



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 2, 2025 – 02:11 PM EDT

PDB ID : 9MSN / pdb\_00009msn  
Title : Crystal structure of MPXV A35R in complex with neutralizing antibody EV35-2  
Authors : Yuan, M.; Zhu, X.; Wilson, I.A.  
Deposited on : 2025-01-10  
Resolution : 2.92 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 Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.45.1

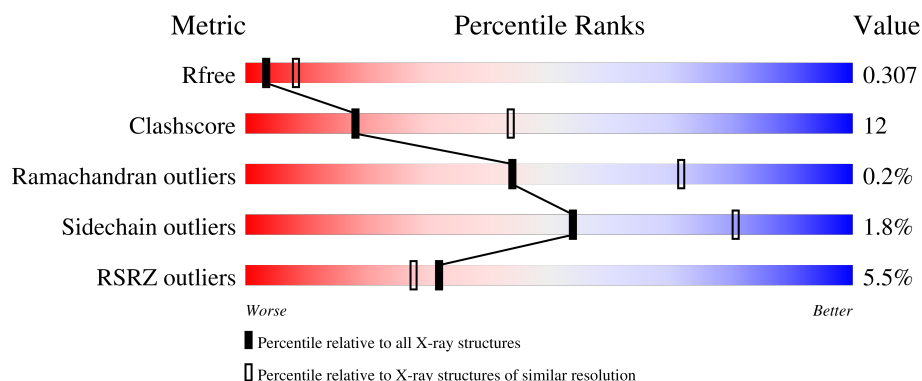
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.92 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))
$R_{free}$	164625	2797 (2.94-2.90)
Clashscore	180529	3049 (2.94-2.90)
Ramachandran outliers	177936	2981 (2.94-2.90)
Sidechain outliers	177891	2983 (2.94-2.90)
RSRZ outliers	164620	2799 (2.94-2.90)

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	A	225	<div> <div>4%</div> <div>65%</div> <div>30%</div> <div>• •</div> </div>
1	H	225	<div> <div>4%</div> <div>67%</div> <div>29%</div> <div>•</div> </div>
2	B	216	<div> <div>6%</div> <div>72%</div> <div>27%</div> <div>•</div> </div>
2	L	216	<div> <div>9%</div> <div>73%</div> <div>25%</div> <div>• •</div> </div>
3	E	100	<div> <div>6%</div> <div>70%</div> <div>16%</div> <div>14%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	100	<div><div></div><div>5%</div><div>71%</div><div>15%</div><div>14%</div></div>
3	J	100	<div><div></div><div>3%</div><div>61%</div><div>24%</div><div>•</div><div>14%</div></div>
3	K	100	<div><div></div><div>3%</div><div>60%</div><div>19%</div><div>•</div><div>17%</div></div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9308 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 EV35-2 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1654	1046	282	316	10			
1	H	217	Total	C	N	O	S	0	0	0
			1650	1044	282	315	9			

- Molecule 2 is a protein called EV35-2 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1639	1027	280	328	4			
2	L	213	Total	C	N	O	S	0	0	0
			1635	1025	279	327	4			

- Molecule 3 is a protein called Protein OPG161.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	86	Total	C	N	O	S	0	0	0
			683	424	108	147	4			
3	K	83	Total	C	N	O	S	0	0	0
			653	406	102	141	4			
3	E	86	Total	C	N	O	S	0	0	0
			683	424	108	147	4			
3	F	86	Total	C	N	O	S	0	0	0
			683	424	108	147	4			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	98	GLY	-	expression tag	UNP A0A7H0DND2
J	99	SER	-	expression tag	UNP A0A7H0DND2
J	100	HIS	-	expression tag	UNP A0A7H0DND2
J	101	HIS	-	expression tag	UNP A0A7H0DND2

