



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 11:45 am BST

PDB ID : 4GPK  
Title : Crystal structure of NprR in complex with its cognate peptide NprX  
Authors : Zouhir, S.; Guimaraes, B.; Perchat, S.; Nicaise, M.; Lereclus, D.; Nessler, S.  
Deposited on : 2012-08-21  
Resolution : 3.20 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

<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  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

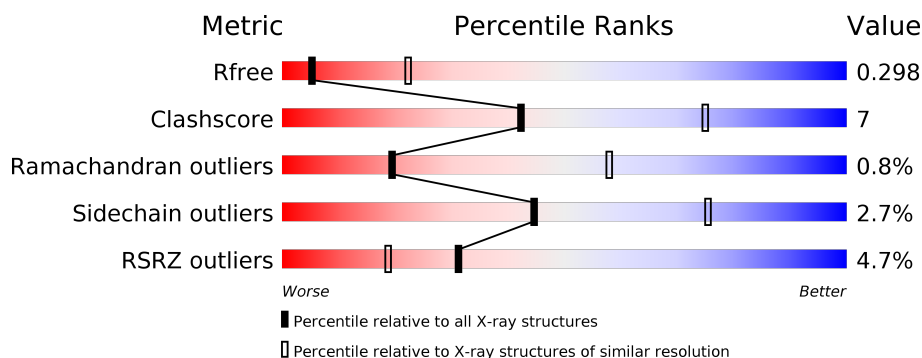
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 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	372	<div> <div>6%</div> <div> <div></div> <div>77%</div> <div>15%</div> <div>• 8%</div> </div> </div>
1	B	372	<div> <div>10%</div> <div> <div></div> <div>69%</div> <div>21%</div> <div>• 8%</div> </div> </div>
1	C	372	<div> <div>4%</div> <div> <div></div> <div>67%</div> <div>22%</div> <div>• 9%</div> </div> </div>
1	D	372	<div> <div>4%</div> <div> <div></div> <div>67%</div> <div>24%</div> <div>• 8%</div> </div> </div>
1	E	372	<div> <div>6%</div> <div> <div></div> <div>74%</div> <div>17%</div> <div>9%</div> </div> </div>
1	F	372	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>14%</div> <div>• 8%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	372	
1	H	372	
1	I	372	
1	J	372	
1	K	372	
1	L	372	
2	M	8	
2	N	8	
2	O	8	
2	P	8	
2	Q	8	
2	R	8	
2	S	8	
2	T	8	
2	U	8	
2	V	8	
2	W	8	
2	X	8	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 35360 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 NprR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	0	0	0
			2896	1882	465	535	14			
1	B	342	Total	C	N	O	S	0	0	0
			2882	1873	462	533	14			
1	C	340	Total	C	N	O	S	0	0	0
			2869	1869	460	526	14			
1	D	342	Total	C	N	O	S	0	0	0
			2883	1876	462	531	14			
1	E	339	Total	C	N	O	S	0	0	0
			2861	1863	459	525	14			
1	F	341	Total	C	N	O	S	0	0	0
			2875	1865	462	534	14			
1	G	345	Total	C	N	O	S	0	0	0
			2911	1893	465	539	14			
1	H	343	Total	C	N	O	S	0	0	0
			2895	1883	463	535	14			
1	I	344	Total	C	N	O	S	0	0	0
			2903	1889	464	536	14			
1	J	347	Total	C	N	O	S	0	0	0
			2929	1902	471	542	14			
1	K	340	Total	C	N	O	S	0	0	0
			2866	1863	460	529	14			
1	L	346	Total	C	N	O	S	0	0	0
			2918	1896	467	541	14			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	MET	-	INITIATING METHIONINE	UNP G5DDY8
A	424	ARG	-	EXPRESSION TAG	UNP G5DDY8
A	425	SER	-	EXPRESSION TAG	UNP G5DDY8
A	426	HIS	-	EXPRESSION TAG	UNP G5DDY8
A	427	HIS	-	EXPRESSION TAG	UNP G5DDY8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	428	HIS	-	EXPRESSION TAG	UNP G5DDY8
A	429	HIS	-	EXPRESSION TAG	UNP G5DDY8
A	430	HIS	-	EXPRESSION TAG	UNP G5DDY8
A	431	HIS	-	EXPRESSION TAG	UNP G5DDY8
B	60	MET	-	INITIATING METHIONINE	UNP G5DDY8
B	424	ARG	-	EXPRESSION TAG	UNP G5DDY8
B	425	SER	-	EXPRESSION TAG	UNP G5DDY8
B	426	HIS	-	EXPRESSION TAG	UNP G5DDY8
B	427	HIS	-	EXPRESSION TAG	UNP G5DDY8
B	428	HIS	-	EXPRESSION TAG	UNP G5DDY8
B	429	HIS	-	EXPRESSION TAG	UNP G5DDY8
B	430	HIS	-	EXPRESSION TAG	UNP G5DDY8
B	431	HIS	-	EXPRESSION TAG	UNP G5DDY8
C	60	MET	-	INITIATING METHIONINE	UNP G5DDY8
C	424	ARG	-	EXPRESSION TAG	UNP G5DDY8
C	425	SER	-	EXPRESSION TAG	UNP G5DDY8
C	426	HIS	-	EXPRESSION TAG	UNP G5DDY8
C	427	HIS	-	EXPRESSION TAG	UNP G5DDY8
C	428	HIS	-	EXPRESSION TAG	UNP G5DDY8
C	429	HIS	-	EXPRESSION TAG	UNP G5DDY8
C	430	HIS	-	EXPRESSION TAG	UNP G5DDY8
C	431	HIS	-	EXPRESSION TAG	UNP G5DDY8
D	60	MET	-	INITIATING METHIONINE	UNP G5DDY8
D	424	ARG	-	EXPRESSION TAG	UNP G5DDY8
D	425	SER	-	EXPRESSION TAG	UNP G5DDY8
D	426	HIS	-	EXPRESSION TAG	UNP G5DDY8
D	427	HIS	-	EXPRESSION TAG	UNP G5DDY8
D	428	HIS	-	EXPRESSION TAG	UNP G5DDY8
D	429	HIS	-	EXPRESSION TAG	UNP G5DDY8
D	430	HIS	-	EXPRESSION TAG	UNP G5DDY8
D	431	HIS	-	EXPRESSION TAG	UNP G5DDY8
E	60	MET	-	INITIATING METHIONINE	UNP G5DDY8
E	424	ARG	-	EXPRESSION TAG	UNP G5DDY8
E	425	SER	-	EXPRESSION TAG	UNP G5DDY8
E	426	HIS	-	EXPRESSION TAG	UNP G5DDY8
E	427	HIS	-	EXPRESSION TAG	UNP G5DDY8
E	428	HIS	-	EXPRESSION TAG	UNP G5DDY8
E	429	HIS	-	EXPRESSION TAG	UNP G5DDY8
E	430	HIS	-	EXPRESSION TAG	UNP G5DDY8
E	431	HIS	-	EXPRESSION TAG	UNP G5DDY8
F	60	MET	-	INITIATING METHIONINE	UNP G5DDY8
F	424	ARG	-	EXPRESSION TAG	UNP G5DDY8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	425	SER	-	EXPRESSION TAG	UNP G5DDY8
F	426	HIS	-	EXPRESSION TAG	UNP G5DDY8
F	427	HIS	-	EXPRESSION TAG	UNP G5DDY8
F	428	HIS	-	EXPRESSION TAG	UNP G5DDY8
F	429	HIS	-	EXPRESSION TAG	UNP G5DDY8
F	430	HIS	-	EXPRESSION TAG	UNP G5DDY8
F	431	HIS	-	EXPRESSION TAG	UNP G5DDY8
G	60	MET	-	INITIATING METHIONINE	UNP G5DDY8
G	424	ARG	-	EXPRESSION TAG	UNP G5DDY8
G	425	SER	-	EXPRESSION TAG	UNP G5DDY8
G	426	HIS	-	EXPRESSION TAG	UNP G5DDY8
G	427	HIS	-	EXPRESSION TAG	UNP G5DDY8
G	428	HIS	-	EXPRESSION TAG	UNP G5DDY8
G	429	HIS	-	EXPRESSION TAG	UNP G5DDY8
G	430	HIS	-	EXPRESSION TAG	UNP G5DDY8
G	431	HIS	-	EXPRESSION TAG	UNP G5DDY8
H	60	MET	-	INITIATING METHIONINE	UNP G5DDY8
H	424	ARG	-	EXPRESSION TAG	UNP G5DDY8
H	425	SER	-	EXPRESSION TAG	UNP G5DDY8
H	426	HIS	-	EXPRESSION TAG	UNP G5DDY8
H	427	HIS	-	EXPRESSION TAG	UNP G5DDY8
H	428	HIS	-	EXPRESSION TAG	UNP G5DDY8
H	429	HIS	-	EXPRESSION TAG	UNP G5DDY8
H	430	HIS	-	EXPRESSION TAG	UNP G5DDY8
H	431	HIS	-	EXPRESSION TAG	UNP G5DDY8
I	60	MET	-	INITIATING METHIONINE	UNP G5DDY8
I	424	ARG	-	EXPRESSION TAG	UNP G5DDY8
I	425	SER	-	EXPRESSION TAG	UNP G5DDY8
I	426	HIS	-	EXPRESSION TAG	UNP G5DDY8
I	427	HIS	-	EXPRESSION TAG	UNP G5DDY8
I	428	HIS	-	EXPRESSION TAG	UNP G5DDY8
I	429	HIS	-	EXPRESSION TAG	UNP G5DDY8
I	430	HIS	-	EXPRESSION TAG	UNP G5DDY8
I	431	HIS	-	EXPRESSION TAG	UNP G5DDY8
J	60	MET	-	INITIATING METHIONINE	UNP G5DDY8
J	424	ARG	-	EXPRESSION TAG	UNP G5DDY8
J	425	SER	-	EXPRESSION TAG	UNP G5DDY8
J	426	HIS	-	EXPRESSION TAG	UNP G5DDY8
J	427	HIS	-	EXPRESSION TAG	UNP G5DDY8
J	428	HIS	-	EXPRESSION TAG	UNP G5DDY8
J	429	HIS	-	EXPRESSION TAG	UNP G5DDY8
J	430	HIS	-	EXPRESSION TAG	UNP G5DDY8

