



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 11:48 AM GMT

PDB ID : 3PNW  
Title : Crystal Structure of the tudor domain of human TDRD3 in complex with an anti-TDRD3 FAB  
Authors : Loppnau, P.; Tempel, W.; Wernimont, A.K.; Lam, R.; Ravichandran, M.; Adams-Cioaba, M.A.; Persson, H.; Sidhu, S.S.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Weigelt, J.; Cossar, D.; Structural Genomics Consortium (SGC)  
Deposited on : 2010-11-19  
Resolution : 2.05 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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.

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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  
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

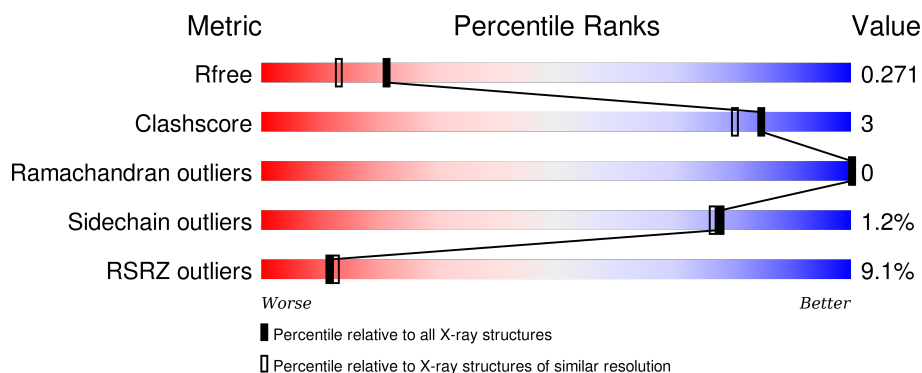
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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	228	<div> <div>6%</div> <div>82% 10% 7%</div> </div>
1	D	228	<div> <div>14%</div> <div>87% 7% 7%</div> </div>
1	G	228	<div> <div>10%</div> <div>89% 7%</div> </div>
1	J	228	<div> <div>10%</div> <div>86% 7% 7%</div> </div>
1	M	228	<div> <div>7%</div> <div>80% 14% 6%</div> </div>

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Mol	Chain	Length	Quality of chain
1	P	228	
1	S	228	
1	V	228	
2	B	246	
2	E	246	
2	H	246	
2	K	246	
2	N	246	
2	Q	246	
2	T	246	
2	W	246	
3	C	77	
3	F	77	
3	I	77	
3	L	77	
3	O	77	
3	R	77	
3	U	77	
3	X	77	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	UNX	B	1872	-	-	-	X
4	UNX	B	1875	-	-	-	X
4	UNX	B	1889	-	-	-	X
4	UNX	B	1906	-	-	-	X
4	UNX	B	1946	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	UNX	E	1814	-	-	X	-
4	UNX	G	1820	-	-	X	-
4	UNX	G	1824	-	-	-	X
4	UNX	G	1885	-	-	-	X
4	UNX	H	1887	-	-	-	X
4	UNX	J	1821	-	-	-	X
4	UNX	J	1866	-	-	-	X
4	UNX	J	1867	-	-	-	X
4	UNX	M	1852	-	-	-	X
4	UNX	N	1822	-	-	-	X
4	UNX	P	1832	-	-	-	X
4	UNX	P	1886	-	-	-	X
4	UNX	Q	1835	-	-	-	X
4	UNX	T	1865	-	-	-	X
4	UNX	T	1890	-	-	-	X
4	UNX	V	1971	-	-	-	X
4	UNX	W	1857	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 31176 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 FAB light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	4	0
			1639	1045	269	320	5			
1	D	213	Total	C	N	O	S	0	2	0
			1619	1028	267	319	5			
1	G	213	Total	C	N	O	S	0	4	0
			1639	1039	271	324	5			
1	J	213	Total	C	N	O	S	0	2	0
			1632	1033	269	325	5			
1	M	214	Total	C	N	O	S	0	4	0
			1648	1049	272	322	5			
1	P	213	Total	C	N	O	S	0	4	0
			1645	1042	271	327	5			
1	S	214	Total	C	N	O	S	0	3	0
			1633	1041	266	321	5			
1	V	212	Total	C	N	O	S	0	1	0
			1602	1021	259	317	5			

- Molecule 2 is a protein called FAB heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	225	Total	C	N	O	S	0	0	0
			1650	1040	275	328	7			
2	E	226	Total	C	N	O	S	0	2	0
			1676	1057	281	331	7			
2	H	218	Total	C	N	O	S	0	3	0
			1624	1029	267	319	9			
2	K	218	Total	C	N	O	S	0	0	0
			1610	1020	267	316	7			
2	N	226	Total	C	N	O	S	0	2	0
			1663	1048	278	330	7			
2	Q	218	Total	C	N	O	S	0	2	0
			1618	1026	268	317	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	225	Total	C	N	O	S	0	2	0
			1654	1047	273	327	7			
2	W	220	Total	C	N	O	S	0	1	0
			1624	1029	267	321	7			

- Molecule 3 is a protein called Tudor domain-containing protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	60	Total	C	N	O	S	0	0	0
			482	316	71	92	3			
3	F	53	Total	C	N	O	S	0	1	0
			434	285	64	83	2			
3	I	55	Total	C	N	O	S	0	0	0
			436	286	64	84	2			
3	L	54	Total	C	N	O	S	0	0	0
			423	275	63	83	2			
3	O	61	Total	C	N	O	S	0	1	0
			482	315	70	95	2			
3	R	61	Total	C	N	O	S	0	1	0
			488	321	70	93	4			
3	U	54	Total	C	N	O	S	0	0	0
			433	284	66	81	2			
3	X	53	Total	C	N	O	S	0	1	0
			404	266	61	75	2			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	539	GLY	-	EXPRESSION TAG	UNP Q9H7E2
F	539	GLY	-	EXPRESSION TAG	UNP Q9H7E2
I	539	GLY	-	EXPRESSION TAG	UNP Q9H7E2
L	539	GLY	-	EXPRESSION TAG	UNP Q9H7E2
O	539	GLY	-	EXPRESSION TAG	UNP Q9H7E2
R	539	GLY	-	EXPRESSION TAG	UNP Q9H7E2
U	539	GLY	-	EXPRESSION TAG	UNP Q9H7E2
X	539	GLY	-	EXPRESSION TAG	UNP Q9H7E2

