



# Full wwPDB X-ray Structure Validation Report ⓘ

May 12, 2021 – 04:08 PM EDT

PDB ID : 4FFV  
Title : Crystal Structure of Dipeptidyl Peptidase IV (DPP4, DPP-IV, CD26) in Complex with 11A19 Fab  
Authors : Wang, Z.; Sudom, A.; Walker, N.P.; Min, X.  
Deposited on : 2012-06-01  
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.

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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  
Xtrriage (Phenix) : 1.13  
EDS : 2.18  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.18

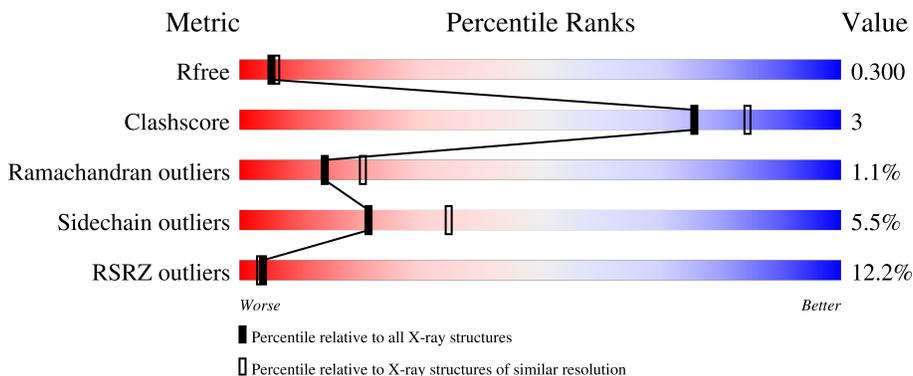
# 1 Overall quality at a glance

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))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	730	
1	B	730	
2	C	210	
2	L	210	
3	D	217	

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Mol	Chain	Length	Quality of chain
3	H	217	 <p>A horizontal bar chart representing the quality of chain H. The bar is divided into three segments: a red segment on the left labeled '20%', a large green segment in the middle labeled '82%', and a yellow/orange segment on the right labeled '11%'. At the far right end of the bar, there are two small black dots.</p>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18423 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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	727	Total 5921	C 3792	N 980	O 1123	S 26	0	0	0
1	B	729	Total 5940	C 3804	N 985	O 1125	S 26	0	0	0

- Molecule 2 is a protein called 11A19 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	207	Total 1579	C 982	N 269	O 321	S 7	0	0	0
2	L	207	Total 1579	C 982	N 269	O 321	S 7	0	0	0

- Molecule 3 is a protein called 11A19 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	209	Total 1596	C 1017	N 259	O 315	S 5	0	0	0
3	H	209	Total 1595	C 1016	N 259	O 315	S 5	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	106	Total 106	O 106	0	0
4	B	100	Total 100	O 100	0	0
4	C	4	Total 4	O 4	0	0
4	D	3	Total 3	O 3	0	0

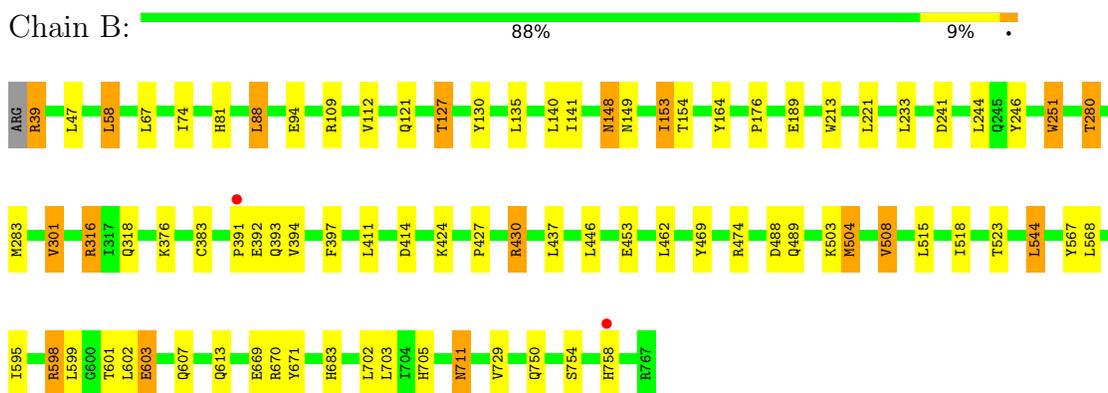
### 3 Residue-property plots [i](#)

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.