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Chain	Residue	Modelled	Actual	Comment	Reference
J	431	HIS	-	EXPRESSION TAG	UNP G5DDY8
K	60	MET	-	INITIATING METHIONINE	UNP G5DDY8
K	424	ARG	-	EXPRESSION TAG	UNP G5DDY8
K	425	SER	-	EXPRESSION TAG	UNP G5DDY8
K	426	HIS	-	EXPRESSION TAG	UNP G5DDY8
K	427	HIS	-	EXPRESSION TAG	UNP G5DDY8
K	428	HIS	-	EXPRESSION TAG	UNP G5DDY8
K	429	HIS	-	EXPRESSION TAG	UNP G5DDY8
K	430	HIS	-	EXPRESSION TAG	UNP G5DDY8
K	431	HIS	-	EXPRESSION TAG	UNP G5DDY8
L	60	MET	-	INITIATING METHIONINE	UNP G5DDY8
L	424	ARG	-	EXPRESSION TAG	UNP G5DDY8
L	425	SER	-	EXPRESSION TAG	UNP G5DDY8
L	426	HIS	-	EXPRESSION TAG	UNP G5DDY8
L	427	HIS	-	EXPRESSION TAG	UNP G5DDY8
L	428	HIS	-	EXPRESSION TAG	UNP G5DDY8
L	429	HIS	-	EXPRESSION TAG	UNP G5DDY8
L	430	HIS	-	EXPRESSION TAG	UNP G5DDY8
L	431	HIS	-	EXPRESSION TAG	UNP G5DDY8

