



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2026 – 12:14 PM JST

PDB ID : 9WJ6 / pdb\_00009wj6  
Title : An integrated in silico-in vitro workflow for discovering high-affinity, selective antibodies to the KRAS(G12D)-MHC I complex  
Authors : Oh, T.S.; Jeong, B.S.; Oh, B.H.  
Deposited on : 2025-08-30  
Resolution : 4.54 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

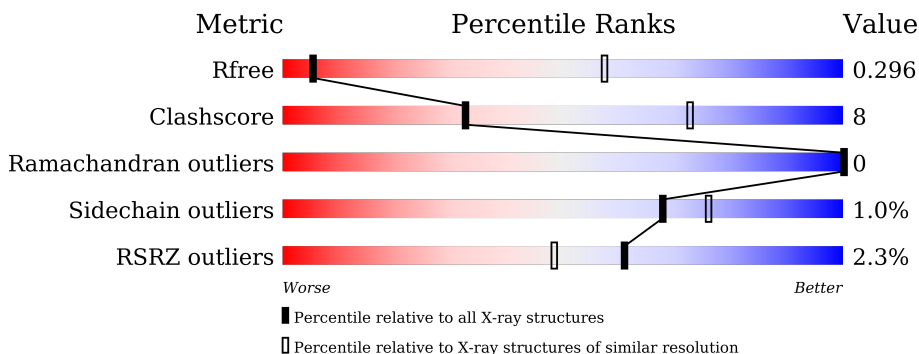
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.54 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.



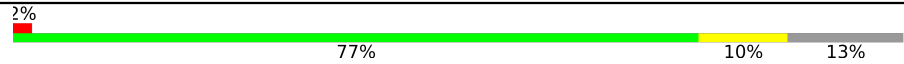

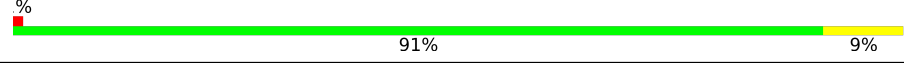
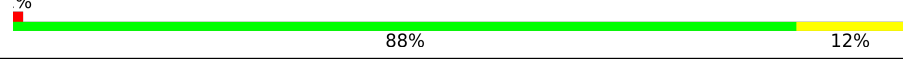
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1131 (5.14-3.90)
Clashscore	190562	1009 (5.14-3.94)
Ramachandran outliers	187476	1061 (5.12-3.90)
Sidechain outliers	187428	1044 (5.12-3.90)
RSRZ outliers	180081	1126 (5.14-3.90)

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 of 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	I	10	
1	P	10	
2	A	234	
2	K	234	
3	E	280	
3	M	280	

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Mol	Chain	Length	Quality of chain
4	B	255	 2% 77% 10% 13%
4	L	255	 2% 76% 11% 13%
5	F	100	 % 91% 9%
5	N	100	 % 88% 12%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12930 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 Peptide from GTPase KRas, N-terminally processed.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	I	10	61	36	11	14	0	0	0
1	P	10	61	36	11	14	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	3	ASP	GLY	engineered mutation	UNP P01116
P	3	ASP	GLY	engineered mutation	UNP P01116

- Molecule 2 is a protein called C8K10D5-1 Fab Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	215	1670	1044	285	335	6	0	0	0
2	K	215	1670	1044	285	335	6	0	0	0

- Molecule 3 is a protein called HLA class I antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	273	2240	1395	414	425	6	0	0	0
3	M	273	2240	1395	414	425	6	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1	MET	-	initiating methionine	UNP C1K0Y1
E	275	HIS	-	expression tag	UNP C1K0Y1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	276	HIS	-	expression tag	UNP C1K0Y1
E	277	HIS	-	expression tag	UNP C1K0Y1
E	278	HIS	-	expression tag	UNP C1K0Y1
E	279	HIS	-	expression tag	UNP C1K0Y1
E	280	HIS	-	expression tag	UNP C1K0Y1
M	1	MET	-	initiating methionine	UNP C1K0Y1
M	275	HIS	-	expression tag	UNP C1K0Y1
M	276	HIS	-	expression tag	UNP C1K0Y1
M	277	HIS	-	expression tag	UNP C1K0Y1
M	278	HIS	-	expression tag	UNP C1K0Y1
M	279	HIS	-	expression tag	UNP C1K0Y1
M	280	HIS	-	expression tag	UNP C1K0Y1

