



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:11 AM UTC

PDB ID : 9HIH / pdb\_00009hih  
Title : Mouse IL-2 fused to S4B6 Fab fragment  
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Deposited on : 2024-11-26  
Resolution : 2.70 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 types of validation reports are described at

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

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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

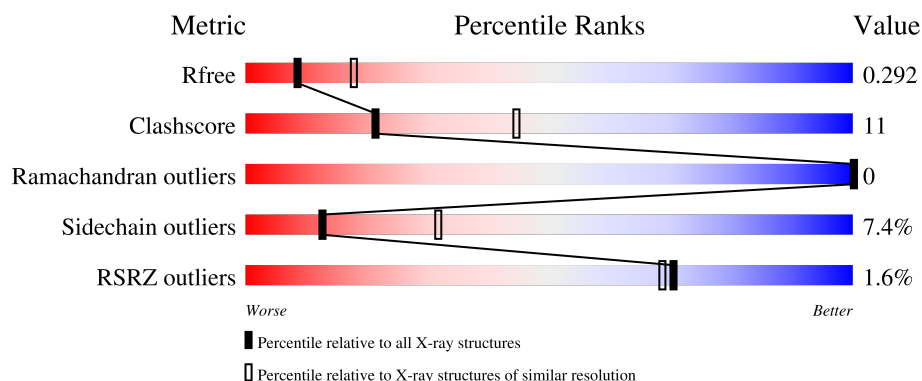
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	H	129	
2	L	196	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4315 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 S4B6 VH\_C1H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	223	Total	C	N	O	S	0	2	0
			1715	1088	281	341	5			

- Molecule 2 is a protein called mIL-2\_LN35\_S4B6\_LC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	323	Total	C	N	O	S	0	3	0
			2560	1603	429	515	13			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	1	ILE	-	expression tag	UNP P04351
L	2	THR	-	expression tag	UNP P04351
L	3	GLY	-	expression tag	UNP P04351
L	153	GLY	-	linker	UNP P04351
L	154	GLY	-	linker	UNP P04351
L	155	GLY	-	linker	UNP P04351
L	156	GLY	-	linker	UNP P04351
L	157	SER	-	linker	UNP P04351
L	158	GLY	-	linker	UNP P04351
L	159	GLY	-	linker	UNP P04351
L	160	GLY	-	linker	UNP P04351
L	161	GLY	-	linker	UNP P04351
L	162	SER	-	linker	UNP P04351
L	163	GLY	-	linker	UNP P04351
L	164	GLY	-	linker	UNP P04351
L	165	GLY	-	linker	UNP P04351
L	166	GLY	-	linker	UNP P04351
L	167	SER	-	linker	UNP P04351
L	168	GLY	-	linker	UNP P04351
L	169	GLY	-	linker	UNP P04351

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Chain	Residue	Modelled	Actual	Comment	Reference
L	170	GLY	-	linker	UNP P04351
L	171	GLY	-	linker	UNP P04351
L	172	SER	-	linker	UNP P04351
L	173	GLY	-	linker	UNP P04351
L	174	GLY	-	linker	UNP P04351
L	175	GLY	-	linker	UNP P04351
L	176	GLY	-	linker	UNP P04351
L	177	SER	-	linker	UNP P04351
L	178	GLY	-	linker	UNP P04351
L	179	GLY	-	linker	UNP P04351
L	180	GLY	-	linker	UNP P04351
L	181	GLY	-	linker	UNP P04351
L	182	SER	-	linker	UNP P04351
L	183	GLY	-	linker	UNP P04351
L	184	GLY	-	linker	UNP P04351
L	185	GLY	-	linker	UNP P04351
L	186	GLY	-	linker	UNP P04351
L	187	SER	-	linker	UNP P04351

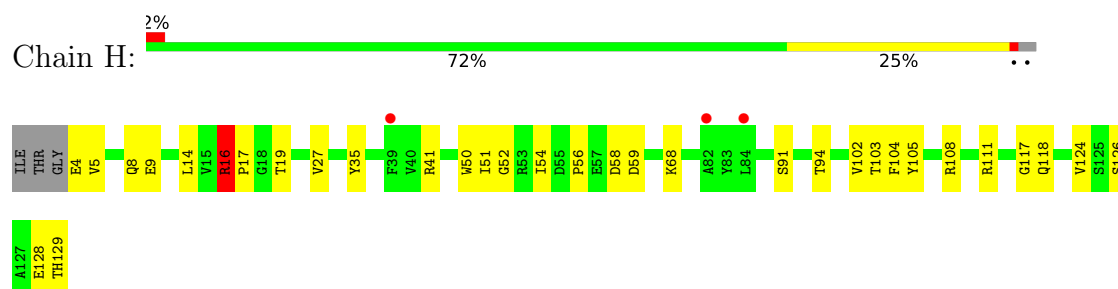
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	13	Total O 13 13	0	0
3	L	27	Total O 27 27	0	0

