



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:05 PM UTC

PDB ID : 6RNN / pdb_00006rnn
Title : P46, an immunodominant surface protein from Mycoplasma hyopneumoniae
Authors : Guasch, A.; Gonzalez-Gonzalez, L.; Fita, I.
Deposited on : 2019-05-09
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

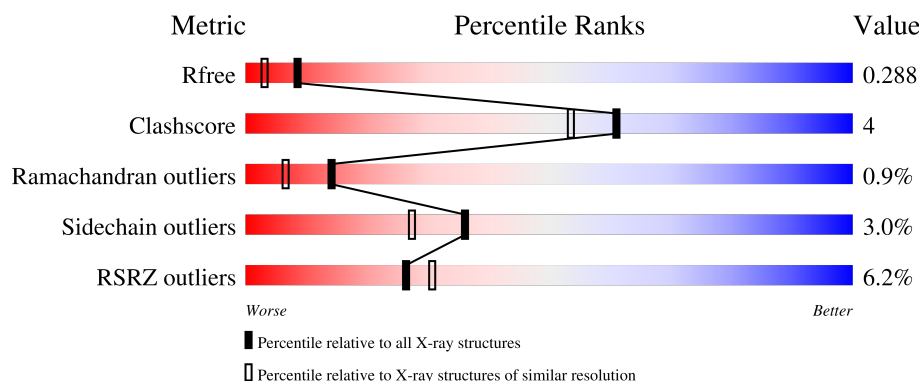
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	C	238	
1	L	238	
2	D	474	
2	H	474	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7125 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 Immunoglobulin light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	215	Total	C	N	O	S	0	1	0
			1677	1049	283	338	7			
1	C	211	Total	C	N	O	S	0	0	0
			1643	1028	276	333	6			

- Molecule 2 is a protein called Immunoglobulin heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	204	Total	C	N	O	S	0	2	0
			1578	1006	255	308	9			
2	H	205	Total	C	N	O	S	0	1	0
			1580	1007	255	310	8			

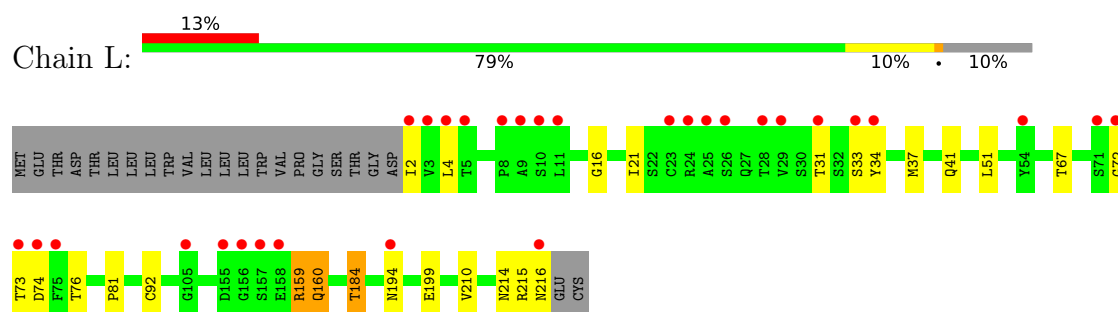
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	140	Total	O	0	0
			140	140		
3	D	166	Total	O	0	0
			166	166		
3	C	181	Total	O	0	0
			181	181		
3	H	160	Total	O	0	0
			160	160		

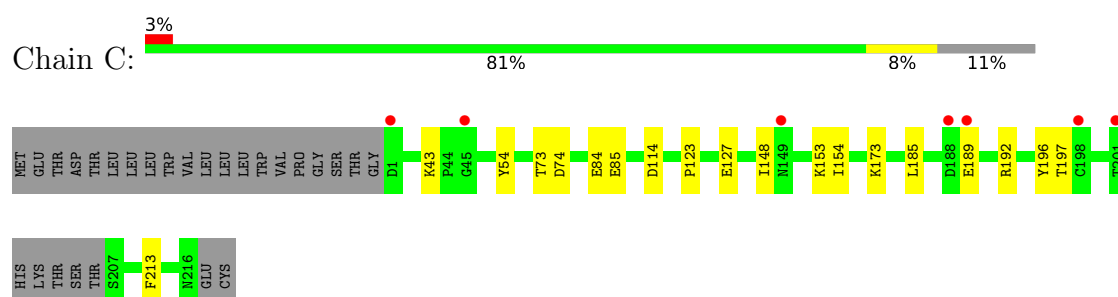
3 Residue-property plots [i](#)

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.