- Molecule 4 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	11	Total	X	0	0
			11	11		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	9	Total X 9 9	0	0
4	J	7	Total X 7 7	0	0
4	Q	8	Total X 8 8	0	0
4	D	5	Total X 5 5	0	0
4	K	6	Total X 6 6	0	0
4	E	11	Total X 11 11	0	0
4	H	16	Total X 16 16	0	0
4	B	12	Total X 12 12	0	0
4	I	1	Total X 1 1	0	0
4	C	2	Total X 2 2	0	0
4	V	7	Total X 7 7	0	0
4	W	10	Total X 10 10	0	0
4	A	7	Total X 7 7	0	0
4	T	12	Total X 12 12	0	0
4	N	12	Total X 12 12	0	0
4	R	1	Total X 1 1	0	0
4	S	2	Total X 2 2	0	0
4	F	1	Total X 1 1	0	0
4	M	3	Total X 3 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	69	Total O 69 69	0	0
5	B	111	Total O 111 111	0	0
5	C	13	Total O 13 13	0	0
5	D	51	Total O 51 51	0	0
5	E	107	Total O 107 107	0	0
5	F	2	Total O 2 2	0	0
5	G	52	Total O 52 52	0	0
5	H	82	Total O 82 82	0	0
5	I	8	Total O 8 8	0	0
5	J	60	Total O 60 60	0	0
5	K	89	Total O 89 89	0	0
5	L	2	Total O 2 2	0	0
5	M	55	Total O 55 55	0	0
5	N	104	Total O 104 104	0	0
5	O	7	Total O 7 7	0	0
5	P	60	Total O 60 60	0	0
5	Q	106	Total O 106 106	0	0
5	R	14	Total O 14 14	0	0
5	S	45	Total O 45 45	0	0
5	T	108	Total O 108 108	0	0
5	U	6	Total O 6 6	0	0
5	V	42	Total O 42 42	0	0

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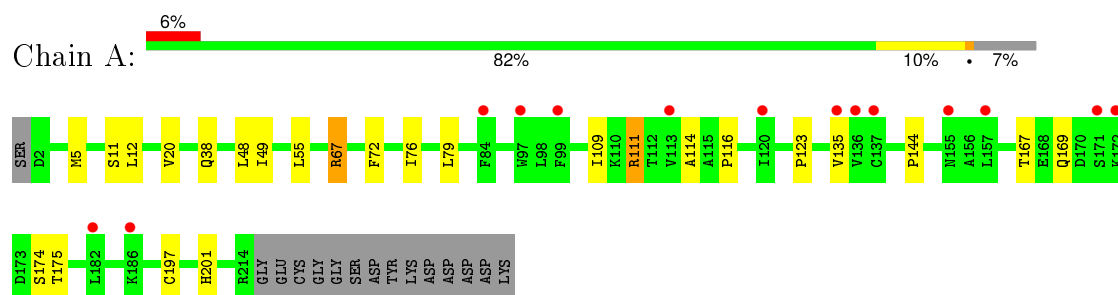
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	W	81	Total	O	0	0
			81	81		
5	X	1	Total	O	0	0
			1	1		

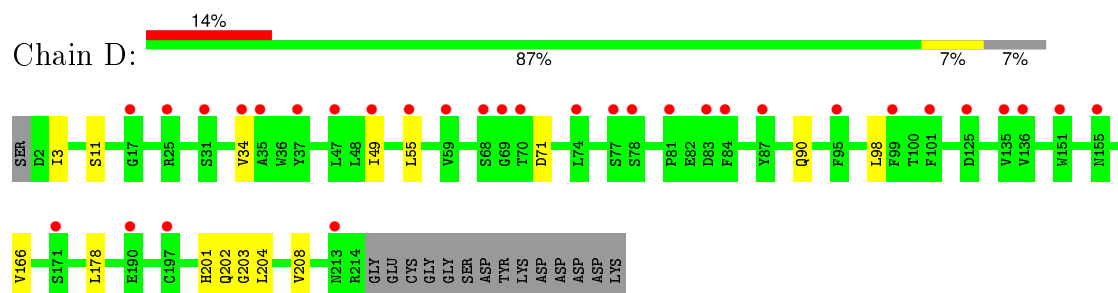
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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.

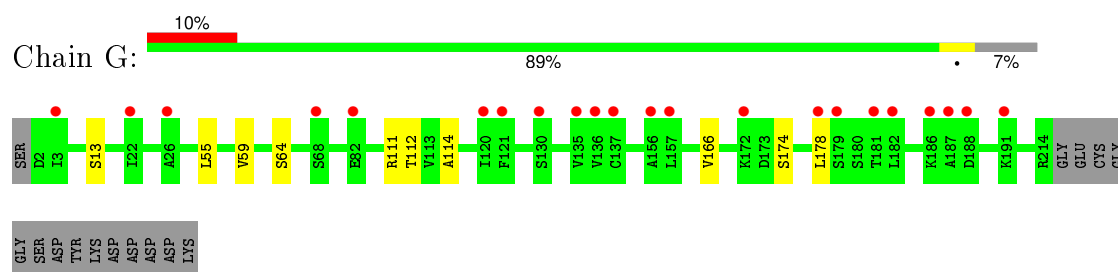
- Molecule 1: FAB light chain



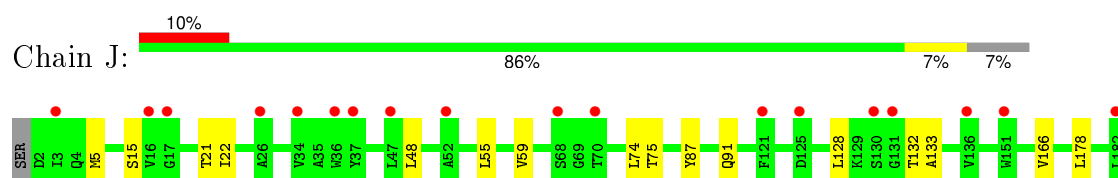
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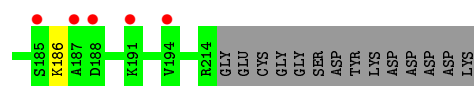


- Molecule 1: FAB light chain

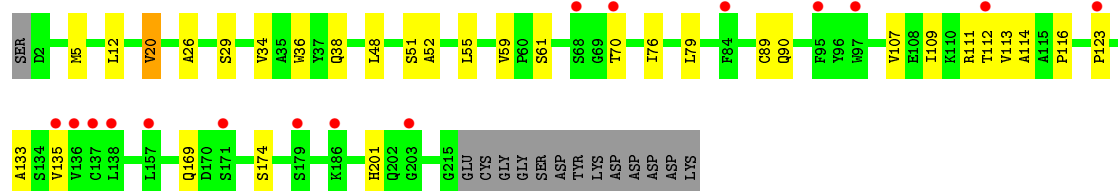
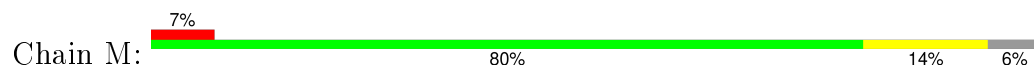


