



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2019 – 01:35 PM EST

PDB ID : 2AP2  
Title : SINGLE CHAIN FV OF C219 IN COMPLEX WITH SYNTHETIC EPITOPE PEPTIDE  
Authors : Van Den Elsen, J.M.H.; Rose, D.R.  
Deposited on : 1999-03-22  
Resolution : 2.40 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.4
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.4

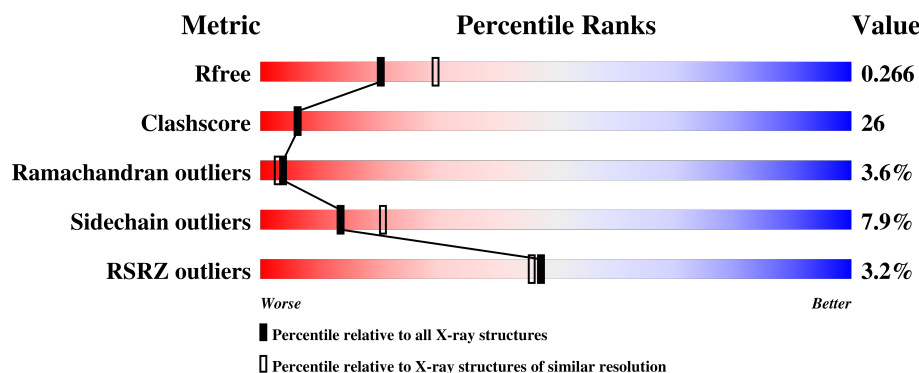
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	111664	3481 (2.40-2.40)
Clashscore	122126	3956 (2.40-2.40)
Ramachandran outliers	120053	3897 (2.40-2.40)
Sidechain outliers	120020	3898 (2.40-2.40)
RSRZ outliers	108989	3386 (2.40-2.40)

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	271	<div> <div>2%</div> <div> <div></div> <div>45%</div> <div>37%</div> <div>6% • 12%</div> </div> </div>
1	C	271	<div> <div>3%</div> <div> <div></div> <div>55%</div> <div>28%</div> <div>6% 11%</div> </div> </div>
2	P	14	<div> <div>7%</div> <div> <div></div> <div>50%</div> <div>36%</div> <div>14%</div> </div> </div>
2	Q	14	<div> <div></div> <div> <div></div> <div>36%</div> <div>50%</div> <div>14%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3954 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 SINGLE CHAIN FV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	239	Total	C	N	O	S	0	0	1
			1844	1161	305	371	7			
1	C	241	Total	C	N	O	S	0	0	1
			1862	1171	308	376	7			

There are 138 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	PHE	-	expression tag	UNP Q6KB05
A	-1	VAL	-	expression tag	UNP Q6KB05
A	0	ARG	-	expression tag	UNP Q6KB05
A	5	THR	ALA	conflict	UNP Q6KB05
A	12	THR	SER	conflict	UNP Q6KB05
A	14	THR	SER	conflict	UNP Q6KB05
A	20	THR	ILE	conflict	UNP Q6KB05
A	33	GLY	ARG	conflict	UNP Q6KB05
A	40	THR	ALA	conflict	UNP Q6KB05
A	49	PRO	SER	conflict	UNP Q6KB05
A	56	TRP	GLY	conflict	UNP Q6KB05
A	98	TYR	HIS	conflict	UNP Q6KB05
A	112	PRO	ILE	conflict	UNP Q6KB05
A	112A	GLY	-	linker	UNP Q6KB05
A	112B	GLY	-	linker	UNP Q6KB05
A	112C	GLY	-	linker	UNP Q6KB05
A	112D	GLY	-	linker	UNP Q6KB05
A	112E	SER	-	linker	UNP Q6KB05
A	112F	GLY	-	linker	UNP Q6KB05
A	112G	GLY	-	linker	UNP Q6KB05
A	112H	GLY	-	linker	UNP Q6KB05
A	112I	GLY	-	linker	UNP Q6KB05
A	112J	SER	-	linker	UNP Q6KB05
A	112K	GLY	-	linker	UNP Q6KB05
A	112L	LYS	-	linker	UNP Q6KB05

