



# Full wwPDB X-ray Structure Validation Report i

Feb 18, 2024 – 08:31 PM EST

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 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 i 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](#) ①) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

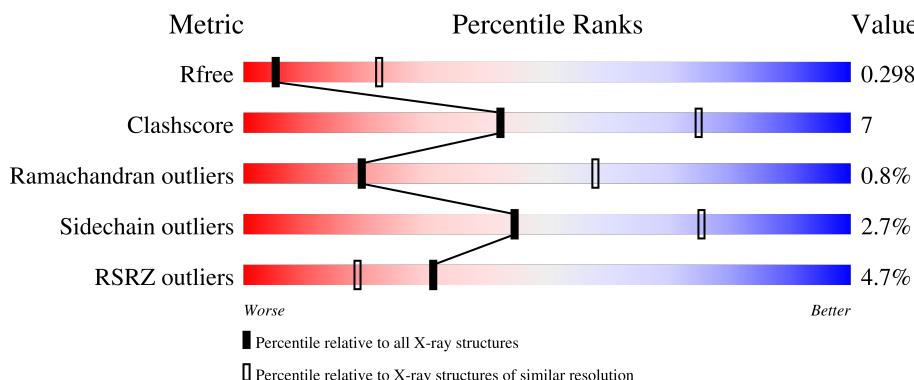
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

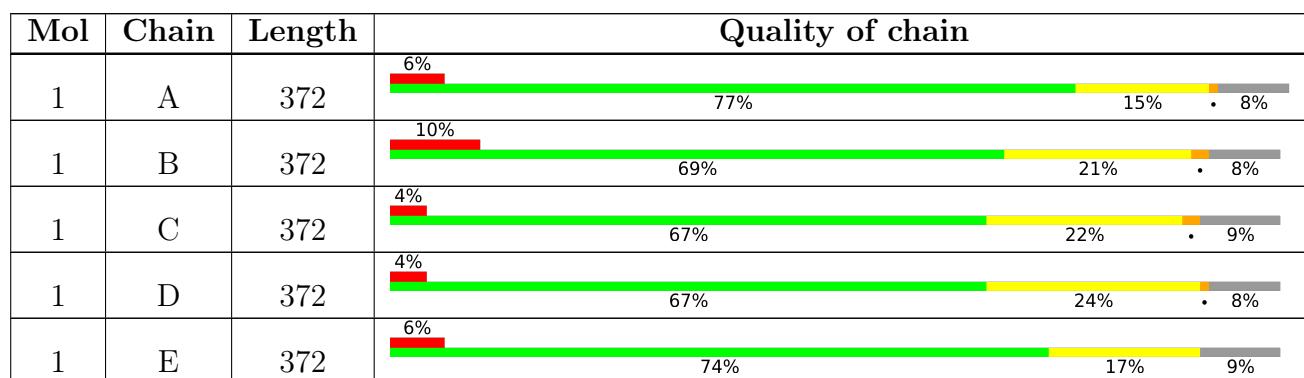
The reported resolution of this entry is 3.20 Å.

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.



