



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:49 PM GMT

PDB ID : 4G42  
Title : Structure of the Chicken MHC Class I Molecule BF2\*0401 complexed to pepitde P8D  
Authors : Zhang, J.; Chen, Y.; Qi, J.; Gao, F.; Liu, J.; Kaufman, J.; Xia, C.; Gao, G.F.  
Deposited on : 2012-07-16  
Resolution : 2.29 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.

---

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

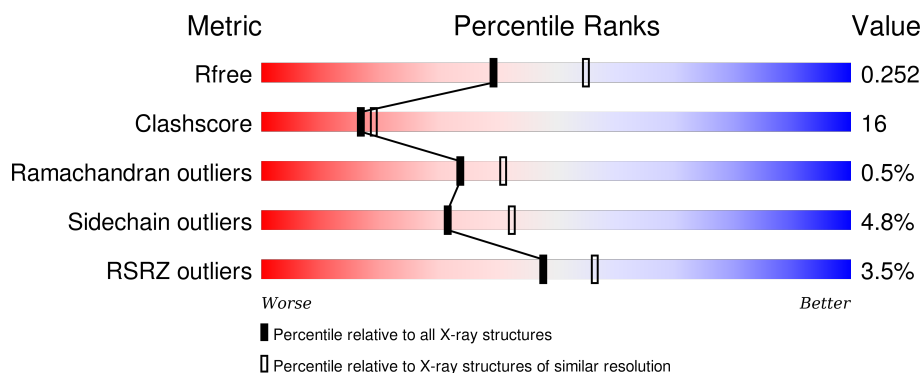
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.29 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	275	<div> <div>4%</div> <div>69% 25% . .</div> </div>
1	D	275	<div> <div>4%</div> <div>76% 19% . . .</div> </div>
2	B	101	<div> <div>2%</div> <div>71% 23% . .</div> </div>
2	E	101	<div> <div>3%</div> <div>72% 21% . .</div> </div>
3	C	8	<div> <div>88% 13%</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	F	8	 63% 38%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6644 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	271	Total	C	N	O	S	1	0	0
			2212	1391	401	413	7			
1	D	272	Total	C	N	O	S	0	0	0
			2220	1397	402	414	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	EXPRESSION TAG	UNP O46790
A	-1	GLU	-	EXPRESSION TAG	UNP O46790
A	0	PHE	-	EXPRESSION TAG	UNP O46790
A	244	GLU	ASP	ENGINEERED MUTATION	UNP O46790
A	271	LYS	-	EXPRESSION TAG	UNP O46790
A	272	LEU	-	EXPRESSION TAG	UNP O46790
D	-2	MET	-	EXPRESSION TAG	UNP O46790
D	-1	GLU	-	EXPRESSION TAG	UNP O46790
D	0	PHE	-	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			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	MET	-	EXPRESSION TAG	UNP P21611
B	-1	GLU	-	EXPRESSION TAG	UNP P21611
B	0	PHE	-	EXPRESSION TAG	UNP P21611
E	-2	MET	-	EXPRESSION TAG	UNP P21611
E	-1	GLU	-	EXPRESSION TAG	UNP P21611
E	0	PHE	-	EXPRESSION TAG	UNP P21611

- Molecule 3 is a protein called 8-MERIC PEPTIDE P8D.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	8	Total	C	N	O	0	0	0
			71	46	10	15			
3	F	8	Total	C	N	O	0	0	0
			71	46	10	15			

