



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 30, 2020 – 07:43 PM JST

PDB ID : 6LHG  
Title : Crystal structure of chicken cCD8aa/pBF2\*04:01  
Authors : Liu, Y.J.; Xia, C.  
Deposited on : 2019-12-08  
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.14.6  
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) : 2.14.6

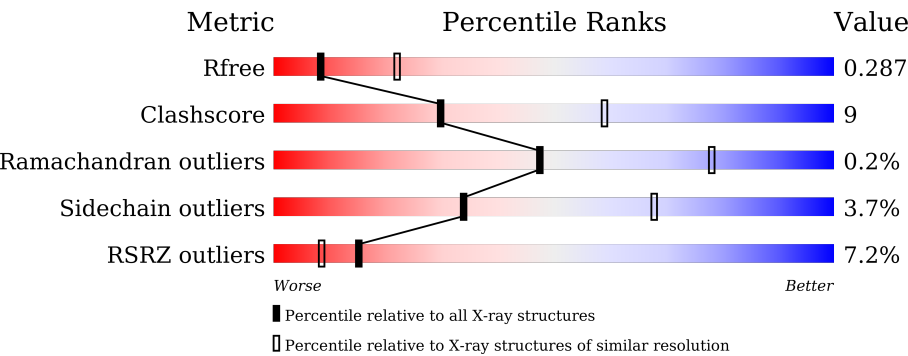
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 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	272	<div><div></div><div>89%11%</div></div>
1	D	272	<div><div>7%</div><div>90%10%</div></div>
2	B	97	<div><div>%</div><div>87%13%</div></div>
2	E	97	<div><div>4%</div><div>80%18%</div></div>
3	C	8	<div><div></div><div>75%25%</div></div>
3	F	8	<div><div></div><div>88%13%</div></div>

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Mol	Chain	Length	Quality of chain
4	G	117	<div><div></div><div>7%</div><div>65%</div><div>30%</div><div></div><div></div></div>
4	H	117	<div><div></div><div>13%</div><div>62%</div><div>30%</div><div></div><div></div></div>
4	I	117	<div><div></div><div>23%</div><div>61%</div><div>35%</div><div></div><div></div></div>
4	J	117	<div><div></div><div>9%</div><div>66%</div><div>26%</div><div></div><div></div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9818 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 MHC class I alpha chain 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	0	0
			2220	1397	402	414	7			
1	D	272	Total	C	N	O	S	0	0	0
			2220	1397	402	414	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	244	GLU	ASP	engineered mutation	UNP O46790
A	271	LYS	-	expression tag	UNP O46790
A	272	LEU	-	expression tag	UNP O46790
D	244	GLU	ASP	engineered mutation	UNP O46790
D	271	LYS	-	expression tag	UNP O46790
D	272	LEU	-	expression tag	UNP O46790

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	97	Total	C	N	O	S	0	0	0
			767	490	125	147	5			
2	E	97	Total	C	N	O	S	0	0	0
			767	490	125	147	5			

- Molecule 3 is a protein called IE8 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	8	Total	C	N	O	0	0	0
			72	47	10	15			
3	F	8	Total	C	N	O	0	0	0
			72	47	10	15			

- Molecule 4 is a protein called CD8 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	112	Total 914	C 579	N 163	O 166	S 6	0	0	0
4	H	112	Total 914	C 579	N 163	O 166	S 6	0	0	0
4	I	112	Total 914	C 579	N 163	O 166	S 6	0	0	0
4	J	112	Total 914	C 579	N 163	O 166	S 6	0	0	0

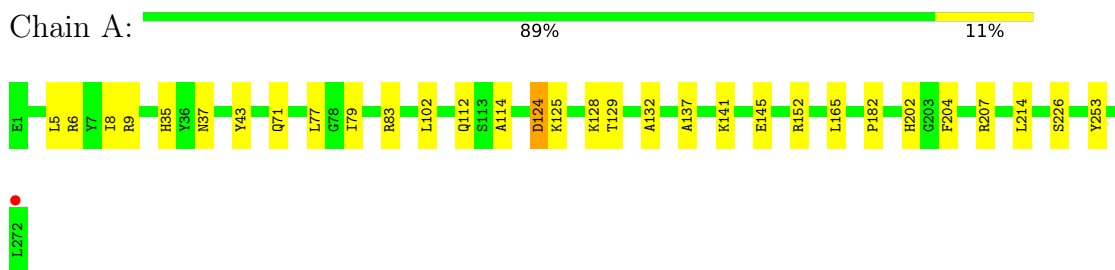
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	17	Total 17	O 17	0	0
5	B	13	Total 13	O 13	0	0
5	G	2	Total 2	O 2	0	0
5	H	2	Total 2	O 2	0	0
5	D	5	Total 5	O 5	0	0
5	E	4	Total 4	O 4	0	0
5	J	1	Total 1	O 1	0	0

