



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:56 PM GMT

PDB ID : 1FG2  
Title : CRYSTAL STRUCTURE OF THE LCMV PEPTIDIC EPITOPE GP33 IN  
COMPLEX WITH THE MURINE CLASS I MHC MOLECULE H-2DB  
Authors : Tissot, A.C.; Ciatto, C.; Mittl, P.R.E.; Gruetter, M.G.; Plueckthun, A.  
Deposited on : 2000-07-27  
Resolution : 2.75 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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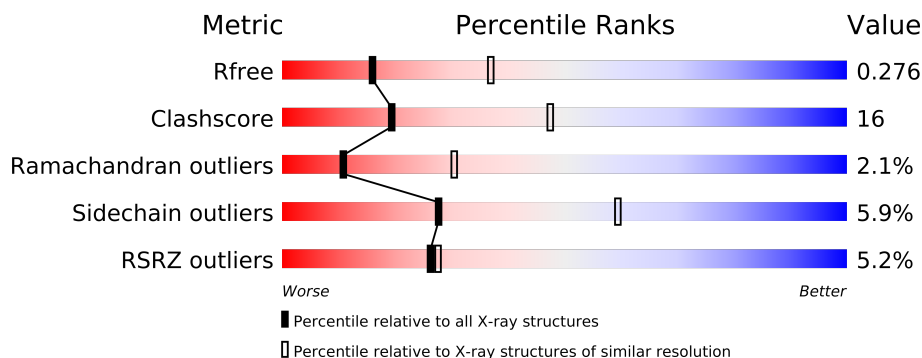
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.75 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))
$R_{free}$	66092	2406 (2.80-2.72)
Clashscore	79885	2995 (2.80-2.72)
Ramachandran outliers	78287	2941 (2.80-2.72)
Sidechain outliers	78261	2944 (2.80-2.72)
RSRZ outliers	66119	2409 (2.80-2.72)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	281	
1	D	281	
1	G	281	
1	J	281	
2	B	100	
2	E	100	
2	H	100	
2	K	100	
3	C	9	
3	F	9	
3	I	9	
3	L	9	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12656 atoms, of which 0 are hydrogen and 0 are deuterium.

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 H-2 CLASS I HISTOCOMPATIBILITY ANTIGEN, D-B ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2244	1418	397	420	9			
1	D	273	Total	C	N	O	S	0	0	0
			2244	1418	397	420	9			
1	G	273	Total	C	N	O	S	0	0	0
			2244	1418	397	420	9			
1	J	273	Total	C	N	O	S	0	0	0
			2244	1418	397	420	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	INITIATING MET	UNP P01899
D	0	MET	-	INITIATING MET	UNP P01899
G	0	MET	-	INITIATING MET	UNP P01899
J	0	MET	-	INITIATING MET	UNP P01899

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			
2	E	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			
2	H	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			
2	K	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	INITIATING MET	UNP P01887
E	0	MET	-	INITIATING MET	UNP P01887
H	0	MET	-	INITIATING MET	UNP P01887
K	0	MET	-	INITIATING MET	UNP P01887

- Molecule 3 is a protein called LCMV PEPTIDIC EPITOPE GP33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			71	46	11	13	1			
3	F	9	Total	C	N	O	S	0	0	0
			71	46	11	13	1			
3	I	9	Total	C	N	O	S	0	0	0
			71	46	11	13	1			
3	L	9	Total	C	N	O	S	0	0	0
			71	46	11	13	1			

- Molecule 4 is water.

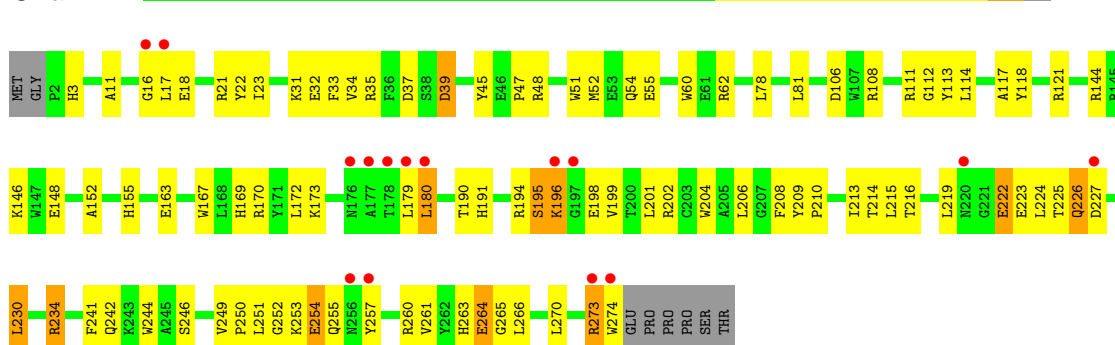
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	16	Total	O	0	0
			16	16		
4	B	14	Total	O	0	0
			14	14		
4	C	2	Total	O	0	0
			2	2		
4	D	14	Total	O	0	0
			14	14		
4	E	13	Total	O	0	0
			13	13		
4	G	15	Total	O	0	0
			15	15		
4	H	8	Total	O	0	0
			8	8		
4	I	1	Total	O	0	0
			1	1		
4	J	18	Total	O	0	0
			18	18		
4	K	9	Total	O	0	0
			9	9		
4	L	2	Total	O	0	0
			2	2		

### 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.

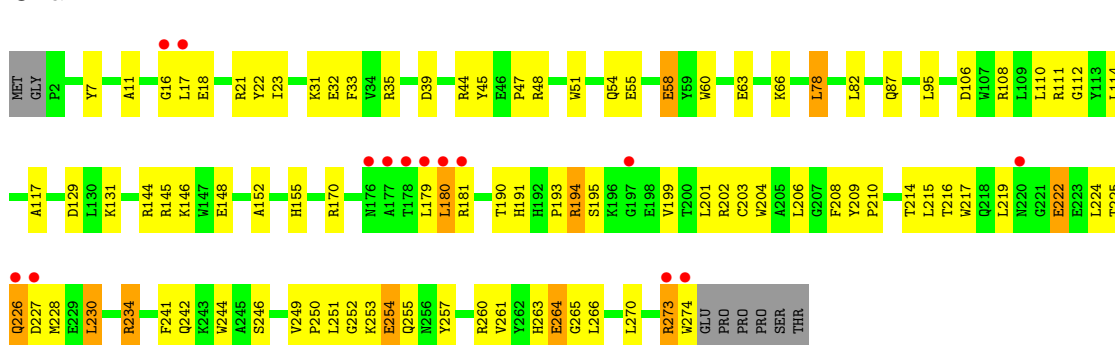
- Molecule 1: H-2 CLASS I HISTOCOMPATIBILITY ANTIGEN, D-B ALPHA CHAIN

Chain A:



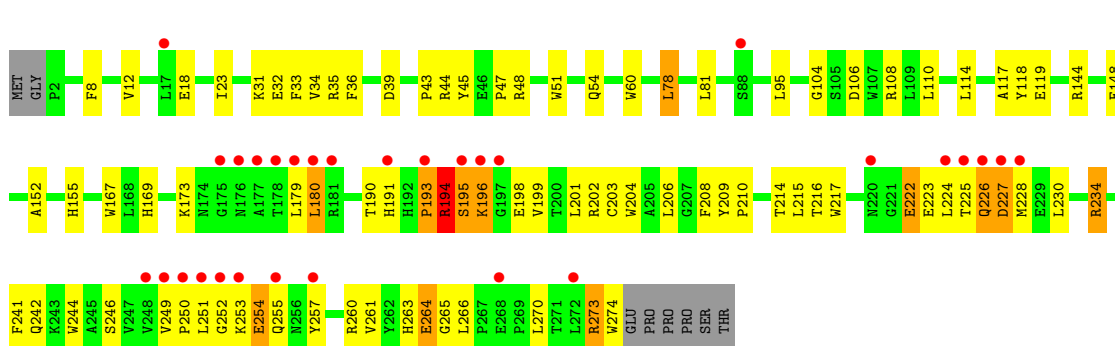
- Molecule 1: H-2 CLASS I HISTOCOMPATIBILITY ANTIGEN, D-B ALPHA CHAIN

Chain D:

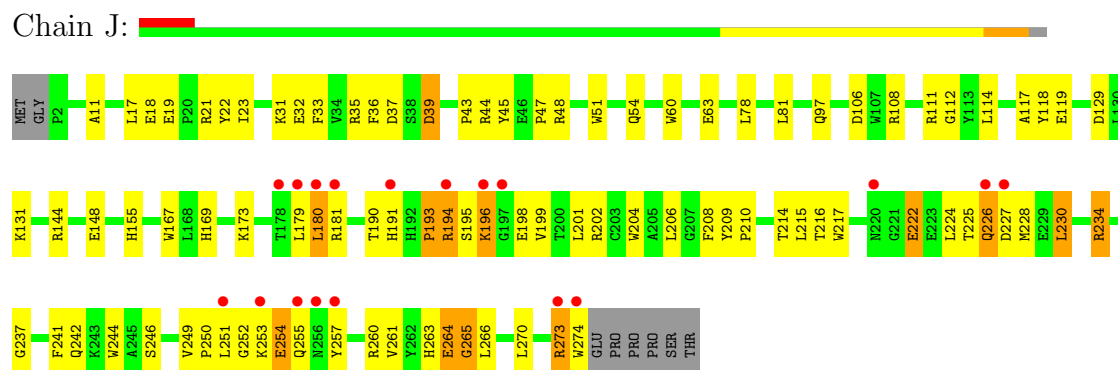


- Molecule 1: H-2 CLASS I HISTOCOMPATIBILITY ANTIGEN, D-B ALPHA CHAIN

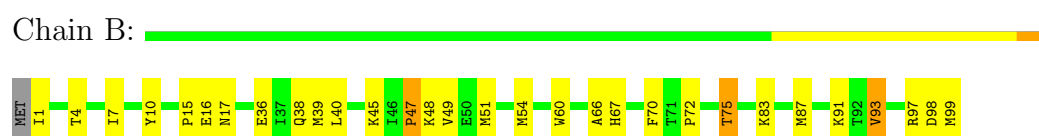
Chain G:



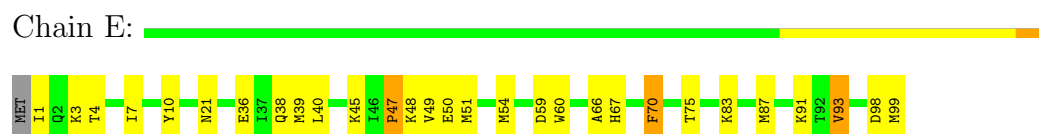
- Molecule 1: H-2 CLASS I HISTOCOMPATIBILITY ANTIGEN, D-B ALPHA CHAIN



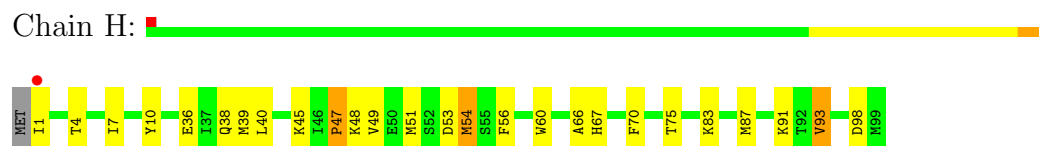
- Molecule 2: BETA-2 MICROGLOBULIN



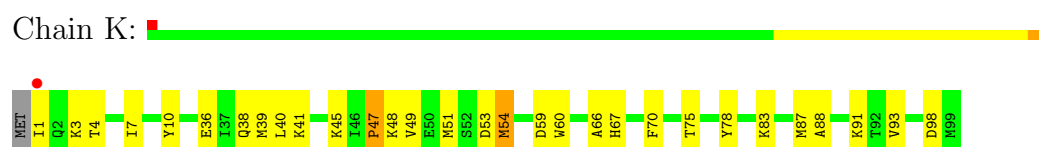
- Molecule 2: BETA-2 MICROGLOBULIN



- Molecule 2: BETA-2 MICROGLOBULIN



- Molecule 2: BETA-2 MICROGLOBULIN



- Molecule 3: LCMV PEPTIDIC EPITOPE GP33

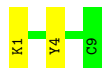


- Molecule 3: LCMV PEPTIDIC EPITOPE GP33



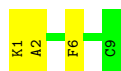
- Molecule 3: LCMV PEPTIDIC EPITOPE GP33

Chain I: 



- Molecule 3: LCMV PEPTIDIC EPITOPE GP33

Chain L: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.53Å 124.77Å 99.56Å 90.00° 103.03° 90.00°	Depositor
Resolution (Å)	30.00 – 2.75 29.84 – 2.75	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.75) 90.3 (29.84-2.75)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.04 (at 2.76Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.236 , 0.276 0.235 , 0.276	Depositor DCC
$R_{free}$ test set	5197 reflections (10.10%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.2	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 19.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 51475 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	12656	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.71% of the height of the origin peak. No significant pseudotranslation is detected.*

