



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:07 PM GMT

PDB ID : 1E4W  
Title : CROSSREACTIVE BINDING OF A CIRCULARIZED PEPTIDE TO AN ANTI-TGFALPHA ANTIBODY FAB-FRAGMENT  
Authors : Hahn, M.; Winkler, D.; Misselwitz, R.; Wessner, H.; Welfle, K.; Zahn, G.; Schneider-Mergener, J.; Hoehne, W.  
Deposited on : 2000-07-12  
Resolution : 1.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

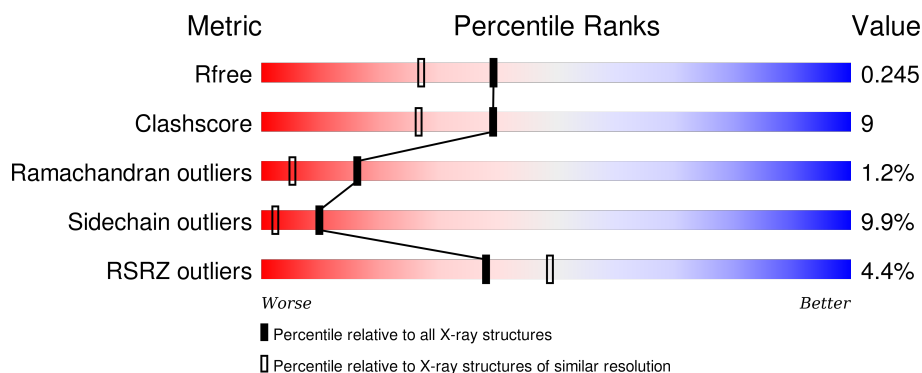
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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	H	213	<div> <div>6%</div> <div>68%</div> <div>22%</div> <div>10%</div> </div>
2	L	214	<div> <div>3%</div> <div>82%</div> <div>14%</div> <div>• •</div> </div>
3	P	7	<div> <div>86%</div> <div>14%</div> </div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3742 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 TAB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	213	Total	C	N	O	S	0	0	0
			1609	1016	264	322	7			

- Molecule 2 is a protein called TAB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	0	0
			1657	1032	276	342	7			

- Molecule 3 is a protein called CYCLIC PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	7	Total	C	N	O	0	0	0
			65	41	10	14			

- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	1	Total	Ni	0	0
			1	1		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	P	1	Total	Cl	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	185	Total	O	0	0
			185	185		

*Continued on next page...*

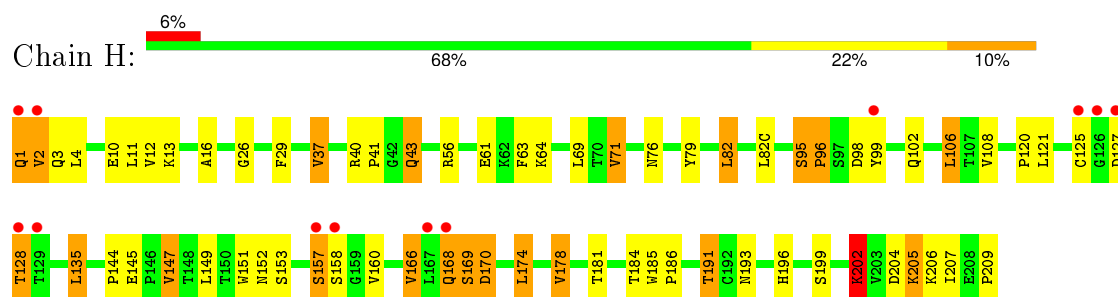
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	219	Total	O	0	0
			219	219		
6	P	5	Total	O	0	0
			5	5		

