



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 07:24 PM GMT

PDB ID : 4R9Y  
Title : Crystal structure of KKOFab in complex with platelet factor 4  
Authors : Cai, Z.; Zhu, Z.; Liu, Q.; Greene, M.I.  
Deposited on : 2014-09-08  
Resolution : 4.11 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 : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
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) : rb-20026982

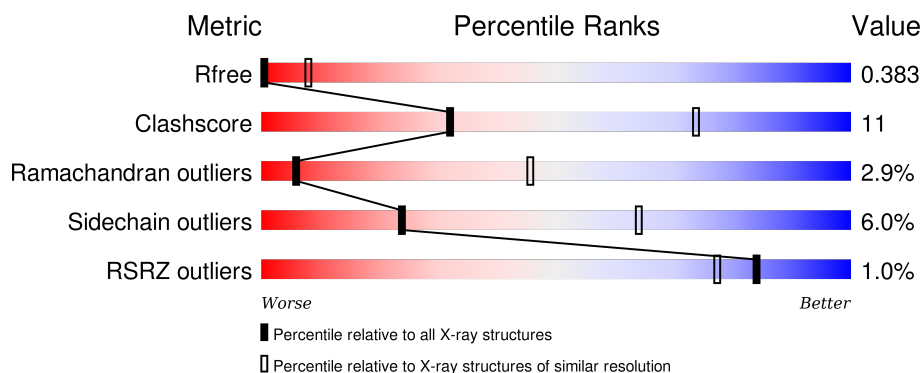
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.11 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	1020 (4.62-3.60)
Clashscore	102246	1119 (4.62-3.60)
Ramachandran outliers	100387	1065 (4.62-3.60)
Sidechain outliers	100360	1051 (4.62-3.60)
RSRZ outliers	91569	1024 (4.62-3.60)

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	70	<div> <div>69%</div> <div>23%</div> <div>7%</div> </div>
1	B	70	<div> <div>53%</div> <div>36%</div> <div>7%</div> </div>
1	C	70	<div> <div>64%</div> <div>26%</div> <div>7%</div> </div>
1	D	70	<div> <div>3%</div> <div>59%</div> <div>33%</div> <div>7%</div> </div>
2	L	214	<div> <div>3%</div> <div>73%</div> <div>25%</div> <div>7%</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	M	214	<div><div></div><div>73%</div><div>24%</div><div></div></div>
3	H	218	<div><div></div><div>72%</div><div>24%</div><div>5%</div></div>
3	N	218	<div><div>%</div><div></div><div>69%</div><div>27%</div><div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8548 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 Platelet factor 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	65	Total	C	N	O	S	0	0	0
			501	319	91	87	4			
1	C	65	Total	C	N	O	S	0	0	0
			501	319	91	87	4			
1	B	65	Total	C	N	O	S	0	0	0
			501	319	91	87	4			
1	A	65	Total	C	N	O	S	0	0	0
			501	319	91	87	4			

- Molecule 2 is a protein called Platelet factor 4 antibody KKO light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	0	0
			1647	1023	275	341	8			
2	M	214	Total	C	N	O	S	0	0	0
			1647	1023	275	341	8			

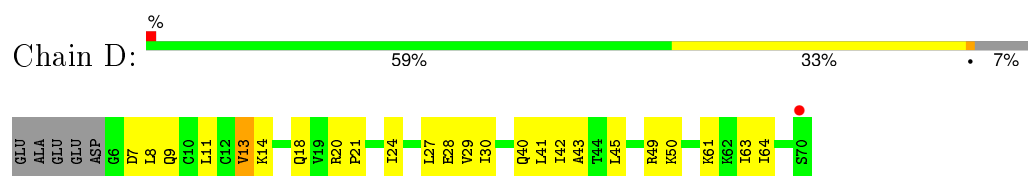
- Molecule 3 is a protein called Platelet factor 4 antibody KKO heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	218	Total	C	N	O	S	0	0	0
			1625	1028	261	329	7			
3	N	218	Total	C	N	O	S	0	0	0
			1625	1028	261	329	7			

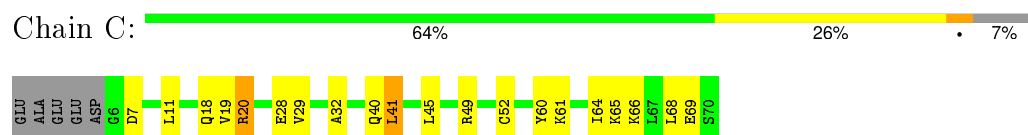
### 3 Residue-property plots [i](#)

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.