- Molecule 1: FAB light chain

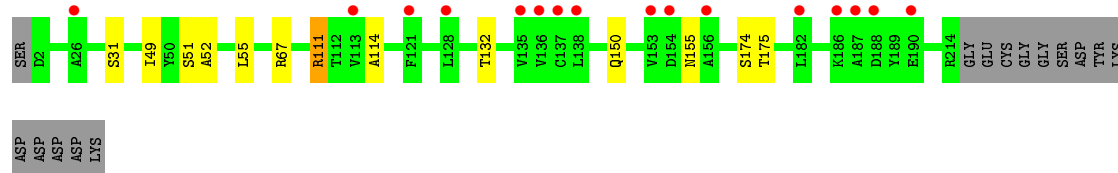
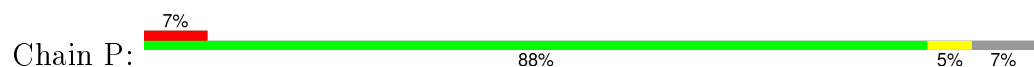




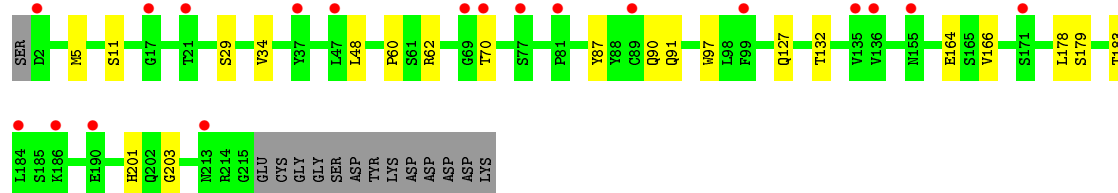
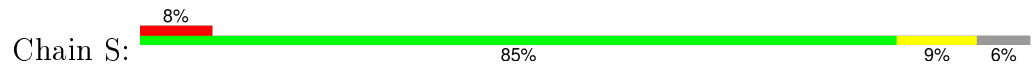
- Molecule 1: FAB light chain



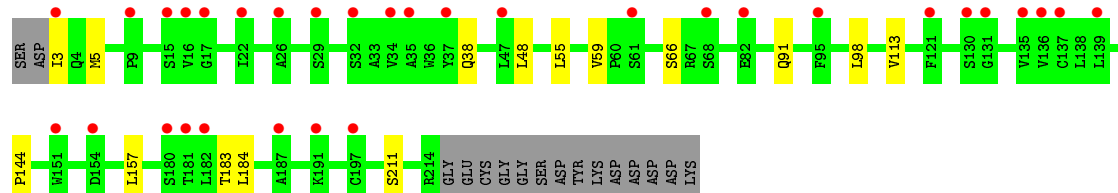
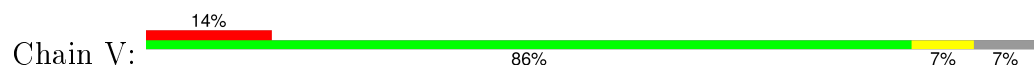
- Molecule 1: FAB light chain



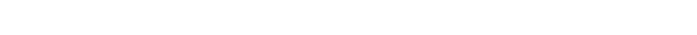
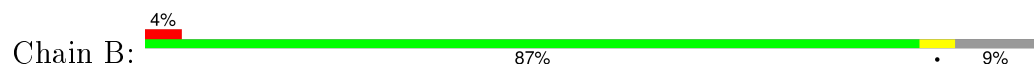
- Molecule 1: FAB light chain

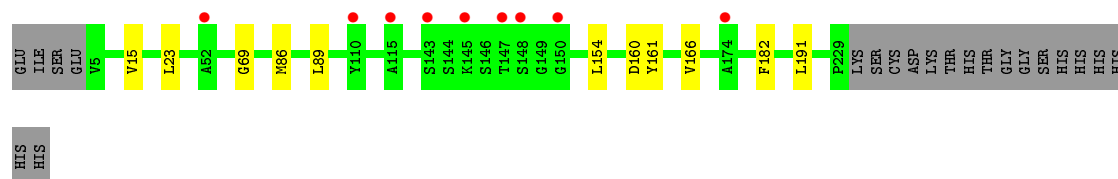


- Molecule 1: FAB light chain

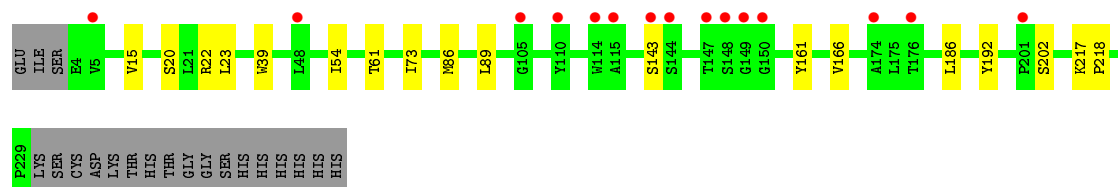
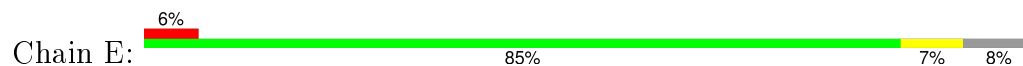


- Molecule 2: FAB heavy chain

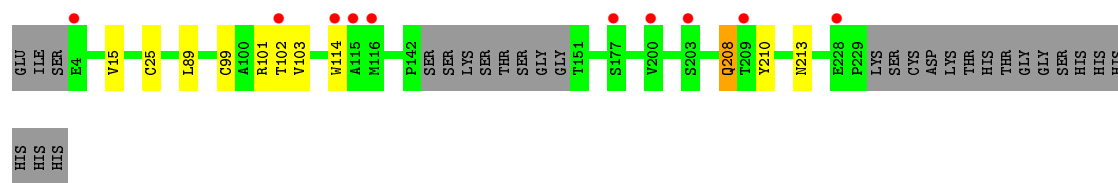
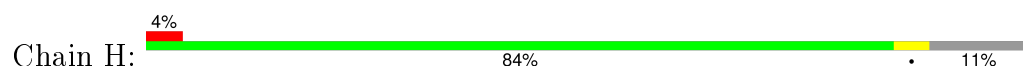




