



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 04:43 pm GMT

PDB ID : 5GGR  
Title : PD-1 in complex with nivolumab Fab  
Authors : Heo, Y.S.  
Deposited on : 2016-06-16  
Resolution : 3.30 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.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

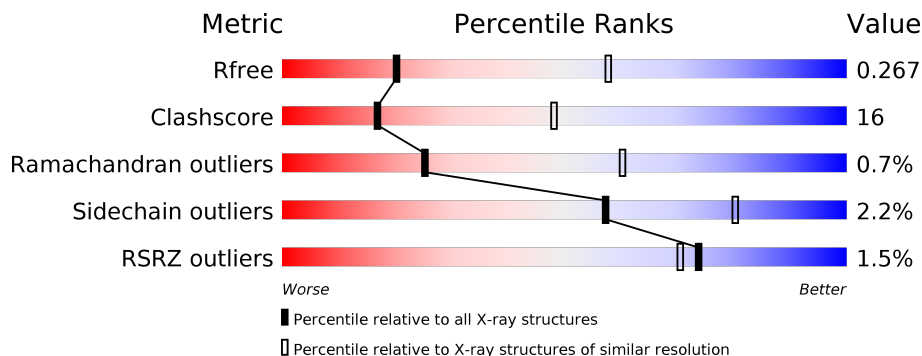
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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))
$R_{free}$	100719	1034 (3.36-3.24)
Clashscore	112137	1100 (3.36-3.24)
Ramachandran outliers	110173	1081 (3.36-3.24)
Sidechain outliers	110143	1080 (3.36-3.24)
RSRZ outliers	101464	1039 (3.36-3.24)

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	225	<div> <div>2%</div> <div> <div></div> <div>64%</div> <div>28%</div> <div>7%</div> </div> </div>
1	H	225	<div> <div></div> <div> <div>63%</div> <div>28%</div> <div>8%</div> </div> </div>
2	B	214	<div> <div></div> <div> <div>68%</div> <div>30%</div> <div>2%</div> </div> </div>
2	L	214	<div> <div>2%</div> <div> <div>67%</div> <div>29%</div> <div>2%</div> </div> </div>
3	Y	125	<div> <div>2%</div> <div> <div>54%</div> <div>37%</div> <div>6%</div> </div> </div>
3	Z	125	<div> <div></div> <div> <div>60%</div> <div>30%</div> <div>6%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8247 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 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	0	0
			1571	990	268	307	6			
1	H	207	Total	C	N	O	S	0	0	0
			1561	985	266	304	6			

- Molecule 2 is a protein called light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	212	Total	C	N	O	S	0	0	0
			1630	1019	278	329	4			
2	L	212	Total	C	N	O	S	0	0	0
			1630	1019	278	329	4			

- Molecule 3 is a protein called Programmed cell death protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Y	118	Total	C	N	O	S	0	0	0
			931	579	169	179	4			
3	Z	117	Total	C	N	O	S	0	0	0
			924	574	168	178	4			

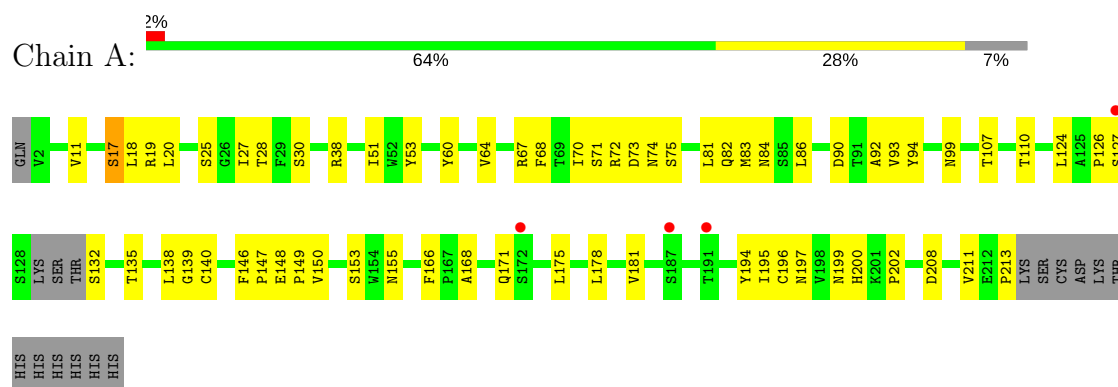
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	93	SER	CYS	engineered mutation	UNP Q15116
Z	93	SER	CYS	engineered mutation	UNP Q15116