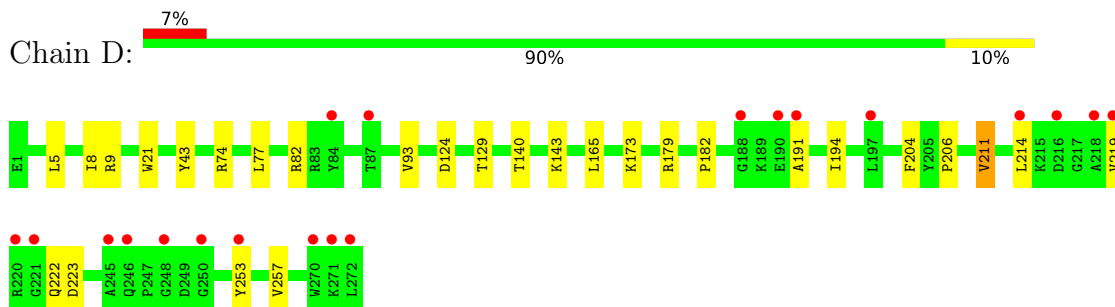
### 3 Residue-property plots [i](#)

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.

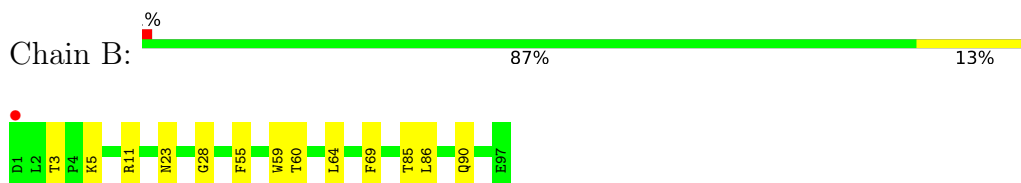
- Molecule 1: MHC class I alpha chain 2



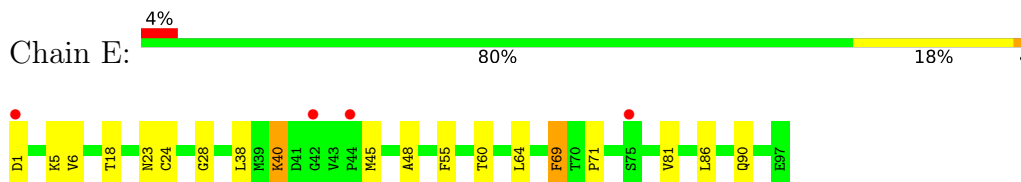
- Molecule 1: MHC class I alpha chain 2




- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin




- Molecule 3: IE8 peptide

Chain C:  75% 25%



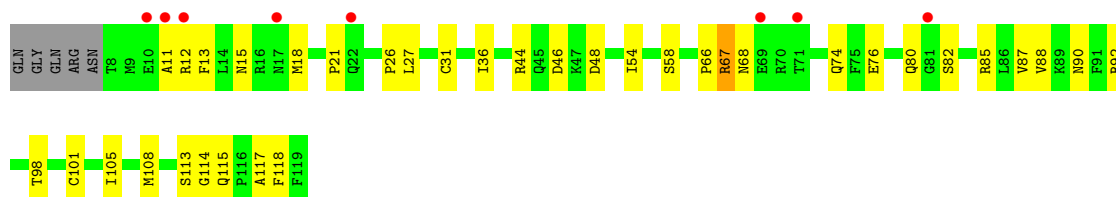
- Molecule 3: IE8 peptide

Chain F:  88% 13%



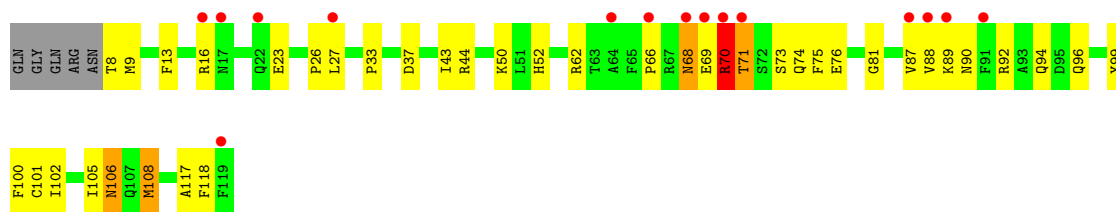
- Molecule 4: CD8 alpha chain

Chain G:  7% 65% 30% ..