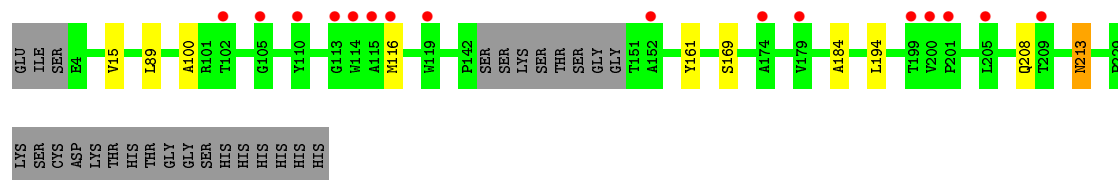
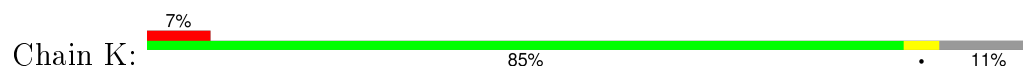
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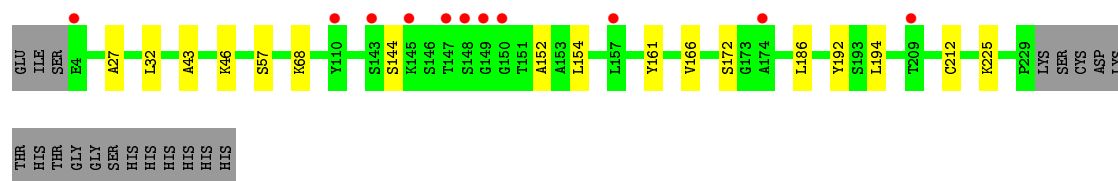
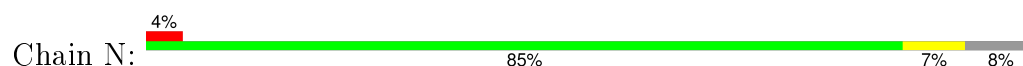
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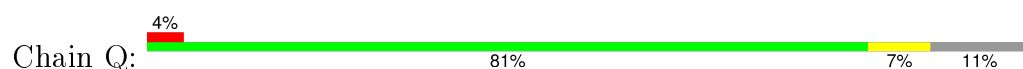
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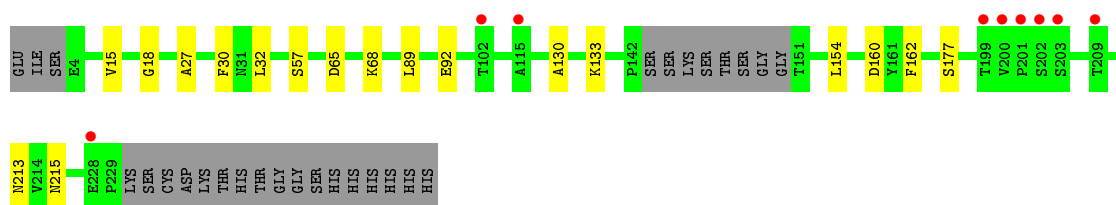


- Molecule 2: FAB heavy chain

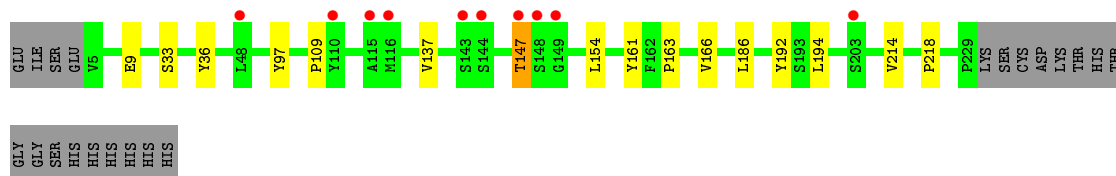
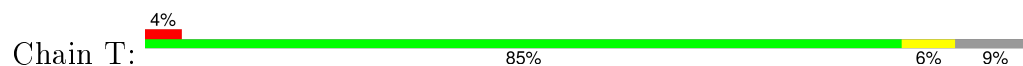


- Molecule 2: FAB heavy chain

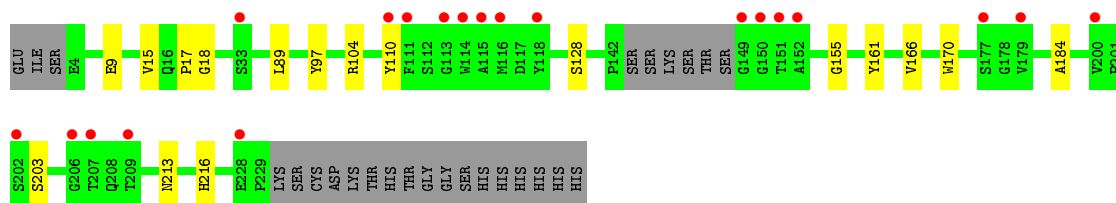
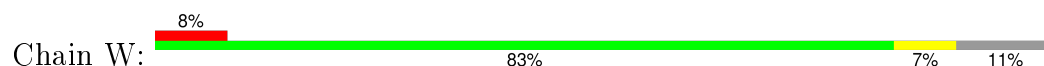




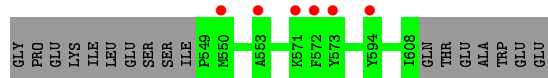
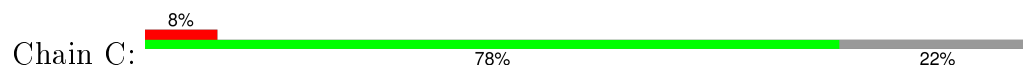
- Molecule 2: FAB heavy chain



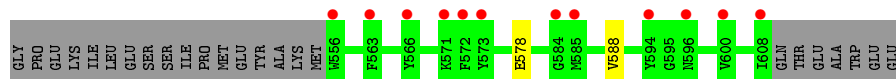
- Molecule 2: FAB heavy chain



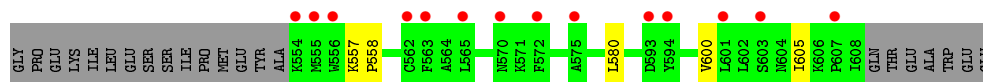
- Molecule 3: Tudor domain-containing protein 3



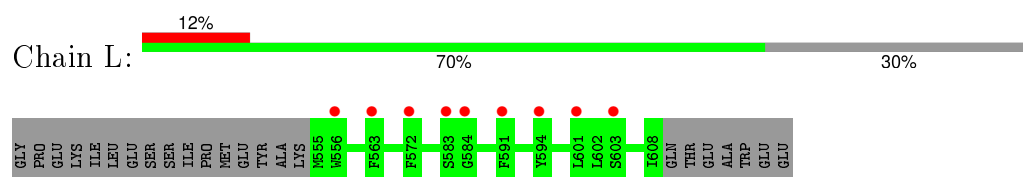
- Molecule 3: Tudor domain-containing protein 3



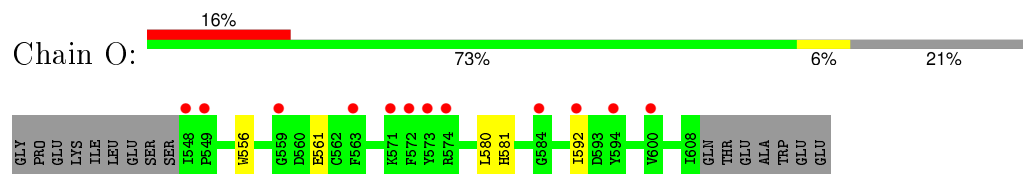
- Molecule 3: Tudor domain-containing protein 3



