



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 15, 2026 – 12:34 AM UTC

PDB ID : 9UDQ / pdb\_00009udq  
Title : Crystal structure of MPXV A35R in complex with a neutralizing antibody MA42  
Authors : Sun, D.; Zhang, N.; Guo, Y.  
Deposited on : 2025-04-07  
Resolution : 2.82 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
Xtriage (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

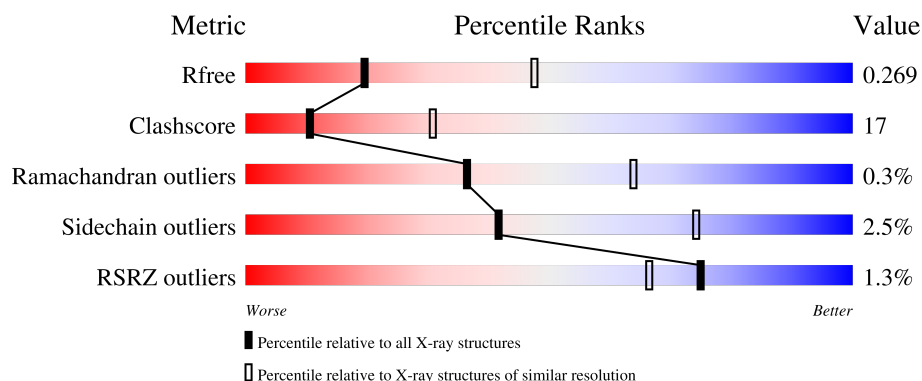
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.82 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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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	B	124	<div> <div>5%</div> <div>40%</div> <div>25%</div> <div>•</div> <div>34%</div> </div>
1	J	124	<div> <div>2%</div> <div>47%</div> <div>19%</div> <div>34%</div> </div>
2	A	215	<div> <div>69%</div> <div>30%</div> </div>
2	C	215	<div> <div>63%</div> <div>36%</div> </div>
3	F	236	<div> <div>58%</div> <div>35%</div> <div>•</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
3	I	236	<div><div></div><div>54%</div><div>39%</div><div>• 6%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7876 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 Protein OPG161.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	J	82	Total	C	N	O	S	0	0	0
			648	403	101	140	4			
1	B	82	Total	C	N	O	S	0	0	0
			648	403	101	140	4			

- Molecule 2 is a protein called Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	215	Total	C	N	O	S	0	0	0
			1640	1029	274	331	6			
2	C	215	Total	C	N	O	S	0	0	0
			1640	1029	274	331	6			

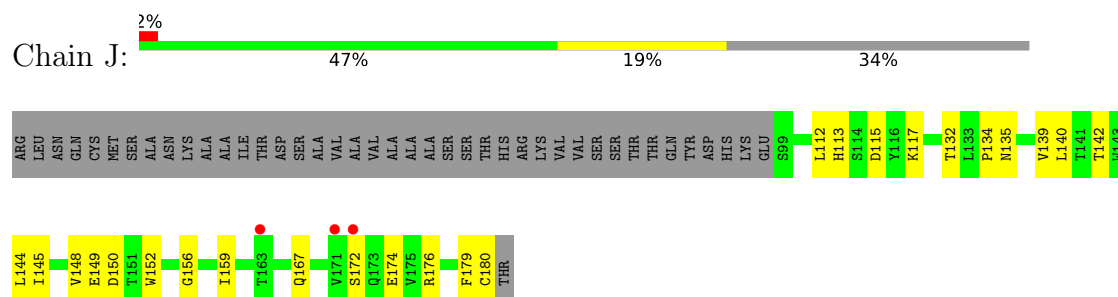
- Molecule 3 is a protein called Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	221	Total	C	N	O	S	0	0	0
			1650	1040	282	321	7			
3	I	221	Total	C	N	O	S	0	0	0
			1650	1040	282	321	7			

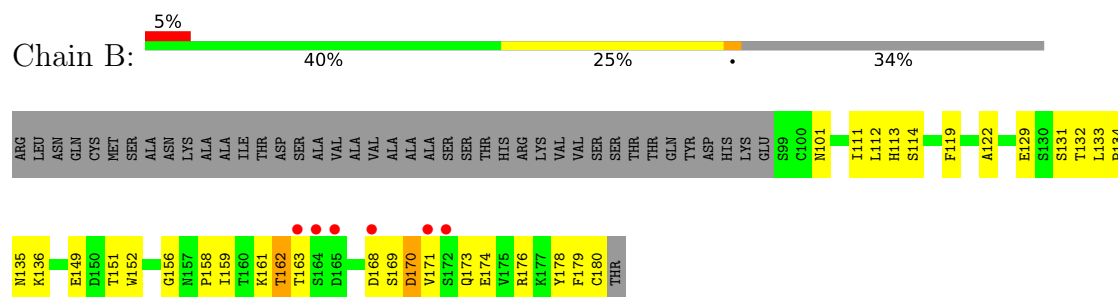
### 3 Residue-property plots

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.