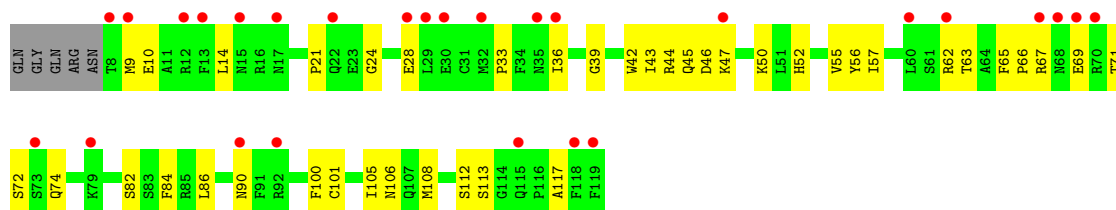
- Molecule 4: CD8 alpha chain

Chain H:  13% 62% 30% ..



- Molecule 4: CD8 alpha chain

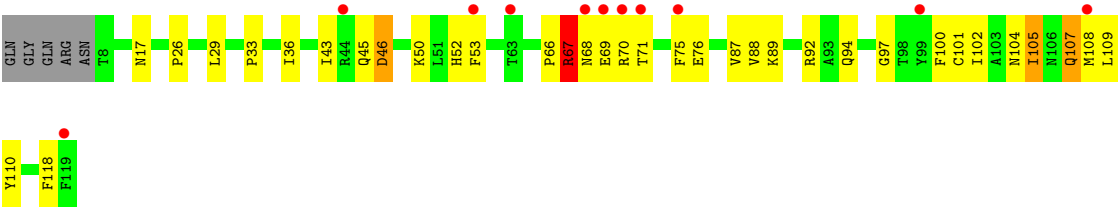
Chain I:  23% 61% 35% .



- Molecule 4: CD8 alpha chain

Chain J:  9% 66% 26% ..







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.58Å 90.82Å 94.87Å 90.00° 98.61° 90.00°	Depositor
Resolution (Å)	29.87 – 2.80 29.85 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.87-2.80) 99.7 (29.85-2.80)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.78 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.252 , 0.288 0.253 , 0.287	Depositor DCC
$R_{free}$ test set	1874 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.6	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 37.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.012 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	9818	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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	0.26	0/2283	0.45	0/3102
1	D	0.28	0/2283	0.48	1/3102 (0.0%)
2	B	0.26	0/791	0.45	0/1076
2	E	0.26	0/791	0.44	0/1076
3	C	0.27	0/74	0.38	0/97
3	F	0.26	0/74	0.34	0/97
4	G	0.33	0/937	0.59	0/1260
4	H	0.34	0/937	0.63	0/1260
4	I	0.36	0/937	0.59	0/1260
4	J	0.37	0/937	0.65	2/1260 (0.2%)
All	All	0.30	0/10044	0.52	3/13590 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	67	ARG	CB-CA-C	6.37	123.14	110.40
1	D	82	ARG	NE-CZ-NH1	5.90	123.25	120.30
4	J	67	ARG	O-C-N	5.33	131.23	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	2220	0	2106	22	1
1	D	2220	0	2106	14	0
2	B	767	0	728	7	0
2	E	767	0	728	11	0
3	C	72	0	62	2	0
3	F	72	0	62	1	0
4	G	914	0	879	24	0
4	H	914	0	879	38	1
4	I	914	0	879	38	0
4	J	914	0	879	56	0
5	A	17	0	0	0	0
5	B	13	0	0	0	0
5	D	5	0	0	0	0
5	E	4	0	0	1	0
5	G	2	0	0	0	0
5	H	2	0	0	0	0
5	J	1	0	0	1	0
All	All	9818	0	9308	180	1

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 9.