- Molecule 2 is a protein called NprX peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	M	8	Total	C	N	O	0	0	0
			56	34	9	13			
2	N	8	Total	C	N	O	0	0	0
			56	34	9	13			
2	O	8	Total	C	N	O	0	0	0
			56	34	9	13			
2	P	8	Total	C	N	O	0	0	0
			56	34	9	13			
2	Q	8	Total	C	N	O	0	0	0
			56	34	9	13			
2	R	8	Total	C	N	O	0	0	0
			56	34	9	13			
2	S	8	Total	C	N	O	0	0	0
			56	34	9	13			
2	T	8	Total	C	N	O	0	0	0
			56	34	9	13			
2	U	8	Total	C	N	O	0	0	0
			56	34	9	13			
2	V	8	Total	C	N	O	0	0	0
			56	34	9	13			

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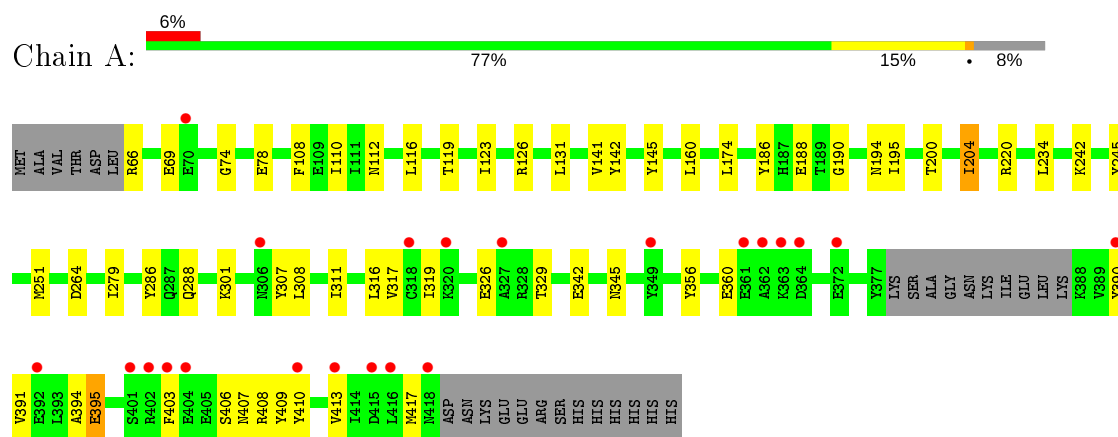
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	W	8	Total	C	N	O	0	0	0
			56	34	9	13			
2	X	8	Total	C	N	O	0	0	0
			56	34	9	13			

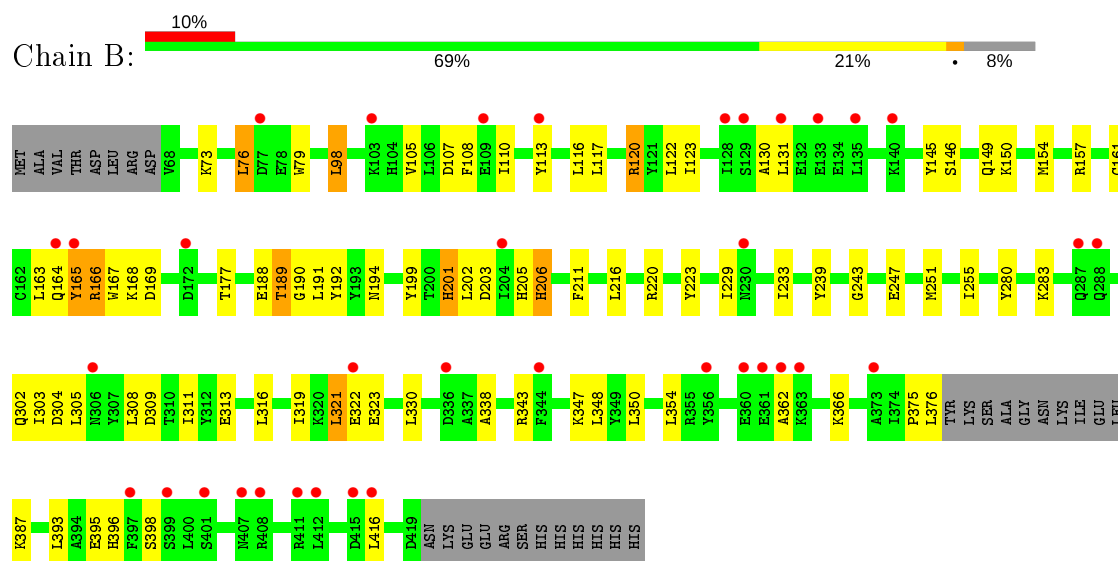
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: NprR