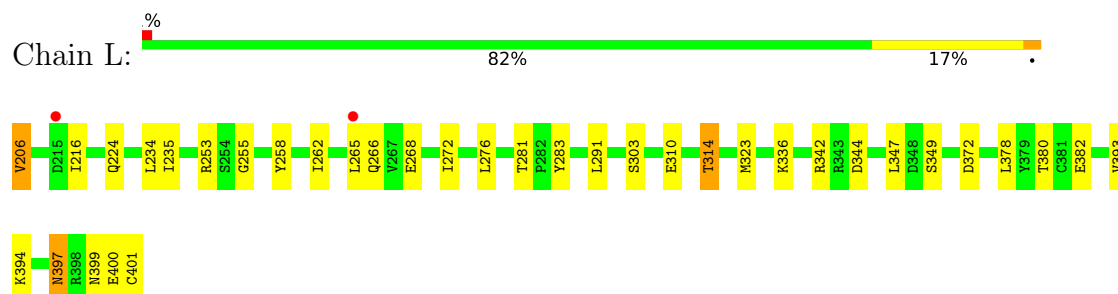
### 3 Residue-property plots [i](#)

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: S4B6 VH\_C1H



#### • Molecule 2: mIL-2\_LN35\_S4B6\_LC



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	42.87Å 77.00Å 169.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	77.00 – 2.70 77.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.1 (77.00-2.70) 98.1 (77.00-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.18 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.235 , 0.276 (Not available) , 0.292	Depositor DCC
$R_{free}$ test set	782 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	63.1	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 51.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4315	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.13% 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	H	0.57	0/1764	1.18	4/2414 (0.2%)
2	L	0.56	0/2610	1.11	7/3534 (0.2%)
All	All	0.56	0/4374	1.14	11/5948 (0.2%)

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	1
2	L	0	1
All	All	0	2

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	87	LEU	N-CA-CB	8.06	122.19	110.58
2	L	88	ASP	CB-CA-C	-7.91	94.90	109.37
1	H	191	THR	OG1-CB-CG2	-7.10	95.10	109.30
1	H	134	VAL	N-CA-CB	-5.75	104.09	110.99
2	L	268	GLU	CB-CG-CD	5.73	122.33	112.60
1	H	4	GLU	CB-CG-CD	5.65	122.20	112.60
2	L	372	ASP	CA-CB-CG	5.54	118.14	112.60
2	L	314	THR	CA-CB-OG1	-5.42	101.47	109.60
2	L	117	SER	CA-C-N	5.18	127.18	120.44
2	L	117	SER	C-N-CA	5.18	127.18	120.44
1	H	128	GLU	CB-CG-CD	5.12	121.31	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	16	ARG	Sidechain
2	L	342	ARG	Sidechain

## 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	1715	0	1675	42	0
2	L	2560	0	2506	58	0
3	H	13	0	0	2	0
3	L	27	0	0	1	0
All	All	4315	0	4181	90	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 11.