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	112M	SER	-	linker	UNP Q6KB05
A	112N	GLY	-	linker	UNP Q6KB05
A	112O	GLY	-	linker	UNP Q6KB05
A	112P	GLY	-	linker	UNP Q6KB05
A	112Q	GLY	-	linker	UNP Q6KB05
A	144	ASP	SER	conflict	UNP Q505N9
A	145	PHE	LEU	conflict	UNP Q505N9
A	162	ARG	TRP	conflict	UNP Q505N9
A	166	ALA	GLU	conflict	UNP Q505N9
A	167	ASN	ASP	conflict	UNP Q505N9
A	168	ASP	GLY	conflict	UNP Q505N9
A	169	ASN	GLU	conflict	UNP Q505N9
A	183	ILE	THR	conflict	UNP Q505N9
A	205	VAL	ILE	conflict	UNP Q505N9
A	211	ARG	ASN	conflict	UNP Q505N9
A	212	GLU	LEU	conflict	UNP Q505N9
A	213	VAL	LEU	conflict	UNP Q505N9
A	215	SER	GLY	conflict	UNP Q505N9
A	216	TYR	GLY	conflict	UNP Q505N9
A	218	SER	-	insertion	UNP Q505N9
A	219	PRO	-	insertion	UNP Q505N9
A	220	LEU	TYR	conflict	UNP Q505N9
A	222	VAL	TYR	conflict	UNP Q505N9
A	225	ALA	GLN	conflict	UNP Q505N9
A	229	VAL	ILE	conflict	UNP Q505N9
A	232	PRO	SER	conflict	UNP Q505N9
A	234	GLY	ALA	conflict	UNP Q505N9
A	241	SER	-	expression tag	UNP Q505N9
A	242	GLU	-	expression tag	UNP Q505N9
A	243	GLN	-	expression tag	UNP Q505N9
A	244	LYS	-	expression tag	UNP Q505N9
A	245	LEU	-	expression tag	UNP Q505N9
A	246	ILE	-	expression tag	UNP Q505N9
A	247	SER	-	expression tag	UNP Q505N9
A	248	GLU	-	expression tag	UNP Q505N9
A	249	GLU	-	expression tag	UNP Q505N9
A	250	ASP	-	expression tag	UNP Q505N9
A	251	LEU	-	expression tag	UNP Q505N9
A	252	ASN	-	expression tag	UNP Q505N9
A	253	HIS	-	expression tag	UNP Q505N9
A	254	HIS	-	expression tag	UNP Q505N9
A	255	HIS	-	expression tag	UNP Q505N9

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	256	HIS	-	expression tag	UNP Q505N9
A	257	HIS	-	expression tag	UNP Q505N9
C	-2	PHE	-	expression tag	UNP Q6KB05
C	-1	VAL	-	expression tag	UNP Q6KB05
C	0	ARG	-	expression tag	UNP Q6KB05
C	5	THR	ALA	conflict	UNP Q6KB05
C	12	THR	SER	conflict	UNP Q6KB05
C	14	THR	SER	conflict	UNP Q6KB05
C	20	THR	ILE	conflict	UNP Q6KB05
C	33	GLY	ARG	conflict	UNP Q6KB05
C	40	THR	ALA	conflict	UNP Q6KB05
C	49	PRO	SER	conflict	UNP Q6KB05
C	56	TRP	GLY	conflict	UNP Q6KB05
C	98	TYR	HIS	conflict	UNP Q6KB05
C	112	PRO	ILE	conflict	UNP Q6KB05
C	112A	GLY	-	linker	UNP Q6KB05
C	112B	GLY	-	linker	UNP Q6KB05
C	112C	GLY	-	linker	UNP Q6KB05
C	112D	GLY	-	linker	UNP Q6KB05
C	112E	SER	-	linker	UNP Q6KB05
C	112F	GLY	-	linker	UNP Q6KB05
C	112G	GLY	-	linker	UNP Q6KB05
C	112H	GLY	-	linker	UNP Q6KB05
C	112I	GLY	-	linker	UNP Q6KB05
C	112J	SER	-	linker	UNP Q6KB05
C	112K	GLY	-	linker	UNP Q6KB05
C	112L	LYS	-	linker	UNP Q6KB05
C	112M	SER	-	linker	UNP Q6KB05
C	112N	GLY	-	linker	UNP Q6KB05
C	112O	GLY	-	linker	UNP Q6KB05
C	112P	GLY	-	linker	UNP Q6KB05
C	112Q	GLY	-	linker	UNP Q6KB05
C	144	ASP	SER	conflict	UNP Q505N9
C	145	PHE	LEU	conflict	UNP Q505N9
C	162	ARG	TRP	conflict	UNP Q505N9
C	166	ALA	GLU	conflict	UNP Q505N9
C	167	ASN	ASP	conflict	UNP Q505N9
C	168	ASP	GLY	conflict	UNP Q505N9
C	169	ASN	GLU	conflict	UNP Q505N9
C	183	ILE	THR	conflict	UNP Q505N9
C	205	VAL	ILE	conflict	UNP Q505N9
C	211	ARG	ASN	conflict	UNP Q505N9

