



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:01 AM GMT

PDB ID : 2VLR  
Title : THE STRUCTURAL DYNAMICS AND ENERGETICS OF AN IMMUNODOMINANT T-CELL RECEPTOR ARE PROGRAMMED BY ITS VBETA DOMAIN  
Authors : Ishizuka, J.; Stewart-Jones, G.; Van Der Merwe, A.; Bell, J.; Mcmichael, A.; Jones, Y.  
Deposited on : 2008-01-15  
Resolution : 2.30 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  
<http://wwpdb.org/validation/2016/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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

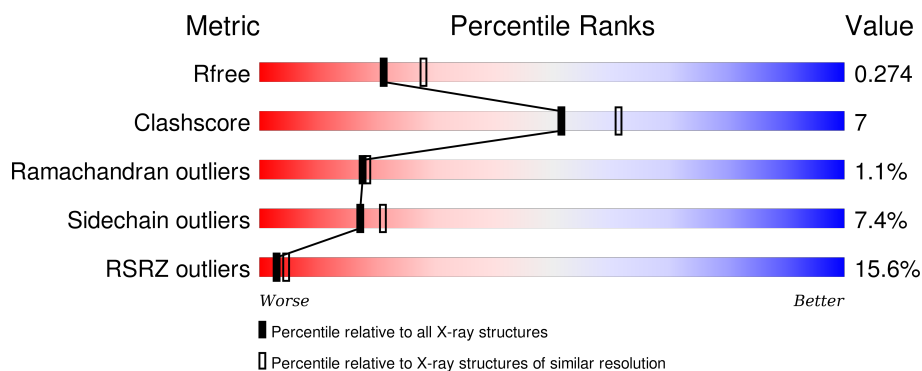
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	276	<div> <div>16%</div> <div>87%</div> <div>12%</div> </div>
1	F	276	<div> <div>27%</div> <div>76%</div> <div>20%</div> </div>
2	B	100	<div> <div>7%</div> <div>81%</div> <div>15%</div> </div>
2	G	100	<div> <div>10%</div> <div>79%</div> <div>17%</div> </div>
3	C	9	<div> <div>33%</div> <div>89%</div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
3	H	9	<div><div></div><div>89%</div><div>11%</div></div>
4	D	201	<div><div>11%</div><div>85%</div><div>12%</div><div>••</div></div>
4	I	201	<div><div>27%</div><div>78%</div><div>18%</div><div>••</div></div>
5	E	244	<div><div>6%</div><div>86%</div><div>10%</div><div>••</div></div>
5	J	244	<div><div>11%</div><div>81%</div><div>15%</div><div>••</div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13819 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 HLA CLASS I HISTOCOMPATIBILITY ANTIGEN, A-2 ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	1	0	0
			2253	1408	410	426	9			
1	F	276	Total	C	N	O	S	1	0	0
			2253	1408	410	426	9			

- Molecule 2 is a protein called BETA-2-MICROGLOBULIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			836	533	141	158	4			
2	G	100	Total	C	N	O	S	0	0	0
			836	533	141	158	4			

- Molecule 3 is a protein called FLU MATRIX PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			68	49	9	10			
3	H	9	Total	C	N	O	0	0	0
			68	49	9	10			

- Molecule 4 is a protein called JM22 TCR ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	199	Total	C	N	O	S	0	0	0
			1530	959	255	310	6			
4	I	199	Total	C	N	O	S	0	0	0
			1530	959	255	310	6			

- Molecule 5 is a protein called JM22 TCR BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	240	Total 1931	C 1218	N 334	O 374	S 5	0	0	0
5	J	240	Total 1931	C 1218	N 334	O 374	S 5	0	0	0

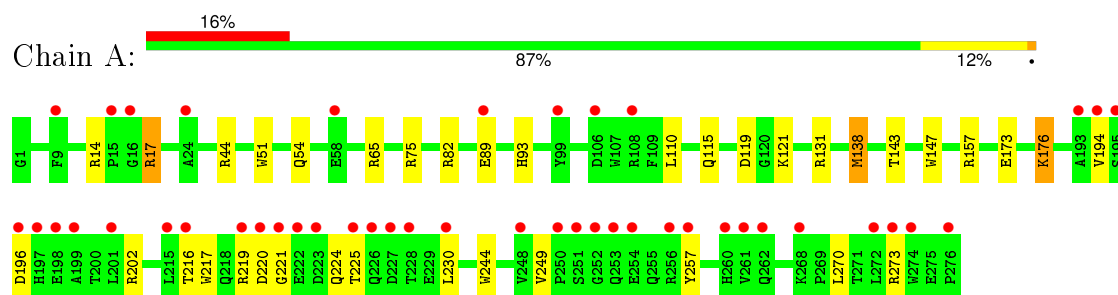
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	90	Total 90	O 90	0	0
6	B	36	Total 36	O 36	0	0
6	C	6	Total 6	O 6	0	0
6	D	75	Total 75	O 75	0	0
6	E	99	Total 99	O 99	0	0
6	F	79	Total 79	O 79	0	0
6	G	36	Total 36	O 36	0	0
6	H	5	Total 5	O 5	0	0
6	I	70	Total 70	O 70	0	0
6	J	87	Total 87	O 87	0	0

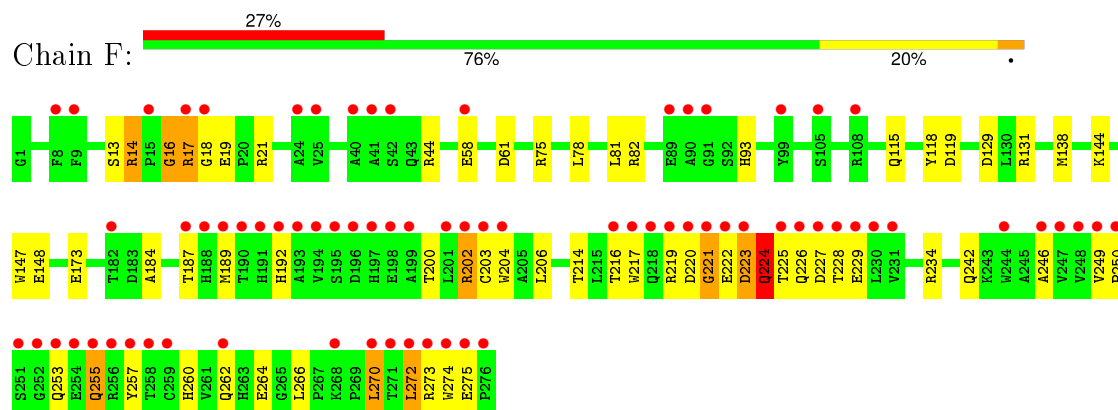
### 3 Residue-property plots

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.

