2	1.83	0.60
2:K:65:GLU:HG2	2:K:65:GLU:O	1.99	0.60
2:I:79:THR:O	2:I:106:VAL:HG11	2.04	0.58
2:K:4:ILE:HD13	2:K:4:ILE:N	2.09	0.58
2:L:79:THR:O	2:L:106:VAL:HG11	2.04	0.58
2:I:80:ARG:HA	2:I:106:VAL:HG12	1.86	0.57
1:F:1:LYS:O	1:F:3:THR:HG23	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:95:LEU:CD1	2:K:30:GLY:HA3	2.35	0.57
2:H:79:THR:O	2:H:106:VAL:HG11	2.04	0.56
1:D:1:LYS:O	1:D:3:THR:HG23	2.05	0.56
2:J:80:ARG:HA	2:J:106:VAL:CG1	2.36	0.56
2:J:68:TYR:N	2:J:68:TYR:CD1	2.72	0.56
2:K:44:ARG:NH2	2:K:56:THR:HG23	2.14	0.55
2:J:24:LEU:HD11	2:J:70:ASN:O	2.07	0.55
2:K:74:LEU:HD12	2:K:74:LEU:C	2.27	0.54
2:K:4:ILE:CD1	2:K:4:ILE:N	2.70	0.54
2:K:41:ALA:O	2:K:44:ARG:HG2	2.08	0.53
1:A:26:GLN:HG2	1:A:27:ASN:N	2.23	0.53
1:F:95:LEU:HD12	2:K:30:GLY:HA3	1.90	0.53
2:J:70:ASN:O	2:J:71:ALA:HB3	2.09	0.52
2:K:55:ILE:HG22	2:K:57:PRO:HD3	1.90	0.51
2:G:17:VAL:HG21	2:G:104:PHE:CD2	2.46	0.50
2:J:35:LYS:HG2	2:J:45:ILE:HD11	1.93	0.50
1:D:5:GLU:OE2	1:E:38:ARG:NH1	2.43	0.50
2:K:75:MET:HE2	2:K:78:VAL:HG22	1.94	0.50
1:E:69:PRO:O	1:E:70:ASN:HB3	2.10	0.50
2:K:83:THR:HG23	2:K:106:VAL:H	1.77	0.49
1:C:3:THR:HG23	1:C:22:HIS:HB2	1.93	0.49
2:K:61:TYR:C	2:K:61:TYR:CD1	2.85	0.49
1:D:0:ALA:HB2	2:L:43:ARG:NH1	2.28	0.49
2:H:83:THR:HG22	2:H:106:VAL:H	1.77	0.49
2:K:11:ALA:HB3	2:K:104:PHE:CZ	2.46	0.49
1:C:47:GLY:HA3	2:G:96:MET:HE1	1.95	0.49
1:C:56:THR:HB	2:G:96:MET:CE	2.43	0.49
2:J:15:LYS:HG3	2:J:16:GLU:H	1.78	0.48
2:K:83:THR:CG2	2:K:106:VAL:H	2.27	0.48
2:K:46:ILE:CD1	2:K:67:ILE:CD1	2.85	0.48
2:K:4:ILE:HG13	2:K:102:GLY:CA	2.43	0.47
1:F:38:ARG:CD	2:K:38:THR:HG21	2.42	0.47
2:K:56:THR:HG23	2:K:56:THR:O	2.15	0.47
2:K:47:GLY:C	2:K:56:THR:HG22	2.35	0.47
1:E:95:LEU:CD1	2:L:30:GLY:HA3	2.45	0.47
1:F:7:THR:HA	1:F:8:PRO:HA	1.76	0.47
2:H:83:THR:HG22	2:H:106:VAL:HB	1.97	0.47
2:K:46:ILE:CG2	2:K:67:ILE:CG1	2.92	0.47
1:C:47:GLY:HA3	2:G:96:MET:CE	2.45	0.47
2:J:5:GLU:OE1	2:J:22:HIS:ND1	2.48	0.46
2:K:46:ILE:CG1	2:K:67:ILE:CD1	2.71	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:LEU:CD1	2:I:30:GLY:HA3	2.45	0.46
2:K:46:ILE:HG23	2:K:67:ILE:CG1	2.45	0.46
2:K:78:VAL:HG13	2:K:79:THR:N	2.31	0.46
2:K:34:TYR:CE1	2:K:44:ARG:HB3	2.51	0.46
2:G:80:ARG:HA	2:G:106:VAL:HG13	1.96	0.46
2:L:27:ASP:N	2:L:28:PRO:CD	2.79	0.46
1:D:95:LEU:CD1	2:H:30:GLY:HA3	2.46	0.46