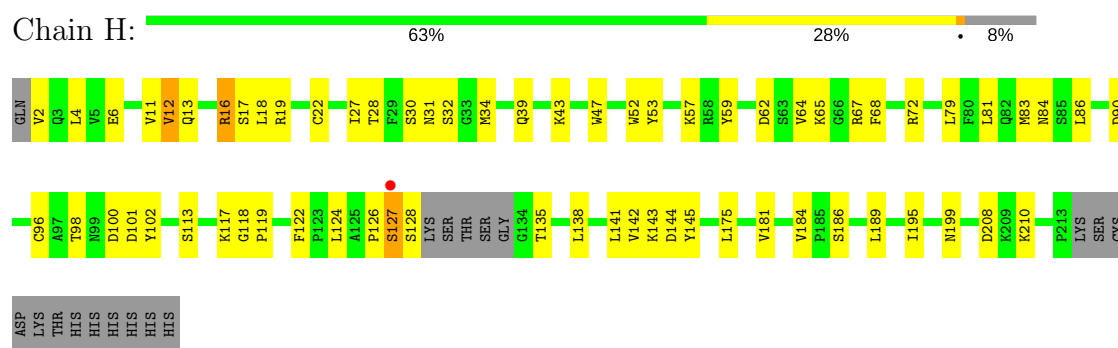
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