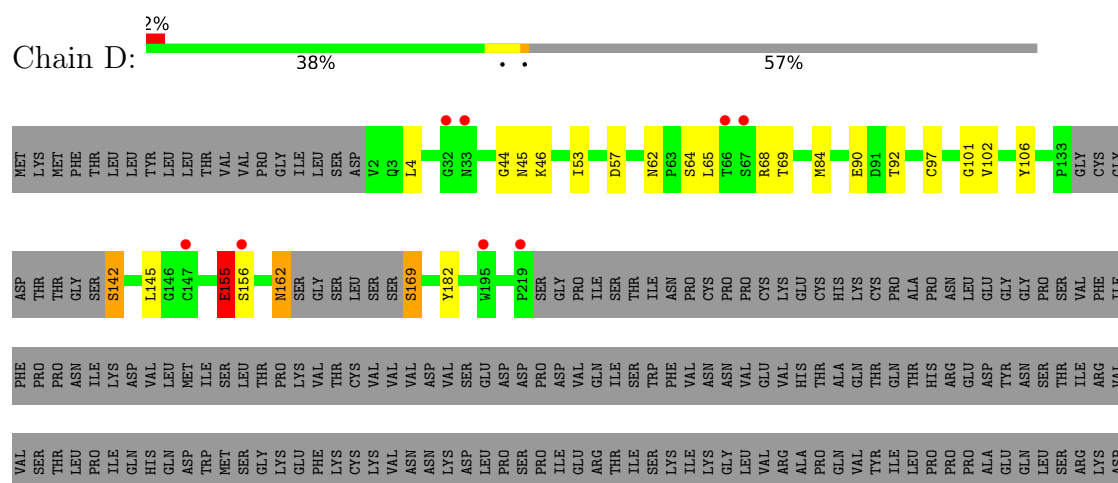
• Molecule 1: Immunoglobulin light chain



• Molecule 1: Immunoglobulin light chain

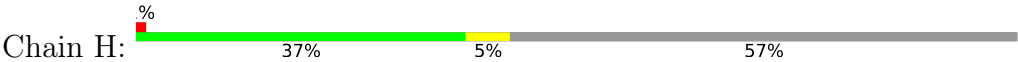


• Molecule 2: Immunoglobulin heavy chain



VAL	SER	THR	CYS	LEU	VAL	VAL	GLY	PHE	LYS	ASN	PRO	GLY	ASP	ILE	VAL	GLU	THR	THR	SER	ASN	GLY	HIS	THR	GLU	GLU	ASN	TYR	LYS	ASP	THR	ALA	PRO	VAL	LEU	ASP	SER	ASP	GLY	SER	TYR	PHE	ILE	TYR	SER	LYS	LEU	ASN	MET	LYS	THR	SER	LYS	TRP	GLY	LYS	THR	ASP	SER
PHE	SER	CYS	ASN	VAL	ARG	HIS	GLU	GLY	LEU	LEU	ASN	TYR	ASP	ILE	LYS	VAL	THR	THR	ILE	SER	ARG	SER	GLY	LYS																																		