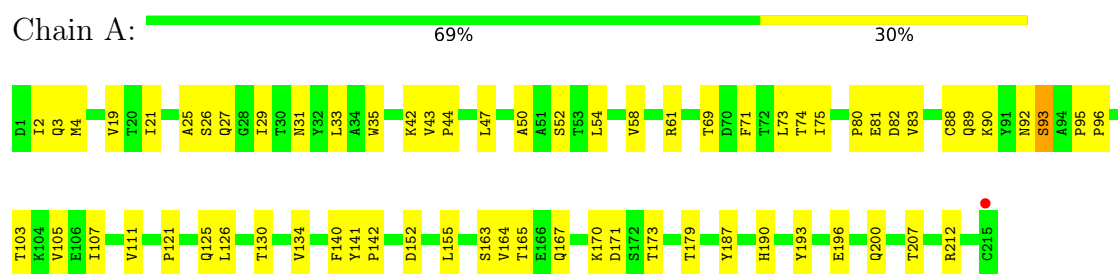
#### • Molecule 1: Protein OPG161



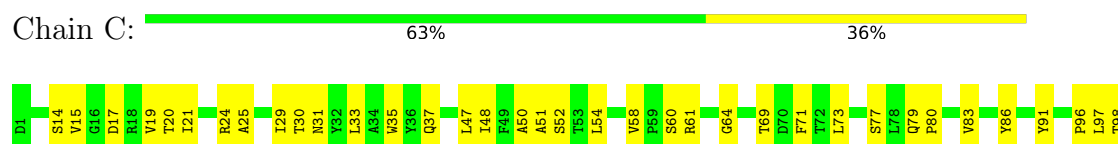
#### • Molecule 1: Protein OPG161

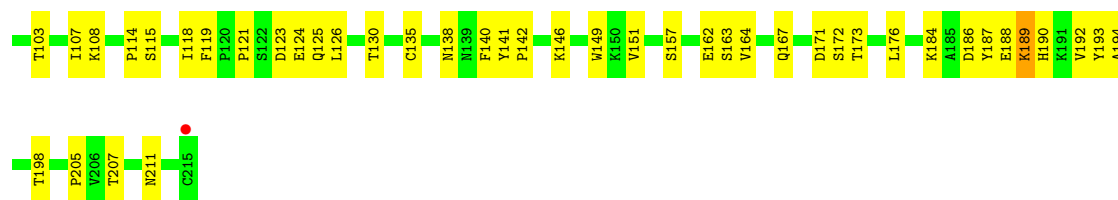


#### • Molecule 2: Light Chain



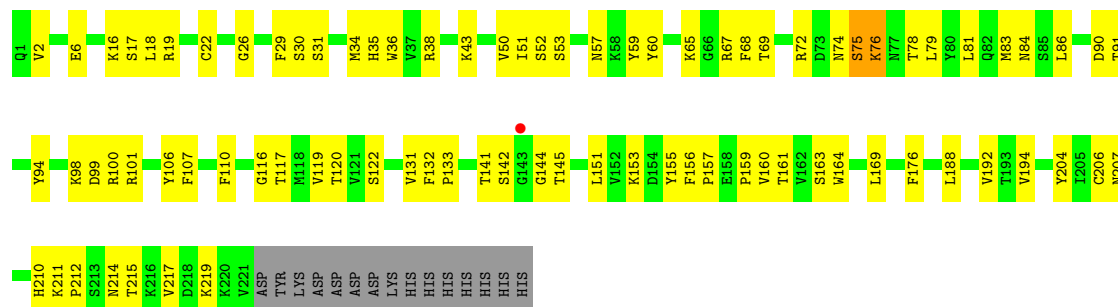
#### • Molecule 2: Light Chain





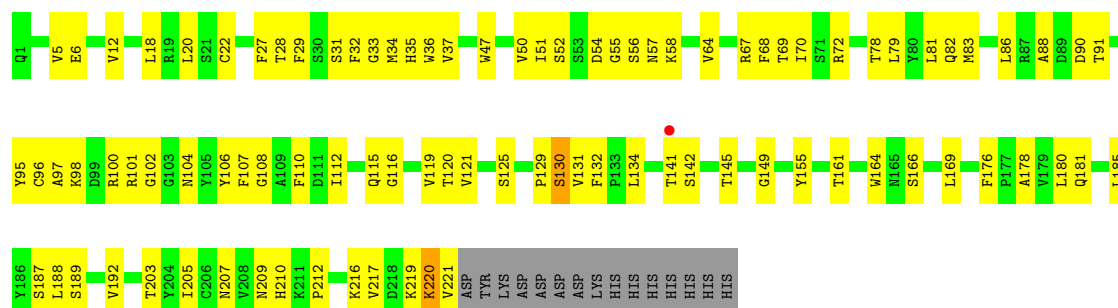
● Molecule 3: Heavy Chain

Chain F: 58% 35% 6%



● Molecule 3: Heavy Chain

Chain I: 54% 39% 6%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	147.48Å 185.99Å 41.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.00 – 2.82 31.00 – 2.82	Depositor EDS
% Data completeness (in resolution range)	97.7 (31.00-2.82) 97.6 (31.00-2.82)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.91 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, $R_{free}$	0.211 , 0.275 0.208 , 0.269	Depositor DCC
$R_{free}$ test set	2000 reflections (6.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.6	Xtriage
Anisotropy	0.577	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 19.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7876	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.01 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.9312e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

### 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	B	0.53	0/663	0.76	0/902
1	J	0.49	0/663	0.70	0/902
2	A	0.46	0/1675	0.66	0/2274
2	C	0.48	0/1675	0.74	5/2274 (0.2%)
3	F	0.48	0/1689	0.79	6/2294 (0.3%)
3	I	0.50	0/1689	0.71	1/2294 (0.0%)
All	All	0.49	0/8054	0.73	12/10940 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	76	LYS	CA-CB-CG	-12.15	89.79	114.10
2	C	189	LYS	CB-CG-CD	-7.11	94.94	111.30
3	I	220	LYS	CG-CD-CE	6.95	127.29	111.30
3	F	76	LYS	CD-CE-NZ	-6.38	91.49	111.90
3	F	76	LYS	CB-CA-C	5.87	119.90	110.09
3	F	75	SER	CA-C-N	-5.86	112.87	122.54
3	F	75	SER	C-N-CA	-5.86	112.87	122.54
2	C	188	GLU	CA-C-N	5.83	128.57	120.29
2	C	188	GLU	C-N-CA	5.83	128.57	120.29
2	C	189	LYS	CA-CB-CG	5.76	125.61	114.10
3	F	76	LYS	CB-CG-CD	5.46	123.85	111.30
2	C	189	LYS	CD-CE-NZ	-5.38	94.70	111.90

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	B	648	0	583	30	0
1	J	648	0	583	18	0
2	A	1640	0	1608	51	0
2	C	1640	0	1608	50	0
3	F	1650	0	1616	56	0
3	I	1650	0	1616	76	0
All	All	7876	0	7614	260	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 17.