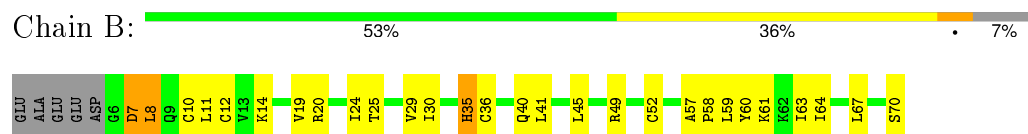
- Molecule 1: Platelet factor 4



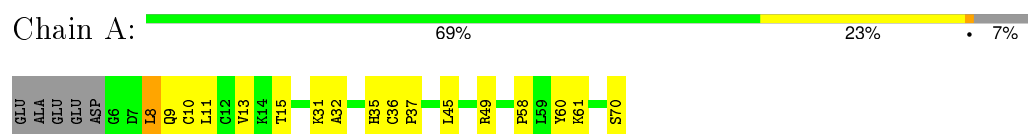
- Molecule 1: Platelet factor 4



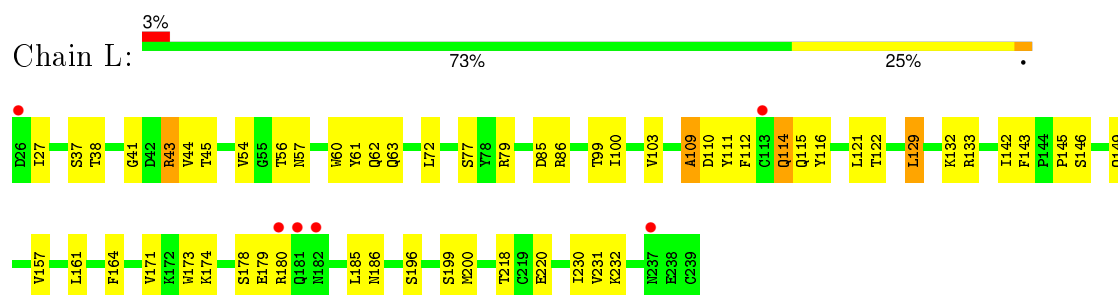
- Molecule 1: Platelet factor 4



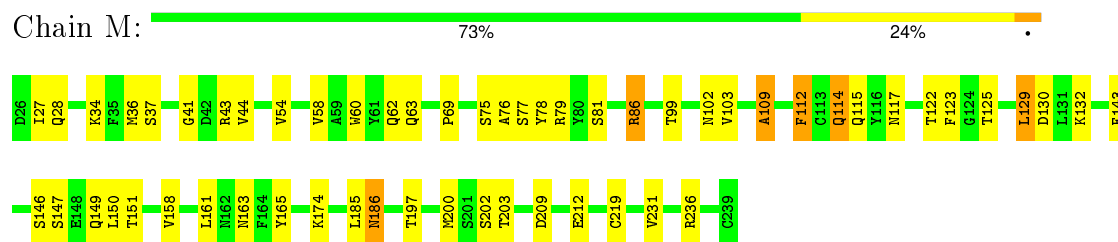
- Molecule 1: Platelet factor 4



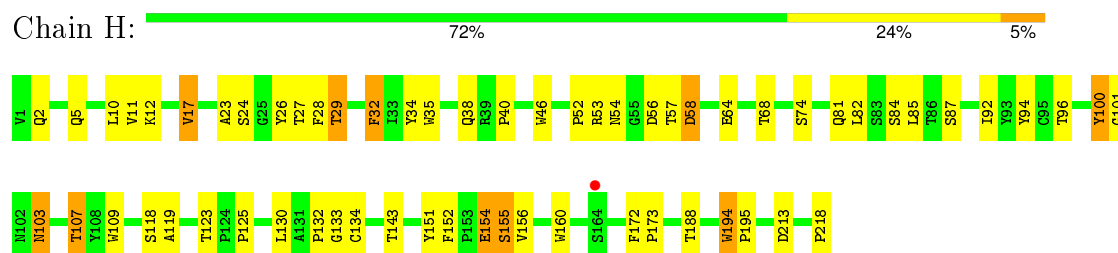
- Molecule 2: Platelet factor 4 antibody KKO light chain