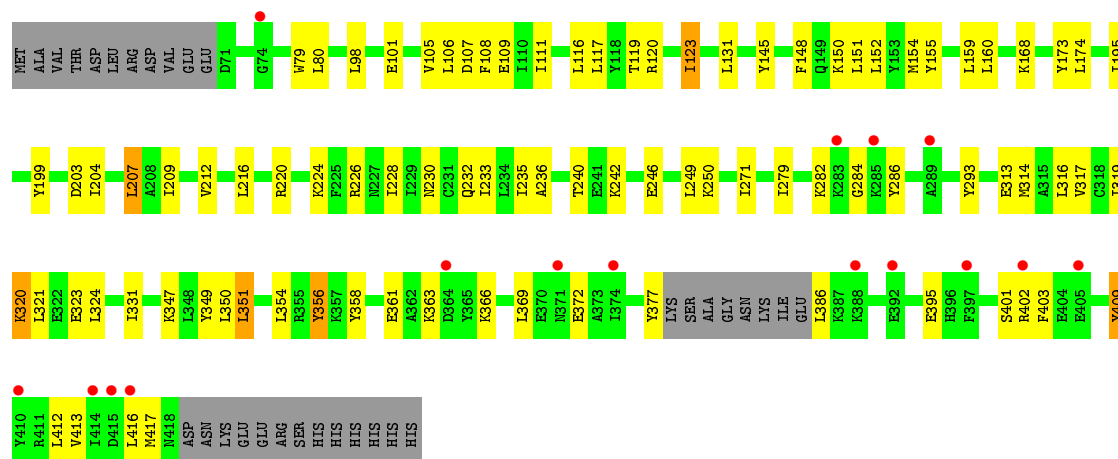


#### • Molecule 1: NprR

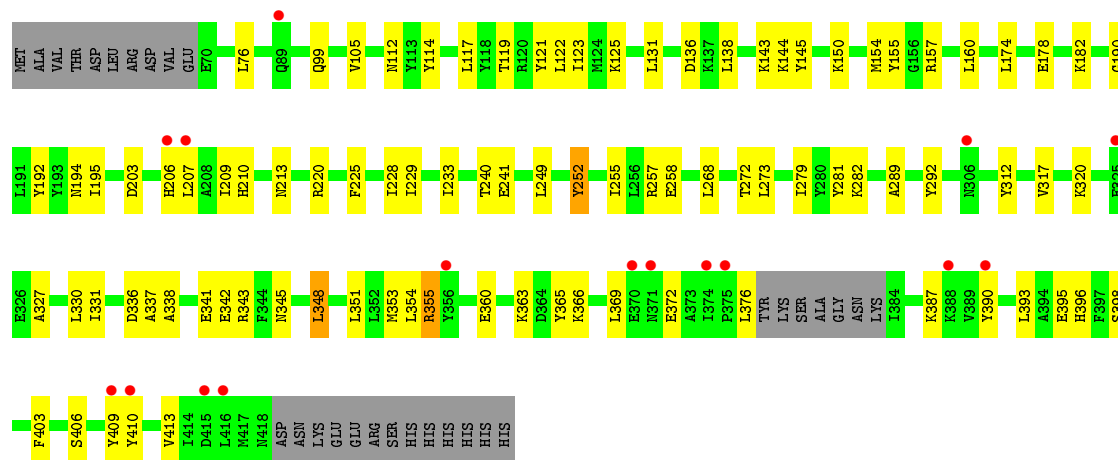


#### • Molecule 1: NprR

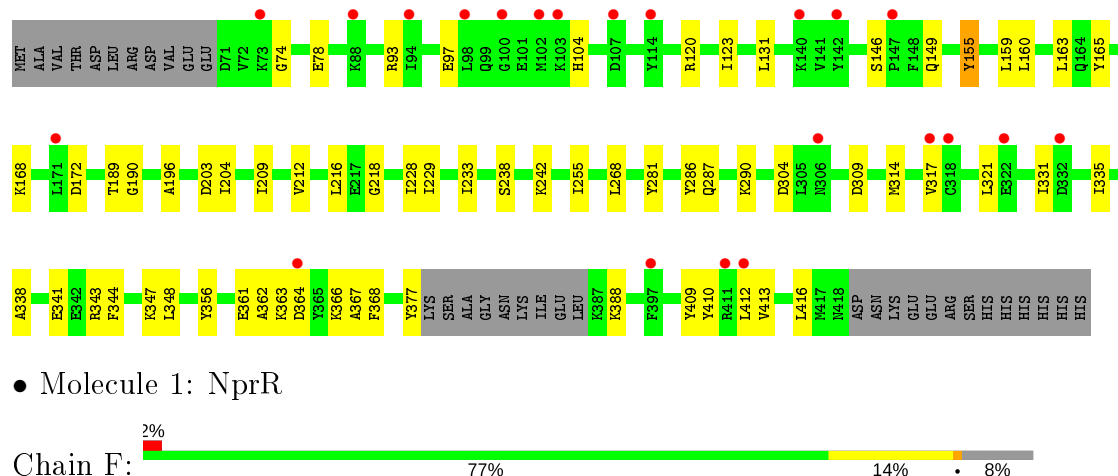
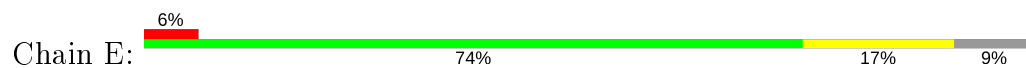