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Chain	Residue	Modelled	Actual	Comment	Reference
J	102	HIS	-	expression tag	UNP A0A7H0DND2
J	103	HIS	-	expression tag	UNP A0A7H0DND2
J	104	HIS	-	expression tag	UNP A0A7H0DND2
J	105	HIS	-	expression tag	UNP A0A7H0DND2
K	98	GLY	-	expression tag	UNP A0A7H0DND2
K	99	SER	-	expression tag	UNP A0A7H0DND2
K	100	HIS	-	expression tag	UNP A0A7H0DND2
K	101	HIS	-	expression tag	UNP A0A7H0DND2
K	102	HIS	-	expression tag	UNP A0A7H0DND2
K	103	HIS	-	expression tag	UNP A0A7H0DND2
K	104	HIS	-	expression tag	UNP A0A7H0DND2
K	105	HIS	-	expression tag	UNP A0A7H0DND2
E	98	GLY	-	expression tag	UNP A0A7H0DND2
E	99	SER	-	expression tag	UNP A0A7H0DND2
E	100	HIS	-	expression tag	UNP A0A7H0DND2
E	101	HIS	-	expression tag	UNP A0A7H0DND2
E	102	HIS	-	expression tag	UNP A0A7H0DND2
E	103	HIS	-	expression tag	UNP A0A7H0DND2
E	104	HIS	-	expression tag	UNP A0A7H0DND2
E	105	HIS	-	expression tag	UNP A0A7H0DND2
F	98	GLY	-	expression tag	UNP A0A7H0DND2
F	99	SER	-	expression tag	UNP A0A7H0DND2
F	100	HIS	-	expression tag	UNP A0A7H0DND2
F	101	HIS	-	expression tag	UNP A0A7H0DND2
F	102	HIS	-	expression tag	UNP A0A7H0DND2
F	103	HIS	-	expression tag	UNP A0A7H0DND2
F	104	HIS	-	expression tag	UNP A0A7H0DND2
F	105	HIS	-	expression tag	UNP A0A7H0DND2

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	9	Total O 9 9	0	0
4	B	3	Total O 3 3	0	0
4	J	2	Total O 2 2	0	0
4	K	1	Total O 1 1	0	0
4	H	7	Total O 7 7	0	0

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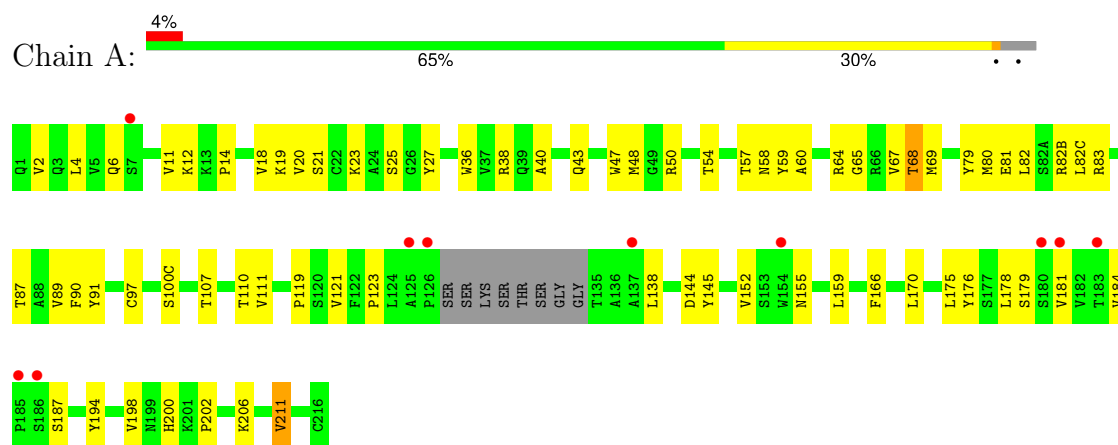
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	4	Total	O	0	0
			4	4		
4	F	2	Total	O	0	0
			2	2		

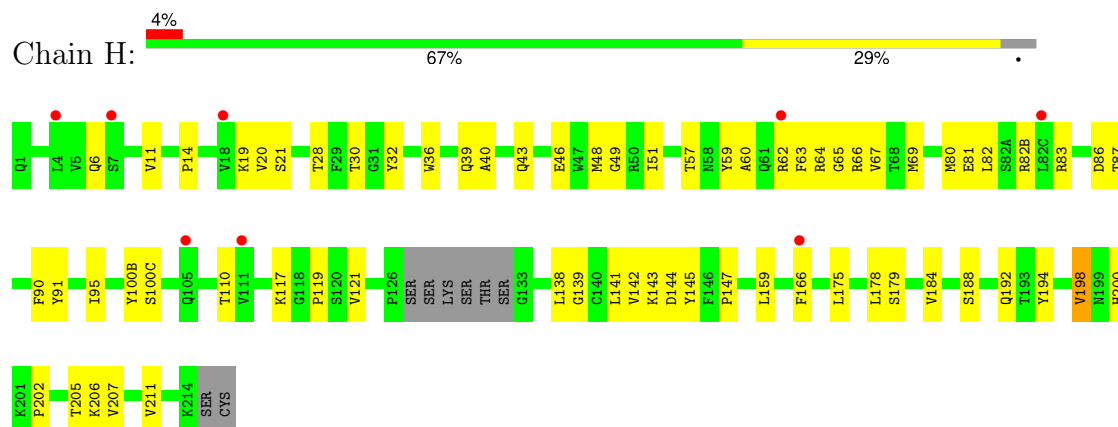
### 3 Residue-property plots

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.