All (260) 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:J:156:GLY:O	3:F:101:ARG:NH2	2.10	0.83
3:F:83:MET:HE1	3:F:119:VAL:HG11	1.61	0.83
2:C:96:PRO:HB2	2:C:98:THR:HG23	1.60	0.81
3:I:32:PHE:HA	3:I:102:GLY:HA2	1.61	0.81
2:A:90:LYS:HG3	2:A:92:ASN:HD22	1.47	0.78
2:A:29:ILE:HB	2:A:92:ASN:HD21	1.46	0.78
2:C:186:ASP:HA	2:C:189:LYS:HD2	1.65	0.78
1:B:168:ASP:HB2	3:I:27:PHE:HB2	1.67	0.76
2:A:47:LEU:HA	2:A:58:VAL:HG21	1.68	0.76
3:I:20:LEU:HG	3:I:83:MET:HE2	1.66	0.75
1:B:134:PRO:HG3	1:B:179:PHE:HB2	1.68	0.74
2:C:126:LEU:HB3	2:C:184:LYS:HE3	1.70	0.73
3:I:22:CYS:HB3	3:I:79:LEU:HB3	1.72	0.72
3:I:51:ILE:HB	3:I:70:ILE:HG12	1.71	0.72
3:I:18:LEU:HB3	3:I:83:MET:HE3	1.71	0.72
3:I:34:MET:HB3	3:I:79:LEU:HD22	1.72	0.71
1:B:169:SER:HB3	3:I:28:THR:HB	1.72	0.71
3:I:181:GLN:HG3	3:I:185:LEU:O	1.90	0.70
2:A:33:LEU:HD22	2:A:71:PHE:CG	2.29	0.67
2:A:90:LYS:NZ	2:A:96:PRO:O	2.28	0.67
2:A:61:ARG:NH1	2:A:82:ASP:OD1	2.27	0.67
3:I:91:THR:HG23	3:I:120:THR:HA	1.76	0.67
3:F:52:SER:O	3:F:72:ARG:NH1	2.27	0.67
2:C:21:ILE:HD13	2:C:103:THR:HB	1.77	0.67
1:J:172:SER:HB3	3:F:101:ARG:NH1	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:SER:O	1:B:171:VAL:N	2.30	0.65
3:I:36:TRP:HD1	3:I:70:ILE:HD12	1.61	0.64
2:C:146:LYS:HB2	2:C:198:THR:OG1	1.97	0.64
3:I:12:VAL:HG11	3:I:86:LEU:HD13	1.79	0.63
1:B:169:SER:HB3	3:I:28:THR:CB	2.29	0.63
1:J:140:LEU:HD23	1:J:145:ILE:HD13	1.79	0.63
1:B:174:GLU:OE2	3:I:104:ASN:HB2	1.99	0.63
3:F:18:LEU:HD12	3:F:19:ARG:H	1.64	0.62
2:A:33:LEU:HD22	2:A:71:PHE:CD1	2.35	0.61
2:C:33:LEU:HD13	2:C:71:PHE:CD1	2.35	0.61
2:C:91:TYR:HA	2:C:97:LEU:HD22	1.81	0.61
3:I:47:TRP:HZ2	3:I:50:VAL:HG12	1.65	0.61
3:F:29:PHE:CE1	3:F:34:MET:HG3	2.36	0.60
2:A:134:VAL:HG22	2:A:179:THR:HG23	1.83	0.60
3:I:209:ASN:OD1	3:I:216:LYS:HG2	2.02	0.60
2:A:35:TRP:CD2	2:A:73:LEU:HB2	2.37	0.60
3:I:29:PHE:O	3:I:72:ARG:NH2	2.35	0.60
3:I:130:SER:HB3	3:I:132:PHE:CZ	2.37	0.60
3:I:52:SER:HB2	3:I:57:ASN:HB2	1.82	0.59
3:I:97:ALA:HB1	3:I:110:PHE:HB3	1.84	0.59
2:A:2:ILE:HG12	2:A:27:GLN:HB2	1.83	0.59
3:F:22:CYS:HB3	3:F:79:LEU:HB3	1.82	0.59
3:F:169:LEU:HD21	3:F:192:VAL:HG21	1.85	0.59
2:A:90:LYS:HE2	2:A:92:ASN:HB2	1.85	0.59
2:A:141:TYR:CD1	2:A:142:PRO:HA	2.38	0.58
3:F:133:PRO:HD3	3:F:219:LYS:HE2	1.85	0.58