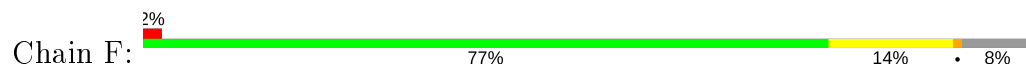
• Molecule 1: NprR

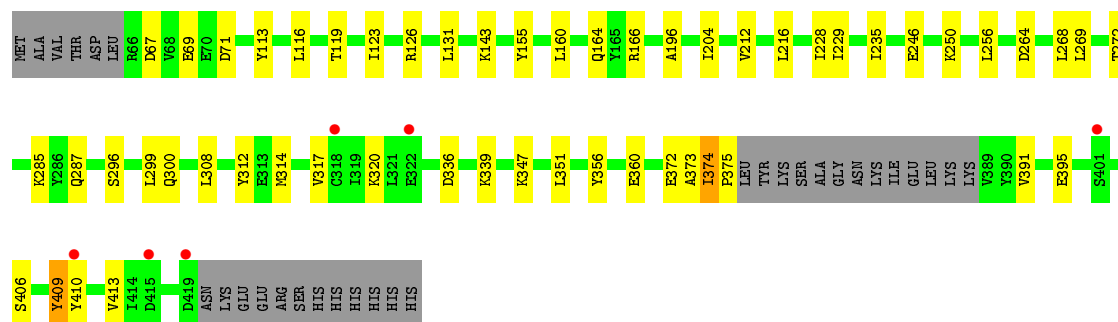


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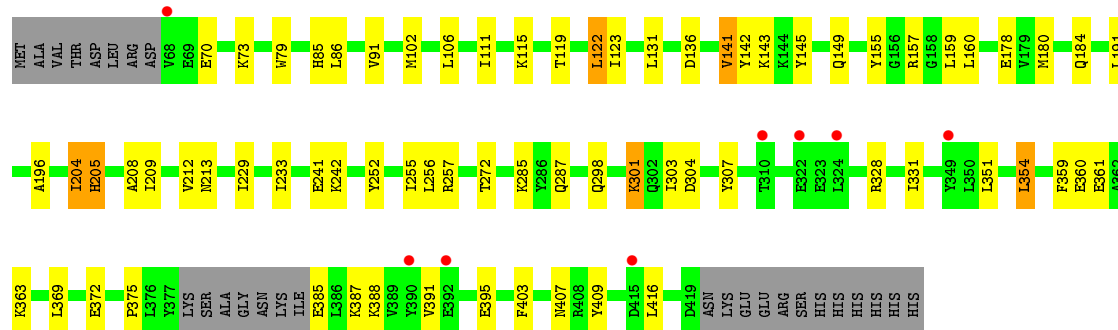
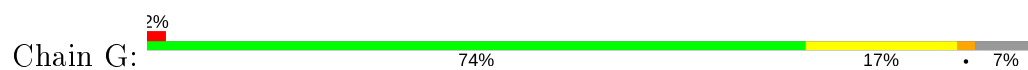


• Molecule 1: NprR

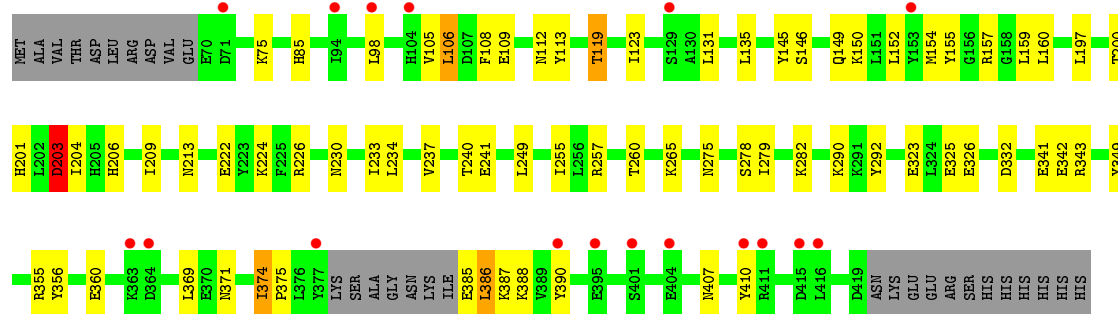
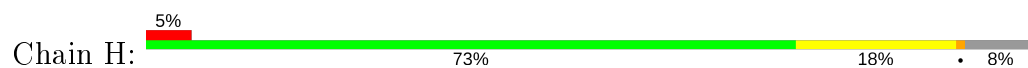