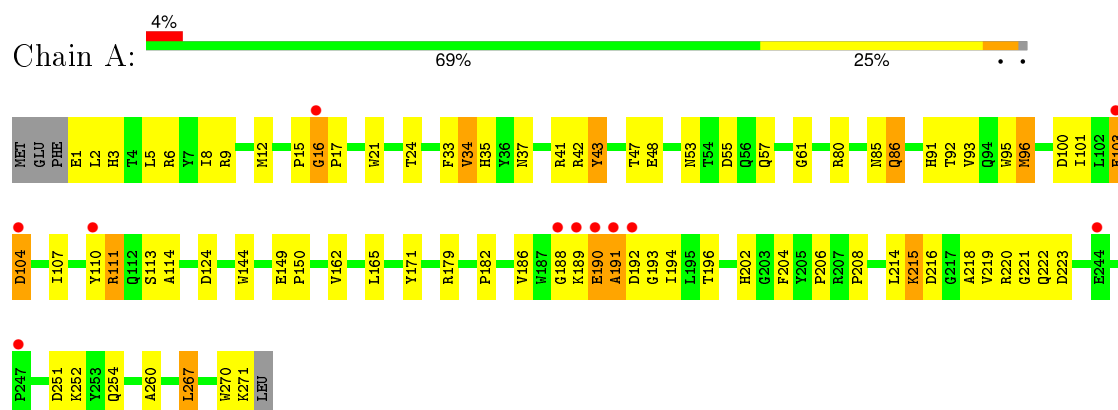
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	221	Total	O	0	0
			221	221		
4	B	59	Total	O	0	0
			59	59		
4	D	177	Total	O	0	0
			177	177		
4	E	68	Total	O	0	0
			68	68		
4	C	6	Total	O	0	0
			6	6		
4	F	5	Total	O	0	0
			5	5		

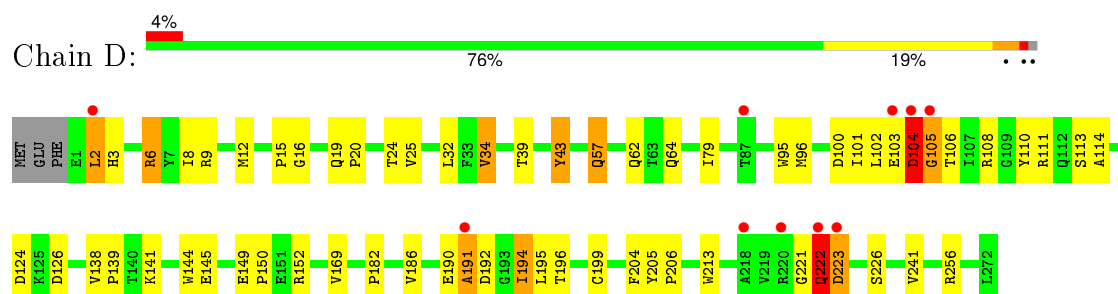
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

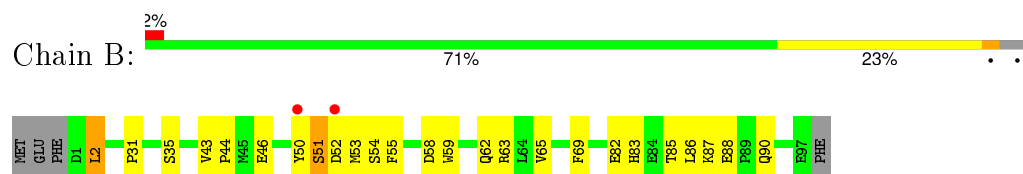
#### • Molecule 1: MHC class I alpha chain 2



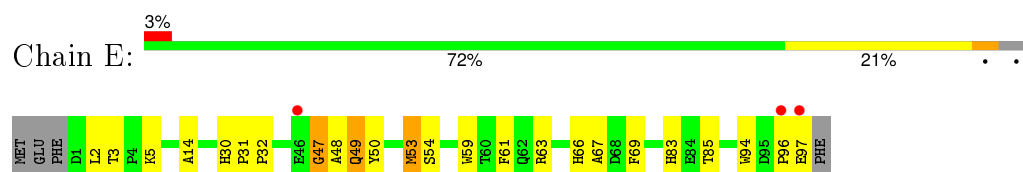
#### • Molecule 1: MHC class I alpha chain 2