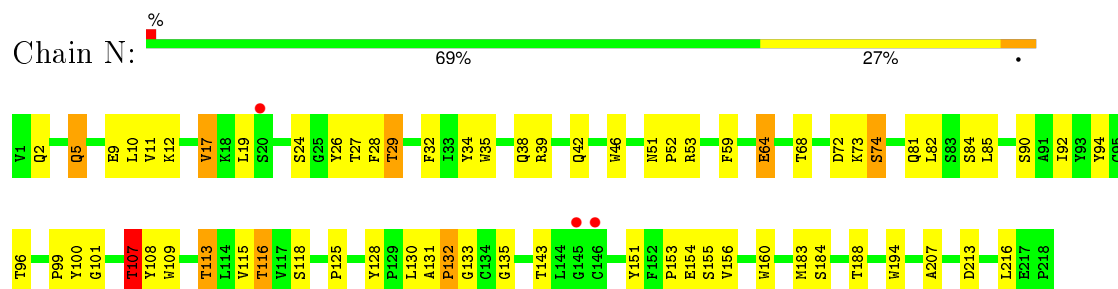
- Molecule 2: Platelet factor 4 antibody KKO light chain



- Molecule 3: Platelet factor 4 antibody KKO heavy chain



- Molecule 3: Platelet factor 4 antibody KKO heavy chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.49 Å 99.34 Å 261.74 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 4.11 19.99 – 4.11	Depositor EDS
% Data completeness (in resolution range)	78.9 (20.00-4.11) 79.1 (19.99-4.11)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.00 (at 4.07 Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.317 , 0.382 0.313 , 0.383	Depositor DCC
$R_{free}$ test set	416 reflections (5.22%)	DCC
Wilson B-factor (Å <sup>2</sup> )	120.2	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.12 , 111.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	1 of 8388 reflections (0.012%)	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	8548	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	269.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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	0.38	0/507	0.54	0/683
1	B	0.41	0/507	0.57	0/683
1	C	0.38	0/507	0.52	0/683
1	D	0.38	0/507	0.51	0/683
2	L	0.44	1/1683 (0.1%)	0.50	0/2290
2	M	0.42	1/1683 (0.1%)	0.50	0/2290
3	H	0.50	3/1669 (0.2%)	0.52	0/2285
3	N	0.50	3/1669 (0.2%)	0.52	0/2285
All	All	0.45	8/8732 (0.1%)	0.52	0/11882

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	35	TRP	CD2-CE2	5.27	1.47	1.41
3	N	35	TRP	CD2-CE2	5.15	1.47	1.41
2	M	60	TRP	CD2-CE2	5.09	1.47	1.41
2	L	173	TRP	CD2-CE2	5.08	1.47	1.41
3	N	160	TRP	CD2-CE2	5.04	1.47	1.41
3	H	109	TRP	CD2-CE2	5.04	1.47	1.41
3	N	109	TRP	CD2-CE2	5.04	1.47	1.41
3	H	160	TRP	CD2-CE2	5.01	1.47	1.41

There are no bond angle outliers.

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	501	0	549	16	0
1	B	501	0	549	23	0
1	C	501	0	549	15	0
1	D	501	0	549	18	0
2	L	1647	0	1540	33	0
2	M	1647	0	1540	34	0
3	H	1625	0	1545	29	0
3	N	1625	0	1545	31	0
All	All	8548	0	8366	180	0

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 11.