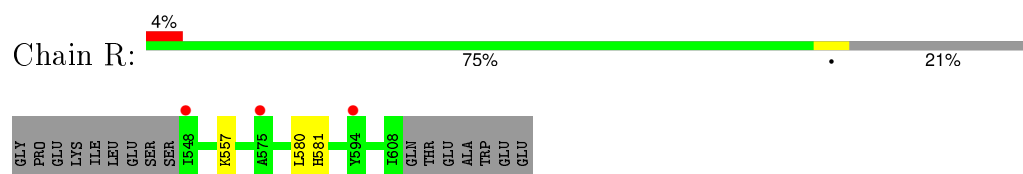
- Molecule 3: Tudor domain-containing protein 3



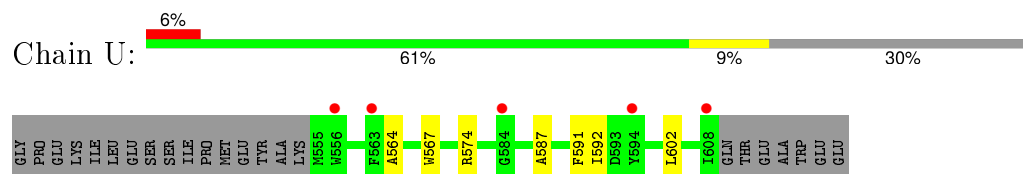
- Molecule 3: Tudor domain-containing protein 3



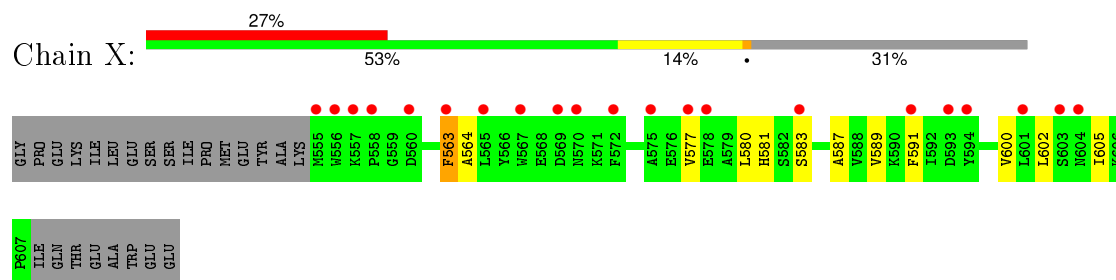
- Molecule 3: Tudor domain-containing protein 3



- Molecule 3: Tudor domain-containing protein 3



- Molecule 3: Tudor domain-containing protein 3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.71Å 93.73Å 159.93Å 80.96° 82.82° 90.06°	Depositor
Resolution (Å)	30.00 – 2.05 30.00 – 2.05	Depositor EDS
% Data completeness (in resolution range)	97.2 (30.00-2.05) 92.6 (30.00-2.05)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.98 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.223 , 0.264 0.231 , 0.271	Depositor DCC
$R_{free}$ test set	2162 reflections (0.82%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.3	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 44.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 266095 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	31176	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 58.12 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.1425e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: UNX

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	0.63	0/1690	0.61	0/2305
1	D	0.63	0/1667	0.61	0/2274
1	G	0.63	0/1693	0.60	0/2307
1	J	0.59	0/1679	0.60	0/2288
1	M	0.63	0/1702	0.61	0/2320
1	P	0.62	0/1698	0.61	0/2315
1	S	0.61	0/1684	0.57	0/2297
1	V	0.62	0/1646	0.60	0/2246
2	B	0.73	0/1692	0.69	0/2312
2	E	0.72	0/1724	0.66	0/2352
2	H	0.74	0/1674	0.70	0/2286
2	K	0.67	0/1651	0.66	0/2256
2	N	0.75	0/1711	0.68	0/2338
2	Q	0.75	0/1665	0.70	0/2275
2	T	0.71	0/1702	0.66	0/2326
2	W	0.76	0/1668	0.66	0/2278
3	C	0.62	0/497	0.56	0/675
3	F	0.56	0/450	0.50	0/612
3	I	0.61	0/449	0.55	0/612
3	L	0.52	0/435	0.49	0/594
3	O	0.59	0/500	0.51	0/683
3	R	0.61	0/506	0.54	0/689
3	U	0.55	0/446	0.51	0/607
3	X	0.61	0/419	0.53	0/573
All	All	0.67	0/30648	0.63	0/41820

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 ⓘ

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	1639	0	1543	17	0
1	D	1619	0	1509	6	0
1	G	1639	0	1559	7	0
1	J	1632	0	1551	11	0
1	M	1648	0	1574	20	0
1	P	1645	0	1559	7	0
1	S	1633	0	1534	13	0
1	V	1602	0	1499	8	0
2	B	1650	0	1573	6	0
2	E	1676	0	1617	12	0
2	H	1624	0	1554	6	0
2	K	1610	0	1537	5	0
2	N	1663	0	1587	9	0
2	Q	1618	0	1552	9	0
2	T	1654	0	1578	9	0
2	W	1624	0	1550	8	0
3	C	482	0	442	0	0
3	F	434	0	400	1	0
3	I	436	0	389	4	0
3	L	423	0	376	0	0
3	O	482	0	417	3	0
3	R	488	0	438	3	0
3	U	433	0	394	4	0
3	X	404	0	352	9	0
4	A	7	0	0	0	0
4	B	12	0	0	0	0
4	C	2	0	0	0	0
4	D	5	0	0	0	0
4	E	11	0	0	2	0
4	F	1	0	0	0	0
4	G	9	0	0	2	0
4	H	16	0	0	0	0
4	I	1	0	0	0	0
4	J	7	0	0	0	0
4	K	6	0	0	0	0
4	M	3	0	0	0	0
4	N	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	P	11	0	0	0	0
4	Q	8	0	0	0	0
4	R	1	0	0	0	0
4	S	2	0	0	0	0
4	T	12	0	0	0	0
4	V	7	0	0	0	0
4	W	10	0	0	0	0
5	A	69	0	0	0	0
5	B	111	0	0	1	0
5	C	13	0	0	0	0
5	D	51	0	0	0	0
5	E	107	0	0	1	0
5	F	2	0	0	0	0
5	G	52	0	0	0	0
5	H	82	0	0	0	0
5	I	8	0	0	0	0
5	J	60	0	0	0	0
5	K	89	0	0	0	0
5	L	2	0	0	0	0
5	M	55	0	0	0	0
5	N	104	0	0	1	0
5	O	7	0	0	0	0
5	P	60	0	0	0	0
5	Q	106	0	0	0	0
5	R	14	0	0	0	0
5	S	45	0	0	0	0
5	T	108	0	0	0	0
5	U	6	0	0	0	0
5	V	42	0	0	0	0
5	W	81	0	0	0	0
5	X	1	0	0	0	0
All	All	31176	0	28084	168	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.