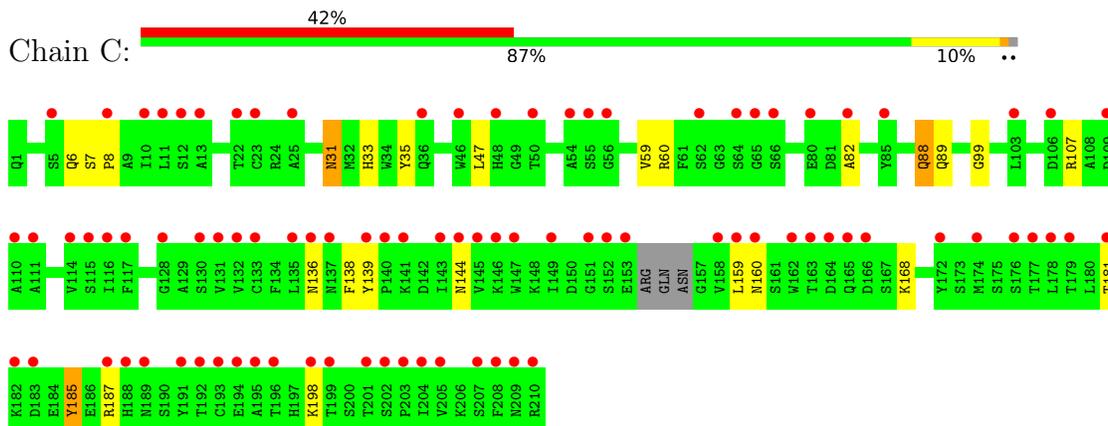
- Molecule 1: Dipeptidyl peptidase 4



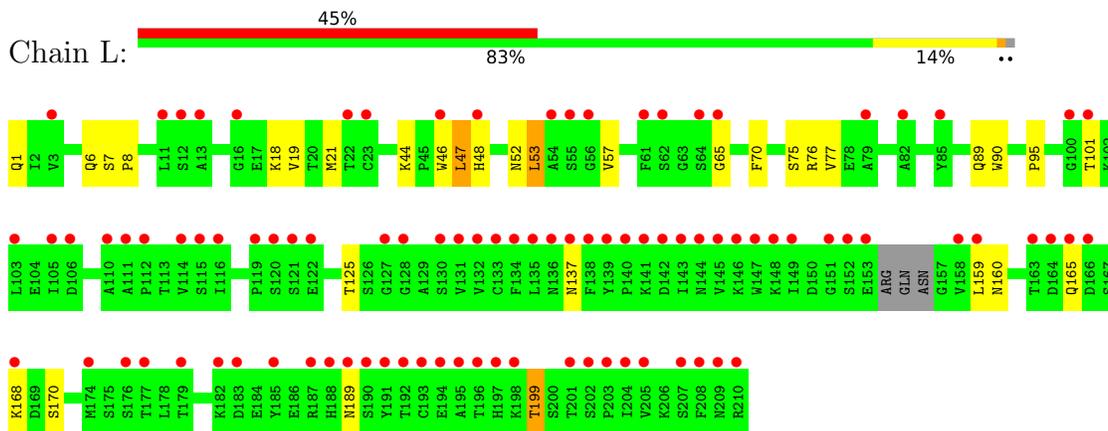
- Molecule 1: Dipeptidyl peptidase 4



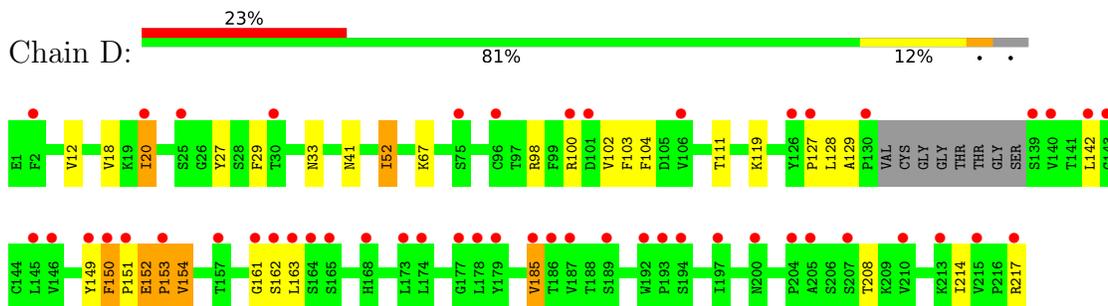
- Molecule 2: 11A19 Fab light chain



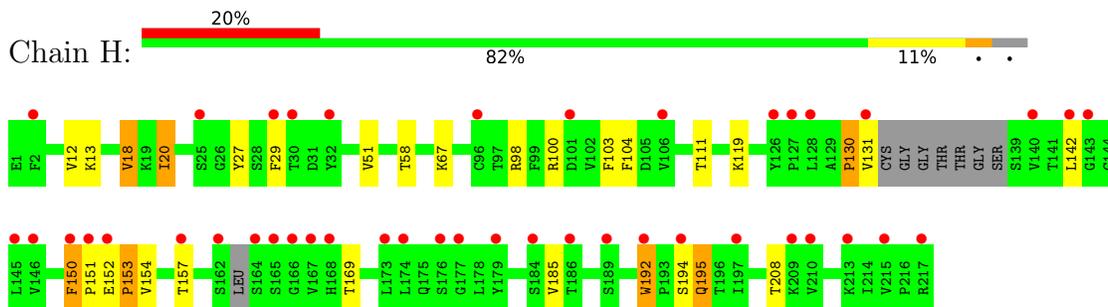
- Molecule 2: 11A19 Fab light chain



- Molecule 3: 11A19 Fab heavy chain



- Molecule 3: 11A19 Fab heavy chain



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.26Å 201.72Å 97.28Å 90.00° 93.71° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 30.01 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.5 (30.00-2.40) 98.5 (30.01-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.18 (at 2.39Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.271 , 0.301 0.272 , 0.300	Depositor DCC
$R_{free}$ test set	7181 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.4	Xtrriage
Anisotropy	0.141	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 10.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.477 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	18423	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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	0.30	0/6090	0.53	0/8280
1	B	0.30	0/6109	0.54	0/8305
2	C	0.30	0/1619	0.48	0/2201
2	L	0.31	0/1619	0.48	0/2201
3	D	0.30	0/1636	0.49	0/2234
3	H	0.30	0/1634	0.47	0/2230
All	All	0.30	0/18707	0.52	0/25451

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
2	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	99	GLY	Peptide

### 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	5921	0	5658	22	0
1	B	5940	0	5682	43	0
2	C	1579	0	1503	6	0
2	L	1579	0	1503	11	0
3	D	1596	0	1571	14	0
3	H	1595	0	1568	16	0
4	A	106	0	0	1	0
4	B	100	0	0	4	0
4	C	4	0	0	0	0
4	D	3	0	0	0	0
All	All	18423	0	17485	110	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 3.