All (180) 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:66:PRO:CA	4:J:108:MET:HE1	1.31	1.58
4:I:66:PRO:HA	4:J:108:MET:CE	1.10	1.55
4:I:66:PRO:HA	4:J:108:MET:HE3	1.23	1.07
4:I:66:PRO:C	4:J:108:MET:HE1	1.74	1.06
4:I:66:PRO:CA	4:J:108:MET:CE	2.03	1.03
4:J:46:ASP:OD2	4:J:50:LYS:NZ	1.92	1.03
4:H:66:PRO:O	4:H:69:GLU:OE1	1.78	1.00
4:J:46:ASP:HB2	4:J:50:LYS:CG	1.92	1.00
4:J:46:ASP:HB2	4:J:50:LYS:HG2	1.40	0.99
4:J:46:ASP:OD2	4:J:50:LYS:CE	2.19	0.90
4:G:67:ARG:HB3	4:G:67:ARG:HH21	1.39	0.88
4:G:67:ARG:HB3	4:G:67:ARG:NH2	1.88	0.87
4:J:46:ASP:HB2	4:J:50:LYS:CD	2.06	0.84
4:G:12:ARG:NH2	4:G:113:SER:O	2.11	0.83
4:G:76:GLU:HB2	4:G:87:VAL:HG22	1.68	0.74
4:G:36:ILE:HD12	4:G:82:SER:HA	1.70	0.74
4:I:10:GLU:HA	4:I:112:SER:HB2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:LEU:HD13	2:B:90:GLN:HG3	1.74	0.70
4:I:56:TYR:CD2	4:J:107:GLN:HG2	2.27	0.69
1:A:226:SER:H	4:H:106:ASN:HD21	1.40	0.69
4:G:26:PRO:HA	4:G:88:VAL:O	1.93	0.69
4:J:67:ARG:N	4:J:67:ARG:HD2	2.07	0.69
4:H:50:LYS:HE3	4:H:52:HIS:NE2	2.08	0.68
4:I:67:ARG:N	4:J:108:MET:HE1	2.08	0.68
4:G:44:ARG:HB2	4:G:54:ILE:HD11	1.75	0.68
4:H:27:LEU:O	4:H:88:VAL:HG13	1.94	0.68
4:G:90:ASN:HD22	4:G:92:ARG:HH21	1.41	0.68
1:D:124:ASP:OD2	1:D:129:THR:OG1	2.12	0.68
1:A:182:PRO:HB3	1:A:204:PHE:HB3	1.75	0.67
4:I:66:PRO:HA	4:J:108:MET:HE1	0.66	0.66
4:I:105:ILE:O	4:I:108:MET:HB2	1.96	0.65
4:J:26:PRO:HA	4:J:88:VAL:O	1.97	0.65
1:D:191:ALA:O	1:D:194:ILE:HG13	1.98	0.64
4:J:46:ASP:CB	4:J:50:LYS:HG2	2.21	0.64
1:D:182:PRO:HB3	1:D:204:PHE:HB3	1.78	0.63
4:I:67:ARG:N	4:J:108:MET:CE	2.62	0.63
1:D:211:VAL:HG12	1:D:257:VAL:HG22	1.81	0.63
4:H:50:LYS:HE3	4:H:52:HIS:CE1	2.33	0.63
4:J:76:GLU:HB2	4:J:87:VAL:HG12	1.83	0.61
1:A:152:ARG:NH2	3:C:4:PHE:O	2.28	0.60
4:J:45:GLN:HA	4:J:50:LYS:O	2.02	0.60
4:G:21:PRO:HG3	4:G:117:ALA:HB1	1.83	0.59
4:J:66:PRO:C	4:J:68:ASN:H	2.06	0.59
4:J:105:ILE:HD12	4:J:105:ILE:C	2.23	0.59
4:I:63:THR:HG1	4:I:65:PHE:HE2	1.51	0.58
4:J:104:ASN:HB2	4:J:109:LEU:HD23	1.85	0.58
4:J:46:ASP:OD2	4:J:50:LYS:CD	2.52	0.58
4:I:10:GLU:HG2	4:I:113:SER:H	1.68	0.57
4:H:105:ILE:HG22	4:H:105:ILE:O	2.05	0.57
4:J:46:ASP:HB2	4:J:50:LYS:HE2	1.87	0.57
4:G:13:PHE:CE1	4:G:115:GLN:HG2	2.40	0.56
1:A:226:SER:H	4:H:106:ASN:ND2	2.03	0.56
4:H:27:LEU:N	4:H:88:VAL:HG22	2.19	0.56
4:J:46:ASP:CG	4:J:50:LYS:HE2	2.25	0.56
1:A:226:SER:N	4:H:106:ASN:HD21	2.04	0.56
4:I:45:GLN:HB2	4:I:100:PHE:HE2	1.70	0.56
4:J:50:LYS:HE3	4:J:52:HIS:CE1	2.41	0.56
4:J:46:ASP:OD2	4:J:50:LYS:HD3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:214:LEU:O	1:D:253:TYR:HA	2.07	0.55