- Molecule 4 is a protein called C8K10D5-1 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	B	223	Total 1657	C 1041	N 282	O 326	S 8	0	0	0
4	L	223	Total 1657	C 1041	N 282	O 326	S 8	0	0	0

- Molecule 5 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	F	100	Total 837	C 533	N 141	O 159	S 4	0	0	0
5	N	100	Total 837	C 533	N 141	O 159	S 4	0	0	0

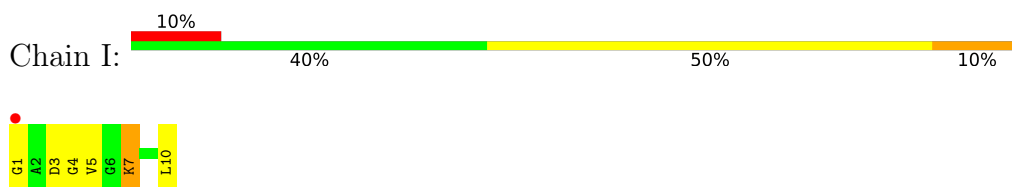
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	0	MET	-	expression tag	UNP P61769
N	0	MET	-	expression tag	UNP P61769

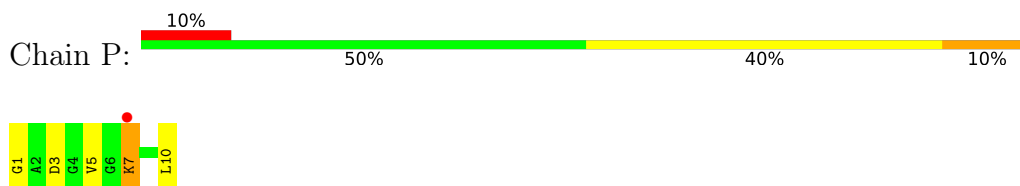
### 3 Residue-property plots [i](#)

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.

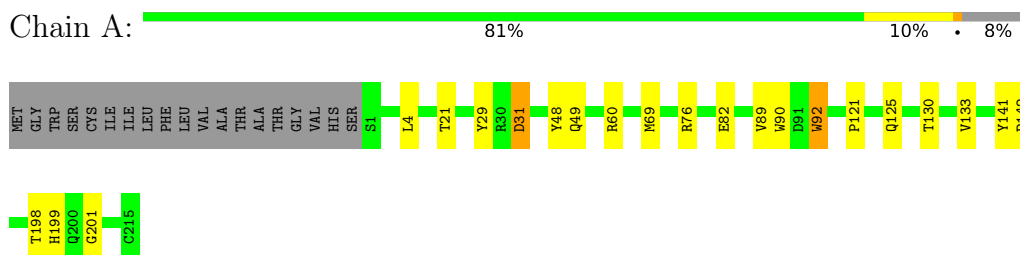
- Molecule 1: Peptide from GTPase KRas, N-terminally processed



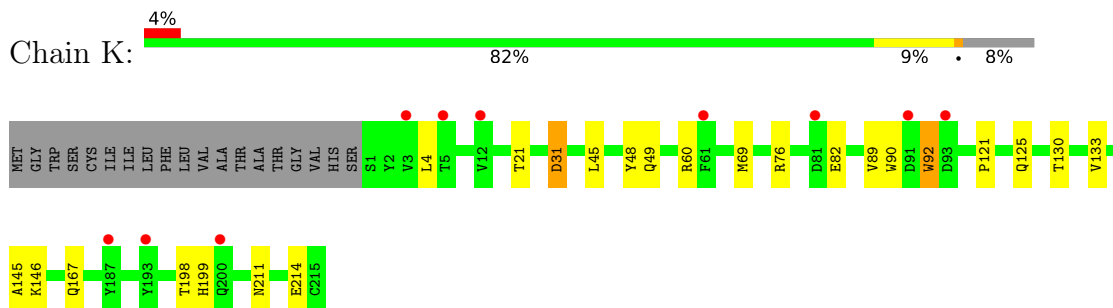
- Molecule 1: Peptide from GTPase KRas, N-terminally processed