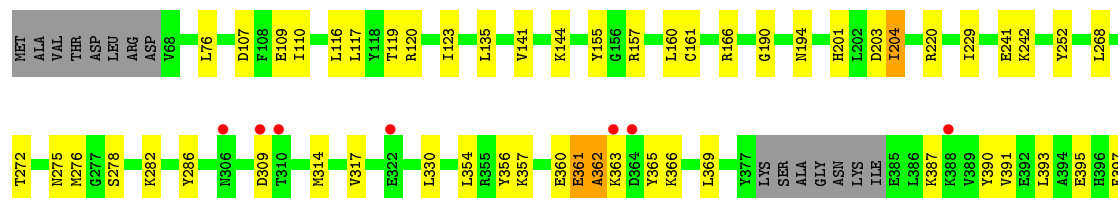
• Molecule 1: NprR

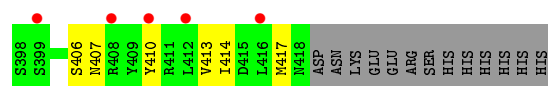


• Molecule 1: NprR

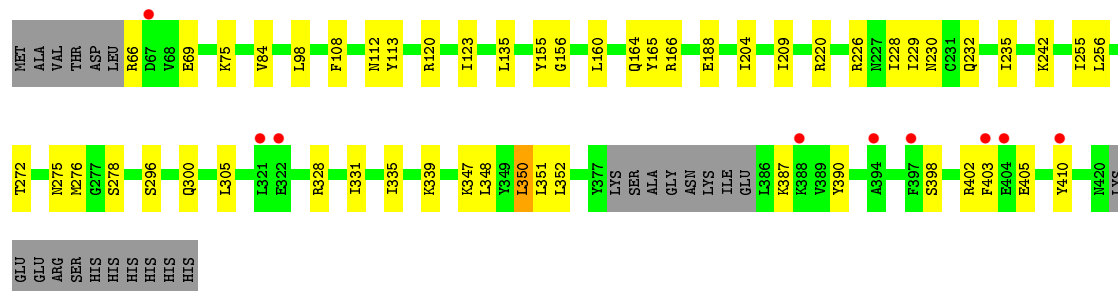
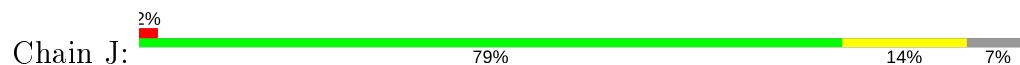


• Molecule 1: NprR

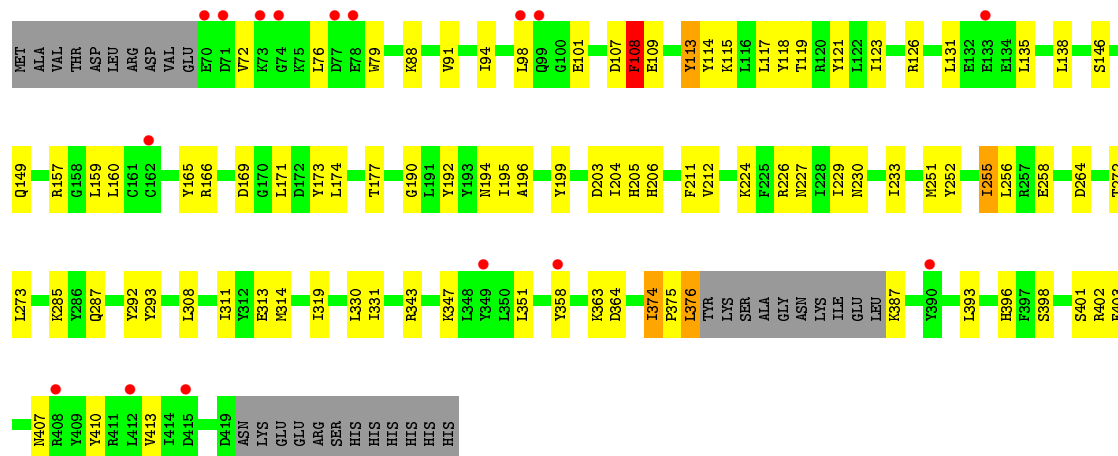




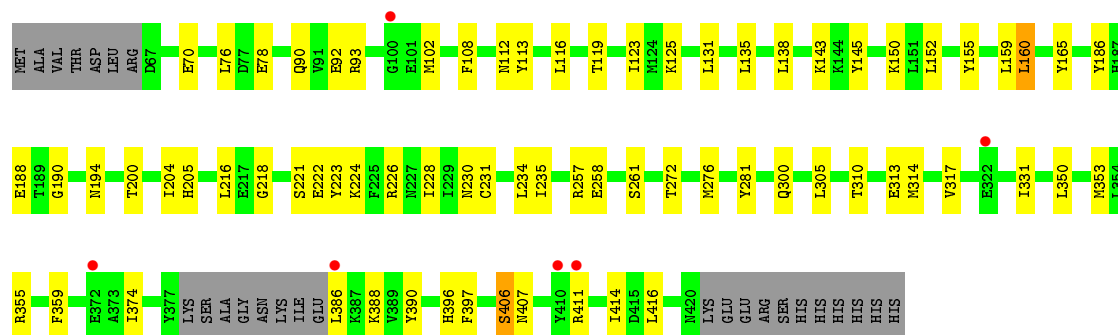
• Molecule 1: NprR



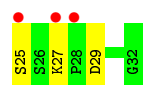
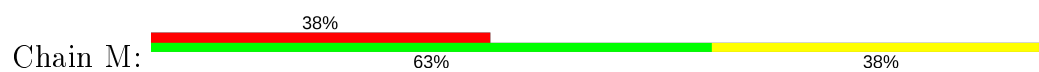
• Molecule 1: NprR



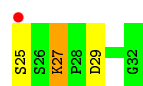
• Molecule 1: NprR



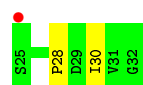
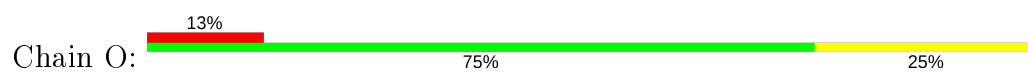
• Molecule 2: NprX peptide



- Molecule 2: NprX peptide



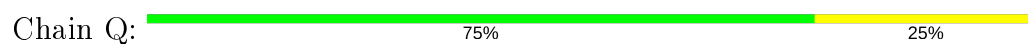
- Molecule 2: NprX peptide



- Molecule 2: NprX peptide



- Molecule 2: NprX peptide



- Molecule 2: NprX peptide



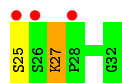
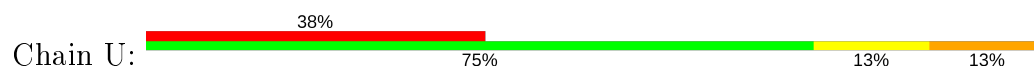
- Molecule 2: NprX peptide