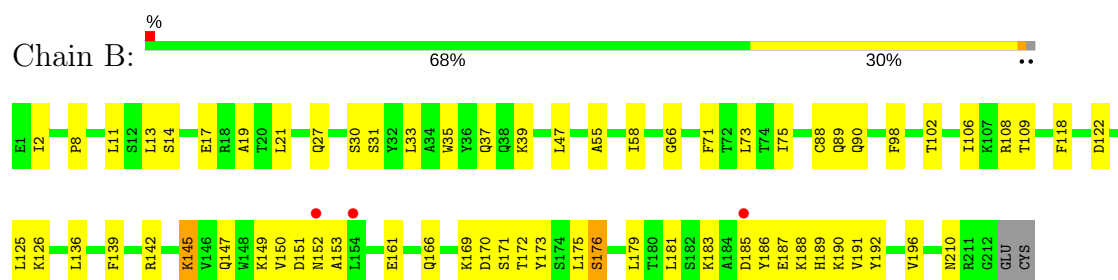
#### • Molecule 1: heavy chain



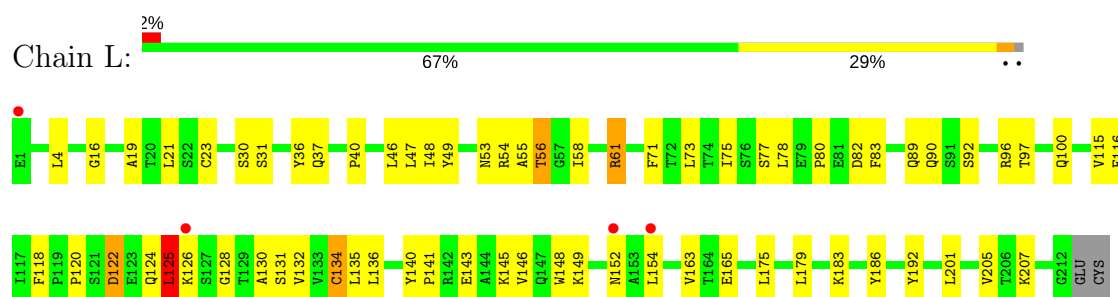
#### • Molecule 1: heavy chain



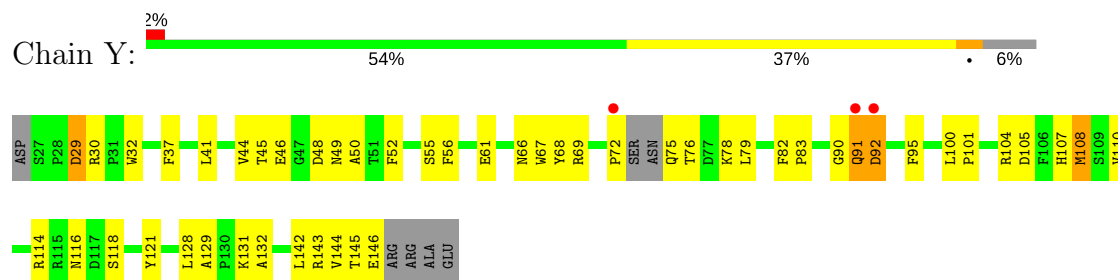
#### • Molecule 2: light chain



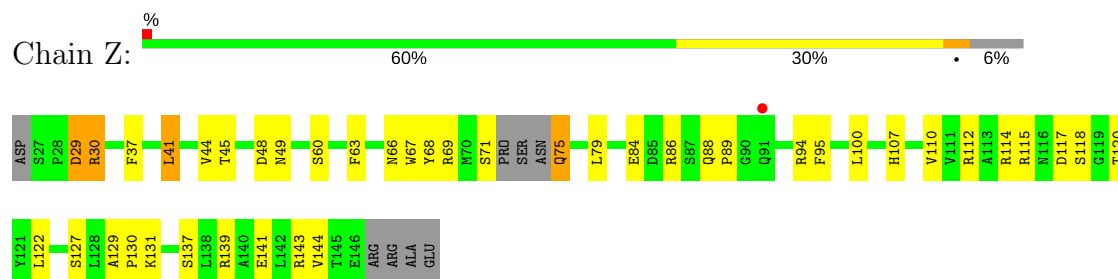
#### • Molecule 2: light chain



• Molecule 3: Programmed cell death protein 1



• Molecule 3: Programmed cell death protein 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.29Å 48.61Å 134.90Å 90.00° 102.12° 90.00°	Depositor
Resolution (Å)	29.75 – 3.30 29.75 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.1 (29.75-3.30) 98.8 (29.75-3.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.16 (at 3.31Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.222 , 0.268 0.223 , 0.267	Depositor DCC
$R_{free}$ test set	897 reflections (5.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.6	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 54.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8247	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	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 90.78 % 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 1.9886e-08. 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	A	0.34	0/1608	0.61	0/2190
1	H	0.39	0/1598	0.67	1/2177 (0.0%)
2	B	0.32	0/1666	0.57	0/2265
2	L	0.41	0/1666	0.67	2/2265 (0.1%)
3	Y	0.35	0/953	0.64	0/1294
3	Z	0.38	0/945	0.62	0/1282
All	All	0.36	0/8436	0.63	3/11473 (0.0%)

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	Y	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	H	16	ARG	CG-CD-NE	6.61	125.68	111.80
2	L	125	LEU	CA-CB-CG	6.56	130.40	115.30
2	L	154	LEU	CA-CB-CG	5.04	126.89	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	Y	90	GLY	Peptide

## 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	1571	0	1536	45	0
1	H	1561	0	1526	51	0
2	B	1630	0	1585	47	0
2	L	1630	0	1587	57	0
3	Y	931	0	898	38	0
3	Z	924	0	889	41	0
All	All	8247	0	8021	255	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 16.