- Molecule 2: C8K10D5-1 Fab Light chain

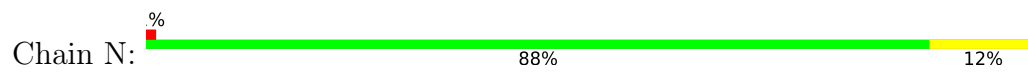


- Molecule 2: C8K10D5-1 Fab Light chain



- Molecule 3: HLA class I antigen





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	164.98Å 164.98Å 426.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.92 – 4.54 29.92 – 4.54	Depositor EDS
% Data completeness (in resolution range)	98.8 (29.92-4.54) 98.3 (29.92-4.54)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.85 (at 4.61Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660, PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.279 , 0.295 0.278 , 0.296	Depositor DCC
$R_{free}$ test set	2000 reflections (9.67%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	118.7	Xtrriage
Anisotropy	0.692	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 193.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.32$ , $\langle L^2 \rangle = 0.15$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.81	EDS
Total number of atoms	12930	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	168.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.24% 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 [i](#)

### 5.1 Standard geometry [i](#)

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	I	0.28	0/60	0.67	0/77
1	P	0.29	0/60	0.66	0/77
2	A	0.16	0/1711	0.38	0/2333
2	K	0.17	0/1711	0.38	0/2333
3	E	0.17	0/2302	0.39	0/3125
3	M	0.18	0/2302	0.43	2/3125 (0.1%)
4	B	0.17	0/1694	0.45	1/2302 (0.0%)
4	L	0.17	0/1694	0.42	0/2302
5	F	0.16	0/860	0.37	0/1162
5	N	0.16	0/860	0.37	0/1162
All	All	0.17	0/13254	0.41	3/17998 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	167	TRP	N-CA-C	6.70	119.44	111.33
4	B	55	SER	N-CA-C	6.05	120.24	112.86
3	M	165	VAL	N-CA-C	-5.69	103.98	111.09