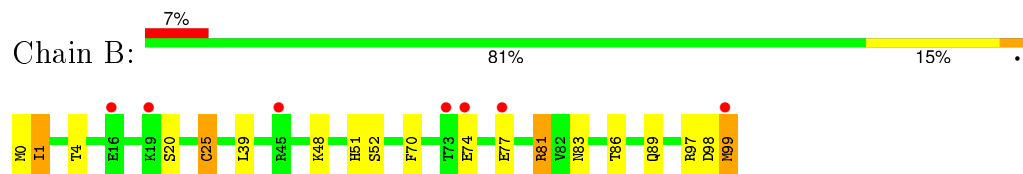
- Molecule 1: HLA CLASS I HISTOCOMPATIBILITY ANTIGEN, A-2 ALPHA CHAIN



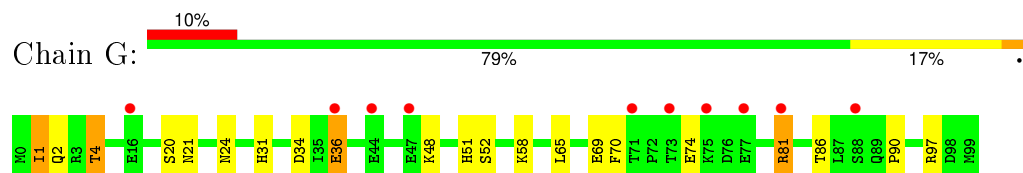
- Molecule 1: HLA CLASS I HISTOCOMPATIBILITY ANTIGEN, A-2 ALPHA CHAIN

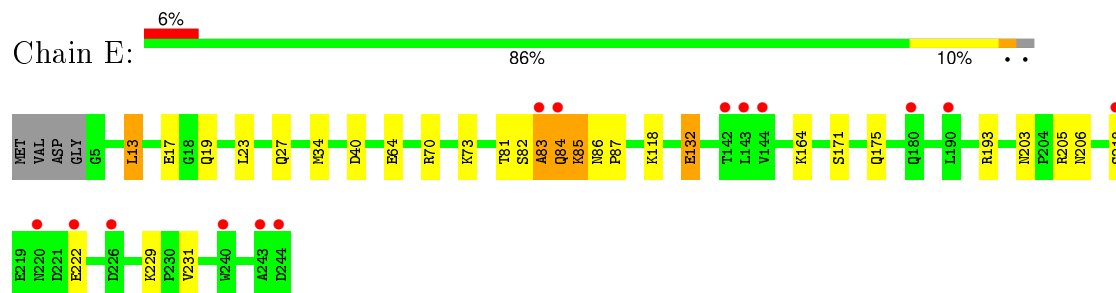
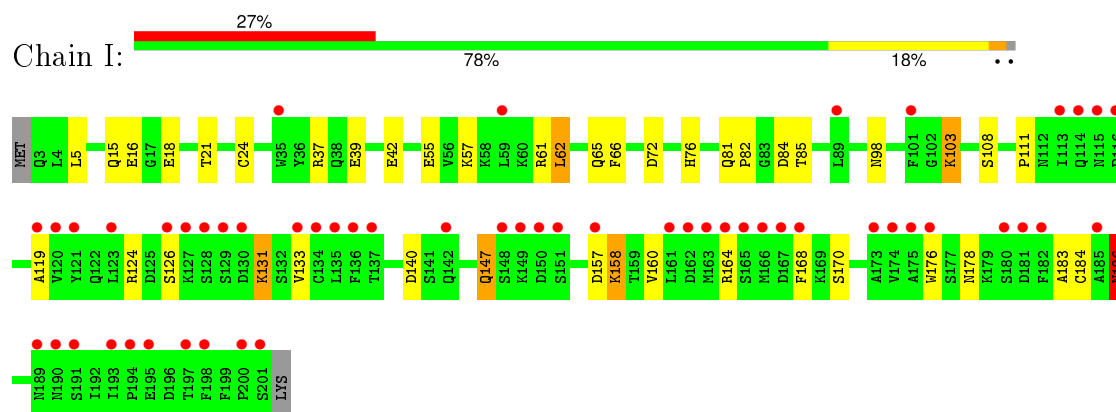
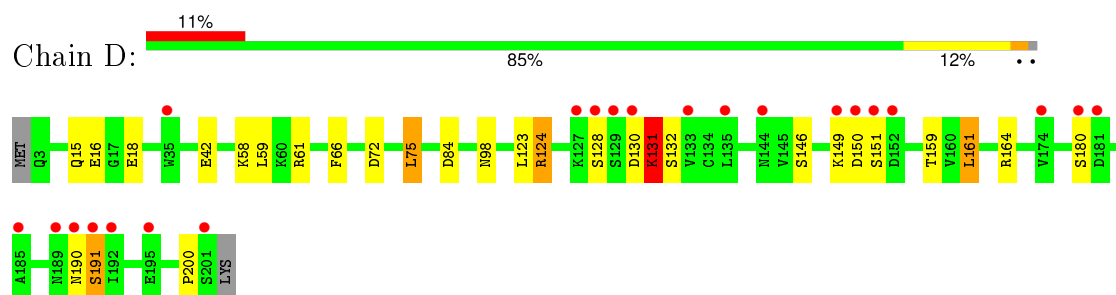
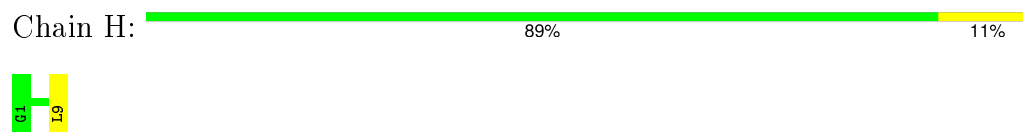
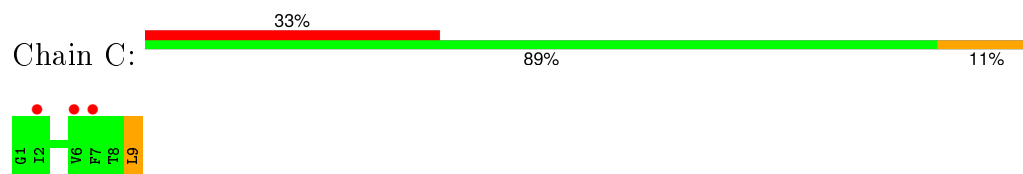