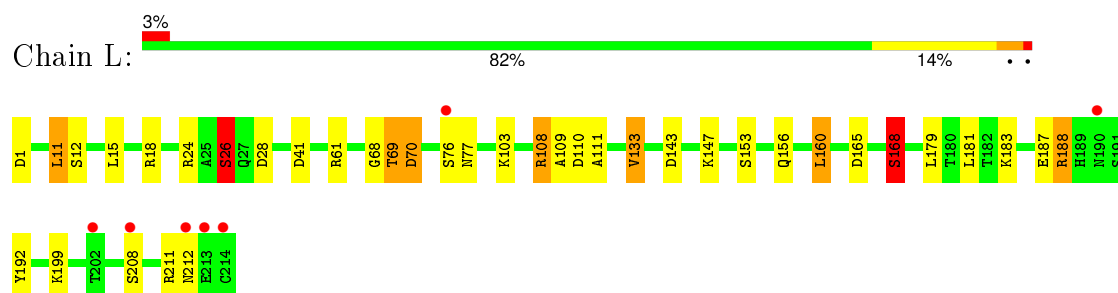
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

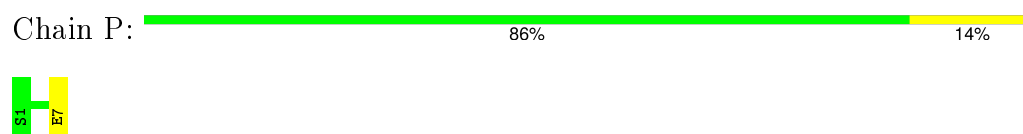
#### • Molecule 1: TAB2



#### • Molecule 2: TAB2



#### • Molecule 3: CYCLIC PEPTIDE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.22Å 94.35Å 121.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.95 38.28 – 1.96	Depositor EDS
% Data completeness (in resolution range)	94.6 (20.00-1.95) 95.8 (38.28-1.96)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.24 (at 1.95Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.204 , 0.269 0.191 , 0.245	Depositor DCC
$R_{free}$ test set	1997 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.6	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 55.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 39908 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3742	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 4.54% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NI, CL

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	H	0.87	1/1651 (0.1%)	1.61	26/2257 (1.2%)
2	L	0.82	1/1694 (0.1%)	1.94	33/2298 (1.4%)
3	P	1.10	1/67 (1.5%)	1.36	0/87
All	All	0.85	3/3412 (0.1%)	1.78	59/4642 (1.3%)

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
1	H	0	2
2	L	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	209	PRO	N-CD	6.75	1.57	1.47
2	L	168	SER	CA-CB	6.28	1.62	1.52
3	P	7	GLU	C-OXT	5.97	1.34	1.23