4:J:46:ASP:CB	4:J:50:LYS:CD	2.82	0.55
4:J:46:ASP:HB2	4:J:50:LYS:CE	2.36	0.54
4:J:46:ASP:CG	4:J:50:LYS:CE	2.75	0.54
4:J:46:ASP:CB	4:J:50:LYS:HE2	2.38	0.54
4:J:43:ILE:HA	4:J:52:HIS:O	2.07	0.54
4:G:105:ILE:O	4:G:108:MET:HB2	2.07	0.53
4:G:80:GLN:OE1	4:G:85:ARG:NH1	2.42	0.53
4:J:105:ILE:O	4:J:105:ILE:HD12	2.07	0.53
4:J:33:PRO:HG2	4:J:36:ILE:HG22	1.89	0.53
2:E:40:LYS:HB2	2:E:45:MET:HG2	1.89	0.53
4:H:75:PHE:CE1	4:H:88:VAL:HB	2.43	0.53
4:J:108:MET:HG2	4:J:110:TYR:OH	2.09	0.53
4:I:36:ILE:HD12	4:I:82:SER:HA	1.91	0.53
4:I:66:PRO:CA	4:J:108:MET:HE3	2.07	0.52
4:G:15:ASN:ND2	4:G:18:MET:HB2	2.25	0.52
4:I:21:PRO:HG3	4:I:117:ALA:HB1	1.92	0.52
1:A:124:ASP:OD2	1:A:129:THR:OG1	2.26	0.52
1:A:102:LEU:HD23	4:H:81:GLY:HA3	1.91	0.51
2:B:23:ASN:HB3	2:B:64:LEU:HD11	1.93	0.51
2:B:28:GLY:HA2	2:B:60:THR:HB	1.93	0.51
2:E:18:THR:O	2:E:71:PRO:HD2	2.10	0.51
4:G:11:ALA:HA	4:G:31:CYS:HA	1.90	0.51
1:A:207:ARG:NH1	4:H:37:ASP:OD1	2.43	0.51
1:D:8:ILE:HB	2:E:55:PHE:CZ	2.45	0.51
4:H:96:GLN:HA	4:H:117:ALA:O	2.11	0.51
4:J:43:ILE:CG1	4:J:100:PHE:HB2	2.41	0.51
4:H:9:MET:HG2	4:H:33:PRO:HA	1.92	0.51
4:H:26:PRO:HA	4:H:88:VAL:O	2.12	0.50
4:I:50:LYS:HE3	4:I:52:HIS:HE1	1.76	0.50
4:H:71:THR:O	4:H:74:GLN:N	2.41	0.50
4:I:43:ILE:HD11	4:J:109:LEU:HD12	1.94	0.50
4:H:44:ARG:HD3	4:H:99:TYR:CZ	2.47	0.49
4:J:46:ASP:CB	4:J:50:LYS:HD3	2.42	0.49
2:E:69:PHE:CZ	2:E:71:PRO:HG3	2.47	0.49
4:H:50:LYS:HE3	4:H:52:HIS:HE2	1.75	0.49
4:J:53:PHE:HD2	4:J:66:PRO:HG3	1.78	0.49
4:H:13:PHE:CE1	4:H:27:LEU:HD11	2.48	0.48
4:G:21:PRO:HD2	4:G:118:PHE:O	2.13	0.48
4:I:55:VAL:HG11	4:I:86:LEU:HD13	1.96	0.48
4:G:11:ALA:C	4:G:12:ARG:HE	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:8:THR:OG1	4:H:9:MET:N	2.47	0.47
1:A:125:LYS:HE2	4:H:16:ARG:HH22	1.79	0.47
4:J:71:THR:HG22	4:J:75:PHE:HB2	1.95	0.47
4:J:76:GLU:HB2	4:J:87:VAL:CG1	2.44	0.47
1:A:8:ILE:HB	2:B:55:PHE:CZ	2.50	0.47
4:G:54:ILE:O	4:G:66:PRO:HD3	2.13	0.47
4:H:13:PHE:CD1	4:H:27:LEU:HD11	2.50	0.47
4:H:27:LEU:H	4:H:88:VAL:HG22	1.79	0.47
1:D:222:GLN:HG2	4:J:104:ASN:ND2	2.29	0.47
4:G:44:ARG:NH1	4:G:46:ASP:OD1	2.48	0.46
4:H:74:GLN:HG2	4:H:92:ARG:HH12	1.81	0.46
4:J:76:GLU:OE2	4:J:89:LYS:HD2	2.16	0.46
2:E:28:GLY:HA2	2:E:60:THR:HB	1.97	0.46
4:J:66:PRO:C	4:J:68:ASN:N	2.69	0.46
1:A:202:HIS:HB3	2:B:11:ARG:O	2.16	0.46
4:I:42:TRP:HB2	4:I:55:VAL:HG12	1.98	0.45
4:J:92:ARG:HB3	4:J:94:GLN:OE1	2.16	0.45
1:A:125:LYS:HB3	4:H:16:ARG:HH12	1.81	0.45
1:A:125:LYS:HE2	4:H:16:ARG:HH12	1.81	0.45
4:H:27:LEU:HB3	4:H:88:VAL:CG1	2.47	0.45
4:I:42:TRP:CD1	4:I:86:LEU:HB2	2.51	0.45