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	I	61	0	63	8	0
1	P	61	0	63	9	0
2	A	1670	0	1592	26	1
2	K	1670	0	1592	34	0
3	E	2240	0	2098	53	0
3	M	2240	0	2098	75	0
4	B	1657	0	1630	22	0
4	L	1657	0	1630	31	3
5	F	837	0	803	9	0
5	N	837	0	803	13	2
All	All	12930	0	12372	200	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (200) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:90:TRP:NE1	2:A:92:TRP:CZ3	2.18	1.11
2:K:92:TRP:HZ2	3:M:155:GLN:HA	1.15	1.10
3:E:142:ILE:HG23	3:M:226:GLN:CG	1.80	1.10
3:E:142:ILE:HG23	3:M:226:GLN:HG3	1.12	1.09
2:K:90:TRP:NE1	2:K:92:TRP:CZ3	2.18	1.09
4:L:100:ARG:HB2	4:L:107:ASP:OD2	1.53	1.07
4:B:100:ARG:HB2	4:B:107:ASP:OD2	1.53	1.07
3:E:170:ARG:NH1	4:B:54:TYR:OH	1.91	1.03
3:E:142:ILE:CG2	3:M:226:GLN:CG	2.37	1.03
4:L:56:LEU:CD1	3:M:166:GLU:HG2	1.89	1.03
3:M:146:LYS:NZ	1:P:10:LEU:O	1.92	1.00
2:K:90:TRP:NE1	2:K:92:TRP:CE3	2.28	1.00
1:I:3:ASP:OD1	3:E:156:ARG:NH1	1.96	0.99
2:K:92:TRP:NE1	3:M:155:GLN:HB2	1.77	0.98
2:A:90:TRP:NE1	2:A:92:TRP:CE3	2.29	0.98
4:L:56:LEU:HD13	3:M:166:GLU:HG2	1.01	0.98
3:E:142:ILE:CG2	3:M:226:GLN:HG2	1.96	0.96
2:K:92:TRP:CZ2	3:M:155:GLN:HA	2.01	0.94
3:E:142:ILE:HG21	3:M:226:GLN:HG2	1.48	0.93
3:M:131:ARG:HG2	3:M:157:ARG:HH11	1.31	0.93
4:L:100:ARG:CB	4:L:107:ASP:OD2	2.17	0.92
4:B:100:ARG:CB	4:B:107:ASP:OD2	2.17	0.92
3:E:131:ARG:HG2	3:E:157:ARG:HH11	1.31	0.91
4:L:56:LEU:HD13	3:M:166:GLU:CG	1.97	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:90:TRP:HE1	2:K:92:TRP:HZ3	1.22	0.88
2:K:92:TRP:HE1	3:M:155:GLN:HB2	1.34	0.88
3:E:142:ILE:CG2	3:M:226:GLN:HG3	1.98	0.88
2:A:90:TRP:HE1	2:A:92:TRP:HZ3	1.22	0.87
3:M:162:GLY:O	3:M:166:GLU:HG3	1.75	0.87
2:A:92:TRP:CE3	2:A:92:TRP:HA	2.10	0.85
2:K:92:TRP:CE3	2:K:92:TRP:HA	2.10	0.85
2:K:92:TRP:HZ2	3:M:155:GLN:CA	1.92	0.83
4:L:56:LEU:HB2	3:M:166:GLU:OE2	1.78	0.82
3:M:192:HIS:HE1	5:N:98:ASP:O	1.62	0.82
2:K:92:TRP:CE2	3:M:155:GLN:HB2	2.16	0.80
2:A:92:TRP:HA	2:A:92:TRP:HE3	1.51	0.75
1:I:3:ASP:CG	3:E:156:ARG:HH11	1.94	0.74
3:M:202:ARG:NH1	5:N:99:MET:O	2.21	0.73
3:M:192:HIS:CE1	5:N:98:ASP:O	2.42	0.72
2:A:31:ASP:N	2:A:31:ASP:OD1	2.21	0.71
2:K:92:TRP:HE1	3:M:155:GLN:CB	2.04	0.71
3:M:192:HIS:NE2	5:N:99:MET:O	2.23	0.70
2:K:92:TRP:HA	2:K:92:TRP:HE3	1.51	0.70
2:K:31:ASP:OD1	2:K:31:ASP:N	2.21	0.69
4:L:54:TYR:OH	3:M:170:ARG:NH1	2.24	0.69
3:E:65:GLN:HB3	3:E:69:ARG:HH11	1.58	0.69
3:E:166:GLU:HG3	4:B:56:LEU:HD13	1.74	0.68
2:K:90:TRP:NE1	2:K:92:TRP:HZ3	1.83	0.68
3:M:65:GLN:HB3	3:M:69:ARG:HH11	1.58	0.68
3:M:155:GLN:NE2	1:P:7:LYS:HE3	2.09	0.66
2:A:90:TRP:NE1	2:A:92:TRP:HZ3	1.84	0.66
3:M:121:LYS:HG3	5:N:1:ILE:HG12	1.77	0.66
2:K:92:TRP:CZ2	3:M:155:GLN:CA	2.74	0.66
3:E:202:ARG:NH1	5:F:99:MET:O	2.29	0.63
3:E:192:HIS:HE1	5:F:98:ASP:O	1.80	0.63
3:E:131:ARG:HG2	3:E:157:ARG:NH1	2.11	0.62
2:K:92:TRP:CZ2	3:M:155:GLN:HB2	2.34	0.61
2:A:92:TRP:HE1	3:E:155:GLN:CA	2.12	0.61
3:M:231:VAL:O	3:M:243:LYS:NZ	2.31	0.61
3:E:166:GLU:CG	4:B:56:LEU:HD13	2.31	0.60
4:L:132:PRO:HD3	4:L:218:LYS:HE2	1.85	0.59
3:E:226:GLN:CD	3:M:142:ILE:HG23	2.28	0.58