All (255) 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:H:16:ARG:HH21	1:H:18:LEU:HB2	1.26	0.99
2:L:49:TYR:HD2	3:Z:131:LYS:HZ2	1.13	0.93
1:H:143:LYS:NZ	2:L:131:SER:OG	2.04	0.91
3:Y:75:GLN:N	3:Y:75:GLN:OE1	2.06	0.88
2:B:190:LYS:HG3	2:B:191:VAL:HG23	1.61	0.81
3:Y:91:GLN:HG2	3:Y:92:ASP:H	1.47	0.78
1:H:28:THR:HG21	3:Z:60:SER:HB2	1.64	0.77
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.66	0.77
3:Z:71:SER:HB3	3:Z:75:GLN:HG2	1.68	0.76
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.69	0.75
1:H:16:ARG:HH21	1:H:18:LEU:CB	2.01	0.72
1:H:22:CYS:HB3	1:H:79:LEU:HB3	1.71	0.71
2:B:33:LEU:HD11	2:B:88:CYS:HB2	1.73	0.70
2:L:55:ALA:HB3	2:L:58:ILE:HG13	1.73	0.70
2:B:150:VAL:HG11	2:B:189:HIS:HD1	1.58	0.69
1:A:148:GLU:HG2	1:A:149:PRO:HA	1.75	0.69
1:H:126:PRO:HG3	1:H:138:LEU:HD23	1.76	0.67
1:H:100:ASP:HB3	3:Z:129:ALA:HB1	1.74	0.67
1:A:20:LEU:HD12	1:A:81:LEU:HD23	1.76	0.66
2:L:56:THR:HB	3:Z:130:PRO:HA	1.77	0.66
2:L:128:GLY:HA2	2:L:183:LYS:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:55:ALA:HB3	2:L:58:ILE:CG1	2.27	0.65
3:Y:44:VAL:HG21	3:Y:50:ALA:HB2	1.78	0.65
2:L:115:VAL:HG13	2:L:207:LYS:HE2	1.79	0.65
3:Y:32:TRP:HE1	3:Y:56:PHE:HZ	1.45	0.65
3:Y:95:PHE:HD1	3:Y:110:VAL:HG22	1.62	0.64
1:H:16:ARG:NH2	1:H:18:LEU:HB2	2.07	0.64
1:A:67:ARG:NH2	1:A:90:ASP:OD2	2.31	0.63
1:A:195:ILE:HD11	1:A:208:ASP:HB3	1.79	0.62
2:B:55:ALA:HB3	2:B:58:ILE:HG13	1.80	0.62
2:L:61:ARG:NH2	2:L:82:ASP:OD2	2.30	0.62
1:A:171:GLN:HG2	1:A:175:LEU:O	1.99	0.62
2:B:66:GLY:HA3	2:B:71:PHE:HA	1.82	0.62
1:H:11:VAL:O	1:H:12:VAL:HB	1.99	0.61
3:Y:41:LEU:HD11	3:Y:143:ARG:HG3	1.82	0.61
1:H:13:GLN:O	1:H:16:ARG:HG2	2.01	0.61
1:A:17:SER:OG	1:A:18:LEU:N	2.31	0.61
1:A:126:PRO:HG2	1:A:213:PRO:HB3	1.83	0.60
3:Z:94:ARG:HH22	3:Z:117:ASP:CG	2.03	0.60
2:L:49:TYR:HB3	3:Z:131:LYS:HG2	1.83	0.60
2:L:100:GLN:OE1	2:L:100:GLN:N	2.35	0.60
3:Z:44:VAL:HG22	3:Z:144:VAL:HG12	1.83	0.60
2:L:49:TYR:CG	3:Z:131:LYS:HG3	2.37	0.59
2:L:21:LEU:HD22	2:L:73:LEU:HD23	1.83	0.59
1:H:62:ASP:HA	1:H:65:LYS:HG3	1.85	0.59
3:Y:104:ARG:HG2	3:Y:105:ASP:OD1	2.03	0.59
1:A:200:HIS:CD2	1:A:202:PRO:HD2	2.37	0.59
3:Z:114:ARG:O	3:Z:144:VAL:HG21	2.02	0.59
3:Z:118:SER:OG	3:Z:144:VAL:HG22	2.03	0.59
1:H:117:LYS:HD3	1:H:118:GLY:N	2.18	0.59
3:Y:48:ASP:OD1	3:Y:49:ASN:N	2.35	0.58
2:L:55:ALA:HB2	3:Z:131:LYS:HE2	1.85	0.58
1:A:124:LEU:HB3	2:B:118:PHE:CD2	2.39	0.58
1:H:195:ILE:HG12	1:H:210:LYS:HA	1.86	0.58
3:Y:46:GLU:HG2	3:Y:146:GLU:HB3	1.86	0.57
2:L:61:ARG:NH1	2:L:77:SER:O	2.37	0.57
3:Y:91:GLN:CG	3:Y:92:ASP:H	2.16	0.57
1:H:2:VAL:HB	1:H:27:ILE:HD11	1.87	0.57
1:A:168:ALA:HB2	1:A:178:LEU:HD23	1.86	0.57
1:H:28:THR:HG21	3:Z:60:SER:CB	2.35	0.56
3:Z:115:ARG:HA	3:Z:144:VAL:CG2	2.35	0.56
1:A:132:SER:OG	1:A:135:THR:O	2.16	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:122:PHE:HB2	1:H:141:LEU:HB3	1.86	0.56
2:L:30:SER:OG	2:L:31:SER:N	2.37	0.56
1:A:19:ARG:HG3	1:A:82:GLN:HA	1.88	0.56
1:H:122:PHE:HD1	1:H:141:LEU:HD23	1.71	0.56
2:L:136:LEU:HD11	2:L:146:VAL:HG11	1.88	0.56
2:B:108:ARG:HG3	2:B:109:THR:O	2.06	0.56
2:B:30:SER:OG	2:B:31:SER:N	2.39	0.55
3:Z:44:VAL:O	3:Z:144:VAL:HA	2.06	0.55
2:B:188:LYS:HG3	2:B:189:HIS:HD2	1.71	0.55
2:L:49:TYR:CD2	3:Z:131:LYS:HG3	2.42	0.55
3:Y:44:VAL:O	3:Y:144:VAL:HA	2.07	0.55
3:Y:66:ASN:ND2	3:Y:78:LYS:HD2	2.21	0.55
1:H:27:ILE:HG22	1:H:28:THR:H	1.72	0.55
2:B:33:LEU:HD12	2:B:89:GLN:O	2.07	0.54
3:Y:68:TYR:CE1	3:Y:78:LYS:HG3	2.43	0.54
1:A:139:GLY:HA2	1:A:181:VAL:HA	1.90	0.54
2:L:125:LEU:HD12	2:L:183:LYS:HG3	1.90	0.54
1:A:82:GLN:HG3	1:A:84:ASN:OD1	2.08	0.54
1:A:60:TYR:CZ	1:A:70:ILE:HG22	2.42	0.54
2:L:90:GLN:HE21	2:L:97:THR:H	1.54	0.53
2:L:149:LYS:HE3	2:L:152:ASN:HA	1.89	0.53
2:B:35:TRP:HB3	2:B:73:LEU:HD12	1.89	0.53
1:A:153:SER:O	1:A:197:ASN:HB2	2.08	0.53
2:L:61:ARG:HH22	2:L:82:ASP:CG	2.12	0.53