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	108	ARG	CD-NE-CZ	32.16	168.63	123.60
2	L	18	ARG	CD-NE-CZ	26.55	160.77	123.60
2	L	108	ARG	NE-CZ-NH2	23.21	131.90	120.30
2	L	18	ARG	NE-CZ-NH1	-17.86	111.37	120.30
2	L	188	ARG	NE-CZ-NH2	-16.66	111.97	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	108	ARG	NH1-CZ-NH2	-13.37	104.69	119.40
2	L	18	ARG	NE-CZ-NH2	12.21	126.40	120.30
2	L	41	ASP	CB-CG-OD2	-10.12	109.20	118.30
2	L	28	ASP	CB-CG-OD1	9.48	126.83	118.30
1	H	157	SER	CA-C-N	9.35	137.76	117.20
1	H	178	VAL	CB-CA-C	-9.17	93.98	111.40
1	H	96	PRO	N-CA-CB	8.60	113.62	103.30
2	L	110	ASP	CB-CG-OD1	8.34	125.80	118.30
1	H	174	LEU	CA-CB-CG	8.31	134.41	115.30
2	L	1	ASP	O-C-N	-8.14	109.68	122.70
2	L	1	ASP	CB-CG-OD1	8.13	125.62	118.30
2	L	41	ASP	CB-CG-OD1	7.84	125.36	118.30
1	H	170	ASP	CB-CG-OD2	7.43	124.99	118.30
1	H	2	VAL	N-CA-CB	7.31	127.57	111.50
1	H	37	VAL	CA-CB-CG2	7.06	121.50	110.90
2	L	11	LEU	CA-CB-CG	6.98	131.35	115.30
1	H	37	VAL	CA-CB-CG1	6.93	121.30	110.90
2	L	211	ARG	NE-CZ-NH2	-6.87	116.87	120.30
1	H	147	VAL	N-CA-CB	-6.78	96.59	111.50
1	H	96	PRO	CA-N-CD	-6.73	102.08	111.50
1	H	56	ARG	NE-CZ-NH2	-6.61	116.99	120.30
2	L	143	ASP	CB-CG-OD1	6.59	124.23	118.30
2	L	1	ASP	OD1-CG-OD2	-6.58	110.81	123.30
2	L	165	ASP	CB-CG-OD2	-6.53	112.42	118.30
1	H	157	SER	CA-C-O	-6.46	106.54	120.10
2	L	61	ARG	CD-NE-CZ	6.24	132.34	123.60
1	H	166	VAL	CG1-CB-CG2	6.21	120.84	110.90
2	L	69	THR	N-CA-CB	-6.18	98.57	110.30
1	H	95	SER	CA-C-O	-6.15	107.19	120.10
1	H	204	ASP	CB-CG-OD2	-6.14	112.78	118.30
2	L	108	ARG	NE-CZ-NH1	6.03	123.32	120.30
2	L	165	ASP	CB-CG-OD1	5.85	123.57	118.30
1	H	178	VAL	CA-CB-CG2	5.85	119.68	110.90
2	L	26	SER	CA-CB-OG	-5.85	95.41	111.20
1	H	204	ASP	CB-CG-OD1	5.84	123.56	118.30
1	H	202	LYS	CA-CB-CG	5.82	126.21	113.40
2	L	1	ASP	CB-CG-OD2	5.81	123.53	118.30
2	L	168	SER	CA-CB-OG	-5.80	95.55	111.20
2	L	168	SER	CB-CA-C	-5.78	99.12	110.10
1	H	71	VAL	N-CA-CB	-5.74	98.86	111.50
2	L	108	ARG	CG-CD-NE	5.62	123.59	111.80
1	H	147	VAL	CB-CA-C	5.61	122.07	111.40

*Continued on next page...*



Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	1	ASP	CA-CB-CG	5.48	125.46	113.40
1	H	79	TYR	CB-CG-CD1	-5.42	117.75	121.00
2	L	153	SER	N-CA-CB	-5.40	102.41	110.50
1	H	99	TYR	CB-CG-CD1	-5.39	117.77	121.00
2	L	188	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	H	43	GLN	CA-CB-CG	5.36	125.20	113.40
2	L	212	ASN	C-N-CA	5.21	134.72	121.70
1	H	166	VAL	N-CA-CB	-5.18	100.10	111.50
2	L	133	VAL	CA-CB-CG1	5.15	118.63	110.90
1	H	128	THR	N-CA-CB	5.14	120.07	110.30
1	H	63	PHE	CB-CG-CD1	-5.12	117.22	120.80
2	L	188	ARG	NH1-CZ-NH2	5.12	125.03	119.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	95	SER	Mainchain,Peptide
2	L	188	ARG	Mainchain

## 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	H	1609	0	1574	42	0
2	L	1657	0	1576	19	0
3	P	65	0	48	0	0
4	L	1	0	0	0	0
5	P	1	0	0	0	0
6	H	185	0	0	3	0
6	L	219	0	0	7	0
6	P	5	0	0	0	0
All	All	3742	0	3198	58	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 9.