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	212	GLU	LEU	conflict	UNP Q505N9
C	213	VAL	LEU	conflict	UNP Q505N9
C	215	SER	GLY	conflict	UNP Q505N9
C	216	TYR	GLY	conflict	UNP Q505N9
C	218	SER	-	insertion	UNP Q505N9
C	219	PRO	-	insertion	UNP Q505N9
C	220	LEU	TYR	conflict	UNP Q505N9
C	222	VAL	TYR	conflict	UNP Q505N9
C	225	ALA	GLN	conflict	UNP Q505N9
C	229	VAL	ILE	conflict	UNP Q505N9
C	232	PRO	SER	conflict	UNP Q505N9
C	234	GLY	ALA	conflict	UNP Q505N9
C	235	SER	-	expression tag	UNP Q505N9
C	236	GLU	-	expression tag	UNP Q505N9
C	237	GLN	-	expression tag	UNP Q505N9
C	238	LYS	-	expression tag	UNP Q505N9
C	239	LEU	-	expression tag	UNP Q505N9
C	240	ILE	-	expression tag	UNP Q505N9
C	241	SER	-	expression tag	UNP Q505N9
C	242	GLU	-	expression tag	UNP Q505N9
C	243	GLU	-	expression tag	UNP Q505N9
C	244	ASP	-	expression tag	UNP Q505N9
C	245	LEU	-	expression tag	UNP Q505N9
C	246	ASN	-	expression tag	UNP Q505N9
C	247	HIS	-	expression tag	UNP Q505N9
C	248	HIS	-	expression tag	UNP Q505N9
C	249	HIS	-	expression tag	UNP Q505N9
C	250	HIS	-	expression tag	UNP Q505N9
C	251	HIS	-	expression tag	UNP Q505N9

- Molecule 2 is a protein called P-GLYCOPROTEIN.

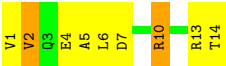
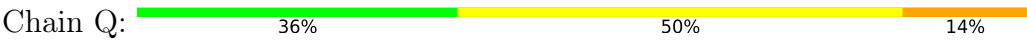
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	12	Total	C	N	O	0	0	1
			74	45	13	16			
2	Q	14	Total	C	N	O	0	0	0
			110	65	22	23			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	31	Total 31	O 31	0	0
3	C	26	Total 26	O 26	0	0
3	P	2	Total 2	O 2	0	0
3	Q	5	Total 5	O 5	0	0







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.79Å 82.66Å 93.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 38.80 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.6 (50.00-2.40) 95.6 (38.80-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.77 (at 2.39Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, $R_{free}$	0.221 , 0.274 0.223 , 0.266	Depositor DCC
$R_{free}$ test set	2112 reflections (9.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.7	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 46.3	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	3954	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.24% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.34	0/1887	0.59	0/2570
1	C	0.33	0/1905	0.59	0/2594
2	P	0.62	0/73	0.52	0/100
2	Q	0.38	0/109	0.59	0/143
All	All	0.35	0/3974	0.59	0/5407

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1844	0	1776	102	0
1	C	1862	0	1790	86	0
2	P	74	0	65	3	0
2	Q	110	0	114	12	0
3	A	31	0	0	5	0
3	C	26	0	0	2	0
3	P	2	0	0	0	0
3	Q	5	0	0	2	0
All	All	3954	0	3745	198	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 26.