The worst 5 of 168 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:E:143:SER:OG	4:E:1814:UNX:UNK	1.42	0.99
1:G:64:SER:OG	4:G:1820:UNX:UNK	1.48	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:29:SER:CB	1:S:70:THR:HG22	2.23	0.69
2:E:143:SER:HG	4:E:1814:UNX:UNK	1.35	0.68
1:M:12[B]:LEU:HD23	1:M:107:VAL:HG13	1.74	0.67

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	215/228 (94%)	209 (97%)	6 (3%)	0	100	100
1	D	213/228 (93%)	204 (96%)	9 (4%)	0	100	100
1	G	215/228 (94%)	204 (95%)	11 (5%)	0	100	100
1	J	213/228 (93%)	204 (96%)	9 (4%)	0	100	100
1	M	216/228 (95%)	208 (96%)	8 (4%)	0	100	100
1	P	215/228 (94%)	205 (95%)	10 (5%)	0	100	100
1	S	215/228 (94%)	203 (94%)	12 (6%)	0	100	100
1	V	211/228 (92%)	201 (95%)	10 (5%)	0	100	100
2	B	223/246 (91%)	220 (99%)	3 (1%)	0	100	100
2	E	226/246 (92%)	222 (98%)	4 (2%)	0	100	100
2	H	217/246 (88%)	212 (98%)	5 (2%)	0	100	100
2	K	214/246 (87%)	209 (98%)	5 (2%)	0	100	100
2	N	226/246 (92%)	223 (99%)	3 (1%)	0	100	100
2	Q	216/246 (88%)	213 (99%)	3 (1%)	0	100	100
2	T	225/246 (92%)	222 (99%)	3 (1%)	0	100	100
2	W	217/246 (88%)	212 (98%)	5 (2%)	0	100	100
3	C	58/77 (75%)	58 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	F	52/77 (68%)	52 (100%)	0	0	100	100
3	I	53/77 (69%)	53 (100%)	0	0	100	100
3	L	52/77 (68%)	52 (100%)	0	0	100	100
3	O	60/77 (78%)	59 (98%)	1 (2%)	0	100	100
3	R	60/77 (78%)	60 (100%)	0	0	100	100
3	U	52/77 (68%)	52 (100%)	0	0	100	100
3	X	52/77 (68%)	50 (96%)	2 (4%)	0	100	100
All	All	3916/4408 (89%)	3807 (97%)	109 (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	A	175/200 (88%)	170 (97%)	5 (3%)	50	42
1	D	173/200 (86%)	170 (98%)	3 (2%)	68	65
1	G	182/200 (91%)	181 (100%)	1 (0%)	92	92
1	J	182/200 (91%)	181 (100%)	1 (0%)	92	92
1	M	181/200 (90%)	179 (99%)	2 (1%)	80	79
1	P	182/200 (91%)	178 (98%)	4 (2%)	60	53
1	S	174/200 (87%)	173 (99%)	1 (1%)	90	90
1	V	171/200 (86%)	169 (99%)	2 (1%)	78	76
2	B	180/205 (88%)	179 (99%)	1 (1%)	90	90
2	E	184/205 (90%)	183 (100%)	1 (0%)	92	92
2	H	178/205 (87%)	176 (99%)	2 (1%)	80	79
2	K	174/205 (85%)	172 (99%)	2 (1%)	80	79
2	N	181/205 (88%)	179 (99%)	2 (1%)	80	79
2	Q	176/205 (86%)	171 (97%)	5 (3%)	51	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	T	178/205 (87%)	175 (98%)	3 (2%)	68	65
2	W	175/205 (85%)	173 (99%)	2 (1%)	80	79
3	C	49/67 (73%)	49 (100%)	0	100	100
3	F	45/67 (67%)	45 (100%)	0	100	100
3	I	43/67 (64%)	43 (100%)	0	100	100
3	L	42/67 (63%)	42 (100%)	0	100	100
3	O	46/67 (69%)	46 (100%)	0	100	100
3	R	48/67 (72%)	48 (100%)	0	100	100
3	U	43/67 (64%)	43 (100%)	0	100	100
3	X	37/67 (55%)	36 (97%)	1 (3%)	52	45
All	All	3199/3776 (85%)	3161 (99%)	38 (1%)	78	76

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	61	SER
1	P	132	THR
2	W	203	SER
2	N	194	LEU
1	P	150	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	215	ASN
2	E	85	GLN
2	E	87	ASN
2	K	180	HIS

### 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](#)

Of 143 ligands modelled in this entry, 143 are unknown - 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 [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 ⓘ

### 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	A	213/228 (93%)	0.48	14 (6%) 22 24	34, 57, 74, 78	0
1	D	213/228 (93%)	0.86	32 (15%) 3 3	44, 63, 88, 98	0
1	G	213/228 (93%)	0.61	22 (10%) 9 9	40, 57, 79, 90	0
1	J	213/228 (93%)	0.74	23 (10%) 8 9	41, 62, 85, 93	0
1	M	214/228 (93%)	0.67	16 (7%) 17 20	41, 61, 76, 88	0
1	P	213/228 (93%)	0.48	16 (7%) 17 20	36, 54, 78, 90	0
1	S	214/228 (93%)	0.69	19 (8%) 12 13	42, 61, 84, 93	0
1	V	212/228 (92%)	0.85	32 (15%) 3 3	41, 61, 82, 90	0
2	B	225/246 (91%)	0.18	9 (4%) 42 48	31, 42, 58, 68	0
2	E	226/246 (91%)	0.29	15 (6%) 22 24	32, 46, 73, 86	0
2	H	218/246 (88%)	0.33	10 (4%) 36 41	32, 44, 65, 78	0
2	K	218/246 (88%)	0.29	16 (7%) 18 21	31, 45, 70, 84	0
2	N	226/246 (91%)	0.21	11 (4%) 33 38	32, 43, 61, 75	0
2	Q	218/246 (88%)	0.23	9 (4%) 41 47	29, 43, 60, 71	0
2	T	225/246 (91%)	0.18	10 (4%) 38 43	32, 44, 67, 80	0
2	W	220/246 (89%)	0.34	20 (9%) 11 12	32, 46, 71, 85	0
3	C	60/77 (77%)	0.26	6 (10%) 9 10	40, 57, 82, 86	0
3	F	53/77 (68%)	1.07	12 (22%) 1 1	57, 81, 102, 110	0
3	I	55/77 (71%)	1.12	14 (25%) 1 0	49, 70, 98, 103	0
3	L	54/77 (70%)	0.87	9 (16%) 2 2	50, 81, 119, 126	0
3	O	61/77 (79%)	1.06	12 (19%) 1 1	50, 74, 103, 111	0
3	R	61/77 (79%)	0.20	3 (4%) 33 38	40, 58, 85, 95	0
3	U	54/77 (70%)	0.72	5 (9%) 11 12	45, 72, 98, 105	0
3	X	53/77 (68%)	1.89	21 (39%) 0 0	60, 91, 120, 130	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
All	All	3932/4408 (89%)	0.51	356 (9%)	11 12	29, 53, 84, 130	0