● Molecule 2: Immunoglobulin heavy chain



MET	LYS	MET	THR	LEU	LEU	TYR	THR	LEU	VAL	PRO	GLY	ILE	SER	LEU	SER	D1	Q16	T17	V18	S28	T31	G32	N33	P43	Y55	S56	L65	T66	T69	T70	I75	N85	A89	E90	G101	Y106	P133	GLY	CYS	GLY	ASP	THR	THR	GLY								
SER	S142	K150	G151	E155	S156	V157	T158	V159	M162	SER	GLY	SER	SER	LEU	SER	SER	S169	L181	Y182	T183	T194	V204	D214	K215	P219	SER	GLY	PRO	ILE	SER	THR	ILE	ASN	CYS	PRO	CYS	GLU	HIS	LYS	CYS	PRO	ALA	ASN	LEU	GLU	GLY						
PRO	SER	VAL	PHE	PHE	PRO	PRO	ASN	ILE	LYS	ASP	VAL	LEU	MET	ILE	SER	LEU	THR	LYS	VAL	VAL	VAL	ASP	VAL	SER	GLU	ASP	PRO	ASP	GLN	ILE	SER	THR	PHE	VAL	ASN	CYS	ASN	VAL	GLU	VAL	HIS	ALA	GLN	THR	THR	GLN	TYR	ASN				
SER	THR	ILE	ARG	VAL	SER	THR	LEU	PRO	GLN	HIS	GLN	ASP	TRP	MET	SER	GLY	LYS	PHE	LYS	VAL	ASN	ASN	LYS	ASP	PRO	PRO	ILE	ARG	THR	ILE	SER	LYS	ILE	LYS	ILE	LYS	ALA	PRO	THR	VAL	GLN	VAL	TYR	LYS	ILE	LEU	ASN	PRO	LYS	THR	ALA	GLN
LEU	SER	ARG	ASP	VAL	SER	LEU	THR	CYS	VAL	GLY	VAL	PHE	ASN	PRO	GLY	ASP	ILE	SER	THR	SER	ASN	GLY	HIS	GLU	ASN	THR	ASP	ALA	PRO	VAL	LEU	ASP	SER	ASP	GLY	SER	THR	PHE	ILE	TYR	LYS	LEU	ASN	MET	LYS	THR	SER	LYS	TRP			
GLU	LYS	THR	ASP	SER	PHE	CYS	VAL	ASN	ARG	HIS	GLU	GLY	LEU	LYS	ASN	TYR	ASP	LEU	LYS	THR	THR	THR	THR	GLU	GLU	ASN	TYR	THR	ALA	PRO	VAL	LEU	ASP	SER	ASP	GLY	SER	THR	PHE	ILE	TYR	LYS	LEU	ASN	MET	LYS	THR	SER	LYS	TRP		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.21Å 88.38Å 123.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.00 – 1.95 61.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.3 (61.00-1.95) 98.3 (61.00-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 1.73Å)	Xtriage
Refinement program	PHENIX (dev_2880: ???)	Depositor
R, R_{free}	0.207 , 0.261 (Not available) , 0.288	Depositor DCC
R_{free} test set	4667 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	22.0	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.025 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7125	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	C	0.33	0/1684	0.55	0/2295
1	L	0.32	0/1723	0.51	0/2349
2	D	0.32	0/1624	0.56	0/2230
2	H	0.30	0/1626	0.54	0/2233
All	All	0.32	0/6657	0.54	0/9107

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	D	0	1
2	H	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	155	GLU	Peptide
2	H	31	THR	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	C	1643	0	1563	12	0
1	L	1677	0	1600	13	0
2	D	1578	0	1539	15	0
2	H	1580	0	1543	15	0
3	C	181	0	0	4	0
3	D	166	0	0	5	0
3	H	160	0	0	3	0
3	L	140	0	0	3	0
All	All	7125	0	6245	53	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 4.