#### • Molecule 2: Beta-2 microglobulin



#### • Molecule 2: Beta-2 microglobulin



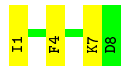
- Molecule 3: 8-MERIC PEPTIDE P8D

Chain C:  88% 13%



- Molecule 3: 8-MERIC PEPTIDE P8D

Chain F:  63% 38%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	165.83Å 40.11Å 130.95Å 90.00° 119.56° 90.00°	Depositor
Resolution (Å)	40.63 – 2.29 40.63 – 2.29	Depositor EDS
% Data completeness (in resolution range)	98.5 (40.63-2.29) 98.5 (40.63-2.29)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.66 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.196 , 0.254 0.198 , 0.252	Depositor DCC
$R_{free}$ test set	1712 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.9	Xtriage
Anisotropy	0.595	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 41.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 33786 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6644	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% 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	0.47	1/2275 (0.0%)	0.64	6/3091 (0.2%)
1	D	0.36	0/2283	0.62	7/3102 (0.2%)
2	B	0.29	0/791	0.48	0/1076
2	E	0.41	0/791	0.64	1/1076 (0.1%)
3	C	0.35	0/73	0.55	0/96
3	F	0.29	0/73	0.51	0/96
All	All	0.40	1/6286 (0.0%)	0.61	14/8537 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	17	PRO	N-CD	9.08	1.60	1.47

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	ASP	N-CA-CB	-7.71	96.71	110.60
1	A	16	GLY	N-CA-C	7.57	132.02	113.10
1	D	2	LEU	N-CA-C	7.34	130.82	111.00
1	D	105	GLY	N-CA-C	-6.87	95.94	113.10
1	D	104	ASP	CB-CA-C	-6.43	97.54	110.40
1	D	222	GLN	C-N-CA	-6.16	106.30	121.70
2	E	47	GLY	N-CA-C	-5.83	98.51	113.10
1	A	218	ALA	N-CA-CB	5.76	118.16	110.10
1	A	17	PRO	CA-N-CD	-5.74	103.47	111.50
1	A	215	LYS	C-N-CA	-5.69	107.48	121.70
1	D	191	ALA	N-CA-C	5.46	125.73	111.00
1	A	104	ASP	N-CA-C	5.43	125.66	111.00
1	D	192	ASP	N-CA-CB	5.16	119.89	110.60
1	D	104	ASP	N-CA-C	5.11	124.81	111.00

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	2212	0	2095	87	0
1	D	2220	0	2106	65	1
2	B	767	0	728	23	0
2	E	767	0	728	26	0
3	C	71	0	60	1	0
3	F	71	0	60	3	0
4	A	221	0	0	9	0
4	B	59	0	0	0	0
4	C	6	0	0	0	0
4	D	177	0	0	7	0
4	E	68	0	0	0	0
4	F	5	0	0	0	0
All	All	6644	0	5777	195	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 16.

All (195) 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)
1:D:2:LEU:O	1:D:2:LEU:HD13	1.11	1.25
1:D:2:LEU:O	1:D:2:LEU:CD1	1.86	1.22
1:D:222:GLN:O	1:D:223:ASP:CB	1.79	1.22
1:D:105:GLY:H	1:D:106:THR:HB	1.00	1.14
1:D:102:LEU:O	4:D:471:HOH:O	1.70	1.10
1:D:222:GLN:O	1:D:222:GLN:HG3	1.48	1.07
2:B:52:ASP:H	2:B:53:MET:HA	1.20	1.06
1:D:191:ALA:O	4:D:469:HOH:O	1.71	1.06
1:D:222:GLN:O	1:D:223:ASP:HB3	1.13	0.94
1:D:105:GLY:H	1:D:106:THR:CB	1.80	0.94
1:D:105:GLY:N	1:D:106:THR:HB	1.81	0.94
1:D:221:GLY:O	1:D:223:ASP:N	2.00	0.93