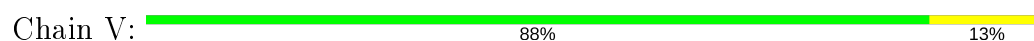
## • Molecule 2: NprX peptide



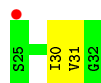
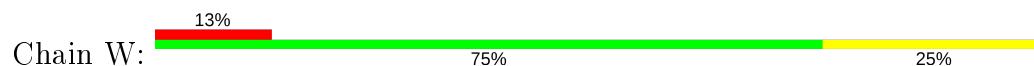
## • Molecule 2: NprX peptide



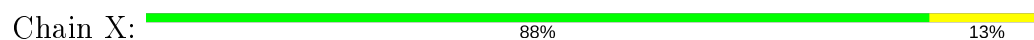
## • Molecule 2: NprX peptide



## • Molecule 2: NprX peptide



## • Molecule 2: NprX peptide



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.24Å 133.35Å 137.50Å 108.25° 104.83° 103.83°	Depositor
Resolution (Å)	29.74 – 3.20 29.74 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.5 (29.74-3.20) 98.5 (29.74-3.20)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 3.18Å)	Xtriage
Refinement program	PHENIX 1.8 _1069, BUSTER-TNT	Depositor
R, $R_{free}$	0.270 , 0.299 0.268 , 0.298	Depositor DCC
$R_{free}$ test set	24330 reflections (20.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	116.6	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 64.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.007 for -h,-l,-k	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	35360	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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	0.21	0/2953	0.36	0/3969
1	B	0.22	0/2938	0.40	0/3948
1	C	0.22	0/2926	0.37	0/3932
1	D	0.21	0/2939	0.38	0/3949
1	E	0.22	0/2918	0.39	0/3921
1	F	0.22	0/2931	0.37	0/3940
1	G	0.22	0/2968	0.37	0/3989
1	H	0.22	0/2952	0.37	0/3967
1	I	0.22	0/2960	0.36	0/3978
1	J	0.22	0/2986	0.36	0/4013
1	K	0.23	0/2922	0.39	0/3926
1	L	0.21	0/2975	0.36	0/3999
2	M	0.23	0/56	0.43	0/73
2	N	0.23	0/56	0.41	0/73
2	O	0.24	0/56	0.46	0/73
2	P	0.20	0/56	0.42	0/73
2	Q	0.36	0/56	0.54	0/73
2	R	0.21	0/56	0.43	0/73
2	S	0.21	0/56	0.36	0/73
2	T	0.24	0/56	0.45	0/73
2	U	0.20	0/56	0.43	0/73
2	V	0.21	0/56	0.36	0/73
2	W	0.24	0/56	0.43	0/73
2	X	0.21	0/56	0.43	0/73
All	All	0.22	0/36040	0.37	0/48407

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	2896	0	2906	34	0
1	B	2882	0	2897	57	0
1	C	2869	0	2892	48	0
1	D	2883	0	2906	50	0
1	E	2861	0	2881	42	0
1	F	2875	0	2877	30	0
1	G	2911	0	2923	35	0
1	H	2895	0	2908	39	0
1	I	2903	0	2919	39	0
1	J	2929	0	2940	31	0
1	K	2866	0	2882	61	0
1	L	2918	0	2927	42	0
2	M	56	0	56	1	0
2	N	56	0	56	2	0
2	O	56	0	56	1	0
2	P	56	0	56	0	0
2	Q	56	0	56	2	0
2	R	56	0	56	2	0
2	S	56	0	56	0	0
2	T	56	0	56	4	0
2	U	56	0	56	2	0
2	V	56	0	56	1	0
2	W	56	0	56	2	0
2	X	56	0	56	0	0
All	All	35360	0	35530	491	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 7.

The worst 5 of 491 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:113:TYR:HB3	1:B:149:GLN:HG2	1.63	0.81
1:B:395:GLU:HA	1:B:398:SER:HB2	1.68	0.76
1:B:313:GLU:OE2	2:N:25:SER:N	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:308:LEU:HD11	1:K:347:LYS:HD3	1.70	0.74
1:D:112:ASN:HD22	1:D:145:TYR:HE1	1.33	0.73

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	339/372 (91%)	323 (95%)	13 (4%)	3 (1%)	17	56
1	B	338/372 (91%)	313 (93%)	21 (6%)	4 (1%)	13	49
1	C	336/372 (90%)	314 (94%)	19 (6%)	3 (1%)	17	56
1	D	338/372 (91%)	316 (94%)	20 (6%)	2 (1%)	25	64
1	E	335/372 (90%)	312 (93%)	20 (6%)	3 (1%)	17	56
1	F	337/372 (91%)	315 (94%)	20 (6%)	2 (1%)	25	64
1	G	341/372 (92%)	323 (95%)	14 (4%)	4 (1%)	13	49
1	H	339/372 (91%)	322 (95%)	13 (4%)	4 (1%)	13	49
1	I	340/372 (91%)	325 (96%)	13 (4%)	2 (1%)	25	64
1	J	343/372 (92%)	326 (95%)	16 (5%)	1 (0%)	41	74
1	K	336/372 (90%)	308 (92%)	24 (7%)	4 (1%)	13	49
1	L	342/372 (92%)	326 (95%)	14 (4%)	2 (1%)	25	64
2	M	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
2	N	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
2	O	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
2	P	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
2	Q	6/8 (75%)	4 (67%)	2 (33%)	0	100	100
2	R	6/8 (75%)	5 (83%)	1 (17%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	S	6/8 (75%)	4 (67%)	2 (33%)	0	100	100
2	T	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
2	U	6/8 (75%)	4 (67%)	2 (33%)	0	100	100
2	V	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
2	W	6/8 (75%)	4 (67%)	2 (33%)	0	100	100
2	X	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
All	All	4136/4560 (91%)	3879 (94%)	223 (5%)	34 (1%)	19	58