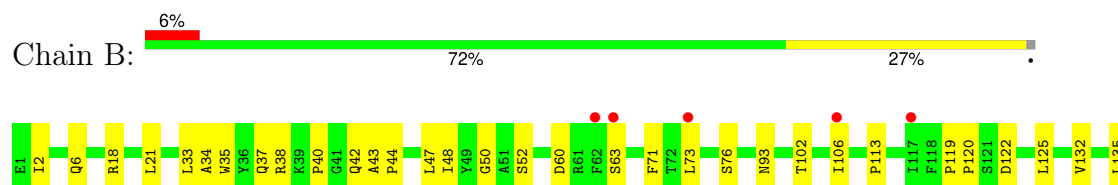
#### • Molecule 1: EV35-2 heavy chain



#### • Molecule 1: EV35-2 heavy chain

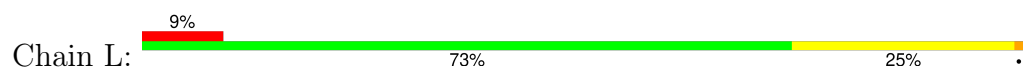


#### • Molecule 2: EV35-2 light chain





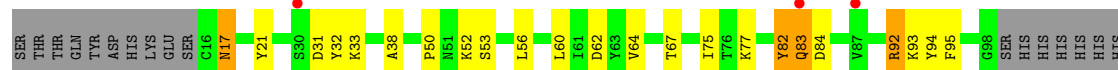
• Molecule 2: EV35-2 light chain



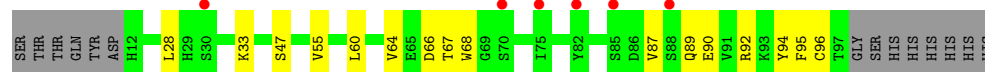
• Molecule 3: Protein OPG161



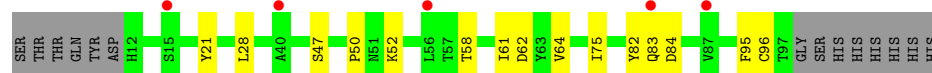
• Molecule 3: Protein OPG161



• Molecule 3: Protein OPG161



• Molecule 3: Protein OPG161





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	114.27Å 130.23Å 100.07Å 90.00° 116.80° 90.00°	Depositor
Resolution (Å)	46.70 – 2.92 46.70 – 2.92	Depositor EDS
% Data completeness (in resolution range)	94.9 (46.70-2.92) 95.2 (46.70-2.92)	Depositor EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.03 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, $R_{free}$	0.280 , 0.307 0.280 , 0.307	Depositor DCC
$R_{free}$ test set	1376 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.6	Xtriage
Anisotropy	0.530	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 20.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	9308	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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	A	0.17	0/1695	0.43	0/2306
1	H	0.15	0/1691	0.44	0/2300
2	B	0.15	0/1676	0.40	0/2278
2	L	0.18	0/1672	0.42	0/2273
3	E	0.16	0/699	0.42	0/950
3	F	0.16	0/699	0.44	0/950
3	J	0.17	0/699	0.53	0/950
3	K	0.33	0/668	0.64	0/909
All	All	0.18	0/9499	0.45	0/12916

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	K	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	K	92	ARG	Sidechain

### 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	A	1654	0	1620	51	0
1	H	1650	0	1616	57	0
2	B	1639	0	1602	38	0
2	L	1635	0	1599	40	0
3	E	683	0	616	12	0
3	F	683	0	616	14	0
3	J	683	0	616	15	0
3	K	653	0	588	19	0
4	A	9	0	0	1	0
4	B	3	0	0	0	0
4	F	2	0	0	0	0
4	H	7	0	0	2	0
4	J	2	0	0	0	0
4	K	1	0	0	0	0
4	L	4	0	0	1	0
All	All	9308	0	8873	218	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 12.