All (198) 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:C:147:HIS:HD2	1:C:159:TRP:HE1	1.11	0.96
1:C:193:LEU:HD13	1:C:195:LEU:HD11	1.49	0.94
1:A:147:HIS:HD2	1:A:159:TRP:HE1	1.17	0.93
1:C:86:ALA:O	1:C:89:LEU:HD23	1.80	0.81
1:A:118:GLN:HE21	1:A:227:THR:HG23	1.45	0.81
1:A:124:VAL:HG21	1:A:198:LEU:HD23	1.61	0.80
1:A:86:ALA:O	1:A:89:LEU:HD22	1.81	0.80
1:C:167:ASN:HD22	1:C:169:ASN:H	1.28	0.80
1:A:154:GLU:O	1:A:155:GLN:HB3	1.81	0.78
1:C:159:TRP:HZ2	1:C:162:ARG:HG2	1.48	0.78
1:A:147:HIS:CD2	1:A:159:TRP:HE1	2.03	0.76
1:A:31:ASN:HD22	1:A:33:GLY:H	1.34	0.74
1:C:167:ASN:ND2	1:C:169:ASN:H	1.86	0.73
1:A:45:LYS:HB2	1:A:48:GLN:OE1	1.89	0.73
1:A:21:MET:HG2	1:A:108:THR:HG21	1.70	0.73
1:C:174:PRO:HA	1:C:177:GLN:HG3	1.72	0.71
1:A:211:ARG:NH1	3:A:301:HOH:O	2.23	0.71
1:C:31:ASN:HB3	1:C:34:ASN:HD21	1.57	0.70
1:A:31:ASN:ND2	1:A:33:GLY:H	1.88	0.70
1:A:31:ASN:HD22	1:A:31:ASN:C	1.92	0.69
1:C:193:LEU:CD1	1:C:195:LEU:HD11	2.22	0.69
1:A:60:ARG:HB2	1:A:60:ARG:HH11	1.58	0.69
1:A:152:ARG:NH1	1:A:201:GLU:HG3	2.07	0.69
1:A:1:ASP:O	1:A:2:ILE:HB	1.91	0.69
1:C:211:ARG:HH11	2:Q:6:LEU:HD21	1.57	0.69
1:C:21:MET:HG2	1:C:108:THR:HG21	1.75	0.68
1:A:118:GLN:NE2	1:A:227:THR:HG23	2.09	0.68
1:A:147:HIS:HD2	1:A:159:TRP:NE1	1.91	0.67
1:C:210:ARG:HD2	1:C:221:ASP:OD1	1.94	0.67
1:C:147:HIS:CD2	1:C:159:TRP:HE1	2.02	0.67
1:C:123:LEU:HD23	1:C:230:THR:HB	1.76	0.66
1:C:14:THR:HG22	1:C:17:GLU:OE2	1.95	0.66
1:C:45:LYS:HG2	1:C:90:ALA:HB2	1.76	0.66
1:A:140:ASN:OD1	1:A:142:LYS:HB3	1.95	0.66
1:A:60:ARG:HB3	1:A:64:VAL:CG2	2.27	0.65
1:A:130:VAL:HG12	1:A:198:LEU:HD21	1.78	0.65
2:Q:1:VAL:N	3:Q:101:HOH:O	2.23	0.65
1:C:31:ASN:HB3	1:C:34:ASN:ND2	2.11	0.65
1:C:8:PRO:HB2	1:C:10:SER:O	1.97	0.64
1:A:124:VAL:HG23	1:A:231:VAL:HG22	1.80	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:SER:O	1:C:11:LEU:HB2	1.99	0.63
1:C:179:LYS:HB2	1:C:179:LYS:NZ	2.13	0.63
1:A:45:LYS:HD3	1:A:90:ALA:HB2	1.80	0.63
1:C:85:GLN:HE21	1:C:85:GLN:HA	1.64	0.63
1:A:163:ILE:O	1:A:165:PRO:HD3	1.99	0.62
1:A:88:ASP:O	1:A:89:LEU:O	2.17	0.62
1:C:141:ILE:HG23	1:C:189:ASN:OD1	1.99	0.62
1:C:99:SER:HA	2:Q:2:VAL:HG23	1.82	0.62
1:A:31:ASN:HB3	1:A:34:ASN:HD21	1.65	0.61