All (90) 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:68:LYS:HA	3:H:301:HOH:O	1.52	1.10
1:H:94:THR:HG22	1:H:124:VAL:H	1.36	0.91
1:H:103:THR:HG22	1:H:105:TYR:H	1.39	0.88
2:L:53:LEU:HB3	2:L:54:PRO:HD2	1.61	0.80
2:L:75:CYS:SG	2:L:123:CYS:HB3	2.27	0.75
1:H:132:PRO:HB3	1:H:158:TYR:HB3	1.70	0.73
2:L:87:LEU:HD13	2:L:100:ALA:HB3	1.73	0.69
2:L:397:ASN:HD22	2:L:399:ASN:H	1.39	0.69
2:L:189:ILE:HD12	2:L:189:ILE:N	2.08	0.68
2:L:118:ASP:OD1	2:L:118:ASP:N	2.20	0.68
1:H:105:TYR:CE1	2:L:58:THR:HB	2.30	0.66
2:L:87:LEU:HD12	2:L:87:LEU:O	1.96	0.66
1:H:148:MET:HE3	1:H:195:THR:HG22	1.78	0.65
2:L:53:LEU:HB2	2:L:55:ARG:HE	1.61	0.64
1:H:184:GLN:HG2	2:L:347:LEU:HD11	1.81	0.63
2:L:68:THR:HG23	2:L:69:GLU:CD	2.24	0.63
2:L:397:ASN:HB2	3:L:523:HOH:O	1.99	0.63
2:L:206:VAL:HG23	2:L:262:ILE:HB	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:198:LEU:HD22	2:L:199:SER:N	2.16	0.60
1:H:221:LYS:NZ	2:L:310[B]:GLU:OE1	2.35	0.59
2:L:54:PRO:HA	2:L:57:LEU:HD13	1.83	0.59
1:H:226:ARG:NH2	2:L:401:CYS:SG	2.75	0.59
1:H:8:GLN:NE2	1:H:118:GLN:OE1	2.35	0.58
2:L:53:LEU:HB3	2:L:54:PRO:CD	2.32	0.58
2:L:53:LEU:HB2	2:L:55:ARG:NE	2.18	0.58
2:L:397:ASN:HD21	2:L:399:ASN:ND2	2.01	0.57
1:H:182:VAL:HG23	2:L:347:LEU:HD13	1.86	0.57
2:L:189:ILE:HD12	2:L:189:ILE:H	1.69	0.57
2:L:216:ILE:HG13	2:L:258:TYR:OH	2.04	0.57
1:H:41:ARG:HB3	1:H:51:ILE:HD11	1.88	0.56
2:L:56:MET:HE2	2:L:88:ASP:OD2	2.06	0.55
2:L:99:ASP:O	2:L:102:ASN:ND2	2.40	0.55
1:H:16:ARG:HG3	1:H:17:PRO:HD2	1.89	0.54
1:H:184:GLN:CG	2:L:347:LEU:HD11	2.37	0.54
1:H:182:VAL:HG21	2:L:347:LEU:HB3	1.88	0.54
1:H:190:LEU:C	1:H:190:LEU:HD12	2.33	0.54
1:H:50:TRP:CH2	1:H:52:GLY:HA2	2.45	0.52
2:L:71:LYS:HD2	2:L:121:PHE:CD1	2.45	0.51
2:L:46:GLU:O	2:L:47:ASN:HB3	2.09	0.51
2:L:87:LEU:O	2:L:87:LEU:CD1	2.59	0.50
2:L:75:CYS:SG	2:L:123:CYS:CB	2.99	0.50
2:L:75:CYS:HG	2:L:123:CYS:CB	2.26	0.49
2:L:397:ASN:ND2	2:L:399:ASN:ND2	2.60	0.49
2:L:380:THR:HG23	2:L:393:VAL:HG13	1.95	0.49
1:H:9:GLU:N	1:H:9:GLU:OE1	2.46	0.48
2:L:66:GLN:HA	2:L:66:GLN:OE1	2.12	0.48
2:L:120:THR:HG21	2:L:255:GLY:H	1.77	0.48
1:H:102:VAL:HA	1:H:111:ARG:O	2.13	0.48
2:L:87:LEU:HD22	2:L:100:ALA:HB1	1.96	0.47
1:H:91:SER:O	1:H:94:THR:HG23	2.15	0.47
1:H:14:LEU:HB2	1:H:160:PRO:HG3	1.98	0.46
1:H:111:ARG:NH2	2:L:79:GLU:OE2	2.49	0.45
2:L:88:ASP:CB	2:L:89:LEU:HD23	2.46	0.45
2:L:27:GLN:O	2:L:30:HIS:HB2	2.16	0.45
1:H:58:ASP:O	1:H:59:ASP:HB2	2.17	0.45
1:H:103:THR:HG22	1:H:105:TYR:N	2.21	0.44
2:L:224:GLN:HB2	2:L:234:LEU:HD11	2.00	0.44
2:L:265:LEU:HD11	2:L:291:LEU:HD21	1.98	0.44
1:H:54:ILE:O	1:H:56:PRO:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:380:THR:CG2	2:L:393:VAL:HG13	2.48	0.44
1:H:154:LEU:HD12	1:H:155:VAL:N	2.33	0.44
2:L:53:LEU:C	2:L:55:ARG:H	2.26	0.44
1:H:16:ARG:O	1:H:19:THR:HG22	2.17	0.44
2:L:87:LEU:CD1	2:L:100:ALA:HB3	2.46	0.43
2:L:42:LEU:HD21	2:L:137:ARG:HG2	2.00	0.43
1:H:16:ARG:HD3	1:H:126:SER:HA	1.99	0.43
1:H:94:THR:HG22	1:H:124:VAL:N	2.18	0.43
2:L:276:LEU:HD11	2:L:283:TYR:HB3	2.00	0.43
1:H:105:TYR:O	2:L:60:LYS:HD3	2.19	0.43
2:L:253:ARG:HD2	2:L:258:TYR:CE2	2.54	0.43
1:H:139:PRO:HD2	1:H:201:TRP:CH2	2.53	0.42
1:H:180:PRO:HD2	2:L:349:SER:OG	2.19	0.42
2:L:198:LEU:HD22	2:L:199:SER:H	1.82	0.42
1:H:153:CYS:SG	1:H:208:CYS:CB	3.07	0.42
1:H:35:TYR:CD2	1:H:103:THR:OG1	2.73	0.42
1:H:157:GLY:HA2	1:H:187:LEU:HB3	2.02	0.42
2:L:115:LYS:HG3	2:L:116:GLY:O	2.20	0.42
2:L:35:LEU:HD13	2:L:143:CYS:HB2	2.02	0.41
2:L:272:ILE:HD12	2:L:272:ILE:N	2.35	0.41
2:L:189:ILE:N	2:L:189:ILE:CD1	2.77	0.41
1:H:177:HIS:HD2	3:H:309:HOH:O	2.03	0.41
1:H:129:THR:HG22	1:H:215:SER:HB3	2.02	0.41
2:L:397:ASN:ND2	2:L:399:ASN:H	2.11	0.41
2:L:88:ASP:HB3	2:L:89:LEU:HD23	2.02	0.41
1:H:9:GLU:OE1	1:H:117:GLY:HA3	2.20	0.41
1:H:104:PHE:CD1	1:H:111:ARG:HD2	2.56	0.41
1:H:221:LYS:HE2	1:H:221:LYS:HB2	1.94	0.41
1:H:108:ARG:O	1:H:111:ARG:HG3	2.20	0.40
1:H:9:GLU:CD	1:H:117:GLY:HA3	2.46	0.40
2:L:68:THR:HG23	2:L:69:GLU:OE2	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	H	223/129 (173%)	215 (96%)	8 (4%)	0	100	100
2	L	318/196 (162%)	310 (98%)	8 (2%)	0	100	100
All	All	541/325 (166%)	525 (97%)	16 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	193/109 (177%)	184 (95%)	9 (5%)	23	51
2	L	296/174 (170%)	269 (91%)	27 (9%)	9	22
All	All	489/283 (173%)	453 (93%)	36 (7%)	13	32