3:I:131:VAL:HB	3:I:217:VAL:HG11	1.85	0.58
2:A:80:PRO:O	2:A:83:VAL:HG23	2.04	0.58
3:F:52:SER:HB3	3:F:57:ASN:HB2	1.85	0.58
2:A:35:TRP:CE2	2:A:73:LEU:HB2	2.38	0.58
1:B:173:GLN:HG2	1:B:176:ARG:NH1	2.19	0.57
1:J:152:TRP:CE2	1:J:176:ARG:HB2	2.38	0.57
1:B:131:SER:HB3	1:B:180:CYS:HB3	1.87	0.57
1:J:172:SER:HB3	3:F:101:ARG:HH11	1.70	0.57
3:F:34:MET:HB3	3:F:79:LEU:HD22	1.87	0.56
2:A:21:ILE:HD13	2:A:103:THR:HB	1.87	0.56
3:F:122:SER:HB3	3:F:156:PHE:HZ	1.70	0.56
2:C:189:LYS:HD3	2:C:190:HIS:CE1	2.39	0.56
2:C:47:LEU:HA	2:C:58:VAL:HG21	1.86	0.56
1:J:112:LEU:HD12	1:J:113:HIS:N	2.21	0.56
3:I:6:GLU:OE2	3:I:96:CYS:N	2.29	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:52:SER:OG	3:I:104:ASN:OD1	2.24	0.55
2:C:15:VAL:CG2	2:C:107:ILE:HD11	2.36	0.55
2:A:90:LYS:HG3	2:A:92:ASN:ND2	2.21	0.55
2:C:15:VAL:HG22	2:C:107:ILE:HD11	1.89	0.55
1:J:148:VAL:HG12	1:J:179:PHE:CD1	2.42	0.55
2:C:25:ALA:HB3	2:C:69:THR:HA	1.88	0.55
3:I:129:PRO:HB3	3:I:155:TYR:HB3	1.88	0.55
2:C:48:ILE:HG13	2:C:54:LEU:HD12	1.89	0.55
3:F:122:SER:HB3	3:F:156:PHE:CZ	2.43	0.54
3:I:33:GLY:H	3:I:102:GLY:HA2	1.73	0.54
3:F:194:VAL:HG11	3:F:204:TYR:CE1	2.43	0.54
2:C:35:TRP:CD2	2:C:73:LEU:HB2	2.44	0.53
2:A:95:PRO:HG2	3:F:59:TYR:CG	2.43	0.53
3:I:35:HIS:CE1	3:I:50:VAL:HB	2.44	0.52
3:I:51:ILE:HG13	3:I:58:LYS:HG2	1.90	0.52
2:A:89:GLN:HG2	2:A:90:LYS:O	2.09	0.52
2:A:4:MET:HE3	2:A:90:LYS:HB2	1.91	0.52
2:A:81:GLU:CD	2:A:81:GLU:H	2.16	0.52
2:C:151:VAL:HG22	2:C:193:TYR:CE1	2.45	0.52
3:I:181:GLN:NE2	3:I:187:SER:OG	2.43	0.52
3:F:50:VAL:HG21	3:F:107:PHE:CE1	2.45	0.52
2:C:192:VAL:HG22	2:C:211:ASN:OD1	2.09	0.52
3:I:67:ARG:NH1	3:I:90:ASP:OD2	2.35	0.52
3:F:75:SER:C	3:F:76:LYS:HG2	2.35	0.51
3:I:51:ILE:HG23	3:I:72:ARG:HH11	1.74	0.51
1:B:152:TRP:CZ2	1:B:176:ARG:HG3	2.45	0.51
2:C:115:SER:HB2	2:C:138:ASN:HB3	1.93	0.51
2:C:125:GLN:HG2	2:C:130:THR:O	2.11	0.51
3:I:169:LEU:HD21	3:I:192:VAL:HG21	1.91	0.51
3:F:68:PHE:CD1	3:F:83:MET:HA	2.46	0.51
2:C:118:ILE:HD12	2:C:119:PHE:H	1.75	0.51
3:I:51:ILE:HD13	3:I:72:ARG:HD2	1.93	0.51
3:F:83:MET:HB3	3:F:86:LEU:HD21	1.93	0.51
3:F:210:HIS:CD2	3:F:212:PRO:HD2	2.45	0.51
2:A:90:LYS:CG	2:A:92:ASN:HD22	2.21	0.50
3:I:6:GLU:HG3	3:I:96:CYS:HB2	1.93	0.50