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	204	ILE
1	B	166	ARG
1	F	373	ALA
1	G	142	TYR
1	H	105	VAL

### 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	309/335 (92%)	304 (98%)	5 (2%)	62	84
1	B	308/335 (92%)	298 (97%)	10 (3%)	39	71
1	C	306/335 (91%)	288 (94%)	18 (6%)	19	54
1	D	308/335 (92%)	299 (97%)	9 (3%)	42	74
1	E	305/335 (91%)	303 (99%)	2 (1%)	84	94
1	F	307/335 (92%)	301 (98%)	6 (2%)	55	80
1	G	311/335 (93%)	300 (96%)	11 (4%)	36	69
1	H	309/335 (92%)	298 (96%)	11 (4%)	35	69
1	I	310/335 (92%)	306 (99%)	4 (1%)	69	87
1	J	313/335 (93%)	309 (99%)	4 (1%)	69	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	306/335 (91%)	297 (97%)	9 (3%)	42	74
1	L	312/335 (93%)	305 (98%)	7 (2%)	52	79
2	M	7/7 (100%)	5 (71%)	2 (29%)	0	1
2	N	7/7 (100%)	5 (71%)	2 (29%)	0	1
2	O	7/7 (100%)	6 (86%)	1 (14%)	3	15
2	P	7/7 (100%)	7 (100%)	0	100	100
2	Q	7/7 (100%)	7 (100%)	0	100	100
2	R	7/7 (100%)	6 (86%)	1 (14%)	3	15
2	S	7/7 (100%)	7 (100%)	0	100	100
2	T	7/7 (100%)	7 (100%)	0	100	100
2	U	7/7 (100%)	6 (86%)	1 (14%)	3	15
2	V	7/7 (100%)	7 (100%)	0	100	100
2	W	7/7 (100%)	7 (100%)	0	100	100
2	X	7/7 (100%)	6 (86%)	1 (14%)	3	15
All	All	3788/4104 (92%)	3684 (97%)	104 (3%)	44	75

5 of 104 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	320	LYS
1	G	205	HIS
2	M	25	SER
1	F	391	VAL
1	G	119	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	396	HIS
1	L	300	GLN
1	E	149	GLN
1	A	194	ASN
1	K	194	ASN

### 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 carbohydrates 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	A	343/372 (92%)	0.32	22 (6%) 19 11	27, 72, 144, 152	0
1	B	342/372 (91%)	0.60	36 (10%) 6 3	36, 90, 143, 162	0
1	C	340/372 (91%)	0.19	16 (4%) 31 19	28, 69, 151, 163	0
1	D	342/372 (91%)	0.18	16 (4%) 31 19	31, 67, 147, 157	0
1	E	339/372 (91%)	0.34	22 (6%) 18 11	18, 76, 149, 159	0
1	F	341/372 (91%)	0.03	6 (1%) 68 55	15, 52, 131, 155	0
1	G	345/372 (92%)	0.16	8 (2%) 60 47	16, 62, 135, 152	0
1	H	343/372 (92%)	0.27	17 (4%) 28 16	19, 79, 147, 157	0
1	I	344/372 (92%)	0.03	12 (3%) 44 28	9, 44, 128, 145	0
1	J	347/372 (93%)	0.09	9 (2%) 56 40	11, 51, 135, 146	0
1	K	340/372 (91%)	0.31	16 (4%) 31 19	13, 72, 134, 146	0
1	L	346/372 (93%)	0.04	6 (1%) 70 57	18, 52, 135, 147	0
2	M	8/8 (100%)	1.57	3 (37%) 0 0	46, 54, 66, 68	0
2	N	8/8 (100%)	1.68	1 (12%) 3 2	57, 61, 65, 72	0
2	O	8/8 (100%)	1.39	1 (12%) 3 2	43, 46, 73, 81	0
2	P	8/8 (100%)	1.51	1 (12%) 3 2	39, 42, 52, 69	0
2	Q	8/8 (100%)	1.13	0 100 100	40, 44, 63, 63	0
2	R	8/8 (100%)	0.86	0 100 100	17, 23, 42, 45	0
2	S	8/8 (100%)	1.43	1 (12%) 3 2	23, 32, 47, 52	0
2	T	8/8 (100%)	1.28	1 (12%) 3 2	36, 47, 53, 74	0
2	U	8/8 (100%)	1.68	3 (37%) 0 0	19, 27, 31, 36	0
2	V	8/8 (100%)	0.88	0 100 100	22, 28, 40, 47	0
2	W	8/8 (100%)	1.40	1 (12%) 3 2	31, 40, 47, 54	0
2	X	8/8 (100%)	0.90	0 100 100	21, 25, 36, 38	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
All	All	4208/4560 (92%)	0.24	198 (4%)	31	19	9, 66, 141, 163	0

The worst 5 of 198 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	410	TYR	6.9
1	J	388	LYS	6.4
1	A	418	ASN	5.9
1	H	415	ASP	5.3
1	H	390	TYR	5.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.