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)
1:B:58:PRO:HA	1:B:61:LYS:HD3	1.31	1.08
1:A:58:PRO:HA	1:A:61:LYS:HD3	1.48	0.96
1:D:28:GLU:HB3	1:C:28:GLU:HB3	1.52	0.89
2:L:79:ARG:HB2	1:A:70:SER:HB2	1.53	0.88
1:D:45:LEU:HD12	1:D:49:ARG:HB3	1.62	0.81
2:L:27:ILE:H	2:L:122:THR:HG21	1.49	0.78
3:N:143:THR:HG22	3:N:188:THR:HA	1.66	0.77
2:M:186:ASN:HB3	2:M:200:MET:SD	2.25	0.77
1:B:58:PRO:CA	1:B:61:LYS:HD3	2.13	0.77
2:M:27:ILE:H	2:M:122:THR:HG21	1.49	0.77
3:H:10:LEU:HD21	3:H:119:ALA:H	1.50	0.76
1:B:58:PRO:HA	1:B:61:LYS:CD	2.14	0.75
1:B:45:LEU:HD12	1:B:49:ARG:HB3	1.73	0.71
2:L:61:TYR:HE1	2:L:114:GLN:HG3	1.57	0.70
3:H:100:TYR:HE2	1:B:12:CYS:HB2	1.56	0.69
1:C:61:LYS:HA	1:C:64:ILE:HD12	1.74	0.69
1:A:8:LEU:HD22	1:A:8:LEU:H	1.57	0.69
1:B:35:HIS:CD2	1:B:36:CYS:H	2.12	0.67
3:N:34:TYR:HD1	3:N:46:TRP:HE1	1.41	0.67
1:A:58:PRO:CA	1:A:61:LYS:HD3	2.24	0.67
2:L:45:THR:HG22	2:L:99:THR:HG22	1.77	0.67
3:H:125:PRO:HA	3:H:151:TYR:HB3	1.78	0.66
3:N:2:GLN:HG2	3:N:24:SER:HB2	1.77	0.65
3:H:143:THR:HG22	3:H:188:THR:HA	1.78	0.65
3:H:123:THR:H	3:H:152:PHE:HB3	1.61	0.64
1:D:29:VAL:HG22	1:D:41:LEU:HG	1.79	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:219:CYS:O	2:M:231:VAL:HG12	1.98	0.63
3:H:34:TYR:HD1	3:H:46:TRP:HE1	1.45	0.63
2:L:54:VAL:HG21	2:L:115:GLN:HB2	1.81	0.63
1:C:45:LEU:HD12	1:C:49:ARG:HB3	1.81	0.62
3:N:28:PHE:O	3:N:52:PRO:HG2	2.00	0.61
1:D:28:GLU:CB	1:C:28:GLU:HB3	2.27	0.59
2:M:146:SER:HB3	2:M:149:GLN:HG2	1.83	0.59
3:H:100:TYR:HE2	1:B:12:CYS:CB	2.16	0.59
2:L:61:TYR:CE1	2:L:114:GLN:HG3	2.36	0.59
1:B:24:ILE:O	1:A:31:LYS:HD3	2.03	0.59
3:N:72:ASP:C	3:N:74:SER:H	2.07	0.58
3:N:17:VAL:O	3:N:81:GLN:HA	2.03	0.58
3:H:2:GLN:O	3:H:23:ALA:HA	2.03	0.57
1:A:32:ALA:HB1	2:M:81:SER:HB2	1.86	0.57
2:M:212:GLU:O	2:M:236:ARG:NH2	2.36	0.57
3:H:82:LEU:HD23	3:H:85:LEU:HG	1.85	0.57
3:N:19:LEU:HD22	3:N:113:THR:HG21	1.86	0.56
1:D:9:GLN:O	1:B:11:LEU:HD12	2.05	0.56
1:A:45:LEU:HD12	1:A:49:ARG:HB3	1.86	0.56
2:M:44:VAL:O	2:M:99:THR:HA	2.06	0.56
1:D:61:LYS:HA	1:D:64:ILE:HD12	1.86	0.55
2:L:41:GLY:H	2:L:103:VAL:CG2	2.19	0.55
3:N:107:THR:HG23	3:N:108:TYR:H	1.72	0.55
1:B:29:VAL:HG22	1:B:41:LEU:HD23	1.89	0.55
3:H:38:GLN:HB3	3:H:92:ILE:HG23	1.89	0.54
1:D:11:LEU:H	1:D:40:GLN:NE2	2.04	0.54
2:L:174:LYS:HB3	2:L:218:THR:HB	1.90	0.54
2:M:143:PHE:HB3	3:N:130:LEU:HD12	1.91	0.53
3:N:82:LEU:HD23	3:N:85:LEU:HG	1.90	0.53
2:L:133:ARG:HD3	2:L:196:SER:HB2	1.90	0.53
3:N:99:PRO:HD3	3:N:107:THR:HG22	1.90	0.53
2:L:146:SER:HB3	2:L:149:GLN:HG2	1.89	0.53
1:D:24:ILE:HD11	1:D:43:ALA:HB1	1.90	0.53
2:M:37:SER:HA	2:M:130:ASP:H	1.74	0.52
2:L:37:SER:HB2	2:L:132:LYS:HE2	1.91	0.52
1:B:57:ALA:HB3	1:B:59:LEU:HD23	1.92	0.52
3:N:38:GLN:HB3	3:N:92:ILE:HG23	1.89	0.52
3:N:5:GLN:HE22	3:N:94:TYR:HA	1.74	0.52
3:N:59:PHE:HB2	3:N:64:GLU:HG2	1.92	0.51
1:D:11:LEU:H	1:D:40:GLN:HE22	1.58	0.51
2:M:109:ALA:H	2:M:129:LEU:HD11	1.76	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:TYR:O	1:C:64:ILE:HG13	2.10	0.51
2:M:63:GLN:HA	2:M:69:PRO:HA	1.93	0.51
1:A:58:PRO:HA	1:A:61:LYS:CD	2.30	0.51
3:N:26:TYR:C	3:N:28:PHE:H	2.13	0.51
2:M:41:GLY:H	2:M:103:VAL:HG23	1.76	0.51
1:D:11:LEU:HD23	1:D:42:ILE:HG21	1.93	0.50
3:N:32:PHE:CZ	3:N:51:ASN:HB2	2.46	0.50
3:H:5:GLN:HE22	3:H:94:TYR:HA	1.76	0.50
2:L:114:GLN:HE21	2:L:115:GLN:H	1.58	0.50
2:L:145:PRO:HG3	2:L:157:VAL:HG22	1.94	0.50
2:L:116:TYR:HA	2:L:121:LEU:HD22	1.93	0.50
2:L:44:VAL:O	2:L:99:THR:HA	2.11	0.49
3:N:125:PRO:HA	3:N:151:TYR:HB3	1.94	0.49
2:M:75:SER:HB2	2:M:78:TYR:CD1	2.48	0.49
3:N:29:THR:HG22	3:N:53:ARG:HG3	1.94	0.49
3:N:9:GLU:O	3:N:115:VAL:HA	2.11	0.49
1:B:24:ILE:HG13	1:B:67:LEU:HD21	1.94	0.49
3:N:153:PRO:HD2	3:N:207:ALA:HB1	1.94	0.49
2:M:36:MET:O	2:M:129:LEU:HA	2.13	0.48
1:C:29:VAL:HG22	1:C:41:LEU:HG	1.94	0.48
2:M:158:VAL:HG12	2:M:203:THR:HA	1.94	0.48
2:L:41:GLY:H	2:L:103:VAL:HG22	1.77	0.48
2:L:60:TRP:O	2:L:72:LEU:HB3	2.13	0.48
2:M:114:GLN:HE21	2:M:115:GLN:N	2.12	0.48
1:C:7:ASP:HB2	1:A:13:VAL:HB	1.96	0.48
3:H:194:TRP:H	3:H:195:PRO:CD	2.27	0.48
2:M:150:LEU:HD12	2:M:151:THR:HG23	1.96	0.48
2:M:132:LYS:HA	2:M:165:TYR:OH	2.13	0.47