All (110) 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:B:112:VAL:HG23	1:B:135:LEU:HD21	1.69	0.75
3:H:150:PHE:HB3	3:H:151:PRO:HD3	1.74	0.69
1:A:191:VAL:HG12	1:A:192:ILE:HD12	1.73	0.69
1:A:607:GLN:NE2	4:A:849:HOH:O	2.29	0.64
1:B:607:GLN:NE2	4:B:838:HOH:O	2.28	0.62
1:A:182:ARG:NH1	1:A:184:THR:O	2.33	0.61
1:A:170:ILE:H	1:A:184:THR:HG22	1.67	0.60
1:B:130:TYR:CZ	1:B:153:ILE:HD11	2.36	0.60
3:H:51:VAL:HG22	3:H:58:THR:HG22	1.83	0.59
3:H:98:ARG:O	3:H:104:PHE:HA	2.03	0.59
1:B:67:LEU:HB3	1:B:74:ILE:HD11	1.84	0.59
1:B:503:LYS:O	1:B:504:MET:HB2	2.03	0.59
1:B:47:LEU:HD22	1:B:750:GLN:HA	1.86	0.57
1:B:518:ILE:HD12	1:B:613:GLN:HG3	1.87	0.56
1:B:94:GLU:OE1	3:D:33:ASN:ND2	2.38	0.56
2:C:35:TYR:HE1	2:C:88:GLN:HE21	1.52	0.56
3:H:154:VAL:HG13	3:H:154:VAL:O	2.06	0.56
1:B:121:GLN:NE2	4:B:897:HOH:O	2.38	0.56
1:A:47:LEU:HD22	1:A:750:GLN:HA	1.87	0.55
1:B:383:CYS:HB3	1:B:397:PHE:CD1	2.41	0.55
3:H:192:TRP:O	3:H:195:GLN:N	2.39	0.54
1:A:169:ASP:OD1	1:A:184:THR:HG23	2.07	0.54
1:B:601:THR:HG23	1:B:602:LEU:N	2.24	0.53
1:B:74:ILE:CG2	1:B:88:LEU:HB3	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:12:VAL:HG11	3:D:18:VAL:HG22	1.91	0.53
1:B:127:THR:HG23	1:B:149:ASN:HA	1.91	0.52
1:B:503:LYS:O	1:B:504:MET:CB	2.57	0.52
1:B:544:LEU:HD12	1:B:568:LEU:HD13	1.90	0.52
2:L:46:TRP:CZ3	2:L:57:VAL:HG13	2.45	0.52
3:H:169:THR:O	3:H:169:THR:CG2	2.59	0.51
3:D:20:ILE:HD12	3:D:111:THR:HB	1.93	0.51
1:B:427:PRO:O	1:B:430:ARG:NH2	2.44	0.50
1:B:148:ASN:HB3	1:B:149:ASN:HD22	1.76	0.50
1:B:711:ASN:C	1:B:711:ASN:HD22	2.16	0.49
3:H:12:VAL:HG11	3:H:18:VAL:HG13	1.94	0.49
1:A:409:GLU:HG3	1:A:462:LEU:HD12	1.95	0.49
1:B:130:TYR:OH	1:B:153:ILE:HD11	2.12	0.49
1:B:233:LEU:HD13	1:B:251:TRP:CD1	2.48	0.49
1:A:544:LEU:HD12	1:A:568:LEU:HD13	1.94	0.49
3:D:12:VAL:HG21	3:D:18:VAL:CG2	2.43	0.49
3:D:151:PRO:O	3:D:152:GLU:HB2	2.13	0.49
3:H:130:PRO:O	3:H:131:VAL:HB	2.13	0.49
3:D:149:TYR:CE2	3:D:154:VAL:HG21	2.48	0.49
1:B:58:LEU:O	1:B:58:LEU:HD23	2.13	0.49
1:B:153:ILE:HG23	1:B:164:TYR:HB3	1.94	0.48
1:B:601:THR:HG23	1:B:602:LEU:HG	1.95	0.48
3:H:194:SER:C	3:H:195:GLN:HE21	2.18	0.47
1:B:141:ILE:HD13	1:B:176:PRO:HB2	1.95	0.47
2:L:165:GLN:HG2	2:L:170:SER:HA	1.96	0.47
1:A:182:ARG:NH1	1:A:185:SER:HA	2.30	0.47
1:B:112:VAL:HG23	1:B:135:LEU:CD2	2.40	0.46
3:D:163:LEU:HD23	3:D:185:VAL:HG21	1.97	0.46
1:B:462:LEU:HD23	1:B:469:TYR:HB3	1.98	0.46
2:C:33:HIS:HB2	2:C:88:GLN:HB3	1.99	0.45
3:D:27:TYR:CE2	3:D:29:PHE:HA	2.51	0.45
1:A:235:GLU:HG2	1:A:251:TRP:HB3	1.98	0.45
1:B:213:TRP:CE2	1:B:301:VAL:HG13	2.52	0.44
3:D:153:PRO:HA	3:D:154:VAL:HB	1.99	0.44
3:D:98:ARG:O	3:D:104:PHE:HA	2.17	0.44