All (58) 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:153:SER:H	1:H:193:ASN:HD21	1.16	0.93
1:H:61:GLU:HG2	1:H:64:LYS:HZ3	1.35	0.90
2:L:108:ARG:NH1	2:L:111:ALA:HB2	1.92	0.85
1:H:157:SER:O	1:H:158:SER:HB3	1.78	0.82
2:L:179:LEU:HG	2:L:181:LEU:HD11	1.64	0.78
1:H:191:THR:HG23	6:H:2139:HOH:O	1.84	0.76
1:H:153:SER:H	1:H:193:ASN:ND2	1.83	0.75
1:H:145:GLU:HG3	6:H:2133:HOH:O	1.86	0.74
1:H:168:GLN:HE21	1:H:168:GLN:H	1.36	0.74
1:H:61:GLU:HG2	1:H:64:LYS:NZ	2.10	0.66
2:L:108:ARG:NE	6:L:2122:HOH:O	2.30	0.65
1:H:169:SER:OG	1:H:170:ASP:N	2.31	0.64
1:H:120:PRO:HD3	1:H:205:LYS:HG2	1.78	0.64
1:H:168:GLN:HB3	2:L:160:LEU:HD21	1.80	0.63
1:H:135:LEU:HG	1:H:207:ILE:HG21	1.80	0.63
2:L:179:LEU:HG	2:L:181:LEU:CD1	2.29	0.62
2:L:108:ARG:NH1	2:L:109:ALA:O	2.33	0.62
1:H:181:THR:OG1	1:H:184:THR:HG23	2.00	0.61
1:H:168:GLN:CB	2:L:160:LEU:HD21	2.30	0.61
1:H:157:SER:O	1:H:158:SER:CB	2.45	0.60
1:H:40:ARG:HB2	1:H:43:GLN:HG2	1.84	0.60
1:H:196:HIS:HD2	1:H:199:SER:OG	1.85	0.58
2:L:103:LYS:HE2	6:L:2116:HOH:O	2.04	0.57
2:L:108:ARG:CZ	6:L:2122:HOH:O	2.53	0.56
1:H:144:PRO:O	1:H:196:HIS:HE1	1.89	0.56
1:H:82:LEU:HB3	1:H:82(C):LEU:HD21	1.88	0.55
2:L:24:ARG:HG2	6:L:2005:HOH:O	2.07	0.54
1:H:168:GLN:NE2	1:H:168:GLN:H	2.05	0.52
1:H:120:PRO:HD3	1:H:205:LYS:CG	2.41	0.51
1:H:152:ASN:ND2	1:H:191:THR:H	2.09	0.51
1:H:10:GLU:HB2	1:H:106:LEU:HD23	1.94	0.50
1:H:12:VAL:HG11	1:H:82(C):LEU:HD12	1.96	0.48
1:H:151:TRP:CE2	1:H:178:VAL:HG22	2.48	0.48
2:L:168:SER:HB2	6:L:2189:HOH:O	2.14	0.47
2:L:183:LYS:NZ	2:L:187:GLU:OE2	2.43	0.47
1:H:191:THR:HB	1:H:206:LYS:HA	1.97	0.46
1:H:168:GLN:HE21	1:H:168:GLN:N	2.06	0.46
1:H:160:VAL:HG22	1:H:178:VAL:HG13	1.97	0.46
2:L:108:ARG:NH2	6:L:2122:HOH:O	2.48	0.46
1:H:12:VAL:CG1	1:H:16:ALA:HB3	2.44	0.46
2:L:26:SER:HB3	6:L:2036:HOH:O	2.16	0.45