2:L:143:PHE:HB3	3:H:130:LEU:HD12	1.95	0.47
1:B:70:SER:HB2	2:M:79:ARG:HB2	1.96	0.47
1:B:30:ILE:HB	1:B:40:GLN:HB2	1.96	0.47
3:H:12:LYS:HA	3:H:119:ALA:HB2	1.96	0.47
2:M:28:GLN:H	2:M:122:THR:HG21	1.79	0.47
3:H:28:PHE:O	3:H:52:PRO:HG2	2.15	0.47
3:N:10:LEU:HG	3:N:116:THR:O	2.15	0.47
1:C:11:LEU:HD13	1:A:11:LEU:HD13	1.96	0.47
2:L:179:GLU:HG2	2:L:180:ARG:N	2.30	0.47
2:L:171:VAL:HG21	2:L:186:ASN:ND2	2.29	0.47
2:M:86:ARG:HG2	2:M:102:ASN:O	2.15	0.47
1:D:21:PRO:HA	1:D:63:ILE:HG12	1.97	0.46
3:N:34:TYR:HD1	3:N:46:TRP:NE1	2.09	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:LYS:HA	1:C:68:LEU:HD12	1.96	0.46
3:H:26:TYR:C	3:H:28:PHE:H	2.19	0.46
3:N:90:SER:HA	3:N:116:THR:HA	1.97	0.46
2:L:142:ILE:H	2:L:232:LYS:HD3	1.81	0.46
2:M:115:GLN:HE21	2:M:122:THR:H	1.62	0.46
1:C:19:VAL:HG22	1:C:20:ARG:N	2.31	0.46
3:N:183:MET:SD	3:N:184:SER:N	2.89	0.46
2:L:99:THR:C	2:L:100:ILE:HG13	2.36	0.45
1:D:30:ILE:HB	1:D:40:GLN:HB2	1.99	0.45
1:D:13:VAL:HG12	1:B:7:ASP:O	2.17	0.45
2:M:163:ASN:HA	2:M:197:THR:HB	1.97	0.45
1:C:11:LEU:H	1:C:40:GLN:NE2	2.15	0.45
1:B:35:HIS:CG	1:B:36:CYS:H	2.35	0.45
3:H:133:GLY:O	3:H:134:CYS:HB3	2.15	0.45
1:B:25:THR:HA	1:A:31:LYS:HG2	1.98	0.45
3:H:2:GLN:HG2	3:H:24:SER:HB2	1.99	0.45
3:N:39:ARG:HG2	3:N:42:GLN:H	1.81	0.45
2:M:143:PHE:HB2	2:M:158:VAL:HG23	1.98	0.45
3:H:123:THR:O	3:H:152:PHE:N	2.50	0.45
2:L:174:LYS:HA	2:L:178:SER:O	2.16	0.45
3:N:90:SER:HB2	3:N:116:THR:HG22	1.99	0.45
3:N:132:PRO:HB2	3:N:133:GLY:H	1.55	0.45
1:B:10:CYS:HA	1:B:36:CYS:HB2	1.98	0.45
2:L:62:GLN:HG3	2:L:111:TYR:CE1	2.52	0.45
2:M:54:VAL:HG23	2:M:117:ASN:HB2	1.98	0.44
1:A:35:HIS:CG	1:A:36:CYS:H	2.35	0.44
2:M:112:PHE:HE1	2:M:123:PHE:HB3	1.82	0.44
1:A:35:HIS:CD2	1:A:36:CYS:H	2.36	0.44
1:D:49:ARG:HG2	1:D:50:LYS:H	1.83	0.44
2:M:146:SER:HB2	3:N:128:TYR:HB3	2.00	0.44
1:C:19:VAL:HG22	1:C:20:ARG:H	1.82	0.44
1:B:60:TYR:O	1:B:64:ILE:HG12	2.17	0.44
3:H:29:THR:HG22	3:H:53:ARG:HG3	2.00	0.44
3:H:38:GLN:HE21	3:H:40:PRO:HB3	1.82	0.44
1:C:11:LEU:H	1:C:40:GLN:HE22	1.65	0.44
2:L:186:ASN:HB3	2:L:200:MET:SD	2.58	0.44
2:L:109:ALA:H	2:L:129:LEU:HD11	1.82	0.43
2:M:54:VAL:HG21	2:M:115:GLN:HB2	2.00	0.43
2:L:230:ILE:H	2:L:230:ILE:HD12	1.84	0.43
2:L:164:PHE:CE2	2:L:199:SER:HA	2.54	0.43
3:N:11:VAL:HG22	3:N:12:LYS:H	1.83	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:54:ASN:HB3	3:H:56:ASP:OD1	2.20	0.42
1:C:66:LYS:HD2	1:C:69:GLU:OE2	2.20	0.42
2:M:158:VAL:HA	2:M:202:SER:O	2.20	0.42
3:H:32:PHE:HB3	3:H:34:TYR:CE2	2.54	0.42
3:N:131:ALA:HB2	3:N:216:LEU:HD12	2.01	0.42
2:L:142:ILE:HB	2:L:232:LYS:HB3	2.02	0.42
2:M:58:VAL:HG11	2:M:76:ALA:HB2	2.02	0.42
3:N:5:GLN:HE21	3:N:113:THR:HG22	1.85	0.42
2:M:37:SER:HB3	2:M:130:ASP:HB3	2.01	0.41
2:M:62:GLN:O	2:M:69:PRO:HA	2.21	0.41
2:M:147:SER:O	2:M:150:LEU:HG	2.21	0.41
3:H:154:GLU:HB3	3:H:155:SER:H	1.66	0.41
1:B:60:TYR:HA	1:B:63:ILE:HB	2.02	0.41
3:H:17:VAL:O	3:H:81:GLN:HA	2.20	0.41
3:H:172:PHE:HA	3:H:173:PRO:HD3	1.93	0.41
1:D:13:VAL:HG13	1:D:14:LYS:HG2	2.02	0.41
1:A:60:TYR:CZ	1:A:61:LYS:HD2	2.56	0.41
1:D:28:GLU:HB3	1:C:28:GLU:CB	2.37	0.41
3:H:194:TRP:HE1	3:H:218:PRO:HG3	1.85	0.41
3:H:103:ASN:N	3:H:103:ASN:OD1	2.54	0.41
2:L:220:GLU:HG2	2:L:231:VAL:CG1	2.51	0.41
2:L:63:GLN:HB3	2:L:110:ASP:HB3	2.03	0.41
1:B:8:LEU:HD22	1:B:8:LEU:H	1.86	0.41
2:L:54:VAL:HG22	2:L:57:ASN:HB2	2.02	0.40
2:L:43:ARG:HA	2:L:100:ILE:O	2.20	0.40
1:A:10:CYS:SG	1:A:37:PRO:HD2	2.61	0.40
2:M:34:LYS:HE3	2:M:125:THR:HB	2.03	0.40
1:D:27:LEU:HD21	1:D:41:LEU:HD21	2.02	0.40
1:B:64:ILE:HG21	1:A:60:TYR:CE2	2.57	0.40
3:H:57:THR:O	3:H:58:ASP:HB2	2.21	0.40
1:D:7:ASP:HB2	1:B:14:LYS:H	1.87	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	63/70 (90%)	52 (82%)	11 (18%)	0	100	100
1	B	63/70 (90%)	52 (82%)	9 (14%)	2 (3%)	5	43
1	C	63/70 (90%)	52 (82%)	10 (16%)	1 (2%)	12	57
1	D	63/70 (90%)	50 (79%)	13 (21%)	0	100	100
2	L	212/214 (99%)	187 (88%)	22 (10%)	3 (1%)	14	59
2	M	212/214 (99%)	188 (89%)	22 (10%)	2 (1%)	21	67
3	H	216/218 (99%)	175 (81%)	29 (13%)	12 (6%)	2	29
3	N	216/218 (99%)	170 (79%)	34 (16%)	12 (6%)	2	29
All	All	1108/1144 (97%)	926 (84%)	150 (14%)	32 (3%)	6	45