2:L:47:LEU:CD2	2:L:53:LEU:HD23	2.48	0.44
1:B:595:ILE:HG21	1:B:603:GLU:HG3	2.00	0.44
1:A:184:THR:HG21	1:A:194:ASN:CB	2.46	0.44
3:H:20:ILE:HD12	3:H:111:THR:CB	2.48	0.44
2:C:31:ASN:HD22	2:C:31:ASN:HA	1.61	0.44
3:H:142:LEU:HD11	3:H:185:VAL:CG1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ARG:HD2	1:B:508:VAL:HG12	1.99	0.43
1:B:488:ASP:O	1:B:489:GLN:HB2	2.18	0.43
3:D:150:PHE:HB3	3:D:151:PRO:HD3	1.99	0.43
1:A:319:ASN:C	1:A:319:ASN:HD22	2.22	0.43
1:A:409:GLU:HG2	1:A:460:VAL:HG13	2.00	0.43
1:B:754:SER:O	1:B:758:HIS:ND1	2.51	0.43
1:B:318:GLN:OE1	1:B:670:ARG:HD3	2.19	0.43
2:L:7:SER:HA	2:L:8:PRO:HA	1.93	0.43
1:A:303:TRP:CE2	1:A:309:ILE:HD12	2.54	0.42
2:L:19:VAL:HG21	2:L:77:VAL:HG21	2.01	0.42
3:H:152:GLU:N	3:H:153:PRO:CD	2.82	0.42
1:B:74:ILE:HG23	1:B:88:LEU:HB3	2.00	0.42
2:L:47:LEU:HD22	2:L:53:LEU:HD23	2.01	0.42
1:A:318:GLN:OE1	1:A:670:ARG:HD3	2.20	0.42
1:A:409:GLU:CG	1:A:462:LEU:HD12	2.49	0.42
1:A:449:ASP:O	1:A:450:LEU:C	2.58	0.42
1:B:241:ASP:HB3	4:B:820:HOH:O	2.20	0.42
1:B:392:GLU:O	1:B:394:VAL:HG23	2.19	0.42
3:D:33:ASN:ND2	3:D:52:ILE:HG22	2.35	0.42
2:L:65:GLY:HA3	2:L:70:PHE:HA	2.01	0.42
2:L:48:HIS:O	2:L:52:ASN:HB2	2.20	0.42
1:B:280:THR:HG22	4:B:821:HOH:O	2.20	0.41
2:C:181:THR:O	2:C:185:TYR:N	2.51	0.41
2:L:21:MET:HG3	2:L:101:THR:HG21	2.02	0.41
3:H:20:ILE:HD12	3:H:111:THR:HB	2.02	0.41
2:C:7:SER:HA	2:C:8:PRO:HA	1.92	0.41
2:L:90:TRP:CG	2:L:95:PRO:HB3	2.56	0.41
2:L:159:LEU:HD23	2:L:160:ASN:N	2.35	0.41
2:C:159:LEU:HD23	2:C:160:ASN:N	2.35	0.41
3:H:169:THR:O	3:H:169:THR:HG22	2.21	0.41
1:B:316:ARG:HD3	1:B:669:GLU:OE1	2.20	0.41
1:B:599:LEU:HD13	1:B:671:TYR:HB3	2.01	0.41
1:B:74:ILE:HG23	1:B:88:LEU:CB	2.51	0.41
1:A:547:VAL:HG21	1:A:636:VAL:HG11	2.02	0.41
3:D:142:LEU:HB2	3:D:214:ILE:HD13	2.03	0.41
1:A:652:ILE:HG23	1:A:702:LEU:HB3	2.03	0.41
1:B:598:ARG:HA	1:B:683:HIS:CD2	2.56	0.41
1:A:43:LEU:HD21	1:A:754:SER:HA	2.02	0.41
3:H:154:VAL:O	3:H:154:VAL:CG1	2.68	0.41
3:H:27:TYR:CE2	3:H:29:PHE:HA	2.57	0.40
3:D:129:ALA:O	3:D:217:ARG:NH2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:ILE:CG2	1:B:164:TYR:HB3	2.52	0.40
1:B:601:THR:CG2	1:B:602:LEU:N	2.85	0.40
1:A:232:PRO:HB2	1:B:246:TYR:CZ	2.56	0.40
1:A:344:ILE:N	1:A:344:ILE:HD12	2.37	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	A	725/730 (99%)	693 (96%)	32 (4%)	0	100	100
1	B	727/730 (100%)	691 (95%)	31 (4%)	5 (1%)	22	32
2	C	203/210 (97%)	186 (92%)	14 (7%)	3 (2%)	10	14
2	L	203/210 (97%)	179 (88%)	20 (10%)	4 (2%)	7	9
3	D	205/217 (94%)	183 (89%)	12 (6%)	10 (5%)	2	1
3	H	203/217 (94%)	187 (92%)	12 (6%)	4 (2%)	7	9
All	All	2266/2314 (98%)	2119 (94%)	121 (5%)	26 (1%)	14	20