1:A:115:GLN:HG2	1:A:137:SER:HB3	1.81	0.61
1:C:147:HIS:HD2	1:C:159:TRP:NE1	1.92	0.61
1:C:92:TYR:O	1:C:107:GLY:HA2	2.00	0.61
1:A:148:TRP:CE2	1:A:193:LEU:HB2	2.36	0.60
1:C:24:LYS:NZ	1:C:76:ASP:HB3	2.16	0.60
2:Q:1:VAL:HG23	2:Q:2:VAL:H	1.66	0.60
1:A:19:VAL:HG21	1:A:81:ILE:HD12	1.83	0.60
1:A:185:ASP:OD1	1:A:187:SER:HB3	2.02	0.60
1:C:19:VAL:HG22	1:C:81:ILE:HB	1.84	0.59
1:A:195:LEU:CB	1:A:198:LEU:HD11	2.33	0.59
1:A:152:ARG:HH12	1:A:201:GLU:HG3	1.65	0.59
1:A:85:GLN:HA	1:A:85:GLN:HE21	1.66	0.59
1:A:30:LEU:HD12	1:A:31:ASN:N	2.18	0.58
1:A:234:GLY:O	1:A:242:GLU:N	2.36	0.58
1:C:13:VAL:HG22	1:C:14:THR:H	1.68	0.58
1:A:67:ARG:CZ	1:A:85:GLN:HG3	2.34	0.58
1:A:154:GLU:C	1:A:155:GLN:HE21	2.07	0.58
1:A:164:ASP:HB3	1:A:167:ASN:OD1	2.03	0.57
1:C:25:SER:O	1:C:75:THR:HG23	2.04	0.57
1:C:164:ASP:HB3	1:C:167:ASN:HD21	1.70	0.56
1:C:129:SER:OG	1:C:196:SER:HA	2.05	0.56
1:A:3:VAL:HB	1:A:26:SER:OG	2.05	0.56
2:P:10:ARG:O	2:P:12:GLY:N	2.38	0.56
2:Q:7:ASP:HA	2:Q:10:ARG:NH1	2.19	0.56
1:C:148:TRP:CE2	1:C:193:LEU:HB2	2.41	0.56
1:C:34:ASN:HD22	1:C:34:ASN:C	2.09	0.56
1:C:193:LEU:HD13	1:C:195:LEU:CD1	2.30	0.55
1:C:19:VAL:CG2	1:C:81:ILE:HB	2.36	0.55
1:C:65:PRO:HG2	1:C:68:PHE:HD2	1.70	0.55
1:A:167:ASN:OD1	1:A:169:ASN:HB2	2.06	0.55
1:A:141:ILE:HD11	1:A:186:THR:HA	1.88	0.55
1:A:106:ALA:O	1:A:155:GLN:OE1	2.25	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:LEU:HD12	1:A:31:ASN:H	1.72	0.55
1:A:155:GLN:N	1:A:155:GLN:HE21	2.05	0.55
1:A:19:VAL:HG22	1:A:81:ILE:HB	1.88	0.55
1:A:195:LEU:HB3	1:A:198:LEU:HD11	1.88	0.55
1:C:15:ALA:HA	1:C:84:VAL:O	2.06	0.54
1:A:163:ILE:HG13	1:A:170:THR:HG22	1.90	0.54
1:C:100:TYR:H	2:Q:1:VAL:CG2	2.21	0.53
1:C:93:TYR:HE1	1:C:155:GLN:HE21	1.56	0.53
1:C:97:ASP:OD1	1:C:211:ARG:NH2	2.42	0.53
1:A:34:ASN:C	1:A:34:ASN:HD22	2.13	0.52
1:A:163:ILE:CG1	1:A:170:THR:HG22	2.39	0.52
1:A:40:THR:HG21	3:A:321:HOH:O	2.08	0.52
1:C:16:GLY:C	1:C:83:SER:HA	2.29	0.52
1:C:151:GLN:O	1:C:204:ALA:HB1	2.10	0.52
1:A:116:LEU:HD22	1:A:134:CYS:SG	2.50	0.51
1:C:14:THR:N	1:C:17:GLU:OE2	2.44	0.51
1:C:85:GLN:HA	1:C:85:GLN:NE2	2.25	0.51
1:A:-2:PHE:N	3:A:303:HOH:O	2.43	0.51
1:C:163:ILE:O	1:C:165:PRO:HD3	2.10	0.51
2:Q:1:VAL:HG23	2:Q:2:VAL:N	2.26	0.51