2:H:83:THR:HG22	2:H:106:VAL:N	2.31	0.46
2:J:74:LEU:HD23	2:J:75:MET:N	2.31	0.46
2:J:74:LEU:CD2	2:J:74:LEU:C	2.85	0.45
2:G:79:THR:C	2:G:106:VAL:HG11	2.37	0.45
2:J:68:TYR:N	2:J:68:TYR:HD1	2.13	0.45
2:K:61:TYR:CD1	2:K:61:TYR:O	2.70	0.45
2:K:17:VAL:HG23	2:K:17:VAL:O	2.15	0.45
2:K:83:THR:HG23	2:K:106:VAL:N	2.31	0.45
2:G:17:VAL:HG21	2:G:104:PHE:CE2	2.53	0.44
2:K:80:ARG:HA	2:K:106:VAL:HG13	1.98	0.44
2:K:65:GLU:CD	2:K:65:GLU:H	2.19	0.44
1:A:54:GLN:HG3	1:B:68:TYR:CD1	2.53	0.44
2:I:83:THR:HG22	2:I:106:VAL:HB	1.98	0.44
2:K:72:SER:O	2:K:73:LEU:C	2.55	0.44
1:D:7:THR:HA	1:D:8:PRO:HA	1.84	0.44
2:K:78:VAL:CG1	2:K:79:THR:N	2.79	0.43
2:K:4:ILE:HG13	2:K:102:GLY:N	2.32	0.43
1:E:68:TYR:CD2	1:E:72:SER:HB2	2.54	0.43
2:G:11:ALA:O	2:G:106:VAL:HG23	2.18	0.43
2:K:67:ILE:N	2:K:67:ILE:CD1	2.63	0.43
2:L:79:THR:C	2:L:106:VAL:HG11	2.39	0.43
2:K:4:ILE:HD12	2:K:100:VAL:HG22	2.00	0.42
2:K:11:ALA:O	2:K:106:VAL:HG23	2.19	0.42
2:J:78:VAL:HG23	2:J:106:VAL:HG21	2.01	0.42
1:C:95:LEU:CD1	2:G:30:GLY:HA3	2.49	0.42
2:G:10:ASN:OD1	2:G:107:HIS:HD2	2.02	0.42
2:I:83:THR:HG22	2:I:106:VAL:N	2.35	0.42
1:A:54:GLN:OE1	1:B:68:TYR:HB3	2.20	0.42
1:A:27:ASN:HB3	1:A:92:LYS:HD2	2.01	0.42
2:J:11:ALA:O	2:J:106:VAL:HG23	2.21	0.41
2:K:1:GLN:HB2	2:K:1:GLN:HE21	1.58	0.41
2:K:30:GLY:HA3	2:K:48:TYR:O	2.20	0.41
1:A:26:GLN:CD	1:A:26:GLN:N	2.72	0.41
1:E:69:PRO:O	1:E:70:ASN:CB	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:83:THR:HG22	2:I:106:VAL:H	1.86	0.41
2:J:83:THR:HG23	2:J:105:SER:HA	2.03	0.41
2:J:66:THR:HG22	2:J:68:TYR:CE1	2.56	0.41
1:A:27:ASN:ND2	1:A:93:SER:OG	2.53	0.41
2:L:38:THR:HG22	2:L:39:VAL:N	2.36	0.41
2:K:30:GLY:CA	2:K:48:TYR:O	2.69	0.41
1:C:56:THR:HB	2:G:96:MET:HE1	2.03	0.41
1:D:31:TYR:CZ	1:D:71:ALA:HB2	2.55	0.41
2:G:78:VAL:HG23	2:G:106:VAL:HG21	2.03	0.41
2:J:79:THR:C	2:J:106:VAL:HG11	2.41	0.41
1:A:25:PRO:HG3	1:A:92:LYS:HD3	2.02	0.40
2:I:7:VAL:HG21	2:I:20:LEU:HD12	2.03	0.40
1:E:69:PRO:CD	1:E:69:PRO:O	2.70	0.40
2:I:12:ALA:H	2:I:15:LYS:HE2	1.86	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:GLU:OE1	2:J:5:GLU:OE2[4_555]	1.08	1.12
1:D:76:GLN:NE2	2:J:5:GLU:CG[4_555]	1.88	0.32
2:I:29:ARG:NH2	2:L:5:GLU:OE1[4_455]	2.18	0.02

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	106/108 (98%)	102 (96%)	4 (4%)	0	100	100