1:H:64:VAL:HB	1:H:68:PHE:CD1	2.43	0.53
2:L:148:TRP:CG	2:L:179:LEU:HD13	2.43	0.53
1:H:143:LYS:NZ	2:L:124:GLN:HE22	2.06	0.53
2:B:8:PRO:HG3	2:B:11:LEU:HD13	1.92	0.52
3:Y:100:LEU:HB3	3:Y:101:PRO:HD2	1.91	0.52
1:A:150:VAL:HG23	1:A:199:ASN:O	2.10	0.52
1:H:12:VAL:HG21	1:H:16:ARG:NH1	2.23	0.52
2:B:183:LYS:O	2:B:187:GLU:HG3	2.08	0.52
3:Z:120:THR:HG21	3:Z:139:ARG:HD2	1.92	0.52
2:B:122:ASP:HA	2:B:125:LEU:HD12	1.91	0.51
2:B:106:ILE:HB	2:B:166:GLN:HE22	1.75	0.51
1:H:101:ASP:OD2	2:L:46:LEU:HD22	2.09	0.51
3:Y:95:PHE:CD1	3:Y:110:VAL:HG22	2.42	0.51
1:H:102:TYR:CE1	3:Z:130:PRO:HD3	2.46	0.51
2:B:188:LYS:HG3	2:B:189:HIS:CD2	2.45	0.51
3:Z:41:LEU:HD21	3:Z:143:ARG:HG3	1.92	0.51
3:Y:55:SER:HA	3:Y:105:ASP:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:PRO:HB3	1:A:138:LEU:HB3	1.93	0.50
1:H:144:ASP:HB3	1:H:175:LEU:HD13	1.93	0.50
3:Y:82:PHE:HA	3:Y:83:PRO:C	2.31	0.50
3:Z:115:ARG:HA	3:Z:144:VAL:HG21	1.92	0.50
1:A:99:ASN:O	3:Y:131:LYS:HD3	2.12	0.50
2:L:49:TYR:CD2	2:L:53:ASN:HB2	2.46	0.50
1:H:67:ARG:NH2	1:H:90:ASP:OD2	2.45	0.50
2:B:106:ILE:HB	2:B:166:GLN:NE2	2.26	0.50
2:B:186:TYR:O	2:B:192:TYR:OH	2.28	0.50
3:Y:114:ARG:O	3:Y:144:VAL:HG21	2.11	0.50
1:A:139:GLY:HA3	1:A:181:VAL:HG12	1.93	0.49
1:A:38:ARG:HB2	1:A:92:ALA:HB1	1.94	0.49
1:H:135:THR:HB	1:H:184:VAL:O	2.12	0.49
2:L:201:LEU:HD13	2:L:205:VAL:HG23	1.93	0.49
1:A:27:ILE:HG22	1:A:28:THR:H	1.78	0.49
1:A:196:CYS:O	1:A:208:ASP:HA	2.12	0.49
1:H:47:TRP:CG	2:L:96:ARG:HB2	2.48	0.49
2:L:122:ASP:O	2:L:126:LYS:HG2	2.12	0.49
3:Y:67:TRP:CH2	3:Y:110:VAL:HG23	2.48	0.49
2:L:186:TYR:O	2:L:192:TYR:OH	2.30	0.49
1:A:67:ARG:HH22	1:A:90:ASP:CG	2.16	0.49
2:B:19:ALA:HB3	2:B:75:ILE:HB	1.95	0.49
2:L:122:ASP:OD1	2:L:126:LYS:HE3	2.13	0.48
3:Y:69:ARG:HD2	3:Y:121:TYR:CZ	2.47	0.48
1:A:51:ILE:HD13	1:A:72:ARG:HG2	1.95	0.48
1:A:25:SER:O	1:A:27:ILE:HG12	2.13	0.48
1:H:32:SER:O	1:H:72:ARG:NH2	2.38	0.48
3:Z:88:GLN:HG3	3:Z:89:PRO:HD2	1.96	0.48
2:L:49:TYR:CE2	2:L:53:ASN:HB2	2.49	0.48
1:A:20:LEU:HB2	1:A:81:LEU:HB3	1.96	0.48
1:H:119:PRO:HB3	1:H:145:TYR:HB3	1.95	0.48
2:L:49:TYR:CE2	2:L:53:ASN:CB	2.97	0.48
2:L:40:PRO:HG3	2:L:165:GLU:OE2	2.14	0.47
1:H:31:ASN:OD1	3:Z:30:ARG:NH1	2.47	0.47
1:H:186:SER:O	1:H:189:LEU:HG	2.14	0.47
3:Y:129:ALA:O	3:Y:132:ALA:HB2	2.14	0.47
2:L:19:ALA:HB3	2:L:75:ILE:HB	1.96	0.47
3:Z:37:PHE:HB2	3:Z:137:SER:HB2	1.97	0.47
3:Y:100:LEU:HD11	3:Y:107:HIS:NE2	2.29	0.47
3:Y:69:ARG:NH2	3:Y:116:ASN:O	2.46	0.47
2:B:150:VAL:CG1	2:B:189:HIS:HD1	2.25	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:GLU:OE2	1:A:168:ALA:HB3	2.14	0.47
2:B:170:ASP:OD2	2:B:172:THR:OG1	2.25	0.47
2:B:191:VAL:HG22	2:B:210:ASN:HD22	1.79	0.47
1:H:30:SER:O	1:H:53:TYR:HB2	2.14	0.47
1:H:83:MET:HB3	1:H:86:LEU:HD21	1.96	0.47
2:B:149:LYS:HG2	2:B:153:ALA:O	2.14	0.47
3:Z:63:PHE:CD1	3:Z:127:SER:HA	2.50	0.47
3:Z:41:LEU:HD11	3:Z:141:GLU:OE1	2.15	0.47
1:H:98:THR:OG1	1:H:100:ASP:HB2	2.15	0.46
1:A:196:CYS:C	1:A:197:ASN:HD22	2.18	0.46
2:B:151:ASP:C	2:B:153:ALA:H	2.19	0.46
3:Y:131:LYS:HG2	3:Y:131:LYS:O	2.15	0.46
3:Z:63:PHE:HD1	3:Z:127:SER:HA	1.80	0.46
2:B:151:ASP:OD1	2:B:190:LYS:HB3	2.16	0.46
2:L:4:LEU:HD22	2:L:23:CYS:SG	2.56	0.46
3:Z:100:LEU:HD21	3:Z:107:HIS:CG	2.51	0.46
3:Z:84:GLU:HG2	3:Z:86:ARG:HG3	1.98	0.46
1:H:19:ARG:HA	1:H:81:LEU:O	2.16	0.46
1:H:181:VAL:HG21	2:L:135:LEU:CD1	2.46	0.46
3:Z:66:ASN:HB3	3:Z:68:TYR:CE1	2.51	0.46
3:Y:118:SER:OG	3:Y:144:VAL:HG22	2.16	0.45
2:B:179:LEU:HG	2:B:181:LEU:HD13	1.98	0.45
3:Y:68:TYR:CD1	3:Y:76:THR:HG23	2.52	0.45
1:H:127:SER:O	1:H:128:SER:CB	2.65	0.45
1:A:53:TYR:HA	1:A:72:ARG:NH1	2.32	0.45
1:H:119:PRO:HB2	1:H:142:VAL:HG13	1.97	0.45
2:B:2:ILE:HB	2:B:90:GLN:HE21	1.81	0.45
2:L:16:GLY:N	2:L:78:LEU:O	2.49	0.45
3:Z:45:THR:O	3:Z:48:ASP:HB2	2.17	0.45
1:A:94:TYR:O	1:A:107:THR:HG22	2.17	0.45
1:A:64:VAL:HB	1:A:68:PHE:CG	2.52	0.44