3:I:205:ILE:CD1	3:I:220:LYS:HB2	2.42	0.50
2:A:29:ILE:CB	2:A:92:ASN:HD21	2.17	0.50
3:F:16:LYS:N	3:F:16:LYS:HD2	2.26	0.50
3:I:134:LEU:HD11	3:I:189:SER:HB3	1.93	0.50
2:A:31:ASN:O	2:A:50:ALA:HA	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:6:GLU:HB3	3:F:117:THR:HB	1.92	0.50
3:F:163:SER:OG	3:F:207:ASN:HB2	2.11	0.50
1:J:115:ASP:OD2	1:J:117:LYS:HG2	2.11	0.50
3:F:65:LYS:O	3:F:67:ARG:N	2.45	0.49
3:I:33:GLY:N	3:I:102:GLY:HA2	2.26	0.49
3:I:88:ALA:HA	3:I:121:VAL:HB	1.95	0.49
3:F:50:VAL:HG21	3:F:107:PHE:HE1	1.77	0.49
2:C:171:ASP:O	2:C:173:THR:HG23	2.12	0.49
1:B:149:GLU:HA	1:B:159:ILE:O	2.12	0.49
3:F:35:HIS:HE2	3:F:99:ASP:HB2	1.78	0.49
1:B:122:ALA:HB1	1:B:178:TYR:CG	2.48	0.49
1:J:139:VAL:O	1:J:142:THR:OG1	2.29	0.49
2:A:152:ASP:OD2	2:A:190:HIS:HB3	2.13	0.48
3:I:83:MET:HE1	3:I:119:VAL:HG21	1.95	0.48
1:B:169:SER:HB3	3:I:28:THR:OG1	2.13	0.48
1:J:115:ASP:OD2	1:J:117:LYS:NZ	2.37	0.48
2:C:80:PRO:HA	2:C:107:ILE:HD12	1.96	0.48
3:I:37:VAL:O	3:I:95:TYR:N	2.32	0.48
1:J:112:LEU:HD12	1:J:113:HIS:H	1.78	0.48
1:J:144:LEU:H	1:J:144:LEU:HD12	1.78	0.48
3:I:166:SER:N	3:I:207:ASN:OD1	2.35	0.48
3:F:141:THR:HG23	3:F:144:GLY:HA3	1.95	0.48
3:F:65:LYS:C	3:F:67:ARG:H	2.21	0.48
2:C:51:ALA:O	2:C:64:GLY:HA3	2.14	0.48
1:B:174:GLU:HB3	3:I:106:TYR:HB2	1.96	0.48
2:A:171:ASP:O	2:A:173:THR:HG23	2.14	0.48
3:F:22:CYS:O	3:F:78:THR:HA	2.14	0.47
1:B:119:PHE:CE1	1:B:156:GLY:HA2	2.50	0.47
3:F:51:ILE:HD13	3:F:72:ARG:HD2	1.96	0.47
3:I:178:ALA:HA	3:I:188:LEU:HB3	1.96	0.47
3:F:30:SER:HB2	3:F:74:ASN:ND2	2.29	0.47
1:B:169:SER:CB	3:I:28:THR:HB	2.44	0.47
2:A:190:HIS:N	2:A:212:ARG:HH21	2.13	0.47
3:F:38:ARG:HD3	3:F:94:TYR:CZ	2.50	0.47
3:I:5:VAL:HG13	3:I:115:GLN:HE22	1.80	0.47
2:C:77:SER:O	2:C:79:GLN:NE2	2.48	0.46
3:F:6:GLU:OE1	3:F:116:GLY:N	2.39	0.46
3:F:159:PRO:HG2	3:F:211:LYS:HE3	1.97	0.46
1:B:101:ASN:O	1:B:111:ILE:HD13	2.15	0.46
2:C:135:CYS:HB2	2:C:149:TRP:CZ2	2.51	0.46
2:C:80:PRO:O	2:C:83:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:60:TYR:OH	3:F:69:THR:HA	2.16	0.46
2:A:187:TYR:HA	2:A:193:TYR:OH	2.16	0.46
3:I:54:ASP:OD1	3:I:56:SER:N	2.21	0.46
1:B:170:ASP:OD1	3:I:31:SER:OG	2.19	0.46
3:I:54:ASP:OD1	3:I:55:GLY:N	2.49	0.46
1:B:119:PHE:CD1	1:B:156:GLY:HA2	2.51	0.46