All (53) 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)
2:D:69:THR:HG22	2:D:84:MET:HG3	1.69	0.74
1:C:114:ASP:O	3:C:302:HOH:O	2.09	0.69
1:C:84:GLU:H	1:C:84:GLU:CD	2.01	0.67
2:D:169:SER:OG	3:D:505:HOH:O	2.13	0.66
1:L:2:ILE:N	3:L:305:HOH:O	2.31	0.63
1:C:127:GLU:OE2	1:C:127:GLU:N	2.30	0.61
1:C:154:ILE:HD12	1:C:196:TYR:CD2	2.36	0.60
2:H:43:PRO:O	3:H:528:HOH:O	2.17	0.60
2:H:101:GLY:HA3	2:H:106:TYR:CE2	2.38	0.59
2:D:162:ASN:O	3:D:514:HOH:O	2.17	0.59
2:H:142:SER:N	3:H:510:HOH:O	2.35	0.58
1:C:185:LEU:HB3	1:C:189:GLU:HG3	1.86	0.57
1:C:54:TYR:OH	3:C:306:HOH:O	2.16	0.57
1:L:21:ILE:HG23	3:L:307:HOH:O	2.05	0.55
1:L:159:ARG:HG3	1:L:160:GLN:N	2.22	0.55
1:C:43:LYS:NZ	1:C:85:GLU:O	2.29	0.55
2:D:64:SER:OG	2:D:65:LEU:HD12	2.07	0.54
2:H:65:LEU:O	2:H:69:THR:HG23	2.08	0.53
2:H:17:THR:HG22	2:H:85:ASN:HB3	1.91	0.53
2:D:4:LEU:HD23	2:D:97[A]:CYS:SG	2.50	0.52
1:L:4:LEU:HD13	1:L:37:MET:HE1	1.92	0.51
2:D:92:THR:HG21	2:H:75:ILE:HD11	1.92	0.51
1:L:16:GLY:HA2	1:L:81:PRO:HB2	1.93	0.51
2:D:101:GLY:HA3	2:D:106:TYR:CE2	2.46	0.50
2:H:33:ASN:HA	2:H:55:TYR:CD1	2.47	0.50
2:D:90:GLU:HB3	3:D:593:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:184:THR:OG1	3:L:302:HOH:O	2.20	0.48
2:H:151:GLY:HA2	2:H:181:LEU:HB3	1.96	0.47
1:L:41:GLN:HB2	1:L:51:LEU:HD11	1.96	0.46
1:C:74:ASP:OD1	3:C:305:HOH:O	2.21	0.46
2:D:44:GLY:O	2:D:45:ASN:HB2	2.16	0.45
2:H:215:LYS:NZ	3:H:518:HOH:O	2.32	0.45
1:L:37:MET:CE	1:L:92:CYS:HB2	2.45	0.45
1:L:199:GLU:HG3	1:L:210:VAL:HG22	1.98	0.45
3:D:558:HOH:O	2:H:28:SER:HB2	2.17	0.44
2:D:68:ARG:NH2	2:D:84:MET:HE2	2.33	0.44
2:D:142:SER:N	3:D:509:HOH:O	2.51	0.44
2:H:65:LEU:HB3	2:H:69:THR:HG21	2.01	0.42
2:H:159:VAL:HG22	2:H:204:VAL:HG22	2.00	0.42
1:L:214:ASN:C	1:L:216:ASN:H	2.27	0.42
2:D:53:ILE:HD11	2:D:57:ASP:OD1	2.19	0.42
2:D:62:ASN:HB3	2:D:65:LEU:HD13	2.01	0.42
2:H:65:LEU:HB3	2:H:69:THR:CG2	2.49	0.42
1:C:123:PRO:HB3	1:C:213:PHE:CE1	2.55	0.42
1:C:153:LYS:HB3	1:C:197:THR:HB	2.02	0.41
1:C:173:LYS:HD3	1:C:173:LYS:HA	1.85	0.41
1:C:192:ARG:NH2	3:C:432:HOH:O	2.53	0.41
1:L:31:THR:HG22	1:L:34:TYR:O	2.21	0.41
2:D:46:LYS:HG3	2:H:56:SER:HB2	2.01	0.41
1:L:37:MET:HE3	1:L:92:CYS:HB2	2.03	0.41
2:D:155:GLU:HG3	2:D:182:TYR:CZ	2.56	0.41
1:L:31:THR:C	1:L:33:SER:H	2.29	0.41
2:H:150:LYS:HG3	2:H:183:THR:OG1	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	200/238 (84%)	193 (96%)	6 (3%)	1 (0%)	24	16
1	L	214/238 (90%)	204 (95%)	8 (4%)	2 (1%)	14	6
2	D	178/474 (38%)	172 (97%)	4 (2%)	2 (1%)	11	4
2	H	200/474 (42%)	193 (96%)	5 (2%)	2 (1%)	12	5
All	All	792/1424 (56%)	762 (96%)	23 (3%)	7 (1%)	14	6