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	136	ASN
3	D	152	GLU
3	D	162	SER
1	B	393	GLN
1	B	504	MET
2	C	139	TYR
3	D	41	ASN
1	B	189	GLU

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Mol	Chain	Res	Type
3	D	150	PHE
3	D	153	PRO
2	L	53	LEU
2	L	75	SER
2	L	199	THR
3	H	130	PRO
3	H	150	PHE
1	B	391	PRO
2	C	82	ALA
2	L	76	ARG
1	B	148	ASN
3	D	127	PRO
3	D	161	GLY
3	H	153	PRO
3	D	102	VAL
3	D	154	VAL
3	D	185	VAL
3	H	192	TRP

### 5.3.2 Protein sidechains [i](#)

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	648/651 (100%)	617 (95%)	31 (5%)	25	41
1	B	650/651 (100%)	613 (94%)	37 (6%)	20	33
2	C	181/184 (98%)	167 (92%)	14 (8%)	13	20
2	L	181/184 (98%)	170 (94%)	11 (6%)	18	30
3	D	184/189 (97%)	176 (96%)	8 (4%)	29	46
3	H	184/189 (97%)	174 (95%)	10 (5%)	22	36
All	All	2028/2048 (99%)	1917 (94%)	111 (6%)	21	35

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LYS
1	A	86	ILE
1	A	88	LEU
1	A	139	GLN
1	A	148	ASN
1	A	174	ILE
1	A	227	ASN
1	A	244	LEU
1	A	248	LYS
1	A	270	ASN
1	A	291	VAL
1	A	319	ASN
1	A	332	THR
1	A	383	CYS
1	A	389	ARG
1	A	416	LEU
1	A	462	LEU
1	A	483	LEU
1	A	489	GLN
1	A	503	LYS
1	A	508	VAL
1	A	515	LEU
1	A	543	LEU
1	A	544	LEU
1	A	567	TYR
1	A	598	ARG
1	A	604	VAL
1	A	702	LEU
1	A	703	LEU
1	A	705	HIS
1	A	711	ASN
1	B	39	ARG
1	B	58	LEU
1	B	81	HIS
1	B	88	LEU
1	B	109	ARG
1	B	127	THR
1	B	140	LEU
1	B	153	ILE
1	B	154	THR
1	B	221	LEU
1	B	244	LEU
1	B	251	TRP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	280	THR
1	B	283	MET
1	B	301	VAL
1	B	316	ARG
1	B	376	LYS
1	B	411	LEU
1	B	414	ASP
1	B	424	LYS
1	B	430	ARG
1	B	437	LEU
1	B	446	LEU
1	B	453	GLU
1	B	474	ARG
1	B	508	VAL
1	B	515	LEU
1	B	523	THR
1	B	544	LEU
1	B	567	TYR
1	B	598	ARG
1	B	603	GLU
1	B	702	LEU
1	B	703	LEU
1	B	705	HIS
1	B	711	ASN
1	B	729	VAL
2	C	6	GLN
2	C	31	ASN
2	C	47	LEU
2	C	59	VAL
2	C	60	ARG
2	C	88	GLN
2	C	89	GLN
2	C	107	ARG
2	C	138	PHE
2	C	144	ASN
2	C	168	LYS
2	C	185	TYR
2	C	187	ARG
2	C	198	LYS
3	D	20	ILE
3	D	52	ILE
3	D	67	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	D	100	ARG
3	D	103	PHE
3	D	119	LYS
3	D	128	LEU
3	D	208	THR
2	L	1	GLN
2	L	6	GLN
2	L	18	LYS
2	L	44	LYS
2	L	47	LEU
2	L	89	GLN
2	L	125	THR
2	L	137	ASN
2	L	168	LYS
2	L	189	ASN
2	L	199	THR
3	H	13	LYS
3	H	18	VAL
3	H	20	ILE
3	H	67	LYS
3	H	100	ARG
3	H	103	PHE
3	H	119	LYS
3	H	157	THR
3	H	195	GLN
3	H	208	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	72	ASN
1	A	81	HIS
1	A	177	HIS
1	A	227	ASN
1	A	270	ASN
1	A	319	ASN
1	A	436	GLN
1	A	442	ASN
1	A	456	GLN
1	A	484	HIS
1	A	573	ASN
1	A	711	ASN

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Mol	Chain	Res	Type
1	B	121	GLN
1	B	149	ASN
1	B	261	ASN
1	B	484	HIS
1	B	489	GLN
1	B	528	GLN
1	B	686	ASN
1	B	711	ASN
2	C	31	ASN
2	C	136	ASN
2	C	144	ASN
3	D	175	GLN
2	L	136	ASN
2	L	189	ASN
3	H	5	GLN
3	H	6	GLN
3	H	175	GLN
3	H	195	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides 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

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	727/730 (99%)	-0.20	1 (0%) 95 95	14, 34, 58, 77	0
1	B	729/730 (99%)	-0.20	2 (0%) 94 93	14, 34, 57, 80	1 (0%)
2	C	207/210 (98%)	2.11	89 (42%) 0 0	41, 90, 146, 162	0
2	L	207/210 (98%)	2.15	94 (45%) 0 0	38, 95, 146, 156	0
3	D	209/217 (96%)	1.23	50 (23%) 0 0	36, 80, 118, 132	0
3	H	209/217 (96%)	1.15	43 (20%) 1 0	38, 77, 117, 124	0
All	All	2288/2314 (98%)	0.47	279 (12%) 4 3	14, 43, 124, 162	1 (0%)