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:GLU:O	1:A:191:ALA:HB2	1.69	0.93
2:B:52:ASP:N	2:B:53:MET:HA	1.82	0.91
1:A:6:ARG:HD3	1:A:110:TYR:OH	1.68	0.91
1:A:1:GLU:HG2	1:A:3:HIS:HD2	1.34	0.91
1:A:16:GLY:O	4:A:412:HOH:O	1.91	0.86
1:A:35:HIS:HE1	1:A:37:ASN:HD22	1.24	0.81
1:A:1:GLU:HG2	1:A:3:HIS:CD2	2.14	0.80
1:A:103:GLU:OE2	4:A:518:HOH:O	2.03	0.77
2:B:52:ASP:HB3	2:B:53:MET:O	1.84	0.76
1:D:102:LEU:HB2	1:D:106:THR:HG23	1.67	0.75
2:E:49:GLN:HG3	2:E:66:HIS:NE2	2.01	0.74
1:A:190:GLU:O	1:A:191:ALA:CB	2.31	0.74
1:A:1:GLU:HA	1:A:2:LEU:C	2.06	0.74
2:E:49:GLN:HG3	2:E:66:HIS:CD2	2.23	0.74
2:E:49:GLN:HG2	2:E:66:HIS:O	1.88	0.73
1:D:221:GLY:C	1:D:223:ASP:N	2.41	0.73
1:D:34:VAL:HG13	1:D:43:TYR:CE2	2.24	0.72
1:D:222:GLN:O	1:D:222:GLN:CG	2.30	0.71
1:A:104:ASP:OD1	4:A:492:HOH:O	2.08	0.70
1:D:221:GLY:C	1:D:223:ASP:H	1.95	0.69
1:D:15:PRO:HG2	1:D:16:GLY:HA2	1.75	0.69
1:A:34:VAL:HG13	1:A:43:TYR:CE2	2.27	0.69
1:A:6:ARG:CD	1:A:110:TYR:OH	2.38	0.68
1:A:15:PRO:HB2	1:A:16:GLY:HA2	1.74	0.68
1:A:103:GLU:HA	1:A:103:GLU:OE1	1.93	0.67
1:A:1:GLU:HB2	1:A:103:GLU:CD	2.14	0.67
1:A:34:VAL:HG13	1:A:43:TYR:HE2	1.59	0.67
1:A:6:ARG:NH2	1:A:110:TYR:OH	2.28	0.66
1:A:214:LEU:HD22	1:A:219:VAL:HG22	1.76	0.66
1:A:194:ILE:O	1:A:194:ILE:CG2	2.44	0.66
2:E:47:GLY:O	2:E:67:ALA:HB1	1.96	0.65
2:E:83:HIS:HD2	2:E:85:THR:OG1	1.80	0.65
1:A:35:HIS:CE1	1:A:37:ASN:HD22	2.11	0.64
1:D:34:VAL:HG13	1:D:43:TYR:HE2	1.60	0.63
2:B:52:ASP:HB3	2:B:53:MET:C	2.18	0.63
1:A:191:ALA:C	1:A:193:GLY:H	2.00	0.63
1:A:114:ALA:HB2	2:B:59:TRP:CE2	2.33	0.63
2:B:87:LYS:HG2	2:B:88:GLU:HG3	1.80	0.63
1:A:103:GLU:CA	1:A:103:GLU:OE1	2.43	0.63
1:A:15:PRO:CB	1:A:16:GLY:HA2	2.27	0.63
1:A:35:HIS:HE1	1:A:37:ASN:ND2	1.96	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:THR:HG22	4:D:471:HOH:O	2.00	0.61
1:D:96:MET:SD	1:D:110:TYR:HE1	2.22	0.61
1:D:9:ARG:HG3	1:D:9:ARG:HH11	1.65	0.61
1:D:2:LEU:HD23	1:D:102:LEU:HG	1.83	0.61