All (218) 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)
3:K:53:SER:HB2	1:H:117:LYS:HD3	1.58	0.85
1:A:67:VAL:HG22	1:A:82:LEU:HD13	1.66	0.78
1:A:87:THR:HG23	1:A:110:THR:HA	1.64	0.77
2:L:50:GLY:HA2	3:E:89:GLN:NE2	2.00	0.75
2:L:35:TRP:HB2	2:L:48:ILE:HB	1.70	0.74
1:H:40:ALA:HB3	1:H:43:GLN:HB2	1.68	0.73
1:A:14:PRO:HG2	3:F:83:GLN:HE22	1.52	0.72
2:B:142:ARG:HD2	2:B:163:VAL:HG21	1.71	0.72
2:B:35:TRP:HB2	2:B:48:ILE:HB	1.72	0.71
1:H:59:TYR:HB2	1:H:64:ARG:HG2	1.73	0.71
3:K:52:LYS:O	3:K:56:LEU:HB2	1.91	0.71
3:E:67:THR:HG23	3:E:94:TYR:HA	1.71	0.70
2:B:155:GLN:HE21	2:B:158:ASN:HD21	1.39	0.69
1:H:49:GLY:HA3	1:H:69:MET:HE1	1.75	0.69
1:H:184:VAL:HG21	1:H:194:TYR:HE2	1.57	0.69
1:A:152:VAL:HG22	1:A:198:VAL:HG12	1.74	0.68
1:A:138:LEU:HD11	1:A:194:TYR:HD2	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:VAL:HG21	1:A:194:TYR:HE2	1.61	0.66
1:H:66:ARG:HH11	1:H:82:LEU:HD21	1.60	0.66
2:L:125:LEU:HD11	2:L:186:TYR:HD2	1.59	0.65
2:L:18:ARG:HD2	2:L:76:SER:HA	1.78	0.65
1:A:144:ASP:HA	1:A:175:LEU:HB3	1.78	0.65
1:H:119:PRO:HB3	1:H:145:TYR:HB3	1.79	0.65
2:B:37:GLN:HB3	2:B:47:LEU:HD11	1.78	0.64
2:B:155:GLN:HB3	2:B:158:ASN:HD21	1.62	0.64
1:A:89:VAL:HG13	1:A:107:THR:H	1.61	0.64
2:B:38:ARG:HH12	2:B:40:PRO:HA	1.63	0.63
3:J:67:THR:HG23	3:J:94:TYR:HA	1.80	0.63
1:H:188:SER:HB3	1:H:192:GLN:HG3	1.80	0.62
1:H:87:THR:HG23	1:H:110:THR:HA	1.81	0.62
2:L:146:VAL:HG22	2:L:196:VAL:HG22	1.81	0.62
3:E:55:VAL:HG23	3:E:60:LEU:HB2	1.82	0.61
3:F:21:TYR:HE2	3:F:58:THR:HB	1.66	0.61
3:K:84:ASP:HB2	1:H:82(B):ARG:HD3	1.83	0.61
1:A:97:CYS:HB3	1:A:100(C):SER:HB2	1.81	0.60
1:A:83:ARG:HH11	3:F:82:TYR:HE1	1.49	0.60
1:A:166:PHE:CE2	2:B:176:SER:HB3	2.37	0.59
1:A:14:PRO:HG2	3:F:83:GLN:NE2	2.17	0.59
1:A:121:VAL:HG21	1:A:198:VAL:HG21	1.83	0.59
2:L:125:LEU:O	2:L:183:LYS:HD3	2.02	0.58
2:L:3:VAL:HG22	2:L:26:SER:HB2	1.83	0.58
3:F:52:LYS:HZ3	3:F:75:ILE:HA	1.68	0.58
2:L:11:LEU:HD22	2:L:13:LEU:HD21	1.84	0.58
1:H:48:MET:HG3	1:H:63:PHE:CD2	2.39	0.57
3:K:50:PRO:HD3	3:K:95:PHE:O	2.03	0.57
1:A:82(B):ARG:NE	1:H:82(B):ARG:HE	2.01	0.57
2:L:120:PRO:HD3	2:L:132:VAL:HG22	1.87	0.56
1:H:83:ARG:HG3	1:H:86:ASP:OD1	2.04	0.56
2:L:167:ASP:HB3	2:L:169:LYS:HD2	1.88	0.56
2:L:163:VAL:HG22	2:L:175:LEU:HG	1.86	0.56
2:L:169:LYS:HD2	2:L:169:LYS:H	1.70	0.55
1:A:54:THR:HB	3:K:32:TYR:CD1	2.42	0.55
1:A:6:GLN:HB2	1:A:21:SER:O	2.07	0.55
1:H:202:PRO:HG3	4:H:301:HOH:O	2.07	0.55
1:H:184:VAL:HG21	1:H:194:TYR:CE2	2.39	0.55
1:A:119:PRO:HB3	1:A:145:TYR:HB3	1.88	0.54