- Molecule 2: BETA-2-MICROGLOBULIN

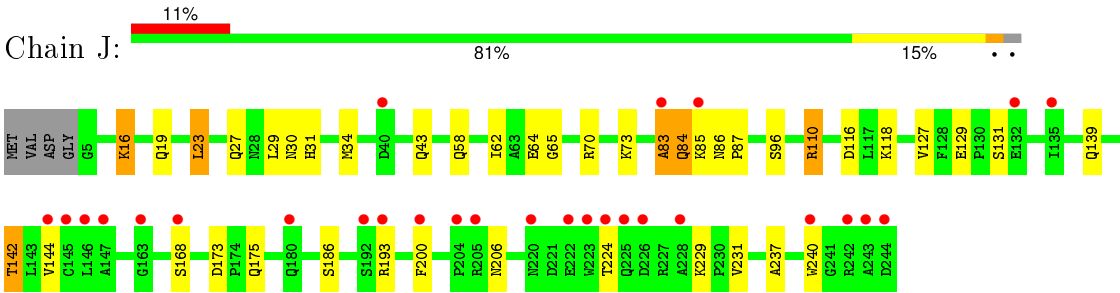


- Molecule 2: BETA-2-MICROGLOBULIN





- Molecule 5: JM22 TCR BETA CHAIN





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.62Å 95.52Å 122.05Å 110.29° 98.64° 93.59°	Depositor
Resolution (Å)	112.51 – 2.30 29.69 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.5 (112.51-2.30) 85.5 (29.69-2.30)	Depositor EDS
$R_{merge}$	0.97	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.94 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.219 , 0.281 0.215 , 0.274	Depositor DCC
$R_{free}$ test set	4402 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.4	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 57.2	EDS
Estimated twinning fraction	0.001 for -h,-k,h+k+l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 87498 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13819	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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	2.71	2/2319 (0.1%)	1.20	5/3149 (0.2%)
1	F	4.06	4/2319 (0.2%)	1.18	6/3149 (0.2%)
2	B	0.78	1/859 (0.1%)	0.72	0/1162
2	G	0.69	0/859	0.68	0/1162
3	C	1.30	0/69	1.03	1/92 (1.1%)
3	H	1.31	0/69	0.93	0/92
4	D	0.93	1/1560 (0.1%)	0.87	3/2113 (0.1%)
4	I	0.90	1/1560 (0.1%)	0.76	1/2113 (0.0%)
5	E	0.95	0/1984	0.82	4/2699 (0.1%)
5	J	0.83	0/1984	0.75	1/2699 (0.0%)
All	All	2.14	9/13582 (0.1%)	0.94	21/18430 (0.1%)

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	F	0	1
5	J	0	1
All	All	0	2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	224	GLN	CA-CB	185.41	5.61	1.53
1	A	224	GLN	CA-CB	118.31	4.14	1.53
1	F	224	GLN	CB-CG	46.03	2.76	1.52
1	A	224	GLN	CB-CG	-39.50	0.46	1.52
4	I	158	LYS	CE-NZ	13.15	1.81	1.49
1	F	224	GLN	CD-OE1	12.90	1.52	1.24
2	B	25	CYS	CB-SG	6.04	1.92	1.82
1	F	224	GLN	CD-NE2	5.59	1.46	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	16	GLU	CG-CD	5.01	1.59	1.51

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	224	GLN	N-CA-CB	-45.82	28.13	110.60
1	A	224	GLN	CA-CB-CG	-43.14	18.49	113.40
1	A	224	GLN	N-CA-CB	-20.84	73.09	110.60
1	F	224	GLN	CB-CA-C	-12.99	84.42	110.40
1	A	224	GLN	CB-CA-C	-12.24	85.92	110.40
1	F	224	GLN	CA-CB-CG	10.71	136.95	113.40
4	D	161	LEU	CA-CB-CG	9.62	137.42	115.30
4	D	75	LEU	CA-CB-CG	7.77	133.17	115.30
1	F	18	GLY	N-CA-C	-6.79	96.13	113.10
1	A	44	ARG	NE-CZ-NH2	-6.59	117.00	120.30
5	E	40	ASP	CB-CG-OD1	6.07	123.76	118.30
5	E	23	LEU	CA-CB-CG	5.91	128.88	115.30
5	J	23	LEU	CA-CB-CG	5.80	128.65	115.30
5	E	13	LEU	CA-CB-CG	5.61	128.20	115.30
1	F	16	GLY	N-CA-C	5.59	127.09	113.10
1	F	129	ASP	CB-CG-OD1	5.41	123.17	118.30
4	I	62	LEU	CA-CB-CG	5.23	127.33	115.30
3	C	9	LEU	CA-CB-CG	5.20	127.27	115.30
1	A	110	LEU	CA-CB-CG	5.19	127.24	115.30
5	E	13	LEU	CB-CG-CD1	-5.15	102.25	111.00
4	D	75	LEU	CB-CG-CD1	5.13	119.71	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	17	ARG	Peptide
5	J	84	GLN	Peptide

## 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	2253	0	2103	17	1
1	F	2253	0	2103	37	2
2	B	836	0	803	13	2
2	G	836	0	803	13	1
3	C	68	0	75	2	0
3	H	68	0	75	1	0
4	D	1530	0	1480	16	0
4	I	1530	0	1480	26	0
5	E	1931	0	1829	24	0
5	J	1931	0	1829	32	0
6	A	90	0	0	7	0
6	B	36	0	0	2	0
6	C	6	0	0	0	0
6	D	75	0	0	1	0
6	E	99	0	0	5	0
6	F	79	0	0	9	0
6	G	36	0	0	2	0
6	H	5	0	0	0	0
6	I	70	0	0	7	0
6	J	87	0	0	7	0
All	All	13819	0	12580	175	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 7.