1:D:182:PRO:HB3	1:D:204:PHE:HB3	1.81	0.61
1:A:1:GLU:H1	1:A:3:HIS:CD2	2.19	0.60
1:D:2:LEU:C	1:D:2:LEU:HD13	2.11	0.60
1:A:221:GLY:O	1:A:223:ASP:N	2.35	0.60
1:D:102:LEU:HB2	1:D:106:THR:CG2	2.33	0.59
2:E:53:MET:CE	2:E:63:ARG:NH1	2.65	0.58
1:D:2:LEU:HA	1:D:101:ILE:O	2.03	0.58
2:B:31:PRO:O	2:B:83:HIS:HE1	1.87	0.57
1:D:114:ALA:HB2	2:E:59:TRP:CE2	2.39	0.57
2:E:47:GLY:O	2:E:67:ALA:CB	2.53	0.57
2:B:35:SER:HB3	2:B:82:GLU:HB2	1.87	0.57
1:A:86:GLN:HG2	1:A:91:HIS:NE2	2.19	0.57
1:A:190:GLU:HB2	1:A:194:ILE:O	2.05	0.57
1:A:191:ALA:C	1:A:193:GLY:N	2.49	0.56
1:A:6:ARG:HG2	1:A:6:ARG:HH21	1.70	0.56
1:A:86:GLN:HG2	1:A:91:HIS:CE1	2.40	0.56
1:A:8:ILE:HD11	2:B:54:SER:HA	1.88	0.56
1:D:57:GLN:NE2	1:D:57:GLN:H	2.04	0.56
1:D:15:PRO:CG	1:D:16:GLY:HA2	2.35	0.56
1:D:8:ILE:HD11	2:E:54:SER:HB2	1.88	0.56
1:A:92:THR:HG23	4:A:369:HOH:O	2.04	0.55
1:A:6:ARG:HD3	1:A:110:TYR:HH	1.69	0.55
1:A:6:ARG:CZ	1:A:110:TYR:OH	2.54	0.55
2:B:53:MET:HE3	2:B:63:ARG:HH11	1.72	0.55
2:E:53:MET:HE2	2:E:63:ARG:NH1	2.22	0.55
2:E:48:ALA:HA	2:E:67:ALA:HB2	1.89	0.54
2:E:96:PRO:HB2	2:E:97:GLU:OE1	2.07	0.54
1:A:215:LYS:HB2	1:A:220:ARG:HG3	1.89	0.53
1:D:222:GLN:O	1:D:223:ASP:HB2	1.99	0.53
1:D:15:PRO:HB2	1:D:19:GLN:HB2	1.89	0.53
2:B:51:SER:CB	2:B:52:ASP:HA	2.38	0.53
1:A:5:LEU:HB2	1:A:165:LEU:HD13	1.90	0.53
1:A:96:MET:SD	1:A:110:TYR:HE1	2.32	0.53
1:D:96:MET:SD	1:D:110:TYR:CE1	3.02	0.52
1:A:194:ILE:HG22	1:A:194:ILE:O	2.08	0.52
1:A:96:MET:SD	1:A:110:TYR:CE1	3.03	0.52
1:D:12:MET:HB2	4:D:319:HOH:O	2.10	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:ILE:HG22	1:D:96:MET:HG2	1.92	0.51
1:A:42:ARG:HG3	4:A:459:HOH:O	2.09	0.51
1:A:8:ILE:HB	2:B:55:PHE:CZ	2.45	0.51
1:A:182:PRO:HA	1:A:202:HIS:O	2.10	0.51
1:D:104:ASP:HB3	1:D:106:THR:HB	1.93	0.51
2:B:53:MET:HE3	2:B:63:ARG:HD2	1.93	0.51
2:B:83:HIS:HD2	2:B:85:THR:OG1	1.93	0.51
1:D:103:GLU:CD	1:D:104:ASP:N	2.65	0.51
1:A:179:ARG:NH1	1:A:260:ALA:HB1	2.26	0.51