2:E:6:VAL:HG21	2:E:81:VAL:HG21	1.98	0.45
4:I:24:GLY:HA2	4:I:90:ASN:OD1	2.17	0.45
4:J:46:ASP:HB2	4:J:50:LYS:HD3	1.95	0.45
1:D:5:LEU:HB2	1:D:165:LEU:HD13	1.98	0.45
1:D:21:TRP:CH2	1:D:74:ARG:HB2	2.52	0.45
4:G:68:ASN:HA	4:H:108:MET:CE	2.47	0.45
4:H:43:ILE:HG13	4:H:100:PHE:HB2	1.99	0.44
4:G:27:LEU:O	4:G:87:VAL:HA	2.18	0.44
4:H:43:ILE:CG1	4:H:100:PHE:HB2	2.47	0.44
4:G:46:ASP:HB2	4:G:48:ASP:OD1	2.17	0.44
4:I:9:MET:O	4:I:10:GLU:HG3	2.18	0.44
1:D:219:VAL:O	4:I:106:ASN:HA	2.18	0.44
4:J:29:LEU:N	5:J:201:HOH:O	2.46	0.43
1:A:214:LEU:O	1:A:253:TYR:HA	2.18	0.43
4:I:67:ARG:HD2	4:I:67:ARG:HA	1.84	0.43
4:H:43:ILE:HD13	4:H:102:ILE:HD11	2.00	0.43
4:I:45:GLN:HA	4:I:50:LYS:O	2.18	0.43
4:I:65:PHE:CZ	4:I:72:SER:OG	2.71	0.43
4:I:42:TRP:HB3	4:I:86:LEU:HD22	1.99	0.43
4:I:67:ARG:N	4:J:108:MET:HE2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:ARG:HH12	4:H:37:ASP:CG	2.21	0.43
1:A:35:HIS:CE1	1:A:37:ASN:HD22	2.35	0.43
1:D:9:ARG:HH12	3:F:2:ASP:CG	2.21	0.43
4:I:14:LEU:HD22	4:I:28:GLU:HG3	2.01	0.43
4:J:43:ILE:HD13	4:J:102:ILE:HD11	1.99	0.43
1:A:132:ALA:HB1	1:A:137:ALA:HB3	2.01	0.43
2:B:3:THR:HG22	2:B:85:THR:HB	2.01	0.42
4:H:96:GLN:HB3	4:H:118:PHE:CD1	2.54	0.42
2:E:86:LEU:HD13	2:E:90:GLN:HG2	2.01	0.42
4:G:12:ARG:HH12	4:G:114:GLY:C	2.22	0.42
1:A:141:LYS:HE3	1:A:145:GLU:OE1	2.20	0.42
2:E:23:ASN:HB3	2:E:64:LEU:HD11	2.01	0.42
4:J:105:ILE:CG1	4:J:105:ILE:O	2.68	0.42
1:D:140:THR:O	1:D:143:LYS:HG2	2.19	0.42
2:E:24:CYS:HB2	2:E:38:LEU:HD21	2.01	0.42
4:I:33:PRO:HG3	4:I:84:PHE:CE1	2.55	0.42
4:H:70:ARG:HD3	4:H:70:ARG:HA	1.43	0.42
4:J:50:LYS:HB2	4:J:52:HIS:HE1	1.84	0.42
4:H:92:ARG:HB3	4:H:94:GLN:OE1	2.19	0.41
4:G:98:THR:HA	4:G:115:GLN:O	2.20	0.41
1:A:9:ARG:HH12	3:C:2:ASP:CG	2.24	0.41
4:H:76:GLU:O	4:H:87:VAL:HG12	2.20	0.41
4:I:44:ARG:NH1	4:I:46:ASP:OD1	2.49	0.41
4:J:97:GLY:HA2	4:J:118:PHE:CZ	2.54	0.41
4:I:69:GLU:HG3	4:I:71:THR:H	1.85	0.41
4:J:104:ASN:CB	4:J:109:LEU:HD23	2.50	0.41
1:D:77:LEU:HD13	1:D:93:VAL:HG23	2.03	0.41
4:H:90:ASN:HB3	4:H:92:ARG:NE	2.35	0.41
4:I:62:ARG:HE	4:I:62:ARG:HB2	1.71	0.41
4:I:67:ARG:H	4:J:108:MET:HE2	1.86	0.41
4:J:66:PRO:O	4:J:68:ASN:N	2.41	0.41
1:A:114:ALA:HB2	2:B:59:TRP:CE2	2.56	0.41
4:G:67:ARG:HB3	4:G:67:ARG:CZ	2.48	0.40
4:H:71:THR:O	4:H:75:PHE:N	2.54	0.40
1:D:179:ARG:HH11	1:D:206:PRO:HD3	1.86	0.40
1:A:5:LEU:HB2	1:A:165:LEU:HD13	2.04	0.40
1:A:79:ILE:O	1:A:83:ARG:HG3	2.22	0.40
2:E:48:ALA:O	5:E:101:HOH:O	2.21	0.40
2:E:1:ASP:H2	4:I:67:ARG:HE	1.70	0.40
4:I:39:GLY:HA3	4:I:57:ILE:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:LYS:CD	4:H:68:ASN:ND2[2_546]	1.71	0.49