2:B:122:ASP:HA	2:B:125:LEU:HB2	1.88	0.54
3:E:28:LEU:HD23	3:F:62:ASP:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:VAL:HG21	1:A:194:TYR:CE2	2.43	0.53
1:H:59:TYR:HB2	1:H:64:ARG:CG	2.36	0.53
2:L:15:PRO:HG3	2:L:106:ILE:HD11	1.90	0.53
1:A:68:THR:HG23	1:A:81:GLU:HB3	1.91	0.53
3:J:13:LYS:HG3	3:J:20:TYR:HD2	1.74	0.53
1:H:166:PHE:HD1	2:L:164:THR:HG23	1.73	0.53
1:A:50:ARG:HG2	1:A:58:ASN:HB2	1.90	0.53
1:A:200:HIS:CD2	1:A:202:PRO:HD2	2.44	0.53
2:L:37:GLN:HB3	2:L:47:LEU:HD11	1.90	0.52
1:A:65:GLY:C	3:K:83:GLN:HA	2.34	0.52
2:B:169:LYS:HG3	2:B:170:ASP:N	2.24	0.52
1:H:19:LYS:HG3	1:H:81:GLU:HB2	1.91	0.52
2:B:2:ILE:HD11	2:B:93:ASN:ND2	2.25	0.52
3:E:66:ASP:HA	3:E:92:ARG:HH21	1.75	0.52
2:L:21:LEU:O	2:L:72:THR:HA	2.09	0.52
1:A:36:TRP:CE2	1:A:80:MET:HB2	2.46	0.51
2:B:145:LYS:HB3	2:B:197:THR:HB	1.92	0.51
2:L:113:PRO:HD3	2:L:198:HIS:CD2	2.45	0.51
2:L:131:SER:HA	2:L:179:LEU:O	2.10	0.51
1:A:82(B):ARG:HE	1:H:82(B):ARG:HE	1.58	0.51
1:H:36:TRP:CE2	1:H:80:MET:HB2	2.47	0.50
1:H:65:GLY:HA3	3:F:83:GLN:HA	1.92	0.50
2:L:2:ILE:HG23	2:L:26:SER:H	1.76	0.50
1:H:166:PHE:CE2	2:L:176:SER:HB3	2.46	0.50
3:J:67:THR:HG21	3:J:95:PHE:HD1	1.77	0.50
1:H:60:ALA:O	1:H:64:ARG:HG3	2.11	0.50
1:H:119:PRO:HB2	1:H:142:VAL:HG23	1.94	0.50
1:H:144:ASP:HA	1:H:175:LEU:HB3	1.93	0.50
3:F:50:PRO:HD3	3:F:95:PHE:O	2.11	0.50
2:B:140:TYR:CD1	2:B:141:PRO:HA	2.47	0.49
1:A:19:LYS:HG3	1:A:81:GLU:HB2	1.95	0.49
3:F:47:SER:HB2	3:F:96:CYS:HB3	1.93	0.49
1:H:66:ARG:HD3	3:F:84:ASP:OD2	2.12	0.49
1:H:200:HIS:HB3	1:H:205:THR:OG1	2.12	0.49
2:L:61:ARG:HD2	2:L:76:SER:HB3	1.93	0.49
1:H:142:VAL:HG13	1:H:178:LEU:HB3	1.93	0.49
2:B:165:GLU:HG3	2:B:166:GLN:H	1.78	0.49
1:A:48:MET:HE1	1:A:90:PHE:HD1	1.77	0.49
2:B:42:GLN:HG2	2:B:43:ALA:H	1.77	0.49
1:A:57:THR:HB	1:A:59:TYR:CE1	2.48	0.48
1:H:121:VAL:HG21	1:H:198:VAL:HG11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:LEU:HA	1:A:23:LYS:O	2.13	0.48
3:K:82:TYR:HA	1:H:83:ARG:HB3	1.94	0.48
2:L:2:ILE:HD11	2:L:93:ASN:OD1	2.13	0.48
2:L:198:HIS:HB3	2:L:201:LEU:HD12	1.94	0.48
2:L:30:SER:HB3	2:L:32:PHE:CE1	2.49	0.48
3:K:83:GLN:OE1	1:H:14:PRO:HG2	2.14	0.48
2:B:2:ILE:HD11	2:B:93:ASN:HD22	1.79	0.48
1:A:19:LYS:HZ3	1:A:81:GLU:HB2	1.79	0.47
3:K:31:ASP:HB2	3:K:33:LYS:HZ3	1.80	0.47
3:E:28:LEU:HB2	3:E:95:PHE:CE2	2.50	0.47
3:J:55:VAL:HG23	3:J:60:LEU:HB2	1.95	0.47
1:H:80:MET:HE1	1:H:82:LEU:HB2	1.97	0.47
1:H:100(B):TYR:CZ	2:L:95:PRO:HB3	2.49	0.47
1:A:144:ASP:HB3	1:A:175:LEU:HD13	1.95	0.47
2:B:113:PRO:HB3	2:B:139:PHE:HB3	1.94	0.47