1:A:1:GLU:HB2	1:A:103:GLU:CG	2.42	0.50
1:A:103:GLU:O	1:A:103:GLU:OE1	2.29	0.49
2:E:5:LYS:HD2	2:E:5:LYS:N	2.27	0.49
2:E:14:ALA:HB3	2:E:96:PRO:O	2.12	0.49
1:A:144:TRP:HB3	1:A:149:GLU:HB2	1.94	0.49
1:A:85:ASN:HB3	2:E:97:GLU:HB2	1.94	0.49
1:A:95:TRP:CZ3	1:A:111:ARG:HD3	2.48	0.49
1:D:190:GLU:HG2	1:D:195:LEU:HD13	1.95	0.48
1:A:221:GLY:C	1:A:223:ASP:H	2.17	0.48
1:A:8:ILE:HG13	1:A:8:ILE:O	2.13	0.48
1:A:15:PRO:HG3	1:A:21:TRP:HA	1.96	0.48
1:A:149:GLU:N	1:A:150:PRO:CD	2.77	0.48
1:A:86:GLN:HB2	4:A:480:HOH:O	2.13	0.48
1:D:194:ILE:HD11	1:D:196:THR:OG1	2.13	0.47
1:A:182:PRO:HB3	1:A:204:PHE:HB3	1.96	0.47
1:A:215:LYS:O	1:A:252:LYS:O	2.32	0.47
1:A:33:PHE:HA	1:A:47:THR:HG23	1.95	0.47
1:D:103:GLU:CD	1:D:104:ASP:H	2.18	0.47
1:D:138:VAL:HB	1:D:139:PRO:HD3	1.96	0.47
1:D:226:SER:HB2	1:D:241:VAL:HG22	1.96	0.47
1:D:205:TYR:CG	1:D:206:PRO:HA	2.50	0.47
1:D:25:VAL:HB	1:D:32:LEU:CD1	2.45	0.47
1:A:2:LEU:HD11	1:A:100:ASP:HB3	1.96	0.47
1:A:15:PRO:HB2	1:A:16:GLY:CA	2.44	0.47
2:E:94:TRP:CE2	2:E:96:PRO:HA	2.50	0.46
1:A:107:ILE:HD12	1:A:162:VAL:HG21	1.96	0.46
1:A:53:ASN:HB3	1:A:171:TYR:CE2	2.51	0.46
1:D:256:ARG:HD2	4:D:302:HOH:O	2.14	0.46
2:B:83:HIS:CD2	2:B:85:THR:H	2.34	0.46
1:A:12:MET:HB3	1:A:92:THR:HG22	1.98	0.46
1:D:100:ASP:HB2	1:D:108:ARG:HB2	1.98	0.46
2:B:43:VAL:HG13	2:B:44:PRO:HD2	1.97	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:50:TYR:CD2	2:E:50:TYR:N	2.84	0.46
2:E:94:TRP:O	2:E:96:PRO:HD3	2.16	0.45
1:D:144:TRP:HB3	1:D:149:GLU:HB2	1.98	0.45
1:A:96:MET:SD	1:A:96:MET:C	2.95	0.45
2:B:2:LEU:HA	2:B:2:LEU:HD12	1.80	0.45
1:A:188:GLY:HA2	1:A:196:THR:O	2.17	0.45
1:A:191:ALA:O	1:A:192:ASP:C	2.53	0.45
1:D:105:GLY:N	1:D:106:THR:CB	2.60	0.44
1:A:221:GLY:C	1:A:223:ASP:N	2.68	0.44
2:B:83:HIS:CD2	2:B:85:THR:HG23	2.52	0.44
1:A:251:ASP:HB2	4:A:403:HOH:O	2.16	0.44
1:A:206:PRO:HB2	1:A:208:PRO:HD2	2.00	0.44
1:D:19:GLN:HA	1:D:20:PRO:HD3	1.90	0.44
1:A:61:GLY:HA3	4:A:502:HOH:O	2.16	0.44