All (175) 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)
4:I:158:LYS:NZ	4:I:158:LYS:CE	1.81	1.41
2:G:81:ARG:HH11	2:G:81:ARG:HG2	0.94	1.09
1:A:17:ARG:NH1	6:A:2007:HOH:O	1.91	1.02
5:E:81:THR:O	5:E:83:ALA:N	1.96	0.98
2:G:81:ARG:NH1	2:G:81:ARG:HG2	1.73	0.95
5:E:86:ASN:HB3	6:E:2053:HOH:O	1.66	0.94
1:F:266:LEU:HD22	1:F:270:LEU:HD23	1.56	0.88
4:D:61:ARG:NH1	4:D:84:ASP:OD2	2.07	0.87
4:I:119:ALA:HB1	6:I:2052:HOH:O	1.74	0.86
5:E:84:GLN:NE2	5:E:85:LYS:H	1.73	0.86
5:J:84:GLN:O	5:J:86:ASN:N	2.07	0.85
1:A:17:ARG:NH2	6:A:2007:HOH:O	2.08	0.84
2:B:81:ARG:HH11	2:B:81:ARG:HG2	1.42	0.83
2:G:81:ARG:NH1	2:G:90:PRO:HB3	1.92	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:124:ARG:HH11	4:D:124:ARG:CG	1.93	0.82
5:E:84:GLN:HE21	5:E:85:LYS:H	1.27	0.81
1:F:216:THR:HA	6:F:2063:HOH:O	1.84	0.78
5:J:65:GLY:HA3	5:J:83:ALA:HA	1.63	0.78
2:G:81:ARG:HH11	2:G:81:ARG:CG	1.87	0.77
1:F:17:ARG:HB3	6:F:2005:HOH:O	1.84	0.76
2:B:4:THR:HG22	2:B:86:THR:OG1	1.86	0.76
1:F:217:TRP:HB2	6:F:2066:HOH:O	1.85	0.76
4:D:124:ARG:HG3	4:D:124:ARG:HH11	1.52	0.74
5:J:116:ASP:OD1	5:J:118:LYS:HG2	1.87	0.74
1:A:17:ARG:CZ	6:A:2007:HOH:O	2.25	0.74
5:E:86:ASN:OD1	6:E:2054:HOH:O	2.07	0.72
5:J:34:MET:HE3	5:J:70:ARG:NE	2.05	0.72
1:F:202:ARG:NH1	1:F:246:ALA:HB2	2.06	0.70
4:D:124:ARG:HD3	4:D:124:ARG:H	1.56	0.70
5:J:34:MET:HE2	5:J:70:ARG:NH2	2.06	0.69
4:I:61:ARG:NH1	4:I:84:ASP:OD2	2.24	0.69
4:I:103:LYS:HE3	6:J:2026:HOH:O	1.92	0.68
2:B:98:ASP:HB2	6:B:2036:HOH:O	1.93	0.68
5:J:142:THR:HG22	6:J:2065:HOH:O	1.93	0.67
2:G:81:ARG:HH12	2:G:90:PRO:HB3	1.57	0.67
2:G:2:GLN:HG2	6:G:2001:HOH:O	1.95	0.67
5:E:84:GLN:HE21	5:E:85:LYS:N	1.93	0.66
4:D:146:SER:H	4:D:191:SER:HB3	1.60	0.66
5:J:16:LYS:H	5:J:19:GLN:HE21	1.40	0.66
4:I:140:ASP:HA	6:I:2055:HOH:O	1.95	0.65
5:E:132:GLU:CD	5:E:132:GLU:H	2.01	0.64
1:F:187:THR:OG1	1:F:272:LEU:HD13	1.97	0.63
1:F:228:THR:HA	1:F:246:ALA:O	1.99	0.63
4:I:111:PRO:HG3	4:I:160:VAL:HG11	1.80	0.62
5:J:34:MET:HE2	5:J:70:ARG:HH21	1.65	0.62
5:J:34:MET:CE	5:J:70:ARG:NE	2.64	0.61
4:D:58:LYS:O	4:D:59:LEU:HD13	2.01	0.60
5:J:58:GLN:HG2	6:J:2028:HOH:O	2.01	0.60
4:D:61:ARG:HH12	4:D:84:ASP:CG	2.01	0.60
5:J:173:ASP:OD1	5:J:193:ARG:NH2	2.35	0.60
5:E:34:MET:HE3	5:E:70:ARG:NE	2.17	0.60
2:B:51:HIS:HD2	2:B:52:SER:O	1.86	0.59
4:I:131:LYS:HG3	6:I:2065:HOH:O	2.02	0.59
4:D:15:GLN:O	4:D:18:GLU:HG3	2.02	0.59
1:F:234:ARG:HE	1:F:242:GLN:HE21	1.48	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:HIS:HD2	1:A:119:ASP:OD2	1.84	0.59
4:D:131:LYS:HA	6:D:2059:HOH:O	2.02	0.59
5:E:81:THR:C	5:E:83:ALA:N	2.56	0.58
2:B:74:GLU:HB2	6:B:2029:HOH:O	2.03	0.58
5:J:34:MET:CE	5:J:70:ARG:HE	2.17	0.58
5:E:19:GLN:NE2	6:E:2008:HOH:O	2.36	0.58
2:B:1:ILE:O	2:B:1:ILE:CG2	2.51	0.58
4:I:158:LYS:NZ	4:I:158:LYS:CD	2.65	0.57
1:F:184:ALA:O	6:F:2052:HOH:O	2.17	0.57
4:I:81:GLN:HB3	4:I:82:PRO:HD2	1.87	0.56
1:F:229:GLU:HA	6:F:2068:HOH:O	2.04	0.56
1:A:65:ARG:NH1	6:A:2027:HOH:O	2.37	0.56
4:I:61:ARG:HH12	4:I:84:ASP:CG	2.09	0.56
1:F:234:ARG:HE	1:F:242:GLN:NE2	2.02	0.56
5:J:229:LYS:HG3	5:J:231:VAL:HG13	1.87	0.56
1:A:75:ARG:HD2	6:A:2010:HOH:O	2.06	0.55
4:I:183:ALA:O	4:I:186:ASN:ND2	2.39	0.55
1:F:14:ARG:NE	1:F:19:GLU:O	2.39	0.55
1:F:214:THR:HB	1:F:262:GLN:HB2	1.88	0.55
4:I:15:GLN:O	4:I:18:GLU:HG3	2.06	0.55
1:F:223:ASP:HA	1:F:224:GLN:HE21	1.72	0.55
5:J:84:GLN:C	5:J:86:ASN:H	2.00	0.55
4:D:124:ARG:CD	4:D:124:ARG:H	2.20	0.55
4:I:147:GLN:H	4:I:147:GLN:HE21	1.55	0.55
5:J:34:MET:HE3	5:J:70:ARG:HE	1.72	0.54
4:I:37:ARG:NH1	4:I:85:THR:O	2.40	0.54
2:B:81:ARG:CG	2:B:81:ARG:HH11	2.13	0.54
1:A:131:ARG:HE	1:A:157:ARG:NH1	2.05	0.54
4:I:119:ALA:CB	6:I:2052:HOH:O	2.43	0.53
5:J:86:ASN:N	5:J:87:PRO:CD	2.72	0.53
1:F:249:VAL:HB	1:F:250:PRO:HD2	1.91	0.53
5:E:229:LYS:HG3	5:E:231:VAL:HG13	1.91	0.52
1:F:260:HIS:HB2	6:F:2062:HOH:O	2.09	0.52
1:F:202:ARG:HD2	1:F:204:TRP:CD1	2.45	0.52