2:K:92:TRP:CZ2	3:M:155:GLN:CB	2.87	0.58
4:L:102:GLU:OE2	3:M:167:TRP:CH2	2.57	0.58
4:L:102:GLU:OE2	3:M:167:TRP:CZ2	2.57	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:121:LYS:HG3	5:F:1:ILE:HG12	1.86	0.58
4:B:132:PRO:HD3	4:B:218:LYS:HE2	1.85	0.57
3:M:121:LYS:NZ	5:N:0:MET:HE3	2.19	0.57
1:I:10:LEU:O	3:E:84:TYR:OH	2.18	0.56
3:M:121:LYS:HZ1	5:N:0:MET:HE3	1.69	0.56
3:M:131:ARG:HG2	3:M:157:ARG:NH1	2.11	0.55
2:K:49:GLN:OE1	3:M:69:ARG:NH2	2.38	0.55
3:M:107:GLY:O	3:M:169:ARG:NH1	2.29	0.55
2:A:92:TRP:HE1	3:E:155:GLN:N	2.05	0.55
3:M:58:GLU:O	3:M:62:ARG:HG3	2.07	0.55
3:E:58:GLU:O	3:E:62:ARG:HG3	2.07	0.54
1:I:1:GLY:O	3:E:159:TYR:OH	2.23	0.54
3:M:159:TYR:CE1	1:P:3:ASP:HA	2.42	0.54
3:M:230:LEU:HD22	3:M:243:LYS:HE3	1.90	0.54
2:A:49:GLN:OE1	3:E:69:ARG:NH2	2.40	0.54
2:K:4:LEU:HD11	2:K:89:VAL:HG22	1.89	0.54
2:A:4:LEU:HD11	2:A:89:VAL:HG22	1.89	0.54
3:E:107:GLY:O	3:E:169:ARG:NH1	2.29	0.53
3:M:159:TYR:CG	1:P:3:ASP:OD2	2.61	0.53
3:E:230:LEU:HD22	3:E:243:LYS:HE3	1.90	0.53
3:E:145:ARG:HH12	3:M:225:THR:HB	1.73	0.53
3:M:106:ASP:OD1	3:M:108:ARG:HG2	2.09	0.52
3:E:106:ASP:OD1	3:E:108:ARG:HG2	2.10	0.52
3:M:5:MET:HB2	3:M:168:LEU:HD13	1.91	0.52
5:F:2:GLN:HB2	5:N:2:GLN:HB2	1.92	0.52
4:B:100:ARG:HB3	4:B:107:ASP:OD2	2.07	0.52
3:E:192:HIS:CE1	5:F:98:ASP:O	2.61	0.52
3:E:145:ARG:NH1	3:M:225:THR:HB	2.25	0.52
3:E:166:GLU:OE1	4:B:56:LEU:HD22	2.10	0.52
3:E:192:HIS:NE2	5:F:99:MET:O	2.42	0.52
4:L:54:TYR:HH	3:M:170:ARG:HH11	1.56	0.51
3:M:7:TYR:CE2	1:P:1:GLY:O	2.63	0.51
3:M:162:GLY:C	3:M:166:GLU:HG3	2.35	0.51
3:E:5:MET:HB2	3:E:168:LEU:HD13	1.92	0.51
1:I:10:LEU:O	3:E:146:LYS:NZ	2.40	0.51
5:F:95:TRP:CZ2	5:F:97:ARG:HB3	2.46	0.51
2:K:82:GLU:HG3	2:K:167:GLN:HB3	1.92	0.51
3:E:166:GLU:CD	4:B:56:LEU:HD13	2.36	0.51
3:E:142:ILE:HD13	3:M:226:GLN:HA	1.92	0.51
3:E:231:VAL:O	3:E:243:LYS:NZ	2.31	0.51
2:K:90:TRP:CD1	2:K:92:TRP:CE3	2.99	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:90:TRP:CD1	2:A:92:TRP:CE3	2.99	0.50
2:K:121:PRO:HD3	2:K:133:VAL:HG22	1.93	0.50
2:A:121:PRO:HD3	2:A:133:VAL:HG22	1.93	0.50
5:N:95:TRP:CZ2	5:N:97:ARG:HB3	2.46	0.50
2:A:82:GLU:HG3	2:A:167:GLN:HB3	1.92	0.50
1:I:7:LYS:HD3	2:A:29:TYR:O	2.11	0.50
4:B:128:PRO:HB3	4:B:154:TYR:HB3	1.94	0.50
4:L:128:PRO:HB3	4:L:154:TYR:HB3	1.93	0.50
1:I:1:GLY:HA3	3:E:167:TRP:CD1	2.48	0.49
2:A:146:LYS:HB3	2:A:198:THR:HB	1.96	0.48
2:K:146:LYS:HB3	2:K:198:THR:HB	1.96	0.48
4:L:102:GLU:CD	3:M:167:TRP:CZ2	2.91	0.48
4:L:54:TYR:HB2	4:L:56:LEU:HD11	1.96	0.47
2:A:92:TRP:CZ2	3:E:155:GLN:HA	2.50	0.47
4:B:100:ARG:HB2	4:B:107:ASP:O	2.15	0.47
4:B:34:MET:HB3	4:B:79:LEU:HD22	1.96	0.46
4:L:34:MET:HB3	4:L:79:LEU:HD22	1.96	0.46
2:A:145:ALA:HB2	2:A:199:HIS:HD2	1.80	0.46
3:E:133:TRP:HB2	3:E:144:GLN:HG3	1.98	0.46
2:A:92:TRP:O	3:E:151:ARG:NH1	2.48	0.46
3:M:139:ALA:O	3:M:142:ILE:HB	2.16	0.46
3:E:226:GLN:CG	3:M:142:ILE:HG23	2.45	0.46
3:M:133:TRP:HB2	3:M:144:GLN:HG3	1.98	0.46
4:L:100:ARG:HB3	4:L:107:ASP:OD2	2.07	0.46
1:I:4:GLY:HA3	4:B:106:MET:HE1	1.97	0.46
4:B:108:GLY:O	4:B:109:MET:HE2	2.16	0.46
4:L:100:ARG:HB2	4:L:107:ASP:O	2.15	0.46