1:D:141:LYS:O	1:D:145:GLU:HG3	2.18	0.44
1:D:9:ARG:HG3	1:D:24:THR:OG1	2.18	0.43
1:A:101:ILE:HG13	1:A:165:LEU:HD23	2.00	0.43
1:A:55:ASP:OD2	1:A:57:GLN:HB2	2.18	0.43
1:D:6:ARG:HD3	1:D:110:TYR:OH	2.19	0.43
1:D:6:ARG:HD2	1:D:96:MET:SD	2.58	0.43
1:A:191:ALA:O	1:A:193:GLY:N	2.50	0.43
2:B:86:LEU:HD13	2:B:90:GLN:HG2	2.01	0.43
1:D:106:THR:N	4:D:471:HOH:O	2.51	0.43
2:E:96:PRO:O	2:E:97:GLU:HG3	2.17	0.43
1:D:152:ARG:NH2	3:F:4:PHE:O	2.52	0.43
2:E:83:HIS:CD2	2:E:85:THR:H	2.37	0.43
1:A:48:GLU:HG2	4:A:450:HOH:O	2.19	0.43
2:E:94:TRP:CZ2	2:E:96:PRO:HA	2.54	0.43
1:A:1:GLU:HB2	1:A:103:GLU:OE2	2.18	0.42
2:E:32:PRO:HD3	2:E:61:PHE:CE2	2.54	0.42
1:A:215:LYS:HB2	1:A:220:ARG:CG	2.49	0.42
1:A:80:ARG:HD2	1:A:93:VAL:HG22	2.00	0.42
2:E:2:LEU:HD13	2:E:30:HIS:HB3	2.00	0.42
1:D:149:GLU:N	1:D:150:PRO:CD	2.82	0.42
1:A:179:ARG:HH11	1:A:260:ALA:HB1	1.85	0.42
1:A:254:GLN:HB3	1:A:267:LEU:CD2	2.50	0.41
1:D:103:GLU:C	4:D:471:HOH:O	2.58	0.41
1:A:6:ARG:NH2	1:A:6:ARG:HG2	2.35	0.41
1:A:1:GLU:HB2	1:A:103:GLU:HG2	2.03	0.41
1:A:95:TRP:CZ3	1:A:113:SER:HB2	2.55	0.41
1:D:199:CYS:HB2	1:D:213:TRP:CZ2	2.55	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ASN:HB3	1:A:171:TYR:CD2	2.55	0.41
2:E:30:HIS:CG	2:E:31:PRO:HA	2.55	0.41
1:D:79:ILE:HD11	3:F:7:LYS:HD2	2.02	0.41
1:A:9:ARG:HG3	1:A:9:ARG:NH1	2.36	0.41
3:C:7:LYS:HE3	3:C:7:LYS:HB2	1.87	0.41
2:E:49:GLN:HG2	2:E:49:GLN:H	1.75	0.41
1:D:9:ARG:NH1	1:D:9:ARG:HG3	2.34	0.41
1:D:3:HIS:CG	1:D:169:VAL:HG21	2.55	0.41
2:E:3:THR:HG22	2:E:85:THR:HB	2.03	0.41
1:A:270:TRP:O	1:A:271:LYS:CB	2.69	0.41
1:D:95:TRP:CD2	1:D:113:SER:HB2	2.56	0.40
1:D:144:TRP:CG	1:D:149:GLU:HG3	2.56	0.40
1:D:103:GLU:CG	1:D:104:ASP:N	2.84	0.40
1:A:114:ALA:HB2	2:B:59:TRP:CD2	2.56	0.40
2:B:52:ASP:N	2:B:53:MET:CA	2.62	0.40
2:B:58:ASP:O	2:B:59:TRP:HB2	2.21	0.40
2:B:50:TYR:HD2	2:B:65:VAL:HG22	1.87	0.40
1:A:9:ARG:HG2	1:A:24:THR:OG1	2.21	0.40
1:D:62:GLN:NE2	3:F:1:ILE:HB	2.37	0.40