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



## 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	0/2310	0.66	0/3136
1	D	0.44	0/2310	0.66	0/3136
1	G	0.45	0/2310	0.68	1/3136 (0.0%)
1	J	0.45	0/2310	0.68	0/3136
2	B	0.46	0/847	0.68	0/1148
2	E	0.46	0/847	0.68	0/1148
2	H	0.48	0/847	0.68	0/1148
2	K	0.47	0/847	0.69	0/1148
3	C	0.74	0/72	0.86	0/95
3	F	0.85	0/72	0.85	0/95
3	I	0.78	0/72	0.86	0/95
3	L	0.67	0/72	0.72	0/95
All	All	0.46	0/12916	0.68	1/17516 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	195	SER	N-CA-C	-5.45	96.29	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2244	0	2118	85	0
1	D	2244	0	2118	84	0
1	G	2244	0	2118	72	0
1	J	2244	0	2118	82	0
2	B	821	0	796	31	0
2	E	821	0	796	25	0
2	H	821	0	796	26	0
2	K	821	0	796	25	0
3	C	71	0	70	8	0
3	F	71	0	70	6	0
3	I	71	0	70	1	0
3	L	71	0	70	3	0
4	A	16	0	0	1	0
4	B	14	0	0	4	0
4	C	2	0	0	1	0
4	D	14	0	0	2	0
4	E	13	0	0	1	0
4	G	15	0	0	0	0
4	H	8	0	0	0	0
4	I	1	0	0	0	0
4	J	18	0	0	2	0
4	K	9	0	0	3	0
4	L	2	0	0	1	0
All	All	12656	0	11936	398	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (398) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:194:ARG:HB2	1:G:196:LYS:H	1.26	0.99
2:B:75:THR:O	4:B:100:HOH:O	1.83	0.97
1:D:263:HIS:O	1:D:264:GLU:HB2	1.66	0.94
1:G:263:HIS:O	1:G:264:GLU:HB2	1.68	0.92
1:A:263:HIS:O	1:A:264:GLU:HB2	1.71	0.91
1:J:263:HIS:O	1:J:264:GLU:HB2	1.69	0.88
1:D:66:LYS:HZ1	3:F:1:LYS:HG2	1.39	0.88
1:G:255:GLN:HE22	1:G:274:TRP:HB3	1.38	0.87
1:J:255:GLN:HE22	1:J:274:TRP:HB3	1.38	0.86
1:A:255:GLN:HE22	1:A:274:TRP:HB3	1.39	0.86
1:D:255:GLN:HE22	1:D:274:TRP:HB3	1.41	0.85
1:G:119:GLU:HB3	2:H:1:ILE:HD13	1.57	0.84
1:G:119:GLU:HB3	2:H:1:ILE:CD1	2.08	0.82