1:C:211:ARG:NH1	3:C:304:HOH:O	2.43	0.50
1:C:154:GLU:HG3	1:C:155:GLN:H	1.75	0.50
1:C:64:VAL:O	1:C:64:VAL:HG23	2.10	0.50
1:A:6:GLN:NE2	1:A:107:GLY:HA2	2.27	0.50
1:A:31:ASN:ND2	1:A:31:ASN:C	2.64	0.50
1:A:32:SER:HA	1:A:35:GLN:NE2	2.27	0.50
1:A:162:ARG:HD3	3:A:301:HOH:O	2.12	0.49
1:A:86:ALA:C	1:A:88:ASP:H	2.16	0.49
1:A:31:ASN:ND2	1:A:33:GLY:N	2.60	0.49
1:A:98:TYR:HD2	1:A:99:SER:HG	1.61	0.49
1:A:12:THR:HA	1:A:111:GLU:HB2	1.95	0.48
1:C:31:ASN:C	1:C:31:ASN:HD22	2.17	0.48
1:C:152:ARG:HB3	1:C:154:GLU:HG2	1.93	0.48
1:C:60:ARG:HB3	1:C:64:VAL:CG2	2.43	0.48
1:C:155:GLN:NE2	1:C:156:GLY:HA2	2.28	0.48
1:A:118:GLN:HB3	1:A:227:THR:CG2	2.43	0.48
1:A:6:GLN:CD	1:A:107:GLY:HA2	2.34	0.48
1:C:210:ARG:CG	1:C:222:VAL:HB	2.44	0.48
1:C:106:ALA:HA	1:C:155:GLN:HE22	1.77	0.48
1:C:40:THR:HG22	3:C:311:HOH:O	2.13	0.48
1:A:124:VAL:CG2	1:A:198:LEU:HD23	2.38	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:PRO:O	1:A:103:THR:HG23	2.14	0.47
1:C:144:ASP:OD2	1:C:212:GLU:HG2	2.15	0.47
1:C:24:LYS:HZ3	1:C:76:ASP:HB3	1.77	0.47
1:C:154:GLU:O	1:C:155:GLN:CB	2.60	0.47
2:Q:1:VAL:O	2:Q:4:GLU:HB2	2.14	0.47
1:C:93:TYR:HE1	1:C:155:GLN:NE2	2.12	0.47
1:C:93:TYR:OH	1:C:155:GLN:HG2	2.15	0.47
1:A:92:TYR:O	1:A:107:GLY:HA2	2.15	0.47
1:A:144:ASP:O	1:A:165:PRO:HD2	2.15	0.47
1:A:195:LEU:HB2	1:A:198:LEU:HD11	1.96	0.47
1:C:39:LEU:HD22	1:C:95:GLN:O	2.15	0.47
1:A:54:ILE:HG23	1:A:59:THR:O	2.15	0.47
1:A:85:GLN:O	1:A:88:ASP:HB2	2.14	0.47
2:Q:2:VAL:O	2:Q:5:ALA:N	2.47	0.47
1:A:114:VAL:HG23	1:A:114:VAL:O	2.15	0.46
1:A:19:VAL:HG13	1:A:84:VAL:HG21	1.97	0.46
1:A:115:GLN:CG	1:A:137:SER:HB3	2.46	0.46
1:A:48:GLN:HB3	1:A:49:PRO:HD2	1.97	0.46
1:A:100:TYR:OH	1:A:162:ARG:NH1	2.49	0.46
1:A:113:GLU:O	1:A:137:SER:O	2.33	0.46
1:A:140:ASN:OD1	1:A:142:LYS:CB	2.64	0.46
3:A:311:HOH:O	2:P:2:VAL:HB	2.15	0.46
1:A:164:ASP:O	1:A:168:ASP:N	2.49	0.46
1:A:19:VAL:CG2	1:A:81:ILE:HB	2.46	0.45
1:C:113:GLU:O	1:C:113:GLU:HG2	2.16	0.45
1:C:100:TYR:H	2:Q:1:VAL:HG21	1.81	0.45
1:A:0:ARG:HB3	1:A:1:ASP:H	1.47	0.45
1:A:14:THR:HG22	1:A:17:GLU:OE1	2.17	0.45
1:C:129:SER:HA	1:C:198:LEU:CD2	2.46	0.45
1:A:31:ASN:HD22	1:A:33:GLY:N	2.09	0.45
1:C:14:THR:O	1:C:17:GLU:HG2	2.16	0.45