All (1) 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:39:THR:OG1	1:D:126:ASP:OD2[1_565]	2.10	0.10

## 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	269/275 (98%)	255 (95%)	12 (4%)	2 (1%)	26 31

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	270/275 (98%)	257 (95%)	11 (4%)	2 (1%)	26	31
2	B	95/101 (94%)	94 (99%)	1 (1%)	0	100	100
2	E	95/101 (94%)	93 (98%)	2 (2%)	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
All	All	741/768 (96%)	711 (96%)	26 (4%)	4 (0%)	34	41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	191	ALA
1	D	222	GLN
1	A	222	GLN
1	D	223	ASP

### 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	228/232 (98%)	215 (94%)	13 (6%)	25	34
1	D	229/232 (99%)	219 (96%)	10 (4%)	35	46
2	B	85/89 (96%)	80 (94%)	5 (6%)	24	32
2	E	85/89 (96%)	82 (96%)	3 (4%)	43	58
3	C	7/7 (100%)	7 (100%)	0	100	100
3	F	7/7 (100%)	7 (100%)	0	100	100
All	All	641/656 (98%)	610 (95%)	31 (5%)	31	42

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	VAL
1	A	41	ARG

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	43	TYR
1	A	86	GLN
1	A	96	MET
1	A	103	GLU
1	A	111	ARG
1	A	124	ASP
1	A	186	VAL
1	A	189	LYS
1	A	190	GLU
1	A	216	ASP
1	A	267	LEU
2	B	2	LEU
2	B	46	GLU
2	B	51	SER
2	B	62	GLN
2	B	69	PHE
1	D	6	ARG
1	D	34	VAL
1	D	43	TYR
1	D	57	GLN
1	D	64	GLN
1	D	104	ASP
1	D	111	ARG
1	D	124	ASP
1	D	186	VAL
1	D	194	ILE
2	E	49	GLN
2	E	53	MET
2	E	69	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	A	67	GLN
1	A	73	ASN
1	A	81	GLN
1	A	86	GLN
1	A	254	GLN
2	B	83	HIS
1	D	57	GLN
1	D	64	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	67	GLN
1	D	73	ASN
1	D	112	GLN
1	D	225	HIS
1	D	254	GLN
2	E	83	HIS
2	E	90	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	271/275 (98%)	-0.03	11 (4%) 41 50	16, 25, 51, 76	1 (0%)
1	D	272/275 (98%)	-0.09	10 (3%) 45 54	18, 26, 45, 64	1 (0%)
2	B	97/101 (96%)	-0.08	2 (2%) 67 74	20, 27, 41, 57	0
2	E	97/101 (96%)	-0.04	3 (3%) 52 62	18, 26, 41, 64	0
3	C	8/8 (100%)	-0.35	0 100 100	18, 19, 24, 36	0
3	F	8/8 (100%)	-0.39	0 100 100	17, 20, 24, 29	0
All	All	753/768 (98%)	-0.07	26 (3%) 48 56	16, 26, 48, 76	2 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	96	PRO	8.4
2	B	52	ASP	7.0
1	A	104	ASP	4.8
1	D	105	GLY	4.5
1	A	247	PRO	4.2
1	D	87	THR	3.7
1	A	191	ALA	3.7
1	D	222	GLN	3.7
1	A	188	GLY	3.7
1	D	104	ASP	3.4
2	E	97	GLU	3.3
1	D	220	ARG	3.3
1	A	16	GLY	3.2
1	D	223	ASP	3.2
1	A	189	LYS	3.0
1	D	218	ALA	2.9
1	A	244	GLU	2.8
1	D	2	LEU	2.8
2	B	50	TYR	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	103	GLU	2.5
1	A	190	GLU	2.5
1	D	103	GLU	2.5
1	A	110	TYR	2.5
1	A	192	ASP	2.4
1	D	191	ALA	2.1
2	E	46	GLU	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.