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.17	0.80
1:G:194:ARG:HA	1:G:198:GLU:O	1.83	0.78
1:J:155:HIS:HB3	3:L:6:PHE:CZ	2.19	0.77
1:J:194:ARG:CD	1:J:194:ARG:H	1.95	0.77
1:J:194:ARG:H	1:J:194:ARG:HD2	1.49	0.76
1:D:66:LYS:HZ1	3:F:1:LYS:CG	2.00	0.74
2:H:1:ILE:O	2:H:1:ILE:HG23	1.89	0.73
1:A:234:ARG:HD3	2:B:10:TYR:CE2	2.24	0.72
1:A:273:ARG:HD3	1:A:273:ARG:H	1.54	0.72
2:K:3:LYS:HE3	4:K:106:HOH:O	1.90	0.71
1:A:194:ARG:HG3	1:A:198:GLU:O	1.90	0.71
2:E:1:ILE:HG23	2:E:1:ILE:O	1.89	0.71
1:G:273:ARG:HD3	1:G:273:ARG:H	1.56	0.71
1:D:263:HIS:O	1:D:264:GLU:CB	2.38	0.71
2:B:1:ILE:HG23	2:B:1:ILE:O	1.91	0.71
1:A:254:GLU:HG3	1:A:255:GLN:HE21	1.55	0.70
1:G:263:HIS:O	1:G:264:GLU:CB	2.40	0.69
1:J:263:HIS:O	1:J:264:GLU:CB	2.41	0.69
1:J:273:ARG:HD3	1:J:273:ARG:H	1.56	0.69
2:K:1:ILE:HG23	2:K:1:ILE:O	1.92	0.69
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.28	0.69
2:B:75:THR:HG23	4:B:100:HOH:O	1.92	0.68
1:D:16:GLY:C	1:D:18:GLU:H	1.97	0.68
1:G:254:GLU:HG3	1:G:255:GLN:HE21	1.59	0.68
1:A:62:ARG:NH1	3:C:1:LYS:HD2	2.09	0.68
1:A:251:LEU:HD23	1:A:252:GLY:N	2.09	0.68
1:A:121:ARG:NH1	2:B:1:ILE:HG13	2.08	0.68
1:J:254:GLU:HG3	1:J:255:GLN:HE21	1.59	0.68
1:D:251:LEU:HD23	1:D:252:GLY:N	2.09	0.67
1:D:254:GLU:HG3	1:D:255:GLN:HE21	1.58	0.67
1:D:193:PRO:O	1:D:194:ARG:HG3	1.95	0.67
1:J:251:LEU:HD23	1:J:252:GLY:N	2.09	0.67
1:G:35:ARG:NH2	2:H:54:MET:O	2.23	0.67
1:D:32:GLU:OE2	1:D:48:ARG:HD2	1.95	0.66
1:A:263:HIS:O	1:A:264:GLU:CB	2.43	0.66
1:D:234:ARG:HD3	2:E:10:TYR:CE2	2.31	0.66
1:G:32:GLU:OE2	1:G:48:ARG:HD2	1.95	0.66
1:J:234:ARG:HD3	2:K:10:TYR:CE2	2.31	0.66
1:D:273:ARG:HD3	1:D:273:ARG:H	1.59	0.66
1:G:251:LEU:HD23	1:G:252:GLY:N	2.09	0.66
1:D:202:ARG:HG2	1:D:204:TRP:NE1	2.11	0.66
1:J:117:ALA:HB2	2:K:60:TRP:CE2	2.32	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:121:ARG:CZ	2:B:1:ILE:CD1	2.75	0.65
2:B:16:GLU:HG3	2:K:88:ALA:HB3	1.77	0.65
1:D:63:GLU:OE2	3:F:1:LYS:HG3	1.98	0.64
1:G:119:GLU:CB	2:H:1:ILE:CD1	2.75	0.64
1:D:66:LYS:NZ	3:F:1:LYS:HG2	2.11	0.63
1:J:43:PRO:O	1:J:44:ARG:HG3	1.97	0.63
1:A:23:ILE:N	1:A:23:ILE:HD12	2.13	0.63
1:D:58:GLU:CD	1:D:58:GLU:H	2.01	0.63
1:A:202:ARG:HG2	1:A:204:TRP:NE1	2.13	0.62
1:J:194:ARG:HG3	1:J:199:VAL:CG1	2.29	0.62
1:J:201:LEU:HD12	1:J:249:VAL:HG21	1.80	0.62
1:A:31:LYS:HD3	1:A:179:LEU:CD2	2.30	0.62
1:G:47:PRO:HG3	1:G:60:TRP:CZ2	2.34	0.62
1:G:264:GLU:O	1:G:266:LEU:N	2.32	0.62
1:G:23:ILE:N	1:G:23:ILE:HD12	2.15	0.62
1:A:31:LYS:HD3	1:A:179:LEU:HD21	1.81	0.61
1:J:23:ILE:HD12	1:J:23:ILE:N	2.14	0.61
1:J:32:GLU:OE2	1:J:48:ARG:HD2	2.00	0.61
2:E:36:GLU:HB2	2:E:83:LYS:HB3	1.82	0.61
1:D:23:ILE:HD12	1:D:23:ILE:N	2.16	0.61
1:J:194:ARG:N	1:J:194:ARG:HD2	2.13	0.61
1:J:202:ARG:HG2	1:J:204:TRP:NE1	2.15	0.61
1:A:201:LEU:HD12	1:A:249:VAL:HG21	1.83	0.61
1:G:234:ARG:HD3	2:H:10:TYR:CE2	2.36	0.61
1:G:202:ARG:HG2	1:G:204:TRP:NE1	2.16	0.61
1:G:144:ARG:O	1:G:148:GLU:HG3	2.01	0.60
1:G:201:LEU:HD12	1:G:249:VAL:HG21	1.83	0.60
1:A:32:GLU:OE2	1:A:48:ARG:HD2	2.02	0.60
2:H:36:GLU:HB2	2:H:83:LYS:HB3	1.83	0.60
1:J:222:GLU:H	1:J:222:GLU:CD	2.05	0.60
1:D:117:ALA:HB2	2:E:60:TRP:CZ2	2.37	0.59
2:K:36:GLU:HB2	2:K:83:LYS:HB3	1.84	0.59
1:J:18:GLU:HG2	1:J:19:GLU:HG2	1.84	0.59
1:D:222:GLU:H	1:D:222:GLU:CD	2.05	0.59
2:B:36:GLU:HB2	2:B:83:LYS:HB3	1.83	0.59
2:K:54:MET:HA	4:K:102:HOH:O	2.02	0.59
1:A:222:GLU:CD	1:A:222:GLU:H	2.06	0.59
1:D:31:LYS:HD3	1:D:179:LEU:CD2	2.33	0.59
1:D:266:LEU:HD21	1:D:270:LEU:HG	1.84	0.59
1:A:202:ARG:HD2	1:A:244:TRP:CD2	2.37	0.59
1:J:31:LYS:HD3	1:J:179:LEU:CD2	2.32	0.59
1:J:31:LYS:HD3	1:J:179:LEU:HD21	1.83	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:202:ARG:HD2	1:J:244:TRP:CD2	2.38	0.58
1:G:31:LYS:HD3	1:G:179:LEU:CD2	2.33	0.58
1:D:201:LEU:HD12	1:D:249:VAL:HG21	1.86	0.58
1:A:250:PRO:HG2	1:A:253:LYS:HB2	1.85	0.58
1:G:202:ARG:HD2	1:G:244:TRP:CD2	2.39	0.57
1:J:250:PRO:HG2	1:J:253:LYS:HB2	1.86	0.57
1:D:31:LYS:HD3	1:D:179:LEU:HD21	1.86	0.57
1:D:191:HIS:NE2	1:D:199:VAL:HG21	2.19	0.57
1:J:194:ARG:HE	1:J:251:LEU:HD12	1.68	0.57
1:G:250:PRO:HG2	1:G:253:LYS:HB2	1.87	0.57
1:G:194:ARG:HB2	1:G:196:LYS:N	2.09	0.57
1:A:266:LEU:HD21	1:A:270:LEU:HG	1.87	0.57
1:G:119:GLU:CB	2:H:1:ILE:HD11	2.34	0.57
1:J:264:GLU:O	1:J:266:LEU:N	2.37	0.57
1:G:222:GLU:CD	1:G:222:GLU:H	2.08	0.57
1:A:264:GLU:O	1:A:266:LEU:N	2.36	0.57
2:H:39:MET:CE	2:H:49:VAL:HG13	2.35	0.57
1:D:264:GLU:O	1:D:266:LEU:N	2.38	0.56
1:A:214:THR:C	1:A:215:LEU:HD12	2.26	0.56
1:G:266:LEU:HD21	1:G:270:LEU:HG	1.87	0.56
2:E:39:MET:HE1	2:E:67:HIS:N	2.21	0.56
1:D:47:PRO:HG3	1:D:60:TRP:CZ2	2.41	0.56
1:A:273:ARG:N	1:A:273:ARG:HD3	2.19	0.56
1:A:32:GLU:OE2	1:A:35:ARG:HD2	2.06	0.56
1:G:264:GLU:C	1:G:266:LEU:N	2.59	0.56
1:J:194:ARG:HA	1:J:198:GLU:O	2.06	0.56
1:G:31:LYS:HD3	1:G:179:LEU:HD21	1.86	0.56
1:D:35:ARG:NH2	2:E:54:MET:O	2.38	0.56
1:G:191:HIS:NE2	1:G:199:VAL:HG21	2.20	0.56
1:D:44:ARG:HG3	1:D:44:ARG:HH11	1.71	0.55
1:D:202:ARG:HD2	1:D:244:TRP:CD2	2.42	0.55
1:J:35:ARG:NH2	2:K:54:MET:O	2.38	0.55
1:J:214:THR:C	1:J:215:LEU:HD12	2.27	0.55
1:A:121:ARG:NH2	2:B:1:ILE:HD12	2.21	0.55
1:D:250:PRO:HG2	1:D:253:LYS:HB2	1.88	0.55
2:E:3:LYS:HE3	4:E:107:HOH:O	2.06	0.55
1:A:167:TRP:CE2	3:C:1:LYS:HG3	2.41	0.55
2:H:39:MET:HE3	2:H:49:VAL:HG13	1.89	0.55
1:J:266:LEU:HD21	1:J:270:LEU:HG	1.88	0.55
1:G:117:ALA:HB2	2:H:60:TRP:CE2	2.42	0.55
1:G:264:GLU:C	1:G:266:LEU:H	2.09	0.54
2:B:39:MET:HE1	2:B:67:HIS:N	2.22	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:40:LEU:HD23	2:H:45:LYS:HA	1.88	0.54
1:J:194:ARG:HG3	1:J:199:VAL:HG12	1.89	0.54
2:K:39:MET:HE1	2:K:67:HIS:N	2.22	0.54
1:A:191:HIS:NE2	1:A:199:VAL:HG21	2.23	0.54
2:B:40:LEU:HD23	2:B:45:LYS:HA	1.90	0.54
1:D:32:GLU:OE2	1:D:35:ARG:HD2	2.08	0.54
2:H:39:MET:HE1	2:H:67:HIS:N	2.23	0.54
1:J:47:PRO:HG3	1:J:60:TRP:CZ2	2.43	0.53
2:K:40:LEU:HD23	2:K:45:LYS:HA	1.90	0.53
2:K:47:PRO:HG2	2:K:48:LYS:H	1.72	0.53
2:E:40:LEU:HD23	2:E:45:LYS:HA	1.90	0.53
1:A:47:PRO:HG3	1:A:60:TRP:CZ2	2.44	0.53
1:G:179:LEU:O	1:G:180:LEU:HB2	2.09	0.53
1:J:237:GLY:HA3	4:K:100:HOH:O	2.07	0.53
1:J:97:GLN:HG2	4:J:285:HOH:O	2.08	0.53
1:G:32:GLU:OE2	1:G:35:ARG:HD2	2.09	0.52
2:E:39:MET:HE1	2:E:66:ALA:C	2.30	0.52
2:E:39:MET:CE	2:E:49:VAL:HG13	2.39	0.52
1:D:16:GLY:C	1:D:18:GLU:N	2.62	0.52
2:B:47:PRO:HG2	2:B:48:LYS:H	1.74	0.52
1:J:119:GLU:HB3	2:K:1:ILE:HD13	1.92	0.52
1:J:195:SER:O	1:J:196:LYS:HB2	2.10	0.52
1:G:119:GLU:CB	2:H:1:ILE:HD13	2.32	0.52
1:J:191:HIS:NE2	1:J:199:VAL:HG21	2.24	0.52
1:A:121:ARG:CZ	2:B:1:ILE:HD12	2.38	0.52
2:K:39:MET:CE	2:K:49:VAL:HG13	2.40	0.52
1:A:213:ILE:HG22	4:A:296:HOH:O	2.09	0.52
1:A:264:GLU:C	1:A:266:LEU:N	2.62	0.52
1:G:273:ARG:N	1:G:273:ARG:HD3	2.20	0.52
1:A:179:LEU:O	1:A:180:LEU:HB2	2.10	0.52
1:J:264:GLU:C	1:J:266:LEU:N	2.62	0.52
1:A:18:GLU:HA	1:A:18:GLU:OE2	2.10	0.52
1:G:119:GLU:HB2	2:H:1:ILE:HD11	1.92	0.52
1:D:214:THR:C	1:D:215:LEU:HD12	2.29	0.52
1:A:152:ALA:O	1:A:155:HIS:HB3	2.10	0.51
1:D:264:GLU:C	1:D:266:LEU:N	2.62	0.51
1:J:167:TRP:CZ2	3:L:1:LYS:HE3	2.46	0.51
1:D:16:GLY:O	1:D:18:GLU:N	2.43	0.51
1:D:51:TRP:O	1:D:54:GLN:HG3	2.11	0.51
2:H:47:PRO:HG2	2:H:48:LYS:H	1.75	0.51
1:J:264:GLU:C	1:J:266:LEU:H	2.15	0.51
1:J:179:LEU:O	1:J:180:LEU:HB2	2.11	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:43:PRO:O	1:G:44:ARG:HG3	2.11	0.50
1:G:195:SER:O	1:G:196:LYS:HB2	2.11	0.50
2:E:47:PRO:HG2	2:E:48:LYS:H	1.76	0.50
1:A:16:GLY:O	1:A:17:LEU:C	2.49	0.50
1:D:264:GLU:C	1:D:266:LEU:H	2.13	0.50
1:A:121:ARG:NE	2:B:1:ILE:HD11	2.26	0.49
1:D:273:ARG:HD3	1:D:273:ARG:N	2.23	0.49
2:H:10:TYR:CD1	2:H:10:TYR:N	2.81	0.49
1:D:179:LEU:O	1:D:180:LEU:HB2	2.11	0.49
1:D:216:THR:OG1	1:D:260:ARG:HB2	2.13	0.49
1:A:264:GLU:C	1:A:266:LEU:H	2.14	0.49
1:A:62:ARG:HH12	3:C:1:LYS:HD2	1.76	0.49
2:E:10:TYR:CD1	2:E:10:TYR:N	2.79	0.49
1:G:8:PHE:HB3	2:H:56:PHE:CE2	2.47	0.49
1:G:214:THR:C	1:G:215:LEU:HD12	2.32	0.49
1:A:190:THR:OG1	1:A:202:ARG:HB3	2.13	0.49
2:B:54:MET:HA	4:B:108:HOH:O	2.13	0.49
1:J:194:ARG:HG3	1:J:199:VAL:HG13	1.93	0.49
1:D:58:GLU:CD	1:D:58:GLU:N	2.66	0.49
2:K:39:MET:HE1	2:K:66:ALA:C	2.33	0.49
1:D:63:GLU:OE2	1:D:66:LYS:HE2	2.13	0.49
2:B:10:TYR:N	2:B:10:TYR:CD1	2.81	0.49
2:K:36:GLU:OE2	2:K:83:LYS:HD3	2.13	0.49
1:J:190:THR:OG1	1:J:202:ARG:HB3	2.12	0.48
1:D:144:ARG:O	1:D:148:GLU:HG3	2.13	0.48
1:A:144:ARG:O	1:A:148:GLU:HG3	2.13	0.48
1:A:216:THR:OG1	1:A:260:ARG:HB2	2.12	0.48
1:A:261:VAL:HB	1:A:270:LEU:HB2	1.95	0.48
2:B:39:MET:HE1	2:B:66:ALA:C	2.34	0.48
1:G:190:THR:OG1	1:G:202:ARG:HB3	2.13	0.48
1:J:206:LEU:HD23	1:J:242:GLN:HB3	1.96	0.48
1:A:111:ARG:HG2	1:A:112:GLY:N	2.28	0.48
1:A:206:LEU:HD23	1:A:242:GLN:HB3	1.95	0.48