## 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	270/272 (99%)	264 (98%)	6 (2%)	0	100	100
1	D	270/272 (99%)	264 (98%)	6 (2%)	0	100	100
2	B	95/97 (98%)	94 (99%)	1 (1%)	0	100	100
2	E	95/97 (98%)	94 (99%)	1 (1%)	0	100	100
3	C	6/8 (75%)	6 (100%)	0	0	100	100
3	F	6/8 (75%)	6 (100%)	0	0	100	100
4	G	110/117 (94%)	106 (96%)	4 (4%)	0	100	100
4	H	110/117 (94%)	105 (96%)	4 (4%)	1 (1%)	17	46
4	I	110/117 (94%)	107 (97%)	3 (3%)	0	100	100
4	J	110/117 (94%)	106 (96%)	3 (3%)	1 (1%)	17	46
All	All	1182/1222 (97%)	1152 (98%)	28 (2%)	2 (0%)	47	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	70	ARG
4	J	69	GLU

### 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	229/229 (100%)	223 (97%)	6 (3%)	46	79
1	D	229/229 (100%)	225 (98%)	4 (2%)	60	87
2	B	85/85 (100%)	83 (98%)	2 (2%)	49	81
2	E	85/85 (100%)	82 (96%)	3 (4%)	36	70
3	C	7/7 (100%)	7 (100%)	0	100	100
3	F	7/7 (100%)	7 (100%)	0	100	100
4	G	100/104 (96%)	96 (96%)	4 (4%)	31	65
4	H	100/104 (96%)	90 (90%)	10 (10%)	7	22
4	I	100/104 (96%)	97 (97%)	3 (3%)	41	75
4	J	100/104 (96%)	93 (93%)	7 (7%)	15	40
All	All	1042/1058 (98%)	1003 (96%)	39 (4%)	34	68