3:E:139:ALA:O	3:E:142:ILE:HB	2.16	0.46
3:E:242:GLN:NE2	5:F:12:ARG:O	2.48	0.46
4:L:105:TYR:HD2	4:L:106:MET:HG3	1.81	0.46
4:L:108:GLY:O	4:L:109:MET:HE2	2.16	0.46
4:L:12:VAL:O	4:L:120:VAL:HA	2.17	0.45
3:M:159:TYR:CE2	1:P:3:ASP:HB2	2.52	0.45
5:N:31:HIS:ND1	5:N:32:PRO:HA	2.32	0.45
3:M:7:TYR:HE2	1:P:1:GLY:O	1.98	0.45
2:K:45:LEU:HB2	4:L:109:MET:O	2.17	0.45
2:A:21:THR:HB	2:A:69:MET:SD	2.58	0.44
4:B:105:TYR:HD2	4:B:106:MET:HG3	1.82	0.44
5:F:31:HIS:ND1	5:F:32:PRO:HA	2.32	0.44
2:K:145:ALA:HB2	2:K:199:HIS:HD2	1.81	0.44
3:E:255:GLN:H	3:E:255:GLN:CD	2.24	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:139:ALA:HA	3:E:142:ILE:HD12	1.99	0.44
4:B:12:VAL:O	4:B:120:VAL:HA	2.16	0.44
2:K:92:TRP:HZ2	3:M:155:GLN:CB	2.26	0.44
2:K:21:THR:HB	2:K:69:MET:SD	2.58	0.44
4:L:20:LEU:HD12	4:L:81:LEU:HD23	2.00	0.44
3:M:229:GLU:O	3:M:245:ALA:HA	2.16	0.44
2:A:125:GLN:HG2	2:A:130:THR:O	2.18	0.43
3:E:86:ASN:ND2	3:M:229:GLU:OE2	2.50	0.43
3:M:255:GLN:H	3:M:255:GLN:CD	2.24	0.43
3:M:139:ALA:HA	3:M:142:ILE:HD12	1.99	0.43
2:K:49:GLN:HE22	3:M:69:ARG:HH21	1.65	0.43
3:M:111:ARG:HG2	3:M:128:GLU:OE2	2.18	0.43
3:E:51:TRP:CD1	3:E:51:TRP:H	2.33	0.43
4:L:161:VAL:HA	4:L:206:ASN:O	2.18	0.43
2:A:90:TRP:CE2	2:A:92:TRP:HZ3	2.37	0.43
2:K:60:ARG:HG2	2:K:76:ARG:NH2	2.34	0.43
4:B:12:VAL:HG11	4:B:86:LEU:HD13	2.01	0.43
4:L:12:VAL:HG11	4:L:86:LEU:HD13	2.01	0.43
4:B:161:VAL:HA	4:B:206:ASN:O	2.19	0.42
4:L:54:TYR:HH	3:M:170:ARG:NH1	2.16	0.42
4:B:20:LEU:HD12	4:B:81:LEU:HD23	2.00	0.42
3:M:51:TRP:CD1	3:M:51:TRP:H	2.33	0.42
2:A:60:ARG:HG2	2:A:76:ARG:NH2	2.34	0.42
2:K:90:TRP:NE1	2:K:92:TRP:HE3	2.05	0.42
2:K:125:GLN:HG2	2:K:130:THR:O	2.19	0.42
3:M:242:GLN:NE2	5:N:12:ARG:O	2.53	0.42
4:B:107:ASP:O	4:B:107:ASP:CG	2.62	0.42
4:L:54:TYR:HB2	4:L:56:LEU:CD1	2.49	0.42
3:E:219:ARG:HD3	3:E:224:GLN:NE2	2.35	0.42
3:M:122:ASP:OD1	5:N:60:TRP:NE1	2.52	0.42
2:K:90:TRP:CE2	2:K:92:TRP:HZ3	2.37	0.42
3:E:111:ARG:HG2	3:E:128:GLU:OE2	2.18	0.42
3:M:159:TYR:CB	1:P:3:ASP:OD2	2.68	0.41
2:A:48:TYR:HD2	2:A:49:GLN:HG3	1.85	0.41
3:E:27:TYR:CE2	3:E:32:GLN:HB2	2.55	0.41
3:M:27:TYR:CE2	3:M:32:GLN:HB2	2.55	0.41
3:E:102:ASP:HB2	3:E:111:ARG:HB2	2.03	0.41
4:B:171:GLY:O	4:B:191:VAL:HA	2.21	0.41
4:L:107:ASP:O	4:L:107:ASP:CG	2.63	0.41
3:M:219:ARG:HD3	3:M:224:GLN:NE2	2.35	0.41
4:B:177:ALA:HA	4:B:187:LEU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:171:GLY:O	4:L:191:VAL:HA	2.21	0.41
3:M:102:ASP:HB2	3:M:111:ARG:HB2	2.03	0.41
4:L:22:CYS:HB3	4:L:79:LEU:HB3	2.03	0.41
3:M:156:ARG:NH1	1:P:3:ASP:OD1	2.51	0.40
2:A:141:TYR:CG	2:A:142:PRO:HA	2.56	0.40
4:L:36:TRP:NE1	4:L:81:LEU:HB2	2.36	0.40
2:A:92:TRP:HZ2	3:E:155:GLN:HA	1.86	0.40
3:M:162:GLY:O	3:M:166:GLU:N	2.51	0.40
5:N:2:GLN:HA	5:N:31:HIS:O	2.21	0.40
2:K:48:TYR:HD2	2:K:49:GLN:HG3	1.85	0.40
2:K:211:ASN:HB2	2:K:214:GLU:CD	2.47	0.40
4:L:177:ALA:HA	4:L:187:LEU:HB3	2.02	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)
4:L:200:THR:CG2	5:N:77:GLU:OE2[8_545]	1.51	0.69
4:L:200:THR:CG2	5:N:77:GLU:CD[8_545]	2.04	0.16
2:A:201:GLY:O	4:L:124:SER:OG[5_555]	2.14	0.06