1:J:32:GLU:OE2	1:J:35:ARG:HD2	2.12	0.48
1:D:261:VAL:HB	1:D:270:LEU:HB2	1.96	0.48
1:D:190:THR:OG1	1:D:202:ARG:HB3	2.12	0.48
2:H:7:ILE:HD12	2:H:7:ILE:N	2.28	0.48
2:H:39:MET:HE1	2:H:67:HIS:CA	2.44	0.48
2:E:39:MET:HE2	2:E:49:VAL:HG13	1.95	0.48
1:J:261:VAL:HB	1:J:270:LEU:HB2	1.95	0.48
1:G:33:PHE:C	1:G:48:ARG:HB2	2.34	0.47
2:H:36:GLU:OE2	2:H:83:LYS:HD3	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:36:GLU:OE2	2:B:83:LYS:HD3	2.13	0.47
3:L:2:ALA:HB1	4:L:11:HOH:O	2.14	0.47
1:D:206:LEU:HD23	1:D:242:GLN:HB3	1.95	0.47
1:G:209:TYR:CD1	1:G:210:PRO:HA	2.49	0.47
1:J:63:GLU:OE1	4:J:287:HOH:O	2.20	0.47
1:D:234:ARG:NH2	2:E:99:MET:OXT	2.47	0.47
1:J:202:ARG:HD2	1:J:244:TRP:CE3	2.49	0.47
2:K:10:TYR:CD1	2:K:10:TYR:N	2.81	0.47
2:E:36:GLU:OE2	2:E:83:LYS:HD3	2.14	0.47
1:A:225:THR:HG22	1:A:225:THR:O	2.14	0.47
1:D:209:TYR:CD1	1:D:210:PRO:HA	2.50	0.47
3:C:1:LYS:NZ	4:C:111:HOH:O	2.47	0.47
1:D:202:ARG:HD3	1:D:246:SER:HB3	1.96	0.47
2:H:1:ILE:O	2:H:1:ILE:CG2	2.61	0.47
1:J:194:ARG:HB3	1:J:198:GLU:C	2.35	0.47
2:B:39:MET:CE	2:B:49:VAL:HG13	2.45	0.47
1:J:224:LEU:C	1:J:226:GLN:H	2.19	0.47
1:J:225:THR:HG22	1:J:225:THR:O	2.15	0.47
2:B:39:MET:HE1	2:B:67:HIS:CA	2.44	0.47
2:B:87:MET:CE	2:B:91:LYS:HB2	2.45	0.47
2:K:39:MET:HE2	2:K:49:VAL:HG13	1.96	0.46
1:G:225:THR:O	1:G:225:THR:HG22	2.15	0.46
2:B:75:THR:C	4:B:100:HOH:O	2.40	0.46
1:A:202:ARG:NH1	2:B:99:MET:HE2	2.30	0.46
2:B:7:ILE:HD12	2:B:7:ILE:N	2.30	0.46
1:D:225:THR:O	1:D:225:THR:HG22	2.14	0.46
1:J:202:ARG:HD3	1:J:246:SER:HB3	1.96	0.46
1:G:202:ARG:HD3	1:G:246:SER:HB3	1.97	0.46
1:A:163:GLU:OE2	3:C:1:LYS:HD3	2.16	0.46
1:D:152:ALA:O	1:D:155:HIS:HB3	2.16	0.46
2:K:7:ILE:N	2:K:7:ILE:HD12	2.31	0.46
1:G:261:VAL:HB	1:G:270:LEU:HB2	1.99	0.45
1:G:35:ARG:NH2	2:H:53:ASP:HB3	2.32	0.45
1:G:216:THR:OG1	1:G:260:ARG:HB2	2.16	0.45
1:G:106:ASP:OD2	1:G:108:ARG:HB2	2.17	0.45
1:G:224:LEU:C	1:G:226:GLN:H	2.19	0.45
1:J:111:ARG:HG2	1:J:112:GLY:N	2.32	0.45
1:D:255:GLN:C	1:D:257:TYR:H	2.20	0.45
1:D:224:LEU:HG	1:D:226:GLN:HB3	1.99	0.45
1:J:208:PHE:CE1	1:J:241:PHE:HB2	2.51	0.45
1:A:62:ARG:NH1	3:C:1:LYS:CD	2.80	0.45
1:A:224:LEU:C	1:A:226:GLN:H	2.19	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:216:THR:OG1	1:J:260:ARG:HB2	2.16	0.45
1:A:55:GLU:CD	1:A:170:ARG:HH21	2.20	0.45
1:D:33:PHE:C	1:D:48:ARG:HB2	2.36	0.45
1:A:195:SER:O	1:A:196:LYS:C	2.55	0.45
1:G:169:HIS:O	1:G:173:LYS:HG3	2.17	0.45
1:A:37:ASP:OD1	1:A:39:ASP:HB2	2.16	0.45
1:G:206:LEU:HD23	1:G:242:GLN:HB3	1.99	0.45
1:J:273:ARG:N	1:J:273:ARG:HD3	2.20	0.45
2:H:87:MET:CE	2:H:91:LYS:HB2	2.47	0.45
1:J:191:HIS:NE2	1:J:199:VAL:HG11	2.32	0.45
2:E:1:ILE:CG2	2:E:1:ILE:O	2.62	0.45
1:J:35:ARG:NH2	2:K:53:ASP:HB3	2.31	0.45
2:K:41:LYS:HE3	2:K:78:TYR:OH	2.17	0.45
1:A:202:ARG:HD3	1:A:246:SER:HB3	1.98	0.44
1:D:234:ARG:HD3	2:E:10:TYR:CZ	2.52	0.44
1:J:33:PHE:C	1:J:48:ARG:HB2	2.37	0.44
1:D:224:LEU:C	1:D:226:GLN:H	2.20	0.44
2:E:87:MET:CE	2:E:91:LYS:HB2	2.47	0.44
1:J:255:GLN:C	1:J:257:TYR:H	2.21	0.44
1:A:33:PHE:C	1:A:48:ARG:HB2	2.37	0.44
1:G:152:ALA:O	1:G:155:HIS:HB3	2.17	0.44
1:J:129:ASP:O	1:J:131:LYS:HG3	2.17	0.44
1:J:194:ARG:HB3	1:J:198:GLU:N	2.33	0.44
1:G:224:LEU:HG	1:G:226:GLN:HB3	1.99	0.44
2:E:7:ILE:N	2:E:7:ILE:HD12	2.31	0.44
1:A:230:LEU:C	1:A:230:LEU:HD12	2.37	0.44
1:J:144:ARG:O	1:J:148:GLU:HG3	2.17	0.44
1:D:201:LEU:O	1:D:246:SER:HA	2.17	0.44
1:D:66:LYS:NZ	3:F:2:ALA:O	2.46	0.44
1:A:224:LEU:HG	1:A:226:GLN:HB3	2.00	0.44
1:J:217:TRP:H	1:J:228:MET:HE2	1.82	0.44
1:D:111:ARG:HG2	1:D:112:GLY:N	2.32	0.44
1:A:255:GLN:C	1:A:257:TYR:H	2.20	0.44
2:K:39:MET:HE1	2:K:67:HIS:CA	2.47	0.44
1:A:51:TRP:CZ3	1:A:52:MET:SD	3.11	0.44
1:A:106:ASP:OD2	1:A:108:ARG:HB2	2.18	0.44
1:G:217:TRP:H	1:G:228:MET:HE2	1.83	0.44
1:G:167:TRP:CE2	3:I:1:LYS:HD2	2.53	0.44
2:H:39:MET:HE1	2:H:66:ALA:C	2.37	0.44
1:D:55:GLU:CD	1:D:170:ARG:HH21	2.21	0.44
1:J:81:LEU:HD13	1:J:118:TYR:CD1	2.53	0.44
1:A:234:ARG:NH2	2:B:99:MET:OXT	2.51	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:202:ARG:HD2	1:G:244:TRP:CE3	2.53	0.43
1:J:37:ASP:OD1	1:J:39:ASP:HB2	2.18	0.43
1:D:11:ALA:HA	1:D:21:ARG:O	2.18	0.43
1:D:217:TRP:H	1:D:228:MET:HE2	1.82	0.43
1:D:63:GLU:OE2	1:D:66:LYS:CE	2.66	0.43
1:D:7:TYR:CE1	3:F:2:ALA:HB2	2.53	0.43
1:A:194:ARG:NH2	1:A:198:GLU:OE1	2.51	0.43
1:J:224:LEU:HG	1:J:226:GLN:HB3	1.99	0.43
1:A:11:ALA:HA	1:A:21:ARG:O	2.18	0.43
1:A:33:PHE:CD2	1:A:34:VAL:HG13	2.53	0.43
1:D:193:PRO:O	1:D:194:ARG:CG	2.65	0.43
1:J:21:ARG:HG2	1:J:23:ILE:HD11	1.99	0.43
1:D:181:ARG:HH11	1:D:181:ARG:HG2	1.83	0.43
1:G:255:GLN:C	1:G:257:TYR:H	2.21	0.43
1:A:202:ARG:HD2	1:A:244:TRP:CE3	2.53	0.43
2:K:41:LYS:HG3	2:K:78:TYR:CE2	2.53	0.43
1:A:191:HIS:NE2	1:A:199:VAL:HG11	2.34	0.43
1:D:202:ARG:HD2	1:D:244:TRP:CE3	2.53	0.43
1:A:16:GLY:O	1:A:18:GLU:N	2.52	0.43
1:A:51:TRP:O	1:A:54:GLN:HG3	2.18	0.43
1:D:110:LEU:HD13	4:D:288:HOH:O	2.18	0.43
1:J:209:TYR:CD1	1:J:210:PRO:HA	2.54	0.42
1:A:234:ARG:HD3	2:B:10:TYR:CZ	2.53	0.42
1:A:234:ARG:NH1	1:A:242:GLN:OE1	2.51	0.42
1:A:81:LEU:HD13	1:A:118:TYR:CD1	2.55	0.42
1:A:208:PHE:CE1	1:A:241:PHE:HB2	2.53	0.42
1:D:202:ARG:HG2	1:D:204:TRP:HE1	1.82	0.42
1:G:81:LEU:HD13	1:G:118:TYR:CD1	2.54	0.42
1:D:106:ASP:OD2	1:D:108:ARG:HB2	2.19	0.42
1:A:62:ARG:HB3	1:A:62:ARG:HE	1.76	0.42
1:J:169:HIS:O	1:J:173:LYS:HG3	2.19	0.42
1:J:230:LEU:HD12	1:J:230:LEU:C	2.40	0.42
1:D:129:ASP:O	1:D:131:LYS:HG3	2.20	0.42
1:A:222:GLU:CD	1:A:222:GLU:N	2.73	0.42
1:G:78:LEU:CD1	1:G:95:LEU:HB2	2.50	0.42
1:D:214:THR:HA	4:D:287:HOH:O	2.19	0.42
1:G:43:PRO:O	1:G:44:ARG:CG	2.68	0.42
1:A:111:ARG:HD2	1:A:113:TYR:CZ	2.55	0.42
2:E:59:ASP:O	2:E:60:TRP:HB2	2.20	0.41
2:E:7:ILE:HB	2:E:93:VAL:HG11	2.02	0.41
2:K:87:MET:CE	2:K:91:LYS:HB2	2.49	0.41
1:G:51:TRP:O	1:G:54:GLN:HG3	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:209:TYR:CD1	1:A:210:PRO:HA	2.55	0.41
1:D:230:LEU:C	1:D:230:LEU:HD12	2.41	0.41
1:A:169:HIS:O	1:A:173:LYS:HG3	2.20	0.41
1:D:82:LEU:HD12	1:D:87:GLN:HB2	2.01	0.41
1:G:208:PHE:CE1	1:G:241:PHE:HB2	2.54	0.41
1:A:254:GLU:H	1:A:254:GLU:HG2	1.73	0.41
1:G:33:PHE:CD2	1:G:34:VAL:HG13	2.55	0.41
1:J:22:TYR:C	1:J:23:ILE:HD12	2.40	0.41
1:G:201:LEU:O	1:G:246:SER:HA	2.20	0.41
1:D:191:HIS:NE2	1:D:199:VAL:HG11	2.34	0.41
2:K:59:ASP:O	2:K:60:TRP:HB2	2.20	0.41
1:J:23:ILE:CD1	1:J:23:ILE:N	2.83	0.41
1:D:203:CYS:HB2	1:D:217:TRP:CZ2	2.55	0.41
1:D:22:TYR:C	1:D:23:ILE:HD12	2.41	0.41
1:G:191:HIS:NE2	1:G:199:VAL:HG11	2.35	0.41
2:B:87:MET:HE1	2:B:91:LYS:HB2	2.01	0.41
1:J:255:GLN:HE22	1:J:274:TRP:CB	2.21	0.41
1:A:163:GLU:OE2	3:C:1:LYS:NZ	2.47	0.41
1:A:22:TYR:C	1:A:23:ILE:HD12	2.41	0.41
1:J:11:ALA:HA	1:J:21:ARG:O	2.20	0.41
2:B:7:ILE:HB	2:B:93:VAL:HG11	2.03	0.41
1:G:203:CYS:HB2	1:G:217:TRP:CZ2	2.56	0.41
1:J:181:ARG:HH11	1:J:181:ARG:HG2	1.84	0.41
1:J:36:PHE:CD1	1:J:36:PHE:C	2.93	0.41
1:G:104:GLY:CA	1:G:110:LEU:HD22	2.51	0.41
1:A:146:LYS:HE2	3:C:8:THR:O	2.21	0.41
1:J:201:LEU:O	1:J:246:SER:HA	2.21	0.41
2:E:50:GLU:HB2	2:E:67:HIS:CE1	2.56	0.41
1:D:44:ARG:HG3	1:D:44:ARG:NH1	2.35	0.41
2:H:7:ILE:HB	2:H:93:VAL:HG11	2.03	0.41
1:D:78:LEU:HD13	1:D:95:LEU:HB2	2.03	0.41
1:J:51:TRP:O	1:J:54:GLN:HG3	2.21	0.41
1:J:106:ASP:OD2	1:J:108:ARG:HB2	2.21	0.41
1:A:201:LEU:O	1:A:246:SER:HA	2.21	0.40
2:B:15:PRO:HG3	2:B:97:ARG:HB2	2.03	0.40
1:J:234:ARG:HD3	2:K:10:TYR:CZ	2.55	0.40
1:D:145:ARG:O	1:D:146:LYS:C	2.60	0.40
1:D:208:PHE:CE1	1:D:241:PHE:HB2	2.56	0.40
1:J:264:GLU:O	1:J:265:GLY:C	2.60	0.40
1:D:219:LEU:HD13	1:D:257:TYR:CZ	2.56	0.40
1:G:23:ILE:N	1:G:23:ILE:CD1	2.84	0.40
1:D:222:GLU:CD	1:D:222:GLU:N	2.72	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:3:HIS:CG	1:A:172:LEU:HD11	2.57	0.40
2:B:17:ASN:HA	2:B:72:PRO:O	2.22	0.40
2:E:21:ASN:HB3	2:E:70:PHE:CE1	2.57	0.40
1:G:12:VAL:O	1:G:12:VAL:HG23	2.22	0.40
1:G:36:PHE:C	1:G:36:PHE:CD1	2.93	0.40
1:A:219:LEU:HD13	1:A:257:TYR:CZ	2.57	0.40
2:E:39:MET:HE1	2:E:67:HIS:CA	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	271/281 (96%)	238 (88%)	26 (10%)	7 (3%)	8	23
1	D	271/281 (96%)	239 (88%)	26 (10%)	6 (2%)	10	29
1	G	271/281 (96%)	238 (88%)	25 (9%)	8 (3%)	7	19
1	J	271/281 (96%)	238 (88%)	26 (10%)	7 (3%)	8	23
2	B	97/100 (97%)	93 (96%)	3 (3%)	1 (1%)	22	56
2	E	97/100 (97%)	93 (96%)	3 (3%)	1 (1%)	22	56
2	H	97/100 (97%)	93 (96%)	3 (3%)	1 (1%)	22	56
2	K	97/100 (97%)	93 (96%)	3 (3%)	1 (1%)	22	56
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	F	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	I	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	L	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	1500/1560 (96%)	1349 (90%)	119 (8%)	32 (2%)	11	30