1	B	106/108 (98%)	102 (96%)	3 (3%)	1 (1%)	17	30
1	C	106/108 (98%)	102 (96%)	4 (4%)	0	100	100
1	D	107/108 (99%)	103 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	106/108 (98%)	101 (95%)	4 (4%)	1 (1%)	17	30
1	F	106/108 (98%)	102 (96%)	4 (4%)	0	100	100
2	G	106/109 (97%)	103 (97%)	3 (3%)	0	100	100
2	H	107/109 (98%)	104 (97%)	3 (3%)	0	100	100
2	I	108/109 (99%)	105 (97%)	3 (3%)	0	100	100
2	J	106/109 (97%)	99 (93%)	5 (5%)	2 (2%)	8	12
2	K	107/109 (98%)	101 (94%)	5 (5%)	1 (1%)	17	30
2	L	107/109 (98%)	103 (96%)	3 (3%)	1 (1%)	17	30
All	All	1278/1302 (98%)	1227 (96%)	45 (4%)	6 (0%)	29	47

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	27	ASN
1	E	70	ASN
2	J	70	ASN
2	K	73	LEU
2	J	69	PRO
2	L	27	ASP

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	91/91 (100%)	89 (98%)	2 (2%)	52	75
1	B	91/91 (100%)	89 (98%)	2 (2%)	52	75
1	C	91/91 (100%)	90 (99%)	1 (1%)	73	88
1	D	92/91 (101%)	91 (99%)	1 (1%)	73	88
1	E	91/91 (100%)	90 (99%)	1 (1%)	73	88
1	F	91/91 (100%)	89 (98%)	2 (2%)	52	75
2	G	95/95 (100%)	93 (98%)	2 (2%)	53	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	95/95 (100%)	93 (98%)	2 (2%)	53	76
2	I	96/95 (101%)	92 (96%)	4 (4%)	30	51
2	J	95/95 (100%)	89 (94%)	6 (6%)	18	32
2	K	95/95 (100%)	81 (85%)	14 (15%)	3	5
2	L	95/95 (100%)	91 (96%)	4 (4%)	30	51
All	All	1118/1116 (100%)	1077 (96%)	41 (4%)	34	57

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	27	ASN
1	B	6	SER
1	B	26	GLN
1	C	6	SER
1	D	6	SER
1	E	6	SER
1	F	6	SER
1	F	27	ASN
2	G	35	LYS
2	G	95	LEU
2	H	80	ARG
2	H	106	VAL
2	I	3	THR
2	I	20	LEU
2	I	106	VAL
2	I	108	CYS
2	J	1	GLN
2	J	5	GLU
2	J	20	LEU
2	J	35	LYS
2	J	74	LEU
2	J	105	SER
2	K	1	GLN
2	K	4	ILE
2	K	22	HIS
2	K	26	GLN
2	K	27	ASP
2	K	53	GLN
2	K	62	SER

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Mol	Chain	Res	Type
2	K	72	SER
2	K	74	LEU
2	K	79	THR
2	K	83	THR
2	K	104	PHE
2	K	105	SER
2	K	108	CYS
2	L	20	LEU
2	L	29	ARG
2	L	93	LEU
2	L	106	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	81	ASN
1	C	77	ASN
1	E	103	GLN
1	F	27	ASN
2	G	77	ASN
2	G	107	HIS
2	H	77	ASN
2	I	107	HIS
2	J	63	ASN
2	K	1	GLN
2	K	77	ASN
2	L	63	ASN
2	L	77	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 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	108/108 (100%)	0.03	0 100 100	37, 49, 61, 80	0