1:F:147:TRP:CZ2	3:H:9:LEU:HD23	2.45	0.52
1:F:93:HIS:HD2	1:F:119:ASP:OD2	1.92	0.52
5:J:34:MET:CE	5:J:73:LYS:O	2.59	0.51
1:F:192:HIS:O	1:F:200:THR:HB	2.11	0.51
4:I:55:GLU:OE1	4:I:57:LYS:HE3	2.10	0.51
4:D:123:LEU:O	4:D:132:SER:HB2	2.11	0.51
5:J:86:ASN:N	5:J:87:PRO:HD2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:118:LYS:NZ	6:E:2068:HOH:O	2.45	0.50
5:E:132:GLU:N	5:E:132:GLU:CD	2.64	0.50
1:A:147:TRP:CZ2	3:C:9:LEU:HD23	2.46	0.50
6:A:2083:HOH:O	2:B:99:MET:HG2	2.10	0.50
2:G:51:HIS:HD2	2:G:52:SER:O	1.95	0.50
4:I:164:ARG:HG2	5:J:168:SER:HB2	1.93	0.49
5:J:34:MET:HE1	5:J:73:LYS:O	2.13	0.49
1:F:13:SER:HB3	1:F:78:LEU:HD13	1.93	0.49
2:B:25:CYS:HB2	2:B:39:LEU:HD21	1.94	0.49
4:D:124:ARG:HH11	4:D:124:ARG:HG2	1.75	0.49
4:I:126:SER:HB3	5:J:129:GLU:HG3	1.95	0.48
1:F:257:TYR:HB2	6:F:2074:HOH:O	2.12	0.48
5:J:200:PHE:O	5:J:206:ASN:ND2	2.33	0.48
2:G:31:HIS:ND1	6:G:2011:HOH:O	2.32	0.48
1:F:202:ARG:HH11	1:F:246:ALA:HB2	1.78	0.48
5:J:64:GLU:OE1	6:J:2039:HOH:O	2.20	0.47
5:E:84:GLN:HG3	5:E:85:LYS:N	2.28	0.47
2:B:1:ILE:O	2:B:1:ILE:HG22	2.14	0.47
1:A:121:LYS:HB2	1:A:121:LYS:HE3	1.65	0.47
4:D:159:THR:HB	5:E:171:SER:OG	2.14	0.47
2:B:4:THR:CG2	2:B:86:THR:OG1	2.61	0.47
4:I:147:GLN:H	4:I:147:GLN:NE2	2.12	0.47
5:E:84:GLN:HE21	5:E:84:GLN:HA	1.80	0.47
1:F:44:ARG:NH2	1:F:61:ASP:OD1	2.48	0.47
1:A:202:ARG:HD3	1:A:244:TRP:CE3	2.50	0.47
5:E:84:GLN:HE21	5:E:84:GLN:CA	2.28	0.47
1:A:173:GLU:OE1	1:A:176:LYS:NZ	2.47	0.47
4:I:168:PHE:HD2	6:I:2063:HOH:O	1.98	0.47
5:E:84:GLN:CG	5:E:85:LYS:N	2.78	0.46
5:E:34:MET:HE2	5:E:70:ARG:NH2	2.30	0.46
1:F:203:CYS:HA	6:F:2054:HOH:O	2.14	0.46
2:G:24:ASN:HB3	2:G:65:LEU:HD11	1.98	0.46
4:I:81:GLN:HB3	4:I:82:PRO:CD	2.46	0.46
5:J:139:GLN:HB2	6:J:2064:HOH:O	2.15	0.46
1:A:219:ARG:O	1:A:221:GLY:N	2.49	0.45
4:I:133:VAL:HG12	4:I:176:TRP:HB3	1.98	0.45
5:J:34:MET:HE2	5:J:70:ARG:CZ	2.46	0.45
1:A:51:TRP:O	1:A:54:GLN:HG2	2.16	0.45
4:I:157:ASP:HB3	6:I:2060:HOH:O	2.15	0.45
1:F:144:LYS:O	1:F:148:GLU:HG3	2.17	0.45
2:B:81:ARG:NH1	2:B:81:ARG:HG2	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:86:ASN:N	5:E:87:PRO:HD3	2.31	0.45
5:J:110:ARG:HD3	6:J:2061:HOH:O	2.17	0.45
4:D:124:ARG:HG3	4:D:124:ARG:NH1	2.24	0.44
2:B:81:ARG:CG	2:B:81:ARG:NH1	2.75	0.44
4:D:159:THR:HG23	6:E:2083:HOH:O	2.17	0.44
5:J:16:LYS:HB3	5:J:16:LYS:NZ	2.33	0.44
1:F:249:VAL:HB	1:F:250:PRO:CD	2.46	0.44
1:F:81:LEU:HD13	1:F:118:TYR:CD1	2.53	0.44
2:G:4:THR:HG23	2:G:86:THR:OG1	2.17	0.44
5:J:16:LYS:H	5:J:19:GLN:NE2	2.11	0.43
5:J:29:LEU:O	5:J:30:ASN:CB	2.66	0.43
2:G:1:ILE:CG2	2:G:1:ILE:O	2.67	0.43
1:F:274:TRP:CG	1:F:275:GLU:N	2.87	0.43
4:D:130:ASP:OD1	4:D:131:LYS:N	2.43	0.43
1:F:14:ARG:NH1	1:F:21:ARG:HB2	2.34	0.42
4:I:16:GLU:HG2	6:I:2008:HOH:O	2.18	0.42
5:E:34:MET:CE	5:E:73:LYS:O	2.66	0.42
2:G:4:THR:CG2	2:G:86:THR:OG1	2.66	0.42
5:J:31:HIS:HB3	5:J:96:SER:O	2.19	0.42
1:F:202:ARG:HH11	1:F:202:ARG:HB2	1.83	0.42
5:E:203:ASN:HB3	5:E:206:ASN:ND2	2.34	0.42
5:J:127:VAL:HG23	5:J:237:ALA:HB3	2.01	0.42
4:I:5:LEU:HD22	4:I:24:CYS:SG	2.60	0.42
5:J:144:VAL:CG2	6:J:2065:HOH:O	2.67	0.41
1:F:202:ARG:NH1	1:F:202:ARG:HB2	2.36	0.41
5:E:34:MET:HE3	5:E:70:ARG:CZ	2.50	0.41
1:A:249:VAL:HG22	6:A:2077:HOH:O	2.20	0.41
2:G:21:ASN:O	2:G:69:GLU:HG3	2.20	0.41
1:F:131:ARG:HB2	1:F:131:ARG:CZ	2.51	0.41
1:A:217:TRP:CZ3	1:A:257:TYR:HB3	2.56	0.41
1:A:176:LYS:NZ	1:A:176:LYS:HB3	2.36	0.41
1:A:143:THR:HG21	3:C:9:LEU:HD22	2.03	0.40
1:F:255:GLN:HG3	1:F:255:GLN:H	1.65	0.40
1:F:219:ARG:O	1:F:221:GLY:N	2.55	0.40
5:E:34:MET:HE2	5:E:73:LYS:O	2.21	0.40
1:F:189:MET:HA	6:F:2058:HOH:O	2.20	0.40
1:F:206:LEU:HD23	1:F:242:GLN:HB3	2.03	0.40
4:I:21:THR:OG1	4:I:76:HIS:HD2	2.05	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:A:138:MET:SD	2:G:36:GLU:OE2[1_544]	1.67	0.53
2:B:81:ARG:NH2	1:F:138:MET:SD[1_444]	2.05	0.15
2:B:81:ARG:CZ	1:F:138:MET:SD[1_444]	2.06	0.14