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	180	LEU
1	A	195	SER
1	A	264	GLU
1	D	180	LEU
1	D	264	GLU
1	G	180	LEU
1	G	194	ARG
1	G	264	GLU
1	J	180	LEU
1	J	264	GLU
1	A	196	LYS
2	B	47	PRO
1	D	17	LEU
1	D	194	ARG
1	G	196	LYS
1	J	193	PRO
1	J	196	LYS
2	K	47	PRO
1	A	227	ASP
1	D	227	ASP
2	E	47	PRO
1	G	193	PRO
2	H	47	PRO
1	J	227	ASP
1	G	227	ASP
1	G	265	GLY
1	A	265	GLY
1	D	265	GLY
1	J	17	LEU
1	A	223	GLU
1	G	223	GLU
1	J	265	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	232/239 (97%)	222 (96%)	10 (4%)	40 74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	232/239 (97%)	220 (95%)	12 (5%)	32	66
1	G	232/239 (97%)	218 (94%)	14 (6%)	27	58
1	J	232/239 (97%)	220 (95%)	12 (5%)	32	66
2	B	94/95 (99%)	87 (93%)	7 (7%)	20	45
2	E	94/95 (99%)	87 (93%)	7 (7%)	20	45
2	H	94/95 (99%)	86 (92%)	8 (8%)	15	38
2	K	94/95 (99%)	86 (92%)	8 (8%)	15	38
3	C	7/7 (100%)	7 (100%)	0	100	100
3	F	7/7 (100%)	7 (100%)	0	100	100
3	I	7/7 (100%)	6 (86%)	1 (14%)	5	12
3	L	7/7 (100%)	7 (100%)	0	100	100
All	All	1332/1364 (98%)	1253 (94%)	79 (6%)	28	59