2:B:138:ASN:HA	2:B:172:THR:OG1	2.14	0.47
3:K:84:ASP:HB2	1:H:82(B):ARG:CD	2.45	0.47
2:B:106:ILE:HG21	2:B:171:SER:HB2	1.97	0.47
1:A:11:VAL:HG13	1:A:110:THR:HB	1.96	0.46
1:A:47:TRP:CE3	1:A:60:ALA:HB2	2.49	0.46
2:B:149:LYS:HB3	2:B:152:ASN:HA	1.96	0.46
1:H:141:LEU:HD21	1:H:143:LYS:HD3	1.97	0.46
2:B:120:PRO:HD3	2:B:132:VAL:HG22	1.96	0.46
1:A:123:PRO:HB3	1:A:211:VAL:HG12	1.98	0.46
1:A:40:ALA:HB3	1:A:43:GLN:HB2	1.98	0.46
3:J:28:LEU:HD23	3:K:62:ASP:HB3	1.96	0.46
3:E:55:VAL:HG21	3:E:64:VAL:HG21	1.97	0.46
2:L:27(A):THR:HG23	2:L:68:GLY:HA2	1.97	0.46
3:J:33:LYS:HE2	3:J:37:ASP:HB3	1.97	0.45
2:L:151:ASP:OD1	2:L:189:HIS:HB3	2.17	0.45
2:B:33:LEU:HG	2:B:71:PHE:CG	2.52	0.45
1:H:6:GLN:HB2	1:H:21:SER:O	2.17	0.45
1:H:28:THR:HG22	1:H:32:TYR:HE1	1.82	0.45
1:H:178:LEU:HD23	1:H:179:SER:N	2.31	0.45
1:H:46:GLU:CD	1:H:62:ARG:HH21	2.25	0.45
3:K:21:TYR:HB2	3:K:60:LEU:HD11	1.98	0.45
1:H:6:GLN:NE2	1:H:20:VAL:HG13	2.32	0.45
1:A:59:TYR:HB2	1:A:64:ARG:HG3	1.99	0.44
2:B:119:PRO:HB3	2:B:209:PHE:CZ	2.51	0.44
3:K:38:ALA:HB1	3:K:94:TYR:CG	2.52	0.44
1:A:83:ARG:NH1	3:F:82:TYR:HE1	2.13	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:GLN:HG2	1:A:20:VAL:HG13	1.98	0.44
1:A:27:TYR:HE2	4:A:301:HOH:O	1.99	0.44
2:L:48:ILE:HD13	2:L:48:ILE:HA	1.92	0.44
3:J:33:LYS:CE	3:J:37:ASP:HB3	2.47	0.44
3:K:32:TYR:CD2	3:K:92:ARG:HA	2.53	0.44
3:E:87:VAL:HA	3:E:90:GLU:OE2	2.17	0.44
2:B:150:VAL:HB	2:B:155:GLN:OE1	2.17	0.44
2:B:147:GLN:HG3	2:B:195:GLU:HB3	2.00	0.44
2:B:6:GLN:NE2	2:B:102:THR:HG23	2.33	0.43
2:B:155:GLN:HE21	2:B:158:ASN:ND2	2.11	0.43
2:L:46:LEU:HG	2:L:55:ALA:HB2	1.99	0.43
2:B:148:TRP:CE3	2:B:179:LEU:HD22	2.54	0.43
3:J:28:LEU:HB2	3:J:95:PHE:CE2	2.53	0.43
3:E:89:GLN:C	3:E:90:GLU:HG2	2.42	0.43
1:H:138:LEU:HD11	1:H:194:TYR:HD2	1.84	0.43
2:L:12:SER:HA	2:L:105:GLU:HG3	1.99	0.43
1:A:166:PHE:HE2	2:B:176:SER:HB3	1.82	0.43
3:J:32:TYR:HB3	3:J:91:VAL:HB	2.00	0.43
3:J:59:TRP:CD1	3:K:17:ASN:HB3	2.53	0.43
1:A:206:LYS:HE3	1:A:206:LYS:HB3	1.76	0.43
3:J:29:HIS:HB3	3:J:31:ASP:OD1	2.18	0.43
1:H:39:GLN:HB3	1:H:91:TYR:HE1	1.84	0.43
1:H:51:ILE:HG13	1:H:57:THR:HG22	2.02	0.42
1:H:139:GLY:O	1:H:211:VAL:HG11	2.19	0.42
3:K:56:LEU:HD13	3:K:56:LEU:O	2.19	0.42
1:H:66:ARG:HH11	1:H:66:ARG:HG2	1.83	0.42
1:H:147:PRO:HG2	4:H:301:HOH:O	2.19	0.42
1:H:159:LEU:HD23	1:H:159:LEU:HA	1.95	0.42
2:L:21:LEU:HD22	2:L:73:LEU:HD12	2.00	0.42
1:A:155:ASN:HD22	1:A:159:LEU:HB2	1.84	0.42
2:B:18:ARG:HD2	2:B:76:SER:HA	2.01	0.42
2:B:125:LEU:HD11	2:B:186:TYR:CD2	2.54	0.42