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1:GLN:HE21	1:H:3:GLN:HE21	1.65	0.45
1:H:185:TRP:CG	1:H:186:PRO:HA	2.52	0.45
1:H:149:LEU:HD23	1:H:149:LEU:C	2.38	0.44
1:H:168:GLN:O	1:H:169:SER:CB	2.65	0.44
2:L:108:ARG:HH11	2:L:111:ALA:HB2	1.79	0.44
2:L:24:ARG:NH2	2:L:70:ASP:OD2	2.51	0.44
1:H:168:GLN:NE2	1:H:168:GLN:N	2.66	0.43
1:H:11:LEU:C	1:H:11:LEU:HD13	2.39	0.43
1:H:1:GLN:H2	1:H:26:GLY:HA3	1.84	0.43
2:L:192:TYR:O	2:L:208:SER:HB2	2.19	0.43
1:H:168:GLN:HB2	2:L:160:LEU:HD21	2.00	0.42
2:L:181:LEU:N	2:L:181:LEU:HD12	2.35	0.42
1:H:61:GLU:HG2	1:H:64:LYS:CE	2.49	0.42
1:H:196:HIS:CD2	1:H:199:SER:OG	2.71	0.41
1:H:202:LYS:HB3	1:H:202:LYS:HE2	1.64	0.41
1:H:102:GLN:HG3	6:H:2100:HOH:O	2.21	0.41
1:H:61:GLU:HA	1:H:64:LYS:NZ	2.35	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	H	211/213 (99%)	201 (95%)	6 (3%)	4 (2%)	10	2
2	L	212/214 (99%)	206 (97%)	5 (2%)	1 (0%)	34	21
3	P	5/7 (71%)	5 (100%)	0	0	100	100
All	All	428/434 (99%)	412 (96%)	11 (3%)	5 (1%)	16	5

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	127	ASP
1	H	169	SER
1	H	2	VAL
2	L	68	GLY
1	H	96	PRO

### 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	H	185/185 (100%)	161 (87%)	24 (13%)	5	1
2	L	190/190 (100%)	176 (93%)	14 (7%)	17	5
3	P	7/7 (100%)	7 (100%)	0	100	100
All	All	382/382 (100%)	344 (90%)	38 (10%)	10	2

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	1	GLN
1	H	4	LEU
1	H	13	LYS
1	H	29	PHE
1	H	37	VAL
1	H	41	PRO
1	H	69	LEU
1	H	71	VAL
1	H	76	ASN
1	H	82	LEU
1	H	98	ASP
1	H	106	LEU
1	H	108	VAL
1	H	121	LEU
1	H	125	CYS
1	H	128	THR
1	H	135	LEU
1	H	147	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	H	166	VAL
1	H	168	GLN
1	H	174	LEU
1	H	191	THR
1	H	202	LYS
1	H	205	LYS
2	L	11	LEU
2	L	12	SER
2	L	15	LEU
2	L	26	SER
2	L	69	THR
2	L	70	ASP
2	L	76	SER
2	L	77	ASN
2	L	133	VAL
2	L	147	LYS
2	L	156	GLN
2	L	160	LEU
2	L	168	SER
2	L	199	LYS

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

Mol	Chain	Res	Type
1	H	3	GLN
1	H	152	ASN
1	H	168	GLN
1	H	193	ASN
1	H	196	HIS
2	L	3	GLN
2	L	77	ASN

### 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

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	H	213/213 (100%)	0.47	12 (5%) 28 39	24, 33, 54, 80	0
2	L	214/214 (100%)	0.33	7 (3%) 50 61	23, 32, 47, 80	0
3	P	7/7 (100%)	0.58	0 100 100	27, 27, 35, 37	0
All	All	434/434 (100%)	0.40	19 (4%) 38 49	23, 32, 52, 80	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	214	CYS	11.1
1	H	129	THR	9.7
1	H	126	GLY	8.5
1	H	128	THR	8.1
1	H	125	CYS	7.0
1	H	127	ASP	5.8
2	L	212	ASN	3.7
1	H	1	GLN	3.7
2	L	190	ASN	3.6
1	H	99	TYR	3.2
2	L	213	GLU	3.2
1	H	168	GLN	3.2
1	H	2	VAL	2.9
1	H	158	SER	2.5
1	H	167	LEU	2.5
1	H	157	SER	2.4
2	L	76	SER	2.1
2	L	208	SER	2.0
2	L	202	THR	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	CL	P	901	1/1	0.99	0.17	0.57	30,30,30,30	0
4	NI	L	901	1/1	0.98	0.14	-	35,35,35,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.