1:A:38:ARG:HA	1:A:93:VAL:O	2.17	0.44
2:B:89:GLN:HB2	2:B:98:PHE:CD1	2.52	0.44
2:B:185:ASP:OD1	2:B:189:HIS:NE2	2.50	0.44
1:H:2:VAL:CB	1:H:27:ILE:HD11	2.47	0.44
2:L:36:TYR:CE2	2:L:46:LEU:HB2	2.53	0.44
2:L:48:ILE:HD13	2:L:54:ARG:HA	2.00	0.44
3:Z:94:ARG:O	3:Z:110:VAL:HA	2.17	0.44
1:A:166:PHE:CE2	2:B:176:SER:HB3	2.53	0.44
2:B:11:LEU:HG	2:B:13:LEU:CD1	2.47	0.44
2:B:145:LYS:HE2	2:B:147:GLN:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:191:VAL:HG22	2:B:210:ASN:ND2	2.32	0.44
3:Y:44:VAL:HG22	3:Y:142:LEU:HD11	1.99	0.44
3:Z:29:ASP:O	3:Z:30:ARG:HB2	2.16	0.44
2:B:35:TRP:CB	2:B:73:LEU:HD12	2.46	0.44
2:L:134:CYS:SG	2:L:135:LEU:N	2.91	0.44
3:Y:128:LEU:HA	3:Y:128:LEU:HD23	1.75	0.44
1:A:30:SER:OG	1:A:74:ASN:ND2	2.50	0.44
2:L:140:TYR:CD1	2:L:141:PRO:HA	2.52	0.44
2:L:163:VAL:HG22	2:L:175:LEU:HD12	1.98	0.44
1:H:57:LYS:HE3	1:H:59:TYR:OH	2.16	0.44
2:B:14:SER:N	2:B:17:GLU:OE2	2.51	0.43
2:B:21:LEU:HD23	2:B:102:THR:HB	1.99	0.43
3:Z:69:ARG:HB2	3:Z:79:LEU:HD11	2.00	0.43
1:H:39:GLN:HG3	1:H:43:LYS:O	2.18	0.43
1:H:181:VAL:HG21	2:L:135:LEU:HD11	2.00	0.43
3:Y:79:LEU:HD23	3:Y:95:PHE:CE2	2.54	0.43
1:A:140:CYS:SG	1:A:211:VAL:HG21	2.59	0.43
2:L:120:PRO:HD3	2:L:132:VAL:HG22	2.00	0.43
1:A:99:ASN:HB3	3:Y:29:ASP:OD1	2.19	0.43
3:Y:52:PHE:HB2	3:Y:108:MET:HB2	2.00	0.43
1:A:147:PRO:O	1:A:200:HIS:NE2	2.52	0.43
2:B:145:LYS:HE2	2:B:147:GLN:CG	2.49	0.43
1:H:124:LEU:HB3	2:L:118:PHE:CD2	2.54	0.43
2:L:128:GLY:HA2	2:L:183:LYS:CB	2.48	0.43
2:L:143:GLU:OE2	2:L:145:LYS:HE3	2.19	0.43
2:B:108:ARG:HD2	2:B:171:SER:O	2.19	0.42
3:Y:66:ASN:HB3	3:Y:68:TYR:CZ	2.53	0.42
1:H:12:VAL:HG21	1:H:16:ARG:HH11	1.84	0.42
3:Z:79:LEU:HD22	3:Z:95:PHE:CD1	2.54	0.42
3:Y:72:PRO:O	3:Y:75:GLN:NE2	2.37	0.42
1:H:16:ARG:NH2	1:H:17:SER:O	2.52	0.42
1:H:34:MET:HB3	1:H:79:LEU:HD22	2.01	0.42
2:B:169:LYS:HB2	2:B:169:LYS:HE2	1.87	0.42
2:B:11:LEU:HG	2:B:13:LEU:HD11	2.01	0.42
1:H:67:ARG:HH22	1:H:90:ASP:CG	2.23	0.42
1:A:51:ILE:HD12	1:A:71:SER:HA	2.01	0.42
1:A:83:MET:HB3	1:A:86:LEU:HD21	2.02	0.42
2:L:46:LEU:HD21	3:Z:131:LYS:HG2	2.02	0.42
3:Z:79:LEU:HD22	3:Z:95:PHE:CE1	2.55	0.42
2:L:80:PRO:HA	2:L:83:PHE:CE2	2.55	0.42
2:L:90:GLN:OE1	2:L:92:SER:OG	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ASN:HD21	1:A:194:TYR:HA	1.85	0.41
3:Z:131:LYS:HA	3:Z:131:LYS:HD2	1.68	0.41
3:Z:67:TRP:HD1	3:Z:122:LEU:O	2.03	0.41
2:B:142:ARG:HB2	2:B:173:TYR:CE1	2.55	0.41
1:H:6:GLU:HG2	1:H:96:CYS:SG	2.60	0.41
2:L:124:GLN:HG2	2:L:130:ALA:H	1.84	0.41
3:Z:75:GLN:N	3:Z:75:GLN:OE1	2.53	0.41
2:B:136:LEU:HD21	2:B:196:VAL:HG21	2.02	0.41
2:L:30:SER:O	2:L:71:PHE:HZ	2.03	0.41
3:Z:94:ARG:HG2	3:Z:112:ARG:NH2	2.35	0.41
1:A:11:VAL:HA	1:A:110:THR:O	2.21	0.41
2:B:39:LYS:HB2	2:B:39:LYS:HE3	1.82	0.41
2:L:54:ARG:NH1	2:L:58:ILE:O	2.54	0.41
2:B:126:LYS:HD2	2:B:126:LYS:HA	1.94	0.41
1:H:52:TRP:O	1:H:72:ARG:NH1	2.54	0.41
1:A:73:ASP:OD1	1:A:75:SER:HB3	2.21	0.41
2:B:161:GLU:OE2	2:B:175:LEU:HD11	2.20	0.41
3:Y:68:TYR:HE1	3:Y:78:LYS:HG3	1.83	0.41
1:H:68:PHE:HD2	1:H:81:LEU:HD11	1.86	0.40
1:H:67:ARG:HB3	1:H:84:ASN:O	2.20	0.40
2:L:116:PHE:HA	2:L:207:LYS:NZ	2.35	0.40
2:L:89:GLN:HG2	2:L:90:GLN:N	2.35	0.40
2:B:139:PHE:O	2:B:172:THR:HB	2.21	0.40
3:Y:45:THR:HA	3:Y:145:THR:OG1	2.21	0.40
1:A:146:PHE:HA	1:A:147:PRO:HA	1.80	0.40
1:A:28:THR:HG22	3:Y:61:GLU:HG3	2.03	0.40
3:Y:91:GLN:CG	3:Y:92:ASP:N	2.84	0.40
3:Z:48:ASP:OD1	3:Z:49:ASN:N	2.46	0.40
2:L:78:LEU:HA	2:L:78:LEU:HD12	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	205/225 (91%)	193 (94%)	11 (5%)	1 (0%)	32	66
1	H	203/225 (90%)	187 (92%)	14 (7%)	2 (1%)	18	53
2	B	210/214 (98%)	192 (91%)	18 (9%)	0	100	100
2	L	210/214 (98%)	192 (91%)	18 (9%)	0	100	100
3	Y	114/125 (91%)	99 (87%)	13 (11%)	2 (2%)	10	42
3	Z	113/125 (90%)	106 (94%)	5 (4%)	2 (2%)	10	42
All	All	1055/1128 (94%)	969 (92%)	79 (8%)	7 (1%)	25	60