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	5	VAL
1	H	16	ARG
1	H	27	VAL
1	H	133	SER
1	H	166	THR
1	H	190	LEU
1	H	202	SER
1	H	209	ASN
1	H	221	LYS
2	L	32	GLU
2	L	44	ARG
2	L	58	THR
2	L	66	GLN
2	L	87	LEU
2	L	88	ASP

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Mol	Chain	Res	Type
2	L	89	LEU
2	L	99	ASP
2	L	118	ASP
2	L	127	ASP
2	L	189	ILE
2	L	198	LEU
2	L	202	LEU
2	L	206	VAL
2	L	235	ILE
2	L	266	GLN
2	L	281	THR
2	L	303	SER
2	L	314	THR
2	L	323	MET
2	L	336	LYS
2	L	344	ASP
2	L	378	LEU
2	L	382	GLU
2	L	394	LYS
2	L	397	ASN
2	L	400	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	8	GLN
1	H	204	GLN
2	L	28	GLN
2	L	29	GLN
2	L	190	GLN
2	L	214	GLN
2	L	218	ASN
2	L	397	ASN

### 5.3.3 RNA ⓘ

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 oligosaccharides 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	H	126/129 (97%)	0.17	3 (2%) 59 56	34, 72, 98, 118	2 (1%)
2	L	196/196 (100%)	-0.05	2 (1%) 79 78	24, 55, 79, 101	3 (1%)
All	All	322/325 (99%)	0.03	5 (1%) 70 68	24, 59, 94, 118	5 (1%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	39	PHE	2.8
1	H	82	ALA	2.6
1	H	84	LEU	2.5
2	L	265	LEU	2.4
2	L	215	ASP	2.1

### 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.