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	132	PRO
3	N	74	SER
3	H	58	ASP
3	H	101	GLY
3	N	27	THR
3	N	73	LYS
3	N	132	PRO
1	C	32	ALA
2	L	77	SER
2	L	109	ALA
3	H	87	SER
3	H	107	THR
2	M	77	SER
2	M	109	ALA
3	N	84	SER
3	N	101	GLY
3	H	27	THR
3	H	74	SER
3	H	84	SER
3	H	118	SER
3	H	154	GLU
3	H	155	SER
1	B	35	HIS
3	N	107	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	N	154	GLU
3	N	155	SER
3	N	194	TRP
3	H	194	TRP
1	B	7	ASP
3	N	118	SER
2	L	56	THR
3	N	135	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	58/62 (94%)	55 (95%)	3 (5%)	29	68
1	B	58/62 (94%)	54 (93%)	4 (7%)	19	59
1	C	58/62 (94%)	54 (93%)	4 (7%)	19	59
1	D	58/62 (94%)	54 (93%)	4 (7%)	19	59
2	L	186/191 (97%)	177 (95%)	9 (5%)	31	70
2	M	186/191 (97%)	176 (95%)	10 (5%)	27	67
3	H	181/186 (97%)	169 (93%)	12 (7%)	21	61
3	N	181/186 (97%)	169 (93%)	12 (7%)	21	61
All	All	966/1002 (96%)	908 (94%)	58 (6%)	24	64