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	43	TYR
1	A	71	GLN
1	A	77	LEU
1	A	112	GLN
1	A	124	ASP
2	B	5	LYS
2	B	69	PHE
4	G	58	SER
4	G	67	ARG
4	G	74	GLN
4	G	101	CYS
4	H	23	GLU
4	H	62	ARG
4	H	68	ASN
4	H	70	ARG
4	H	71	THR
4	H	73	SER
4	H	89	LYS
4	H	101	CYS

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Mol	Chain	Res	Type
4	H	106	ASN
4	H	108	MET
1	D	43	TYR
1	D	173	LYS
1	D	211	VAL
1	D	223	ASP
2	E	5	LYS
2	E	40	LYS
2	E	69	PHE
4	I	47	LYS
4	I	74	GLN
4	I	101	CYS
4	J	17	ASN
4	J	46	ASP
4	J	67	ARG
4	J	70	ARG
4	J	101	CYS
4	J	105	ILE
4	J	107	GLN

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

Mol	Chain	Res	Type
1	A	35	HIS
2	B	62	GLN
4	G	90	ASN
4	H	106	ASN
4	I	52	HIS
4	J	52	HIS

### 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 monosaccharides 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	272/272 (100%)	-0.21	1 (0%) 92 91	37, 53, 91, 117	0
1	D	272/272 (100%)	0.32	20 (7%) 14 8	40, 73, 131, 174	0
2	B	97/97 (100%)	-0.22	1 (1%) 82 77	37, 49, 69, 91	0
2	E	97/97 (100%)	0.26	4 (4%) 37 27	55, 76, 112, 129	0
3	C	8/8 (100%)	0.07	0 100 100	47, 48, 59, 67	0
3	F	8/8 (100%)	0.19	0 100 100	48, 70, 76, 79	0
4	G	112/117 (95%)	0.47	8 (7%) 16 9	56, 91, 122, 135	0
4	H	112/117 (95%)	0.83	15 (13%) 3 1	50, 87, 126, 147	0
4	I	112/117 (95%)	1.40	27 (24%) 0 0	95, 131, 152, 157	0
4	J	112/117 (95%)	0.79	11 (9%) 7 4	72, 98, 146, 172	0
All	All	1202/1222 (98%)	0.36	87 (7%) 15 8	37, 76, 136, 174	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	J	68	ASN	10.7
4	J	71	THR	8.5
1	D	248	GLY	8.2
1	D	272	LEU	6.8
4	H	68	ASN	6.3
4	J	70	ARG	6.2
1	D	246	GLN	6.2
4	I	119	PHE	6.1
4	I	35	ASN	5.6
4	H	66	PRO	5.5
4	I	68	ASN	5.0
2	E	75	SER	4.9
2	E	1	ASP	4.7

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Mol	Chain	Res	Type	RSRZ
1	D	190	GLU	4.4
4	H	71	THR	4.4
4	H	69	GLU	4.3
4	J	69	GLU	4.3
4	I	73	SER	4.2
4	G	71	THR	4.1
4	I	12	ARG	4.0
4	J	119	PHE	4.0
4	I	92	ARG	3.9
1	A	272	LEU	3.8
1	D	191	ALA	3.7
4	I	67	ARG	3.6
4	I	13	PHE	3.5
1	D	219	VAL	3.4
4	G	17	ASN	3.4
1	D	188	GLY	3.2
4	J	44	ARG	3.1
4	H	16	ARG	3.1
4	G	11	ALA	3.0
4	I	60	LEU	2.9
1	D	197	LEU	2.9
1	D	270	TRP	2.9
4	I	29	LEU	2.8
4	H	119	PHE	2.8
1	D	245	ALA	2.7
4	I	79	LYS	2.7
4	G	12	ARG	2.7
2	E	44	PRO	2.7
4	H	17	ASN	2.6
4	I	115	GLN	2.6
1	D	87	THR	2.6
4	H	87	VAL	2.6
4	H	27	LEU	2.6
4	I	28	GLU	2.6
4	J	53	PHE	2.5
4	I	47	LYS	2.5
4	I	32	MET	2.5
4	I	22	GLN	2.5
4	I	69	GLU	2.5
4	H	88	VAL	2.5
4	J	108	MET	2.5
1	D	253	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
4	H	70	ARG	2.4
4	H	91	PHE	2.4
1	D	216	ASP	2.4
2	B	1	ASP	2.4
4	H	64	ALA	2.4
4	J	75	PHE	2.4
4	G	81	GLY	2.4
4	I	70	ARG	2.4
4	I	17	ASN	2.3
2	E	42	GLY	2.3
4	I	62	ARG	2.3
4	I	36	ILE	2.3
1	D	220	ARG	2.3
1	D	250	GLY	2.3
1	D	221	GLY	2.3
1	D	271	LYS	2.3
4	G	10	GLU	2.3
1	D	218	ALA	2.3
4	I	30	GLU	2.2
4	G	69	GLU	2.2
4	I	118	PHE	2.1
1	D	214	LEU	2.1
4	J	99	TYR	2.1
4	I	9	MET	2.1
4	I	8	THR	2.1
4	G	22	GLN	2.1
4	H	89	LYS	2.1
4	I	90	ASN	2.1
4	J	63	THR	2.0
4	I	15	ASN	2.0
4	H	22	GLN	2.0
1	D	84	TYR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.