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	Y	29	ASP
1	A	127	SER
1	H	12	VAL
1	H	127	SER
3	Z	29	ASP
3	Y	30	ARG
3	Z	30	ARG

### 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	176/192 (92%)	175 (99%)	1 (1%)	89	93
1	H	175/192 (91%)	171 (98%)	4 (2%)	56	79
2	B	184/186 (99%)	180 (98%)	4 (2%)	57	80
2	L	184/186 (99%)	179 (97%)	5 (3%)	50	77
3	Y	104/110 (94%)	100 (96%)	4 (4%)	38	70
3	Z	103/110 (94%)	101 (98%)	2 (2%)	62	81
All	All	926/976 (95%)	906 (98%)	20 (2%)	57	80

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	SER
2	B	27	GLN
2	B	145	LYS
2	B	152	ASN
2	B	176	SER
1	H	4	LEU
1	H	113	SER
1	H	199	ASN
1	H	208	ASP
2	L	56	THR
2	L	61	ARG
2	L	122	ASP
2	L	125	LEU
2	L	134	CYS
3	Y	37	PHE
3	Y	91	GLN
3	Y	92	ASP
3	Y	108	MET
3	Z	41	LEU
3	Z	75	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	155	ASN
1	A	197	ASN
2	B	158	ASN
2	B	210	ASN
2	L	124	GLN
3	Y	75	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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