The worst 5 of 356 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	608	ILE	6.0
2	E	147	THR	5.9
1	G	187	ALA	5.8
3	I	594	TYR	5.8
3	X	575	ALA	5.6

## 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(Å <sup>2</sup> )	Q<0.9
4	UNX	N	1822	1/1	0.94	0.35	13.36	30,30,30,30	0
4	UNX	B	1906	1/1	0.94	0.18	8.78	30,30,30,30	0
4	UNX	B	1946	1/1	0.87	0.27	7.85	30,30,30,30	0
4	UNX	B	1872	1/1	0.98	0.35	7.51	30,30,30,30	0
4	UNX	W	1857	1/1	0.94	0.20	7.27	30,30,30,30	0
4	UNX	J	1866	1/1	0.83	0.26	6.97	30,30,30,30	0
4	UNX	J	1821	1/1	0.91	0.30	6.67	30,30,30,30	0
4	UNX	B	1889	1/1	0.71	0.34	5.86	30,30,30,30	0
4	UNX	J	1867	1/1	0.96	0.39	5.16	30,30,30,30	0
4	UNX	P	1886	1/1	0.78	0.19	5.06	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	UNX	B	1875	1/1	0.73	0.18	4.02	30,30,30,30	0
4	UNX	Q	1835	1/1	0.94	0.26	3.30	30,30,30,30	0
4	UNX	G	1885	1/1	0.95	0.32	3.29	30,30,30,30	0
4	UNX	T	1890	1/1	0.88	0.18	3.06	30,30,30,30	0
4	UNX	P	1832	1/1	0.97	0.18	3.03	30,30,30,30	0
4	UNX	M	1852	1/1	0.96	0.18	2.86	30,30,30,30	0
4	UNX	H	1887	1/1	0.96	0.12	2.40	30,30,30,30	0
4	UNX	V	1971	1/1	0.94	0.30	2.09	30,30,30,30	0
4	UNX	G	1824	1/1	0.78	0.14	2.05	30,30,30,30	0
4	UNX	T	1865	1/1	0.96	0.16	2.00	30,30,30,30	0
4	UNX	V	1879	1/1	0.91	0.19	1.91	30,30,30,30	0
4	UNX	H	1850	1/1	0.97	0.25	1.76	30,30,30,30	0
4	UNX	E	1815	1/1	0.96	0.39	1.56	30,30,30,30	0
4	UNX	H	1963	1/1	0.90	0.23	1.42	30,30,30,30	0
4	UNX	G	1829	1/1	0.96	0.20	1.31	30,30,30,30	0
4	UNX	B	1871	1/1	0.88	0.17	1.30	30,30,30,30	0
4	UNX	Q	1926	1/1	0.95	0.15	1.30	30,30,30,30	0
4	UNX	E	1893	1/1	0.88	0.15	1.27	30,30,30,30	0
4	UNX	J	1816	1/1	0.96	0.25	1.24	30,30,30,30	0
4	UNX	E	1942	1/1	0.95	0.17	1.16	30,30,30,30	0
4	UNX	T	1830	1/1	0.92	0.23	1.11	30,30,30,30	0
4	UNX	D	1939	1/1	0.90	0.18	1.02	30,30,30,30	0
4	UNX	A	1843	1/1	0.98	0.14	1.01	30,30,30,30	0
4	UNX	P	1828	1/1	0.96	0.15	1.00	30,30,30,30	0
4	UNX	A	1956	1/1	0.94	0.13	0.99	30,30,30,30	0
4	UNX	B	1949	1/1	0.87	0.12	0.97	30,30,30,30	0
4	UNX	H	1870	1/1	0.86	0.15	0.76	30,30,30,30	0
4	UNX	J	1936	1/1	0.82	0.13	0.73	30,30,30,30	0
4	UNX	G	1916	1/1	0.88	0.21	0.56	30,30,30,30	0
4	UNX	N	1899	1/1	0.92	0.15	0.53	30,30,30,30	0
4	UNX	T	1910	1/1	0.91	0.17	0.49	30,30,30,30	0
4	UNX	K	1849	1/1	0.97	0.12	0.42	30,30,30,30	0
4	UNX	N	1877	1/1	0.96	0.20	0.27	30,30,30,30	0
4	UNX	W	1883	1/1	0.88	0.23	0.13	30,30,30,30	0
4	UNX	W	1874	1/1	0.87	0.11	0.04	30,30,30,30	0
4	UNX	J	1908	1/1	0.75	0.11	-0.22	30,30,30,30	0
4	UNX	E	1965	1/1	0.95	0.23	-0.37	30,30,30,30	0
4	UNX	Q	1861	1/1	0.92	0.13	-0.40	30,30,30,30	0
4	UNX	W	1862	1/1	0.96	0.10	-0.44	30,30,30,30	0
4	UNX	H	1839	1/1	0.93	0.12	-0.51	30,30,30,30	0
4	UNX	N	1894	1/1	0.86	0.12	-0.54	30,30,30,30	0
4	UNX	T	1921	1/1	0.96	0.12	-0.65	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	UNX	H	1920	1/1	0.90	0.11	-0.67	30,30,30,30	0
4	UNX	B	1844	1/1	0.96	0.14	-0.69	30,30,30,30	0
4	UNX	R	1896	1/1	0.86	0.10	-0.83	30,30,30,30	0
4	UNX	I	1819	1/1	0.88	0.12	-0.87	30,30,30,30	0
4	UNX	H	1948	1/1	0.91	0.11	-0.89	30,30,30,30	0
4	UNX	T	1848	1/1	0.85	0.12	-0.90	30,30,30,30	0
4	UNX	C	1873	1/1	0.95	0.09	-0.93	30,30,30,30	0
4	UNX	W	1845	1/1	0.93	0.09	-1.16	30,30,30,30	0
4	UNX	K	1882	1/1	0.94	0.09	-1.21	30,30,30,30	0
4	UNX	J	1868	1/1	0.94	0.10	-1.23	30,30,30,30	0
4	UNX	Q	1842	1/1	0.97	0.08	-1.33	30,30,30,30	0
4	UNX	B	1947	1/1	0.94	0.11	-1.35	30,30,30,30	0
4	UNX	A	1860	1/1	0.96	0.08	-1.36	30,30,30,30	0
4	UNX	M	1966	1/1	0.93	0.10	-1.42	30,30,30,30	0
4	UNX	P	1903	1/1	0.94	0.11	-1.58	30,30,30,30	0