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	156	SER
2	H	156	SER
1	L	215	ARG
1	L	72	GLY
2	D	155	GLU
2	H	16	GLN
1	C	148	ILE

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	C	187/212 (88%)	186 (100%)	1 (0%)	81	82
1	L	192/212 (91%)	184 (96%)	8 (4%)	26	16
2	D	184/431 (43%)	178 (97%)	6 (3%)	33	24
2	H	184/431 (43%)	177 (96%)	7 (4%)	29	19
All	All	747/1286 (58%)	725 (97%)	22 (3%)	36	29

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

Mol	Chain	Res	Type
1	L	67	THR
1	L	73	THR
1	L	74	ASP
1	L	76	THR

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Mol	Chain	Res	Type
1	L	159	ARG
1	L	160	GLN
1	L	184	THR
1	L	194	ASN
2	D	102	VAL
2	D	142	SER
2	D	145	LEU
2	D	155	GLU
2	D	162	ASN
2	D	169	SER
1	C	73	THR
2	H	18	VAL
2	H	69	THR
2	H	70	THR
2	H	75	ILE
2	H	155	GLU
2	H	157	VAL
2	H	214	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	171	HIS
1	C	57	ASN
1	C	80	HIS
1	C	161	ASN
2	H	33	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 oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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, 95th 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 ²)	Q<0.9
1	C	211/238 (88%)	0.31	7 (3%) 49 55	12, 26, 44, 54	0
1	L	215/238 (90%)	0.91	30 (13%) 6 7	17, 33, 53, 75	1 (0%)
2	D	204/474 (43%)	0.33	8 (3%) 43 50	12, 26, 47, 68	2 (0%)
2	H	205/474 (43%)	0.59	7 (3%) 48 54	16, 32, 49, 60	1 (0%)
All	All	835/1424 (58%)	0.54	52 (6%) 26 31	12, 29, 51, 75	4 (0%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	156	GLY	5.6
1	L	9	ALA	4.2
1	L	3	VAL	4.2
1	L	5	THR	4.2
1	L	25	ALA	4.0
1	L	23	CYS	3.8
1	L	29	VAL	3.5
1	L	28	THR	3.5
1	L	74	ASP	3.4
1	L	34	TYR	3.2
1	L	105	GLY	3.2
1	L	72	GLY	3.1
2	H	32	GLY	3.0
1	L	4	LEU	3.0
1	C	45	GLY	3.0
2	D	156	SER	2.9
2	H	156	SER	2.9
1	L	31	THR	2.8
2	D	195	TRP	2.8
2	H	194	THR	2.8
2	D	67	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	L	54	TYR	2.6
1	L	73	THR	2.6
1	C	201	THR	2.6
1	L	8	PRO	2.6
1	L	155	ASP	2.6
1	C	1	ASP	2.5
2	H	90	GLU	2.5
1	L	157	SER	2.5
1	L	71	SER	2.4
2	D	147[A]	CYS	2.4
1	L	33	SER	2.4
1	L	75	PHE	2.4
1	L	194	ASN	2.4
1	L	10	SER	2.4
1	L	26	SER	2.4
1	C	149	ASN	2.3
1	L	11	LEU	2.3
2	D	219	PRO	2.3
1	L	216	ASN	2.2
1	L	24	ARG	2.2
2	H	17	THR	2.2
1	C	198	CYS	2.2
1	C	188	ASP	2.2
2	D	32	GLY	2.2
1	C	189	GLU	2.1
2	D	33	ASN	2.1
1	L	2	ILE	2.1
2	H	66	THR	2.1
1	L	158	GLU	2.0
2	D	66	THR	2.0
2	H	89	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.