All (279) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	195	ALA	13.9
2	C	201	THR	12.1
2	L	195	ALA	10.9
2	C	191	TYR	8.8
2	L	145	VAL	8.4
2	L	23	CYS	7.6
3	D	101	ASP	7.6
2	L	201	THR	7.5
3	D	194	SER	7.4
2	L	110	ALA	7.3
2	C	147	TRP	7.3
2	C	56	GLY	7.2
2	C	110	ALA	7.1
3	D	140	VAL	7.1
2	C	149	ILE	7.1
2	L	205	VAL	7.0
2	C	111	ALA	6.7
2	C	196	THR	6.7
3	H	184	SER	5.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	L	56	GLY	5.9
3	D	200	ASN	5.9
2	C	13	ALA	5.6
2	C	131	VAL	5.6
2	L	147	TRP	5.6
2	L	179	THR	5.6
2	C	179	THR	5.6
3	H	140	VAL	5.4
2	L	208	PHE	5.4
2	C	139	TYR	5.4
2	L	103	LEU	5.4
2	C	205	VAL	5.3
3	H	164	SER	5.2
3	H	101	ASP	5.2
2	L	192	THR	5.1
2	C	189	ASN	5.1
2	L	193	CYS	5.0
2	L	13	ALA	5.0
2	L	194	GLU	5.0
3	H	177	GLY	5.0
2	L	111	ALA	4.9
3	H	106	VAL	4.9
3	H	126	TYR	4.9
2	C	55	SER	4.8
3	D	192	TRP	4.8
2	L	22	THR	4.8
2	L	131	VAL	4.7
2	C	183	ASP	4.7
2	L	209	ASN	4.7
2	C	145	VAL	4.6
2	L	128	GLY	4.6
2	L	140	PRO	4.6
3	D	162	SER	4.6
2	L	207	SER	4.6
2	L	196	THR	4.5
2	L	149	ILE	4.5
2	C	22	THR	4.5
2	L	127	GLY	4.5
2	C	11	LEU	4.4
3	D	2	PHE	4.4
3	H	166	GLY	4.4
2	L	11	LEU	4.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	L	136	ASN	4.4
3	H	131	VAL	4.4
2	C	152	SER	4.3
2	C	202	SER	4.3
2	L	183	ASP	4.2
2	C	192	THR	4.2
2	L	139	TYR	4.2
2	L	189	ASN	4.2
2	L	146	LYS	4.2
2	L	191	TYR	4.1
2	L	168	LYS	4.1
2	C	23	CYS	4.1
2	L	204	ILE	4.0
3	H	179	TYR	4.0
3	D	187	VAL	4.0
2	C	208	PHE	4.0
2	C	62	SER	4.0
2	L	133	CYS	4.0
2	L	148	LYS	3.9
2	L	210	ARG	3.9
2	L	55	SER	3.9
3	D	145	LEU	3.9
2	C	182	LYS	3.9
2	L	143	ILE	3.8
2	C	204	ILE	3.8
3	H	168	HIS	3.8
3	H	174	LEU	3.8
2	L	100	GLY	3.8
2	C	194	GLU	3.8
3	D	106	VAL	3.8
3	D	163	LEU	3.7
2	C	203	PRO	3.7
2	C	210	ARG	3.7
2	C	188	HIS	3.7
3	H	96	CYS	3.7
3	H	213	LYS	3.6
2	C	103	LEU	3.6
2	C	136	ASN	3.6
2	L	115	SER	3.6
3	H	25	SER	3.6
2	L	16	GLY	3.6
2	C	132	VAL	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	C	137	ASN	3.6
2	C	82	ALA	3.6
2	L	79	ALA	3.6
2	L	135	LEU	3.5
3	D	168	HIS	3.5
2	C	128	GLY	3.5
3	H	2	PHE	3.5
2	L	165	GLN	3.5
3	H	165	SER	3.5
3	D	185	VAL	3.5
2	C	117	PHE	3.4
3	D	173	LEU	3.4
3	D	151	PRO	3.4
2	C	8	PRO	3.3
2	L	12	SER	3.3
2	L	159	LEU	3.3
2	C	144	ASN	3.3
3	D	25	SER	3.3
2	C	163	THR	3.3
2	L	62	SER	3.3
3	H	210	VAL	3.3
3	D	193	PRO	3.3
2	C	199	THR	3.3
2	L	144	ASN	3.3
2	L	151	GLY	3.3
3	H	215	VAL	3.2
3	H	162	SER	3.2
2	C	143	ILE	3.2
3	D	197	ILE	3.2
3	D	179	TYR	3.2
2	C	159	LEU	3.2
3	D	150	PHE	3.2
3	H	197	ILE	3.2
2	L	203	PRO	3.2
2	C	187	ARG	3.2
3	D	153	PRO	3.1
2	C	64	SER	3.1
2	L	153	GLU	3.1
2	L	142	ASP	3.1
2	C	165	GLN	3.1