3:F:43:LYS:HD3	3:F:43:LYS:N	2.31	0.46
3:I:100:ARG:HD3	3:I:108:GLY:O	2.16	0.46
3:F:31:SER:HA	3:F:53:SER:HB2	1.97	0.45
3:I:205:ILE:HD11	3:I:220:LYS:HB2	1.98	0.45
2:A:170:LYS:HE3	2:C:19:VAL:HA	1.97	0.45
2:C:124:GLU:OE1	3:I:219:LYS:HE3	2.16	0.45
3:I:18:LEU:HA	3:I:18:LEU:HD12	1.73	0.45
1:B:132:THR:O	1:B:180:CYS:HA	2.17	0.45
2:C:114:PRO:HB3	2:C:140:PHE:HB3	1.99	0.45
2:C:163:SER:OG	3:I:176:PHE:HB3	2.17	0.45
3:F:98:LYS:O	3:F:110:PHE:HA	2.16	0.45
3:I:6:GLU:CD	3:I:116:GLY:H	2.24	0.45
3:I:68:PHE:HA	3:I:82:GLN:O	2.16	0.44
2:A:107:ILE:HG22	2:A:167:GLN:OE1	2.18	0.44
3:I:36:TRP:NE1	3:I:81:LEU:HB2	2.31	0.44
3:I:98:LYS:HB3	3:I:112:ILE:HB	1.99	0.44
2:A:35:TRP:CZ3	2:A:88:CYS:HB3	2.52	0.44
3:F:2:VAL:HA	3:F:26:GLY:HA3	2.00	0.44
2:C:31:ASN:O	2:C:50:ALA:HA	2.18	0.44
2:A:93:SER:O	2:A:95:PRO:HD3	2.18	0.44
2:A:125:GLN:HG2	2:A:130:THR:O	2.17	0.44
2:C:24:ARG:HA	2:C:69:THR:O	2.18	0.44
2:A:61:ARG:HH11	2:A:82:ASP:CG	2.24	0.44
2:A:140:PHE:O	2:A:173:THR:HB	2.18	0.44
2:C:83:VAL:HG22	2:C:107:ILE:HB	1.98	0.44
3:F:188:LEU:HD12	3:F:188:LEU:C	2.43	0.44
2:C:33:LEU:HD22	2:C:71:PHE:CG	2.52	0.44
3:I:22:CYS:O	3:I:78:THR:HA	2.18	0.44
1:B:112:LEU:HD12	1:B:113:HIS:N	2.32	0.44
1:B:135:ASN:O	1:B:136:LYS:C	2.61	0.44
1:B:174:GLU:HA	3:I:101:ARG:HD3	2.00	0.44
2:C:61:ARG:HG2	2:C:61:ARG:HH11	1.83	0.44
2:A:3:GLN:H	2:A:26:SER:HB3	1.83	0.44
2:A:21:ILE:HD11	2:A:105:VAL:HG23	2.00	0.44
3:F:215:THR:HG22	3:F:217:VAL:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:36:TRP:NE1	3:F:81:LEU:HB2	2.32	0.43
2:C:54:LEU:HD12	2:C:54:LEU:HA	1.83	0.43
2:A:212:ARG:HH11	2:A:212:ARG:HG2	1.82	0.43
1:B:161:LYS:O	1:B:163:THR:N	2.51	0.43
2:C:123:ASP:HA	2:C:126:LEU:HD12	2.00	0.43
3:I:51:ILE:HD13	3:I:72:ARG:CD	2.48	0.43
1:J:149:GLU:HA	1:J:159:ILE:O	2.19	0.43
1:J:135:ASN:ND2	2:C:205:PRO:O	2.45	0.43
2:C:50:ALA:O	2:C:52:SER:N	2.43	0.43
3:F:155:TYR:CE2	3:F:160:VAL:HG13	2.53	0.43
1:B:151:THR:O	1:B:158:PRO:HA	2.18	0.43
2:A:19:VAL:HB	2:A:75:ILE:HB	2.00	0.43
1:B:113:HIS:NE2	1:B:129:GLU:OE2	2.51	0.43
2:C:162:GLU:HG2	2:C:176:LEU:HD21	2.00	0.43
3:I:50:VAL:HG21	3:I:107:PHE:CE1	2.53	0.43
3:I:203:THR:HG23	3:I:220:LYS:HD2	1.99	0.43
3:F:35:HIS:CE1	3:F:110:PHE:CE1	3.07	0.42
3:F:132:PHE:HB2	3:F:151:LEU:HB3	2.00	0.42