## 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	I	8/10 (80%)	8 (100%)	0	0	100	100
1	P	8/10 (80%)	8 (100%)	0	0	100	100
2	A	213/234 (91%)	210 (99%)	3 (1%)	0	100	100
2	K	213/234 (91%)	210 (99%)	3 (1%)	0	100	100
3	E	271/280 (97%)	259 (96%)	12 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	M	271/280 (97%)	259 (96%)	12 (4%)	0	100	100
4	B	221/255 (87%)	214 (97%)	7 (3%)	0	100	100
4	L	221/255 (87%)	214 (97%)	7 (3%)	0	100	100
5	F	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
5	N	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
All	All	1622/1758 (92%)	1576 (97%)	46 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	I	5/5 (100%)	3 (60%)	2 (40%)	0	1
1	P	5/5 (100%)	3 (60%)	2 (40%)	0	1
2	A	187/202 (93%)	185 (99%)	2 (1%)	65	74
2	K	187/202 (93%)	185 (99%)	2 (1%)	65	74
3	E	229/236 (97%)	227 (99%)	2 (1%)	70	76
3	M	229/236 (97%)	227 (99%)	2 (1%)	70	76
4	B	184/212 (87%)	183 (100%)	1 (0%)	81	81
4	L	184/212 (87%)	183 (100%)	1 (0%)	81	81
5	F	95/95 (100%)	95 (100%)	0	100	100
5	N	95/95 (100%)	95 (100%)	0	100	100
All	All	1400/1500 (93%)	1386 (99%)	14 (1%)	68	76