1:C:167:ASN:HD22	1:C:167:ASN:C	2.19	0.45
1:C:31:ASN:HD22	1:C:33:GLY:H	1.64	0.45
1:C:65:PRO:HG2	1:C:68:PHE:CD2	2.50	0.45
1:A:37:ASN:O	1:A:56:TRP:HA	2.17	0.45
1:A:13:VAL:HG21	1:A:84:VAL:HG21	1.99	0.44
1:C:195:LEU:N	1:C:195:LEU:HD12	2.32	0.44
1:C:72:GLY:HA3	1:C:77:PHE:HA	2.00	0.44
1:C:89:LEU:O	1:C:110:LEU:HB2	2.17	0.44
1:C:174:PRO:O	1:C:177:GLN:HG3	2.17	0.44
1:A:119:SER:HB3	1:A:133:SER:OG	2.17	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:GLN:HG2	1:C:96:ASN:N	2.33	0.44
1:A:179:LYS:O	1:A:195:LEU:HA	2.18	0.44
1:A:198:LEU:HA	1:A:202:ASP:OD2	2.18	0.44
1:C:179:LYS:HE3	1:C:196:SER:O	2.18	0.44
1:C:13:VAL:HG22	1:C:14:THR:N	2.32	0.43
1:C:167:ASN:HD22	1:C:169:ASN:N	2.07	0.43
1:A:82:SER:O	1:A:83:SER:CB	2.66	0.43
2:Q:13:ARG:O	2:Q:14:THR:HB	2.18	0.43
1:A:141:ILE:HG23	1:A:189:ASN:CG	2.39	0.43
1:A:217:TYR:CG	1:A:218:SER:N	2.87	0.43
1:C:179:LYS:HB2	1:C:179:LYS:HZ2	1.82	0.43
1:A:211:ARG:HD3	2:P:6:LEU:HD21	1.99	0.43
1:A:150:LYS:HB2	1:A:160:ILE:HD11	2.00	0.43
1:C:203:THR:O	1:C:204:ALA:HB2	2.18	0.43
1:A:1:ASP:O	1:A:2:ILE:CB	2.63	0.43
1:C:34:ASN:ND2	1:C:36:LYS:HB2	2.34	0.43
1:C:26:SER:C	1:C:27:GLN:HG3	2.40	0.42
1:C:44:GLN:HG3	1:C:48:GLN:O	2.20	0.42
1:A:230:THR:HG22	1:A:232:PRO:HD3	2.02	0.42
1:C:132:LEU:N	1:C:132:LEU:CD1	2.83	0.42
2:Q:2:VAL:HB	3:Q:105:HOH:O	2.19	0.42
1:A:12:THR:HA	1:A:111:GLU:O	2.20	0.42
1:A:64:VAL:HG23	1:A:64:VAL:O	2.19	0.41
1:A:61:GLU:O	1:A:64:VAL:HG22	2.20	0.41
1:C:211:ARG:HB2	1:C:220:LEU:HD23	2.01	0.41
1:C:24:LYS:NZ	1:C:76:ASP:CB	2.82	0.41
1:A:29:LEU:HD23	1:A:39:LEU:HD23	2.02	0.41
1:A:123:LEU:HD13	1:A:123:LEU:C	2.41	0.41
1:A:97:ASP:OD1	1:A:211:ARG:NH2	2.53	0.41
1:A:87:GLU:H	1:A:87:GLU:HG3	1.68	0.41
1:A:213:VAL:O	1:A:213:VAL:HG23	2.21	0.40
1:A:82:SER:O	1:A:83:SER:HB3	2.21	0.40
1:A:140:ASN:OD1	1:A:142:LYS:N	2.54	0.40
1:C:130:VAL:HG22	1:C:131:LYS:N	2.37	0.40
1:C:24:LYS:HA	1:C:75:THR:O	2.22	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	235/271 (87%)	210 (89%)	15 (6%)	10 (4%)	3	2
1	C	237/271 (88%)	215 (91%)	16 (7%)	6 (2%)	6	6
2	P	10/14 (71%)	9 (90%)	0	1 (10%)	0	0
2	Q	12/14 (86%)	11 (92%)	0	1 (8%)	1	0
All	All	494/570 (87%)	445 (90%)	31 (6%)	18 (4%)	4	3