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	8	LEU
1	D	13	VAL
1	D	18	GLN
1	D	20	ARG
1	C	18	GLN
1	C	20	ARG
1	C	41	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	52	CYS
2	L	38	THR
2	L	43	ARG
2	L	85	ASP
2	L	86	ARG
2	L	112	PHE
2	L	114	GLN
2	L	129	LEU
2	L	161	LEU
2	L	185	LEU
3	H	11	VAL
3	H	17	VAL
3	H	29	THR
3	H	32	PHE
3	H	64	GLU
3	H	68	THR
3	H	96	THR
3	H	100	TYR
3	H	103	ASN
3	H	107	THR
3	H	156	VAL
3	H	213	ASP
1	B	8	LEU
1	B	19	VAL
1	B	20	ARG
1	B	52	CYS
1	A	8	LEU
1	A	9	GLN
1	A	15	THR
2	M	43	ARG
2	M	86	ARG
2	M	112	PHE
2	M	114	GLN
2	M	129	LEU
2	M	161	LEU
2	M	174	LYS
2	M	185	LEU
2	M	186	ASN
2	M	209	ASP
3	N	5	GLN
3	N	17	VAL
3	N	29	THR

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
3	N	64	GLU
3	N	68	THR
3	N	96	THR
3	N	100	TYR
3	N	107	THR
3	N	113	THR
3	N	116	THR
3	N	156	VAL
3	N	213	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	9	GLN
1	D	18	GLN
1	D	40	GLN
1	C	18	GLN
1	C	40	GLN
2	L	31	GLN
2	L	114	GLN
2	L	115	GLN
2	L	149	GLN
2	L	186	ASN
2	L	237	ASN
3	H	5	GLN
3	H	38	GLN
1	B	9	GLN
1	B	35	HIS
1	A	9	GLN
2	M	31	GLN
2	M	114	GLN
2	M	115	GLN
2	M	149	GLN
2	M	186	ASN
3	N	5	GLN
3	N	170	HIS