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ASP
1	A	45	TYR
1	A	78	LEU
1	A	114	LEU
1	A	222	GLU
1	A	226	GLN
1	A	230	LEU
1	A	234	ARG
1	A	254	GLU
1	A	273	ARG
2	B	4	THR
2	B	38	GLN
2	B	51	MET
2	B	70	PHE
2	B	75	THR
2	B	93	VAL
2	B	98	ASP
1	D	39	ASP
1	D	45	TYR
1	D	58	GLU
1	D	78	LEU
1	D	114	LEU

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Mol	Chain	Res	Type
1	D	195	SER
1	D	222	GLU
1	D	226	GLN
1	D	230	LEU
1	D	234	ARG
1	D	254	GLU
1	D	273	ARG
2	E	4	THR
2	E	38	GLN
2	E	51	MET
2	E	70	PHE
2	E	75	THR
2	E	93	VAL
2	E	98	ASP
1	G	18	GLU
1	G	39	ASP
1	G	45	TYR
1	G	78	LEU
1	G	114	LEU
1	G	193	PRO
1	G	194	ARG
1	G	222	GLU
1	G	226	GLN
1	G	227	ASP
1	G	230	LEU
1	G	234	ARG
1	G	254	GLU
1	G	273	ARG
2	H	4	THR
2	H	38	GLN
2	H	51	MET
2	H	54	MET
2	H	70	PHE
2	H	75	THR
2	H	93	VAL
2	H	98	ASP
3	I	4	TYR
1	J	39	ASP
1	J	45	TYR
1	J	78	LEU
1	J	114	LEU
1	J	193	PRO