## 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	274/276 (99%)	258 (94%)	15 (6%)	1 (0%)	39	48
1	F	274/276 (99%)	252 (92%)	15 (6%)	7 (3%)	7	4
2	B	98/100 (98%)	91 (93%)	7 (7%)	0	100	100
2	G	98/100 (98%)	95 (97%)	2 (2%)	1 (1%)	19	21
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	H	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
4	D	197/201 (98%)	190 (96%)	5 (2%)	2 (1%)	19	21
4	I	197/201 (98%)	177 (90%)	17 (9%)	3 (2%)	13	12
5	E	238/244 (98%)	229 (96%)	7 (3%)	2 (1%)	24	27
5	J	238/244 (98%)	222 (93%)	14 (6%)	2 (1%)	24	27
All	All	1628/1660 (98%)	1526 (94%)	84 (5%)	18 (1%)	17	18

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	82	SER
5	E	83	ALA
1	F	224	GLN
5	J	83	ALA
5	J	85	LYS
4	D	131	LYS
1	F	16	GLY

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Mol	Chain	Res	Type
1	F	220	ASP
1	F	222	GLU
1	F	226	GLN
1	A	220	ASP
4	I	186	ASN
1	F	223	ASP
2	G	97	ARG
4	I	131	LYS
4	I	184	CYS
4	D	200	PRO
1	F	221	GLY

### 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	232/232 (100%)	218 (94%)	14 (6%)	24	31
1	F	232/232 (100%)	216 (93%)	16 (7%)	19	24
2	B	95/95 (100%)	84 (88%)	11 (12%)	7	7
2	G	95/95 (100%)	85 (90%)	10 (10%)	8	9
3	C	7/7 (100%)	7 (100%)	0	100	100
3	H	7/7 (100%)	7 (100%)	0	100	100
4	D	175/177 (99%)	159 (91%)	16 (9%)	12	13
4	I	175/177 (99%)	161 (92%)	14 (8%)	15	18
5	E	211/214 (99%)	198 (94%)	13 (6%)	23	30
5	J	211/214 (99%)	199 (94%)	12 (6%)	25	34
All	All	1440/1450 (99%)	1334 (93%)	106 (7%)	17	21

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	17	ARG

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Mol	Chain	Res	Type
1	A	82	ARG
1	A	89	GLU
1	A	115	GLN
1	A	138	MET
1	A	176	LYS
1	A	194	VAL
1	A	196	ASP
1	A	216	THR
1	A	225	THR
1	A	230	LEU
1	A	270	LEU
1	A	273	ARG
2	B	0	MET
2	B	1	ILE
2	B	20	SER
2	B	48	LYS
2	B	70	PHE
2	B	77	GLU
2	B	81	ARG
2	B	83	ASN
2	B	89	GLN
2	B	97	ARG
2	B	99	MET
4	D	42	GLU
4	D	66	PHE
4	D	72	ASP
4	D	75	LEU
4	D	98	ASN
4	D	124	ARG
4	D	128	SER
4	D	131	LYS
4	D	149	LYS
4	D	150	ASP
4	D	151	SER
4	D	161	LEU
4	D	164	ARG
4	D	180	SER
4	D	190	ASN
4	D	191	SER
5	E	13	LEU
5	E	17	GLU
5	E	27	GLN