### 5.3.3 RNA ⓘ

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	65/70 (92%)	-0.61	0 100 100	124, 158, 199, 223	0
1	B	65/70 (92%)	-0.53	0 100 100	117, 148, 207, 219	0
1	C	65/70 (92%)	-0.38	0 100 100	178, 265, 374, 445	0
1	D	65/70 (92%)	-0.46	1 (1%) 76 67	165, 247, 374, 457	0
2	L	214/214 (100%)	-0.15	6 (2%) 56 45	201, 300, 384, 438	0
2	M	214/214 (100%)	-0.43	0 100 100	126, 212, 314, 355	0
3	H	218/218 (100%)	-0.16	1 (0%) 91 88	166, 297, 418, 515	0
3	N	218/218 (100%)	-0.15	3 (1%) 78 69	194, 334, 458, 509	0
All	All	1124/1144 (98%)	-0.28	11 (0%) 84 77	117, 274, 413, 515	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	182	ASN	4.6
2	L	181	GLN	4.0
2	L	180	ARG	3.9
2	L	26	ASP	3.7
1	D	70	SER	3.6
3	H	164	SER	2.9
3	N	146	CYS	2.4
2	L	237	ASN	2.4
2	L	113	CYS	2.2
3	N	20	SER	2.2
3	N	145	GLY	2.1

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

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

There are no such residues in this entry.