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	5	VAL
1	I	7	LYS

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Mol	Chain	Res	Type
2	A	31	ASP
2	A	92	TRP
3	E	143	THR
3	E	273	ARG
4	B	56	LEU
2	K	31	ASP
2	K	92	TRP
4	L	56	LEU
3	M	143	THR
3	M	273	ARG
1	P	5	VAL
1	P	7	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
5	F	8	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 oligosaccharides 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

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	I	10/10 (100%)	0.84	1 (10%) 12 17	146, 165, 175, 176	0
1	P	10/10 (100%)	0.48	1 (10%) 12 17	142, 150, 153, 154	0
2	A	215/234 (91%)	0.29	0 100 100	142, 156, 173, 194	0
2	K	215/234 (91%)	0.64	10 (4%) 36 33	132, 183, 210, 231	0
3	E	273/280 (97%)	0.46	8 (2%) 53 42	130, 161, 190, 208	0
3	M	273/280 (97%)	0.40	4 (1%) 72 57	128, 163, 264, 288	0
4	B	223/255 (87%)	0.31	6 (2%) 56 44	144, 159, 176, 206	0
4	L	223/255 (87%)	0.43	6 (2%) 56 44	118, 147, 235, 258	0
5	F	100/100 (100%)	0.20	1 (1%) 79 64	135, 153, 173, 185	0
5	N	100/100 (100%)	0.44	1 (1%) 79 64	147, 196, 232, 246	0
All	All	1642/1758 (93%)	0.41	38 (2%) 61 48	118, 160, 230, 288	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	61	PHE	4.0
3	M	225	THR	4.0
4	L	102	GLU	3.9
3	E	103	LEU	3.7
4	L	107	ASP	3.7
2	K	12	VAL	3.5
2	K	187	TYR	3.2
4	B	2	VAL	3.1
2	K	193	TYR	3.0
3	E	226	GLN	2.8
3	E	194	VAL	2.8
5	F	33	SER	2.8
3	M	215	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
4	B	102	GLU	2.7
2	K	91	ASP	2.7
3	E	183	GLU	2.6
4	L	122	SER	2.4
2	K	200	GLN	2.3
3	M	74	ASP	2.3
1	I	1	GLY	2.3
4	L	179	LEU	2.3
2	K	3	VAL	2.3
3	M	274	TRP	2.2
4	B	139	SER	2.2
2	K	93	ASP	2.2
4	B	130	VAL	2.2
4	B	146	ALA	2.2
2	K	5	THR	2.2
2	K	81	ASP	2.2
3	E	74	ASP	2.2
3	E	181	ARG	2.1
1	P	7	LYS	2.1
3	E	147	TRP	2.1
5	N	82	VAL	2.1
4	B	31	GLN	2.0
4	L	125	THR	2.0
4	L	96	CYS	2.0
3	E	148	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 oligosaccharides 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.