2:C:14:SER:O	2:C:17:ASP:HB2	2.20	0.42
3:I:33:GLY:H	3:I:102:GLY:CA	2.31	0.42
3:F:151:LEU:HG	3:F:153:LYS:HB2	2.00	0.42
3:F:157:PRO:HD2	3:F:212:PRO:HB2	2.01	0.42
2:A:164:VAL:HG22	2:A:165:THR:O	2.19	0.42
2:C:141:TYR:CG	2:C:142:PRO:HA	2.55	0.42
3:I:69:THR:HB	3:I:82:GLN:HB3	2.01	0.42
2:A:25:ALA:HB3	2:A:69:THR:HA	2.00	0.42
2:C:167:GLN:HE21	2:C:172:SER:HB3	1.84	0.42
2:A:111:VAL:O	2:C:24:ARG:NH2	2.53	0.42
2:A:141:TYR:CG	2:A:142:PRO:HA	2.54	0.42
2:C:33:LEU:HD22	2:C:71:PHE:CD2	2.54	0.42
2:A:81:GLU:OE1	2:A:81:GLU:N	2.48	0.42
3:F:67:ARG:HH22	3:F:90:ASP:CG	2.28	0.42
2:C:194:ALA:HB1	2:C:207:THR:HG22	2.01	0.42
3:I:64:VAL:HB	3:I:68:PHE:CD2	2.54	0.42
3:F:131:VAL:HG21	3:F:217:VAL:HB	2.01	0.42
2:C:37:GLN:HB2	2:C:86:TYR:CE2	2.55	0.42
1:J:132:THR:O	1:J:180:CYS:HA	2.20	0.41
3:F:91:THR:HG23	3:F:120:THR:HA	2.01	0.41
1:B:161:LYS:O	1:B:162:THR:C	2.61	0.41
3:I:35:HIS:ND1	3:I:50:VAL:HB	2.35	0.41
3:I:134:LEU:HB2	3:I:149:GLY:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:25:ALA:N	2:A:69:THR:O	2.41	0.41
3:F:17:SER:OG	3:F:84:ASN:HA	2.20	0.41
1:B:158:PRO:HG3	1:B:176:ARG:CZ	2.50	0.41
1:B:174:GLU:CD	3:I:104:ASN:HB2	2.46	0.41
1:J:174:GLU:HB3	3:F:106:TYR:HB2	2.02	0.41
1:B:151:THR:HB	1:B:178:TYR:HA	2.02	0.41
3:I:32:PHE:CA	3:I:102:GLY:HA2	2.40	0.41
3:I:210:HIS:CD2	3:I:212:PRO:HD2	2.55	0.41
2:C:121:PRO:HG2	2:C:187:TYR:CZ	2.56	0.41
3:I:68:PHE:CE1	3:I:83:MET:HB3	2.56	0.41
3:F:214:ASN:O	3:F:214:ASN:CG	2.64	0.41
3:I:161:THR:HG23	3:I:209:ASN:HB3	2.02	0.41
1:J:117:LYS:HA	1:J:117:LYS:HD3	1.82	0.41
1:J:134:PRO:HG3	1:J:179:PHE:HB2	2.03	0.41
2:A:54:LEU:HD12	2:A:54:LEU:HA	1.87	0.41
2:C:164:VAL:HG22	2:C:176:LEU:HD12	2.02	0.41
2:C:187:TYR:HA	2:C:193:TYR:OH	2.20	0.41
1:B:133:LEU:HD21	1:B:178:TYR:HB2	2.02	0.40
2:A:163:SER:OG	3:F:176:PHE:HB3	2.21	0.40
3:F:164:TRP:CH2	3:F:206:CYS:HB3	2.56	0.40
2:A:196:GLU:HG3	2:A:207:THR:OG1	2.22	0.40
3:I:149:GLY:HA2	3:I:164:TRP:CH2	2.57	0.40
2:A:43:VAL:HG22	2:A:44:PRO:HD2	2.03	0.40
2:A:121:PRO:HB2	2:A:126:LEU:HD21	2.03	0.40
2:A:190:HIS:C	2:A:212:ARG:NH2	2.80	0.40
2:C:29:ILE:O	2:C:30:THR:C	2.65	0.40
3:I:34:MET:SD	3:I:98:LYS:HA	2.61	0.40
3:I:50:VAL:HG21	3:I:107:PHE:HE1	1.86	0.40
2:A:50:ALA:C	2:A:52:SER:H	2.30	0.40
3:I:5:VAL:O	3:I:22:CYS:HA	2.21	0.40