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Mol	Chain	Res	Type
1	J	194	ARG
1	J	222	GLU
1	J	226	GLN
1	J	230	LEU
1	J	234	ARG
1	J	254	GLU
1	J	273	ARG
2	K	4	THR
2	K	38	GLN
2	K	51	MET
2	K	54	MET
2	K	70	PHE
2	K	75	THR
2	K	93	VAL
2	K	98	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	87	GLN
1	A	97	GLN
1	A	220	ASN
1	A	255	GLN
2	B	31	HIS
3	C	5	ASN
1	D	54	GLN
1	D	87	GLN
1	D	97	GLN
1	D	220	ASN
1	D	255	GLN
2	E	2	GLN
3	F	5	ASN
1	G	42	ASN
1	G	54	GLN
1	G	87	GLN
1	G	97	GLN
1	G	220	ASN
1	G	255	GLN
2	H	2	GLN
2	H	34	HIS
3	I	5	ASN

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Mol	Chain	Res	Type
1	J	54	GLN
1	J	97	GLN
1	J	220	ASN
1	J	255	GLN
2	K	31	HIS
3	L	5	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

### 5.8 Polymer linkage issues

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	273/281 (97%)	0.01	15 (5%) 24 26	11, 38, 98, 100	0
1	D	273/281 (97%)	0.00	14 (5%) 27 28	12, 39, 99, 100	0
1	G	273/281 (97%)	0.31	30 (10%) 6 6	12, 43, 100, 100	0
1	J	273/281 (97%)	0.10	18 (6%) 18 18	12, 41, 100, 100	0
2	B	99/100 (99%)	-0.24	0 100 100	12, 32, 75, 98	0
2	E	99/100 (99%)	-0.21	0 100 100	15, 38, 72, 85	0
2	H	99/100 (99%)	-0.20	1 (1%) 79 81	18, 36, 73, 99	0
2	K	99/100 (99%)	-0.31	1 (1%) 79 81	15, 35, 66, 98	0
3	C	9/9 (100%)	-0.17	0 100 100	25, 30, 43, 46	0
3	F	9/9 (100%)	-0.30	0 100 100	18, 24, 51, 54	0
3	I	9/9 (100%)	0.23	0 100 100	17, 28, 46, 59	0
3	L	9/9 (100%)	0.18	0 100 100	21, 28, 54, 64	0
All	All	1524/1560 (97%)	0.01	79 (5%) 26 27	11, 38, 98, 100	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	178	THR	8.3
1	J	178	THR	7.6
1	J	179	LEU	5.4
1	D	17	LEU	5.4
1	G	251	LEU	5.0
1	G	179	LEU	4.8
1	D	177	ALA	4.8
1	J	180	LEU	4.3
1	D	220	ASN	4.3
1	D	178	THR	4.3
1	D	16	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
1	G	177	ALA	4.2
1	D	180	LEU	4.2
1	A	227	ASP	3.8
1	D	179	LEU	3.7
1	J	251	LEU	3.6
1	D	274	TRP	3.6
1	J	227	ASP	3.6
1	A	177	ALA	3.6
1	G	250	PRO	3.4
1	G	176	ASN	3.4
1	G	197	GLY	3.3
1	A	179	LEU	3.3
1	J	197	GLY	3.3
1	D	227	ASP	3.3
1	A	180	LEU	3.2
1	D	273	ARG	3.2
1	A	17	LEU	3.2
1	G	227	ASP	3.2
1	A	16	GLY	3.2
1	G	255	GLN	3.2
1	J	220	ASN	3.2
1	J	256	ASN	3.2
1	D	226	GLN	3.1
1	A	197	GLY	3.1
1	J	226	GLN	3.0
1	J	253	LYS	3.0
1	A	256	ASN	2.9
1	J	194	ARG	2.9
1	A	273	ARG	2.8
1	G	248	VAL	2.8
1	J	181	ARG	2.8
1	A	220	ASN	2.7
1	D	197	GLY	2.7
2	K	1	ILE	2.6
1	J	257	TYR	2.6
1	D	176	ASN	2.6
1	J	255	GLN	2.6
1	A	196	LYS	2.6
1	A	176	ASN	2.6
1	A	274	TRP	2.6
2	H	1	ILE	2.5
1	J	274	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	J	273	ARG	2.5
1	A	178	THR	2.5
1	G	272	LEU	2.4
1	G	193	PRO	2.4
1	J	191	HIS	2.4
1	G	181	ARG	2.4
1	G	220	ASN	2.4
1	A	257	TYR	2.4
1	G	195	SER	2.4
1	G	257	TYR	2.4
1	G	228	MET	2.4
1	G	196	LYS	2.4
1	G	226	GLN	2.3
1	G	175	GLY	2.3
1	G	268	GLU	2.3
1	G	180	LEU	2.3
1	J	196	LYS	2.3
1	G	88	SER	2.3
1	G	17	LEU	2.3
1	G	249	VAL	2.2
1	D	181	ARG	2.2
1	G	224	LEU	2.2
1	G	191	HIS	2.2
1	G	252	GLY	2.1
1	G	225	THR	2.1
1	G	253	LYS	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.