2	C	177	THR	3.1
2	L	190	SER	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	C	193	CYS	3.0
2	L	164	ASP	3.0
3	D	174	LEU	3.0
3	D	205	ALA	3.0
3	D	149	TYR	3.0
2	L	114	VAL	3.0
3	D	126	TYR	3.0
2	C	207	SER	2.9
2	C	176	SER	2.9
3	D	207	SER	2.9
3	D	127	PRO	2.9
2	C	140	PRO	2.9
2	L	188	HIS	2.9
3	D	213	LYS	2.9
2	L	177	THR	2.9
3	H	142	LEU	2.8
3	D	165	SER	2.8
3	H	150	PHE	2.8
2	L	137	ASN	2.8
3	H	128	LEU	2.8
2	L	130	SER	2.8
2	C	151	GLY	2.7
3	D	186	THR	2.7
2	C	198	LYS	2.7
3	D	96	CYS	2.7
3	H	192	TRP	2.7
3	H	152	GLU	2.7
3	D	130	PRO	2.7
3	H	167	VAL	2.7
2	C	181	THR	2.7
2	L	176	SER	2.7
2	C	115	SER	2.7
3	D	100	ARG	2.7
3	D	177	GLY	2.7
2	C	25	ALA	2.7
3	D	215	VAL	2.7
3	H	157	THR	2.6
3	D	157	THR	2.6
3	H	186	THR	2.6
3	H	173	LEU	2.6
2	L	166	ASP	2.6
2	L	82	ALA	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	C	46	TRP	2.6
2	C	114	VAL	2.6
2	L	163	THR	2.6
3	D	210	VAL	2.6
2	C	209	ASN	2.6
3	D	75	SER	2.6
2	C	85	TYR	2.6
2	C	178	LEU	2.5
2	C	65	GLY	2.5
2	C	54	ALA	2.5
3	D	142	LEU	2.5
2	L	105	ILE	2.5
3	D	161	GLY	2.5
2	L	152	SER	2.5
2	L	141	LYS	2.5
3	H	151	PRO	2.5
2	L	158	VAL	2.5
2	L	61	PHE	2.5
3	D	20	ILE	2.5
2	L	112	PRO	2.5
2	C	158	VAL	2.4
2	L	197	HIS	2.4
2	L	198	LYS	2.4
2	L	120	SER	2.4
2	C	116	ILE	2.4
2	C	135	LEU	2.4
3	D	139	SER	2.4
2	L	85	TYR	2.4
3	H	127	PRO	2.4
2	C	146	LYS	2.4
2	C	80	GLU	2.4
3	H	146	VAL	2.4
2	L	48	HIS	2.3
2	C	10	ILE	2.3
2	C	164	ASP	2.3
2	L	101	THR	2.3
2	L	3	VAL	2.3
2	L	119	PRO	2.3
3	H	29	PHE	2.3
2	L	185	TYR	2.3
3	H	194	SER	2.3
2	C	48	HIS	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	C	162	TRP	2.3
2	C	133	CYS	2.3
2	L	54	ALA	2.3
3	H	145	LEU	2.3
2	L	64	SER	2.3
3	H	32	TYR	2.3
2	L	132	VAL	2.3
3	H	209	LYS	2.3
2	C	153	GLU	2.3
2	L	187	ARG	2.2
3	D	217	ARG	2.2
2	C	160	ASN	2.2
2	L	106	ASP	2.2
3	H	30	THR	2.2
2	C	106	ASP	2.2
2	C	109	ASP	2.2
2	L	121	SER	2.2
2	C	166	ASP	2.2
2	C	172	TYR	2.2
3	D	146	VAL	2.2
3	H	217	ARG	2.2
2	L	46	TRP	2.2
2	L	182	LYS	2.2
2	L	65	GLY	2.2
3	D	30	THR	2.2
2	C	66	SER	2.2
3	H	143	GLY	2.1
3	H	176	SER	2.1
2	L	122	GLU	2.1
3	D	204	PRO	2.1
3	D	164	SER	2.1
2	C	174	MET	2.1
2	L	134	PHE	2.1
2	C	130	SER	2.1
2	L	138	PHE	2.1
1	B	758	HIS	2.1
2	C	5	SER	2.1
2	C	12	SER	2.1
3	H	189	SER	2.1
3	D	143	GLY	2.1
2	C	50	THR	2.1
3	D	189	SER	2.1

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Mol	Chain	Res	Type	RSRZ
3	D	178	LEU	2.1
1	B	391	PRO	2.0
2	L	116	ILE	2.0
2	C	36	GLN	2.0
2	C	141	LYS	2.0
2	L	202	SER	2.0
1	A	68	TYR	2.0
2	L	174	MET	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 monosaccharides 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.