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Mol	Chain	Res	Type
5	E	64	GLU
5	E	84	GLN
5	E	85	LYS
5	E	132	GLU
5	E	164	LYS
5	E	175	GLN
5	E	193	ARG
5	E	205	ARG
5	E	218	SER
5	E	222	GLU
1	F	14	ARG
1	F	58	GLU
1	F	75	ARG
1	F	82	ARG
1	F	115	GLN
1	F	173	GLU
1	F	202	ARG
1	F	224	GLN
1	F	225	THR
1	F	227	ASP
1	F	253	GLN
1	F	255	GLN
1	F	264	GLU
1	F	270	LEU
1	F	272	LEU
1	F	273	ARG
2	G	1	ILE
2	G	4	THR
2	G	20	SER
2	G	34	ASP
2	G	36	GLU
2	G	48	LYS
2	G	58	LYS
2	G	70	PHE
2	G	74	GLU
2	G	81	ARG
4	I	39	GLU
4	I	42	GLU
4	I	62	LEU
4	I	65	GLN
4	I	66	PHE
4	I	72	ASP

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Mol	Chain	Res	Type
4	I	98	ASN
4	I	103	LYS
4	I	108	SER
4	I	124	ARG
4	I	147	GLN
4	I	170	SER
4	I	178	ASN
4	I	186	ASN
5	J	16	LYS
5	J	23	LEU
5	J	27	GLN
5	J	43	GLN
5	J	62	ILE
5	J	110	ARG
5	J	131	SER
5	J	142	THR
5	J	175	GLN
5	J	186	SER
5	J	224	THR
5	J	240	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	HIS
1	A	242	GLN
2	B	2	GLN
2	B	51	HIS
2	B	83	ASN
4	D	76	HIS
4	D	98	ASN
4	D	114	GLN
4	D	142	GLN
5	E	27	GLN
5	E	43	GLN
5	E	84	GLN
5	E	175	GLN
5	E	233	GLN
1	F	3	HIS
1	F	72	GLN
1	F	93	HIS
1	F	115	GLN

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Mol	Chain	Res	Type
1	F	224	GLN
1	F	242	GLN
1	F	253	GLN
2	G	51	HIS
4	I	76	HIS
4	I	98	ASN
4	I	142	GLN
4	I	147	GLN
4	I	186	ASN
5	J	19	GLN
5	J	27	GLN
5	J	43	GLN
5	J	233	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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, 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	276/276 (100%)	0.93	45 (16%) 2 4	22, 35, 76, 95	1 (0%)
1	F	276/276 (100%)	1.63	74 (26%) 1 1	21, 38, 81, 94	1 (0%)
2	B	100/100 (100%)	0.44	7 (7%) 19 27	26, 40, 52, 65	0
2	G	100/100 (100%)	0.50	10 (10%) 9 14	26, 40, 54, 64	0
3	C	9/9 (100%)	1.72	3 (33%) 0 0	21, 22, 23, 23	0
3	H	9/9 (100%)	1.01	0 100 100	17, 22, 24, 24	0
4	D	199/201 (99%)	0.73	22 (11%) 7 11	18, 35, 57, 65	0
4	I	199/201 (99%)	1.34	54 (27%) 1 1	19, 36, 82, 84	0
5	E	240/244 (98%)	0.44	14 (5%) 26 35	20, 34, 51, 62	0
5	J	240/244 (98%)	0.70	28 (11%) 6 10	20, 42, 60, 67	0
All	All	1648/1660 (99%)	0.92	257 (15%) 3 4	17, 37, 77, 95	2 (0%)

All (257) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	190	THR	12.6
1	F	220	ASP	12.4
1	F	256	ARG	11.6
1	A	194	VAL	11.4
1	F	199	ALA	10.7
1	F	193	ALA	9.9
1	F	272	LEU	9.8
1	F	276	PRO	9.4
1	F	221	GLY	9.3
1	F	271	THR	9.2
1	F	196	ASP	8.7
1	A	276	PRO	8.6
1	A	196	ASP	8.4

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Mol	Chain	Res	Type	RSRZ
1	F	249	VAL	8.3
1	F	252	GLY	8.2
1	F	273	ARG	8.0
1	F	226	GLN	7.7
1	A	197	HIS	7.5
1	A	199	ALA	7.5
1	F	275	GLU	7.2
1	F	250	PRO	7.0
4	I	166	MET	7.0
1	F	258	THR	6.9
4	I	129	SER	6.9
1	F	195	SER	6.7
4	D	129	SER	6.6
1	F	248	VAL	6.5
5	J	243	ALA	6.5
1	F	228	THR	6.5
1	F	254	GLU	6.4
4	I	135	LEU	6.4
1	A	193	ALA	6.4
1	A	222	GLU	6.1
1	F	201	LEU	6.1
1	F	191	HIS	6.1
1	A	221	GLY	6.1
1	A	195	SER	5.9
1	F	198	GLU	5.9
1	F	274	TRP	5.8
4	I	201	SER	5.8
1	F	255	GLN	5.8
1	F	192	HIS	5.8
4	I	133	VAL	5.8
4	D	180	SER	5.7
4	I	114	GLN	5.7
1	F	259	CYS	5.7
4	I	149	LYS	5.6
1	A	228	THR	5.6
1	F	225	THR	5.6
1	F	246	ALA	5.5
5	J	224	THR	5.5
1	F	217	TRP	5.4
1	A	225	THR	5.3
4	D	190	ASN	5.3
1	F	197	HIS	5.3

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Mol	Chain	Res	Type	RSRZ
5	E	244	ASP	5.2
1	A	274	TRP	5.2
1	F	251	SER	5.1
4	I	181	ASP	4.9
4	I	134	CYS	4.9
1	F	229	GLU	4.9
4	I	167	ASP	4.7
4	I	180	SER	4.7
5	J	240	TRP	4.7
4	D	128	SER	4.7
1	F	194	VAL	4.6
5	J	220	ASN	4.6
5	J	204	PRO	4.6
4	I	130	ASP	4.6
1	F	189	MET	4.5
1	F	247	VAL	4.5
1	A	223	ASP	4.5
5	E	220	ASN	4.5
1	A	227	ASP	4.5
1	F	219	ARG	4.4
4	I	174	VAL	4.4
5	J	144	VAL	4.4
4	I	126	SER	4.4
5	J	200	PHE	4.3
1	F	204	TRP	4.3
4	D	130	ASP	4.3
1	A	250	PRO	4.2
4	D	151	SER	4.2
1	F	257	TYR	4.2
1	F	253	GLN	4.1
4	I	164	ARG	4.0
4	D	201	SER	4.0
1	F	216	THR	4.0
4	I	185	ALA	4.0
1	F	17	ARG	4.0
1	A	268	LYS	4.0
4	I	194	PRO	3.9
1	A	273	ARG	3.8
4	D	149	LYS	3.8
4	I	151	SER	3.8
4	I	123	LEU	3.7
5	E	240	TRP	3.7