## 5.5 Carbohydrates [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	209/225 (92%)	-0.23	4 (1%) 67 65	21, 38, 60, 78	0
1	H	207/225 (92%)	-0.24	1 (0%) 90 90	23, 39, 58, 83	0
2	B	212/214 (99%)	-0.12	3 (1%) 75 73	28, 43, 72, 101	0
2	L	212/214 (99%)	-0.08	4 (1%) 67 65	27, 44, 68, 93	0
3	Y	118/125 (94%)	-0.05	3 (2%) 58 54	30, 43, 76, 94	0
3	Z	117/125 (93%)	-0.09	1 (0%) 84 83	27, 43, 69, 87	0
All	All	1075/1128 (95%)	-0.15	16 (1%) 74 70	21, 41, 69, 101	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	127	SER	3.5
3	Y	92	ASP	3.1
2	B	152	ASN	3.0
2	L	152	ASN	2.9
3	Y	91	GLN	2.9
2	L	154	LEU	2.9
1	A	191	THR	2.6
2	B	154	LEU	2.6
2	L	126	LYS	2.5
1	A	187	SER	2.4
1	A	172	SER	2.3
1	H	127	SER	2.2
2	B	185	ASP	2.2
2	L	1	GLU	2.2
3	Y	72	PRO	2.2
3	Z	91	GLN	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 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.