3:K:64:VAL:HG12	3:K:75:ILE:HG21	2.00	0.42
3:E:33:LYS:HA	3:E:33:LYS:HD3	1.81	0.42
3:K:50:PRO:CG	3:K:95:PHE:HB2	2.49	0.42
1:A:20:VAL:HG22	1:A:107:THR:HG21	2.02	0.42
1:A:170:LEU:HD13	1:A:176:TYR:CE1	2.55	0.42
2:L:169:LYS:HG2	2:L:170:ASP:N	2.34	0.42
1:A:18:VAL:HG12	1:A:82(C):LEU:HD11	2.02	0.42
1:H:66:ARG:NH1	1:H:82:LEU:HD21	2.31	0.42
1:H:166:PHE:HE2	2:L:176:SER:HB3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:35:TRP:CE2	2:L:73:LEU:HB2	2.54	0.42
1:H:206:LYS:HE3	1:H:206:LYS:HB3	1.79	0.42
1:A:69:MET:HA	1:A:79:TYR:O	2.19	0.42
1:H:95:ILE:HD11	1:H:100(C):SER:H	1.85	0.42
2:B:158:ASN:OD1	2:B:179:LEU:HD11	2.20	0.41
1:H:63:PHE:HB3	1:H:67:VAL:CG2	2.50	0.41
2:L:8:PRO:HD3	2:L:22:SER:HB3	2.01	0.41
1:A:12:LYS:O	1:A:111:VAL:HA	2.19	0.41
2:B:34:ALA:HA	2:B:48:ILE:O	2.20	0.41
3:F:61:ILE:HD12	3:F:61:ILE:H	1.85	0.41
2:B:21:LEU:HD21	2:B:102:THR:OG1	2.19	0.41
2:B:50:GLY:HA2	3:J:89:GLN:HE22	1.86	0.41
3:K:67:THR:HG22	3:K:93:LYS:HB2	2.02	0.41
2:L:21:LEU:HB2	2:L:73:LEU:HB3	2.02	0.41
1:H:57:THR:HB	1:H:59:TYR:CE1	2.56	0.41
1:H:198:VAL:HG13	1:H:207:VAL:HB	2.01	0.41
1:A:2:VAL:HA	1:A:25:SER:O	2.20	0.41
1:A:178:LEU:HD23	1:A:179:SER:N	2.36	0.41
3:J:35:PHE:HB2	3:J:68:TRP:CZ3	2.55	0.41
2:L:33:LEU:HB3	2:L:51:ALA:HB2	2.03	0.41
2:L:125:LEU:HD13	2:L:183:LYS:HG2	2.03	0.41
1:A:91:TYR:CE2	2:B:44:PRO:HD3	2.56	0.41
1:H:48:MET:HE1	1:H:90:PHE:HD1	1.85	0.41
3:E:68:TRP:NE1	3:E:92:ARG:HB2	2.36	0.41
3:F:61:ILE:HA	3:F:64:VAL:HG22	2.02	0.41
1:H:142:VAL:CG1	1:H:178:LEU:HB3	2.51	0.41
3:F:28:LEU:HB2	3:F:95:PHE:CE2	2.56	0.40
2:B:179:LEU:HA	2:B:179:LEU:HD12	1.82	0.40
3:E:47:SER:HB2	3:E:96:CYS:HB3	2.03	0.40
1:A:181:VAL:HG21	2:B:135:LEU:HD13	2.04	0.40
2:B:63:SER:O	2:B:73:LEU:HD12	2.21	0.40
3:J:61:ILE:HG21	3:J:77:LYS:HG2	2.03	0.40
1:H:63:PHE:HB3	1:H:67:VAL:HG21	2.03	0.40
2:L:11:LEU:HG	4:L:302:HOH:O	2.20	0.40
3:J:19:LEU:HB2	3:J:26:TYR:HB2	2.04	0.40
1:A:89:VAL:HA	1:A:107:THR:O	2.22	0.40
2:L:166:GLN:HG3	2:L:171:SER:HA	2.03	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	213/225 (95%)	206 (97%)	7 (3%)	0	100	100
1	H	213/225 (95%)	209 (98%)	4 (2%)	0	100	100
2	B	212/216 (98%)	202 (95%)	10 (5%)	0	100	100
2	L	211/216 (98%)	203 (96%)	8 (4%)	0	100	100
3	E	84/100 (84%)	79 (94%)	5 (6%)	0	100	100
3	F	84/100 (84%)	78 (93%)	6 (7%)	0	100	100
3	J	84/100 (84%)	76 (90%)	7 (8%)	1 (1%)	11	33
3	K	81/100 (81%)	75 (93%)	5 (6%)	1 (1%)	11	33
All	All	1182/1282 (92%)	1128 (95%)	52 (4%)	2 (0%)	44	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	J	23	GLY
3	K	82	TYR