There are no symmetry-related clashes.

## 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	B	80/124 (64%)	72 (90%)	6 (8%)	2 (2%)	4	15
1	J	80/124 (64%)	75 (94%)	5 (6%)	0	100	100
2	A	213/215 (99%)	203 (95%)	10 (5%)	0	100	100
2	C	213/215 (99%)	205 (96%)	8 (4%)	0	100	100
3	F	219/236 (93%)	211 (96%)	8 (4%)	0	100	100
3	I	219/236 (93%)	211 (96%)	7 (3%)	1 (0%)	24	53
All	All	1024/1150 (89%)	977 (95%)	44 (4%)	3 (0%)	36	64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	162	THR
1	B	170	ASP
3	I	142	SER

### 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	B	74/108 (68%)	73 (99%)	1 (1%)	59	84
1	J	74/108 (68%)	72 (97%)	2 (3%)	39	72
2	A	187/187 (100%)	182 (97%)	5 (3%)	39	72
2	C	187/187 (100%)	183 (98%)	4 (2%)	47	78
3	F	183/198 (92%)	179 (98%)	4 (2%)	45	77
3	I	183/198 (92%)	177 (97%)	6 (3%)	33	67
All	All	888/986 (90%)	866 (98%)	22 (2%)	42	74

All (22) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	J	150	ASP
1	J	167	GLN
2	A	42	LYS
2	A	74	THR
2	A	93	SER
2	A	155	LEU
2	A	200	GLN
3	F	100	ARG
3	F	142	SER
3	F	145	THR
3	F	161	THR
1	B	114	SER
2	C	20	THR
2	C	60	SER
2	C	108	LYS
2	C	157	SER
3	I	125	SER
3	I	130	SER
3	I	141	THR
3	I	145	THR
3	I	180	LEU
3	I	221	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	J	106	GLN
2	A	79	GLN
2	A	92	ASN
2	A	190	HIS
3	F	57	ASN
3	F	82	GLN
3	F	209	ASN
1	B	106	GLN
2	C	37	GLN
3	I	115	GLN
3	I	181	GLN

### 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 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	B	82/124 (66%)	0.21	6 (7%)	21 15	28, 40, 75, 96	0
1	J	82/124 (66%)	0.16	3 (3%)	45 36	32, 42, 93, 99	0
2	A	215/215 (100%)	-0.21	1 (0%)	87 82	28, 37, 63, 102	0
2	C	215/215 (100%)	-0.21	1 (0%)	87 82	23, 35, 68, 108	0
3	F	221/236 (93%)	-0.01	1 (0%)	87 82	28, 46, 65, 82	0
3	I	221/236 (93%)	-0.18	1 (0%)	87 82	25, 40, 66, 92	0
All	All	1036/1150 (90%)	-0.10	13 (1%)	75 66	23, 40, 68, 108	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	171	VAL	3.8
3	F	143	GLY	3.5
1	B	171	VAL	3.4
1	B	164	SER	3.3
1	J	172	SER	3.2
1	B	163	THR	3.0
1	B	168	ASP	3.0
1	B	165	ASP	2.8
3	I	141	THR	2.8
1	J	163	THR	2.5
2	A	215	CYS	2.5
1	B	172	SER	2.1
2	C	215	CYS	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.