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Mol	Chain	Res	Type	RSRZ
5	J	132	GLU	3.7
5	J	85	LYS	3.7
5	J	163	GLY	3.7
1	A	254	GLU	3.6
1	A	201	LEU	3.6
2	B	99	MET	3.6
4	D	152	ASP	3.6
5	J	244	ASP	3.5
4	I	173	ALA	3.5
2	B	77	GLU	3.5
4	D	127	LYS	3.4
4	I	189	ASN	3.4
1	A	260	HIS	3.4
1	F	222	GLU	3.3
4	I	182	PHE	3.3
5	J	222	GLU	3.3
1	F	188	HIS	3.3
2	G	73	THR	3.3
2	G	77	GLU	3.3
1	F	270	LEU	3.3
5	E	144	VAL	3.3
1	A	257	TYR	3.2
4	I	168	PHE	3.2
5	J	242	ARG	3.2
5	E	222	GLU	3.2
4	I	163	MET	3.2
5	J	135	ILE	3.1
5	E	226	ASP	3.1
4	I	175	ALA	3.1
4	I	165	SER	3.1
5	J	146	LEU	3.1
5	E	218	SER	3.1
1	A	251	SER	3.1
1	A	253	GLN	3.1
1	F	58	GLU	3.1
5	E	143	LEU	3.0
4	D	181	ASP	3.0
1	F	90	ALA	3.0
1	A	252	GLY	3.0
4	I	150	ASP	3.0
1	F	262	GLN	3.0
5	E	243	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
4	D	135	LEU	3.0
1	F	202	ARG	3.0
2	G	81	ARG	3.0
4	I	198	PHE	3.0
1	F	231	VAL	2.9
1	F	9	PHE	2.9
4	I	193	ILE	2.9
1	F	99	TYR	2.9
1	A	215	LEU	2.9
2	B	16	GLU	2.9
1	A	226	GLN	2.9
5	J	205	ARG	2.8
1	A	261	VAL	2.8
4	I	137	THR	2.8
1	A	219	ARG	2.7
2	G	88	SER	2.7
4	I	191	SER	2.7
1	F	203	CYS	2.7
4	I	136	PHE	2.7
1	A	256	ARG	2.7
1	A	272	LEU	2.7
4	D	185	ALA	2.7
1	F	187	THR	2.7
5	J	145	CYS	2.6
1	F	223	ASP	2.6
1	F	227	ASP	2.6
1	F	108	ARG	2.6
2	G	47	GLU	2.6
4	I	176	TRP	2.6
2	B	19	LYS	2.6
4	I	127	LYS	2.6
1	A	262	GLN	2.6
1	F	105	SER	2.6
1	A	248	VAL	2.6
4	I	195	GLU	2.6
4	D	35	TRP	2.6
1	F	268	LYS	2.6
1	F	89	GLU	2.5
1	A	220	ASP	2.5
4	I	120	VAL	2.5
5	J	225	GLN	2.5
5	J	223	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	41	ALA	2.5
1	F	18	GLY	2.5
2	G	16	GLU	2.5
4	I	162	ASP	2.5
4	I	89	LEU	2.5
4	I	116	PRO	2.5
5	J	226	ASP	2.5
2	G	71	THR	2.5
2	G	44	GLU	2.5
1	A	230	LEU	2.5
4	I	128	SER	2.4
5	J	193	ARG	2.4
4	I	35	TRP	2.4
1	A	9	PHE	2.4
5	E	142	THR	2.4
4	D	189	ASN	2.4
4	D	191	SER	2.4
5	J	192	SER	2.4
1	A	58	GLU	2.4
5	J	228	ALA	2.4
2	G	75	LYS	2.4
3	C	2	ILE	2.4
4	I	119	ALA	2.4
1	A	106	ASP	2.3
4	I	115	ASN	2.3
1	A	198	GLU	2.3
4	I	121	TYR	2.3
5	J	180	GLN	2.3
1	F	25	VAL	2.3
5	J	83	ALA	2.3
3	C	7	PHE	2.3
5	J	168	SER	2.3
4	I	161	LEU	2.3
4	D	174	VAL	2.3
5	E	83	ALA	2.3
4	I	200	PRO	2.2
4	D	195	GLU	2.2
1	F	15	PRO	2.2
1	A	24	ALA	2.2
1	A	99	TYR	2.2
1	F	42	SER	2.2
4	I	142	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
4	I	190	ASN	2.2
1	F	8	PHE	2.2
4	I	148	SER	2.2
4	D	150	ASP	2.2
1	F	230	LEU	2.2
4	I	59	LEU	2.2
1	F	218	GLN	2.2
1	A	216	THR	2.2
1	F	24	ALA	2.2
2	B	74	GLU	2.2
4	I	101	PHE	2.1
2	B	73	THR	2.1
4	D	192	ILE	2.1
4	I	113	ILE	2.1
4	D	133	VAL	2.1
4	D	144	ASN	2.1
5	E	190	LEU	2.1
5	E	84	GLN	2.1
1	F	244	TRP	2.1
2	G	36	GLU	2.1
1	F	40	ALA	2.1
3	C	6	VAL	2.1
4	I	157	ASP	2.1
4	I	197	THR	2.1
2	B	45	ARG	2.1
1	A	89	GLU	2.1
1	A	15	PRO	2.1
1	F	91	GLY	2.0
1	F	182	THR	2.0
5	J	147	ALA	2.0
5	E	180	GLN	2.0
1	A	16	GLY	2.0
5	J	40	ASP	2.0
1	A	108	ARG	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 carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.