1	B	108/108 (100%)	0.02	1 (0%) 84 86	36, 47, 67, 84	0
1	C	108/108 (100%)	0.08	1 (0%) 84 86	41, 54, 67, 94	0
1	D	108/108 (100%)	0.07	1 (0%) 84 86	36, 46, 59, 82	0
1	E	108/108 (100%)	0.22	4 (3%) 41 45	36, 57, 102, 112	0
1	F	108/108 (100%)	0.10	0 100 100	41, 54, 84, 96	0
2	G	108/109 (99%)	0.29	2 (1%) 66 70	48, 70, 117, 141	0
2	H	109/109 (100%)	0.02	0 100 100	37, 53, 84, 116	0
2	I	109/109 (100%)	0.26	0 100 100	41, 61, 104, 131	0
2	J	108/109 (99%)	0.80	13 (12%) 4 4	53, 82, 140, 170	0
2	K	109/109 (100%)	1.52	34 (31%) 0 0	63, 111, 170, 187	0
2	L	109/109 (100%)	0.80	13 (11%) 4 4	62, 86, 109, 120	0
All	All	1300/1302 (99%)	0.35	69 (5%) 26 28	36, 59, 119, 187	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	61	TYR	9.1
2	K	104	PHE	6.8
2	K	80	ARG	6.4
2	K	68	TYR	5.0
2	K	106	VAL	4.6
2	J	11	ALA	4.3
2	K	17	VAL	4.3
2	J	106	VAL	4.2
2	K	83	THR	4.1
2	K	8	PRO	4.0
2	K	105	SER	4.0

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Mol	Chain	Res	Type	RSRZ
2	L	91	ILE	3.9
2	L	27	ASP	3.8
2	K	108	CYS	3.7
2	K	26	GLN	3.7
2	K	84	GLY	3.6
2	L	7	VAL	3.5
2	K	51	SER	3.5
2	K	19	LEU	3.4
2	K	49	VAL	3.4
2	K	6	ALA	3.2
2	K	73	LEU	3.1
2	K	81	ASN	3.0
2	L	11	ALA	3.0
2	K	0	ALA	2.9
2	J	108	CYS	2.9
1	C	0	ALA	2.9
2	K	74	LEU	2.9
2	K	75	MET	2.9
2	J	76	ARG	2.9
2	J	1	GLN	2.8
2	K	46	ILE	2.7
2	L	69	PRO	2.7
2	J	73	LEU	2.7
2	K	7	VAL	2.6
2	L	25	PRO	2.6
2	K	77	ASN	2.5
2	K	11	ALA	2.5
2	J	107	HIS	2.5
2	K	18	LEU	2.5
2	G	17	VAL	2.5
2	L	51	SER	2.5
2	K	14	GLY	2.5
2	K	60	ALA	2.4
1	E	51	GLY	2.4
2	L	31	TYR	2.4
2	L	68	TYR	2.3
2	J	20	LEU	2.2
2	K	55	ILE	2.2
2	J	83	THR	2.2
1	E	54	GLN	2.2
2	J	12	ALA	2.2
2	K	10	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
2	J	17	VAL	2.2
2	J	5	GLU	2.2
1	E	0	ALA	2.2
2	K	62	SER	2.2
1	D	0	ALA	2.1
2	K	69	PRO	2.1
2	J	104	PHE	2.1
2	L	30	GLY	2.1
2	K	82	ASP	2.1
2	G	108	CYS	2.1
2	L	108	CYS	2.1
2	L	55	ILE	2.0
2	L	106	VAL	2.0
1	B	26	GLN	2.0
1	E	93	SER	2.0
2	K	76	ARG	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 carbohydrates 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(Å ²)	Q<0.9
3	NI	A	202	1/1	0.79	0.09	120,120,120,120	0
3	NI	B	201	1/1	0.97	0.27	46,46,46,46	0
3	NI	A	201	1/1	0.98	0.26	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.