4	UNX	A	1859	1/1	0.97	0.11	-1.63	30,30,30,30	0
4	UNX	V	1841	1/1	0.98	0.07	-1.68	30,30,30,30	0
4	UNX	V	1964	1/1	0.95	0.09	-1.85	30,30,30,30	0
4	UNX	G	1820	1/1	0.95	0.09	-1.93	30,30,30,30	0
4	UNX	P	1851	1/1	0.98	0.07	-2.06	30,30,30,30	0
4	UNX	W	1913	1/1	0.88	0.07	-2.24	30,30,30,30	0
4	UNX	K	1888	1/1	0.89	0.10	-2.28	30,30,30,30	0
4	UNX	D	1925	1/1	0.95	0.07	-2.35	30,30,30,30	0
4	UNX	N	1876	1/1	0.98	0.08	-2.46	30,30,30,30	0
4	UNX	H	1941	1/1	0.94	0.09	-2.57	30,30,30,30	0
4	UNX	D	1834	1/1	0.96	0.07	-2.91	30,30,30,30	0
4	UNX	P	1934	1/1	0.93	0.08	-3.53	30,30,30,30	0
4	UNX	E	1904	1/1	0.92	0.07	-3.62	30,30,30,30	0
4	UNX	W	1951	1/1	0.84	0.24	-	30,30,30,30	0
4	UNX	H	1954	1/1	0.86	0.27	-	30,30,30,30	0
4	UNX	N	1969	1/1	0.83	0.10	-	30,30,30,30	0
4	UNX	B	1927	1/1	0.95	0.14	-	30,30,30,30	0
4	UNX	S	1864	1/1	0.90	0.19	-	30,30,30,30	0
4	UNX	P	1827	1/1	0.92	0.11	-	30,30,30,30	0
4	UNX	W	1884	1/1	0.91	0.08	-	30,30,30,30	0
4	UNX	H	1900	1/1	0.95	0.07	-	30,30,30,30	0
4	UNX	H	1944	1/1	0.78	0.21	-	30,30,30,30	0
4	UNX	D	1881	1/1	0.95	0.08	-	30,30,30,30	0
4	UNX	N	1937	1/1	0.93	0.16	-	30,30,30,30	0
4	UNX	K	1891	1/1	0.89	0.08	-	30,30,30,30	0
4	UNX	T	1924	1/1	0.96	0.22	-	30,30,30,30	0
4	UNX	M	1952	1/1	0.92	0.16	-	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	UNX	T	1898	1/1	0.85	0.11	-	30,30,30,30	0
4	UNX	H	1953	1/1	0.98	0.16	-	30,30,30,30	0
4	UNX	T	1846	1/1	0.97	0.04	-	30,30,30,30	0
4	UNX	G	1918	1/1	0.90	0.16	-	30,30,30,30	0
4	UNX	H	1919	1/1	0.87	0.11	-	30,30,30,30	0
4	UNX	E	1897	1/1	0.97	0.08	-	30,30,30,30	0
4	UNX	B	1914	1/1	0.83	0.21	-	30,30,30,30	0
4	UNX	W	1854	1/1	0.95	0.08	-	30,30,30,30	0
4	UNX	T	1928	1/1	0.88	0.24	-	30,30,30,30	0
4	UNX	V	1932	1/1	0.98	0.09	-	30,30,30,30	0
4	UNX	A	1972	1/1	0.88	0.19	-	30,30,30,30	0
4	UNX	T	1940	1/1	0.96	0.22	-	30,30,30,30	0
4	UNX	Q	1901	1/1	0.84	0.14	-	30,30,30,30	0
4	UNX	V	1856	1/1	0.95	0.19	-	30,30,30,30	0
4	UNX	P	1826	1/1	0.91	0.07	-	30,30,30,30	0
4	UNX	A	1950	1/1	0.95	0.11	-	30,30,30,30	0
4	UNX	N	1968	1/1	0.92	0.12	-	30,30,30,30	0
4	UNX	Q	1961	1/1	0.90	0.10	-	30,30,30,30	0
4	UNX	C	1855	1/1	0.81	0.12	-	30,30,30,30	0
4	UNX	S	1915	1/1	0.81	0.14	-	30,30,30,30	0
4	UNX	H	1858	1/1	0.97	0.12	-	30,30,30,30	0
4	UNX	H	1935	1/1	0.86	0.17	-	30,30,30,30	0
4	UNX	E	1814	1/1	0.89	0.31	-	30,30,30,30	0
4	UNX	K	1836	1/1	0.94	0.12	-	30,30,30,30	0
4	UNX	Q	1917	1/1	0.88	0.09	-	30,30,30,30	0
4	UNX	V	1823	1/1	0.80	0.12	-	30,30,30,30	0
4	UNX	P	1817	1/1	0.93	0.06	-	30,30,30,30	0
4	UNX	N	1958	1/1	0.90	0.13	-	30,30,30,30	0
4	UNX	G	1880	1/1	0.93	0.18	-	30,30,30,30	0
4	UNX	N	1938	1/1	0.87	0.19	-	30,30,30,30	0
4	UNX	E	1905	1/1	0.85	0.16	-	30,30,30,30	0
4	UNX	P	1929	1/1	0.95	0.09	-	30,30,30,30	0
4	UNX	H	1962	1/1	0.80	0.21	-	30,30,30,30	0
4	UNX	E	1957	1/1	0.95	0.11	-	30,30,30,30	0
4	UNX	N	1967	1/1	0.94	0.12	-	30,30,30,30	0
4	UNX	B	1902	1/1	0.94	0.08	-	30,30,30,30	0
4	UNX	G	1931	1/1	0.94	0.11	-	30,30,30,30	0
4	UNX	K	1863	1/1	0.98	0.05	-	30,30,30,30	0
4	UNX	A	1943	1/1	0.94	0.11	-	30,30,30,30	0
4	UNX	E	1923	1/1	0.97	0.11	-	30,30,30,30	0
4	UNX	F	1847	1/1	0.97	0.07	-	30,30,30,30	0
4	UNX	G	1818	1/1	0.88	0.10	-	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	UNX	W	1907	1/1	0.90	0.24	-	30,30,30,30	0
4	UNX	E	1945	1/1	0.95	0.14	-	30,30,30,30	0
4	UNX	P	1909	1/1	0.81	0.15	-	30,30,30,30	0
4	UNX	Q	1895	1/1	0.86	0.30	-	30,30,30,30	0
4	UNX	D	1955	1/1	0.81	0.18	-	30,30,30,30	0
4	UNX	T	1959	1/1	0.95	0.17	-	30,30,30,30	0
4	UNX	N	1878	1/1	0.85	0.13	-	30,30,30,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.