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	0	ARG
1	A	89	LEU
1	C	11	LEU
1	C	90	ALA
1	C	155	GLN
2	P	11	GLU
2	Q	2	VAL
1	A	155	GLN
1	A	241	SER
1	C	89	LEU
1	A	2	ILE
1	C	167	ASN
1	A	74	GLY
1	A	83	SER
1	A	87	GLU
1	A	154	GLU
1	A	138	GLY
1	C	74	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	205/225 (91%)	186 (91%)	19 (9%)	10	14
1	C	207/225 (92%)	193 (93%)	14 (7%)	17	27
2	P	6/11 (54%)	6 (100%)	0	100	100
2	Q	11/11 (100%)	10 (91%)	1 (9%)	10	15
All	All	429/472 (91%)	395 (92%)	34 (8%)	13	21

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ASP
1	A	20	THR
1	A	29	LEU
1	A	31	ASN
1	A	34	ASN
1	A	53	LEU
1	A	60	ARG
1	A	66	ASP
1	A	79	LEU
1	A	85	GLN
1	A	89	LEU
1	A	96	ASN
1	A	155	GLN
1	A	162	ARG
1	A	168	ASP
1	A	183	ILE
1	A	193	LEU
1	A	198	LEU
1	A	210	ARG
1	C	29	LEU
1	C	31	ASN
1	C	34	ASN
1	C	40	THR
1	C	79	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	96	ASN
1	C	123	LEU
1	C	152	ARG
1	C	162	ARG
1	C	167	ASN
1	C	179	LYS
1	C	193	LEU
1	C	198	LEU
1	C	210	ARG
2	Q	10	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	34	ASN
1	A	85	GLN
1	A	115	GLN
1	A	118	GLN
1	A	147	HIS
1	A	155	GLN
1	A	177	GLN
1	C	31	ASN
1	C	34	ASN
1	C	35	GLN
1	C	85	GLN
1	C	115	GLN
1	C	147	HIS
1	C	155	GLN
1	C	167	ASN
1	C	169	ASN
1	C	194	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 [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	A	239/271 (88%)	0.05	6 (2%) 57 55	14, 31, 56, 73	0
1	C	241/271 (88%)	0.13	9 (3%) 41 40	19, 34, 60, 75	0
2	P	12/14 (85%)	0.09	1 (8%) 11 10	28, 43, 66, 68	0
2	Q	14/14 (100%)	-0.21	0 100 100	15, 27, 34, 47	0
All	All	506/570 (88%)	0.08	16 (3%) 47 46	14, 33, 60, 75	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	84	VAL	4.4
1	A	155	GLN	3.9
1	C	155	GLN	3.6
1	C	83	SER	3.3
1	A	114	VAL	3.3
1	C	238	LYS	3.1
1	C	19	VAL	3.0
1	A	142	LYS	2.8
1	A	12	THR	2.8
1	C	89	LEU	2.6
1	C	10	SER	2.6
1	A	154	GLU	2.6
1	C	90	ALA	2.5
1	A	140	ASN	2.4
2	P	1	VAL	2.4
1	C	119	SER	2.2

### 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.