### 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	184/190 (97%)	180 (98%)	4 (2%)	47	76
1	H	182/190 (96%)	179 (98%)	3 (2%)	58	83
2	B	185/187 (99%)	182 (98%)	3 (2%)	58	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	185/187 (99%)	182 (98%)	3 (2%)	58	83
3	E	78/91 (86%)	78 (100%)	0	100	100
3	F	78/91 (86%)	78 (100%)	0	100	100
3	J	78/91 (86%)	75 (96%)	3 (4%)	28	61
3	K	74/91 (81%)	71 (96%)	3 (4%)	26	58
All	All	1044/1118 (93%)	1025 (98%)	19 (2%)	54	81

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	68	THR
1	A	187	SER
1	A	211	VAL
2	B	52	SER
2	B	60	ASP
2	B	182	SER
3	J	48	THR
3	J	57	THR
3	J	67	THR
3	K	17	ASN
3	K	77	LYS
3	K	83	GLN
1	H	11	VAL
1	H	30	THR
1	H	198	VAL
2	L	53	SER
2	L	164	THR
2	L	169	LYS

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

Mol	Chain	Res	Type
1	A	52	ASN
1	A	53	ASN
1	A	192	GLN
2	B	42	GLN
2	B	124	GLN
2	B	138	ASN

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Mol	Chain	Res	Type
2	B	155	GLN
1	H	164	HIS
1	H	192	GLN
2	L	31	ASN
2	L	138	ASN
2	L	160	GLN
2	L	198	HIS
3	E	41	ASN
3	E	89	GLN
3	F	83	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 [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	217/225 (96%)	0.61	10 (4%) 38 32	30, 54, 89, 95	0
1	H	217/225 (96%)	0.52	8 (3%) 45 39	33, 51, 67, 85	0
2	B	214/216 (99%)	0.82	12 (5%) 31 27	37, 71, 94, 102	0
2	L	213/216 (98%)	0.86	19 (8%) 17 15	34, 63, 82, 102	0
3	E	86/100 (86%)	0.88	6 (6%) 24 21	42, 64, 114, 122	0
3	F	86/100 (86%)	0.85	5 (5%) 30 26	34, 58, 97, 115	0
3	J	86/100 (86%)	0.87	3 (3%) 47 41	53, 76, 111, 121	0
3	K	83/100 (83%)	0.81	3 (3%) 46 40	30, 59, 87, 94	0
All	All	1202/1282 (93%)	0.74	66 (5%) 32 28	30, 61, 92, 122	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	K	83	GLN	4.4
2	B	196	VAL	4.4
3	F	83	GLN	4.1
2	B	62	PHE	3.7
2	L	47	LEU	3.6
2	L	130	ALA	3.6
2	B	209	PHE	3.6
2	L	11	LEU	3.5
1	A	183	THR	3.4
3	F	87	VAL	3.3
2	B	204	PRO	3.2
2	L	48	ILE	3.2
2	B	194	CYS	3.2
1	H	166	PHE	3.1
2	B	197	THR	3.0
2	L	76	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	H	4	LEU	2.9
1	H	18	VAL	2.9
1	H	7	SER	2.9
2	B	63	SER	2.8
1	A	137	ALA	2.8
1	A	181	VAL	2.8
1	H	62	ARG	2.8
1	A	126	PRO	2.8
2	L	127	SER	2.8
2	L	78	LEU	2.7
3	F	56	LEU	2.7
3	E	75	ILE	2.7
3	E	82	TYR	2.7
2	L	62	PHE	2.6
2	L	154	LEU	2.6
1	H	82(C)	LEU	2.5
2	L	59	PRO	2.5
2	B	143	GLU	2.5
2	L	120	PRO	2.4
1	A	7	SER	2.3
3	E	30	SER	2.3
1	A	185	PRO	2.3
3	E	88	SER	2.3
3	F	15	SER	2.3
2	L	16	GLY	2.3
2	B	117	ILE	2.3
3	E	85	SER	2.3
1	H	111	VAL	2.2
2	L	87	TYR	2.2
2	B	106	ILE	2.2
3	K	87	VAL	2.2
3	F	40	ALA	2.2
1	A	186	SER	2.2
3	E	70	SER	2.2
3	J	12	HIS	2.2
2	L	73	LEU	2.2
3	J	78	THR	2.1
1	H	105	GLN	2.1
2	L	124	GLN	2.1
1	A	180	SER	2.1
3	J	88	SER	2.1
2	L	77	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
2	L	129	THR	2.1
1	A	154	TRP	2.1
2	L	125	LEU	2.1
2	L	79	GLU	2.1
2	B	150	VAL	2.1
1	A	125	ALA	2.0
3	K	30	SER	2.0
2	B	73	LEU	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.