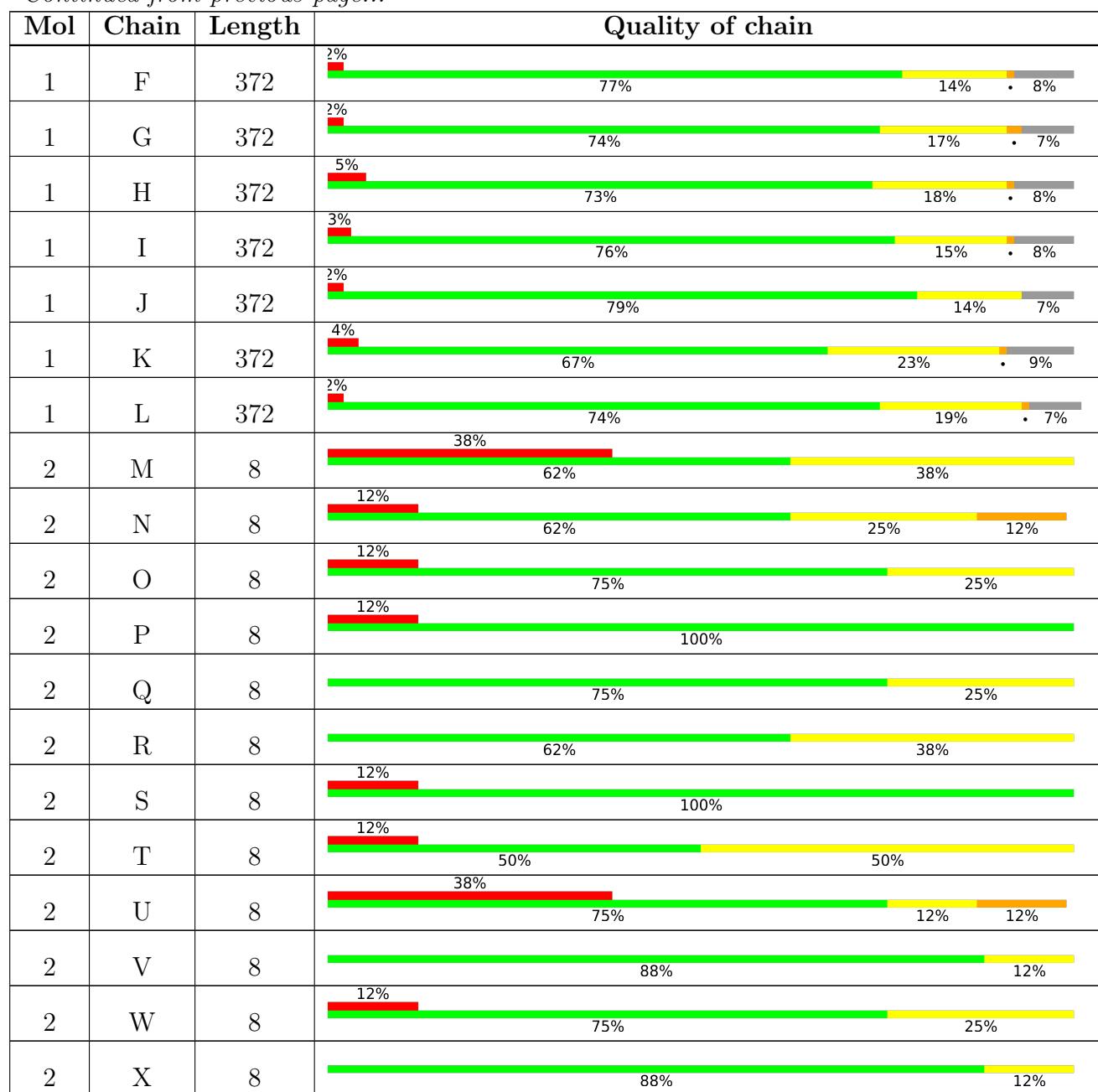
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 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 <=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.



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## 2 Entry composition [\(i\)](#)

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

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 56 34 9 13	0	0	0
2	N	8	Total C N O 56 34 9 13	0	0	0
2	O	8	Total C N O 56 34 9 13	0	0	0
2	P	8	Total C N O 56 34 9 13	0	0	0
2	Q	8	Total C N O 56 34 9 13	0	0	0
2	R	8	Total C N O 56 34 9 13	0	0	0
2	S	8	Total C N O 56 34 9 13	0	0	0
2	T	8	Total C N O 56 34 9 13	0	0	0
2	U	8	Total C N O 56 34 9 13	0	0	0
2	V	8	Total C N O 56 34 9 13	0	0	0

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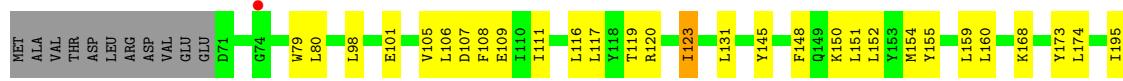
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	W	8	Total C N O 56 34 9 13	0	0	0
2	X	8	Total C N O 56 34 9 13	0	0	0

### 3 Residue-property plots (i)

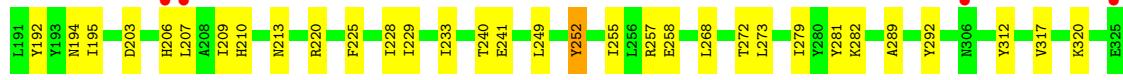
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: NprR

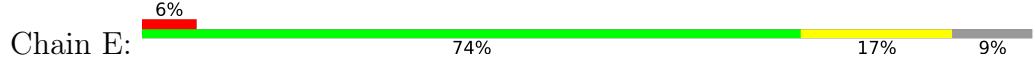




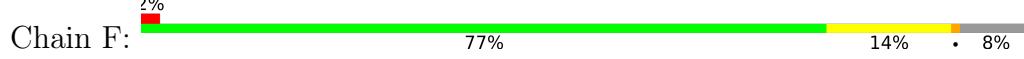
- Molecule 1: NprR

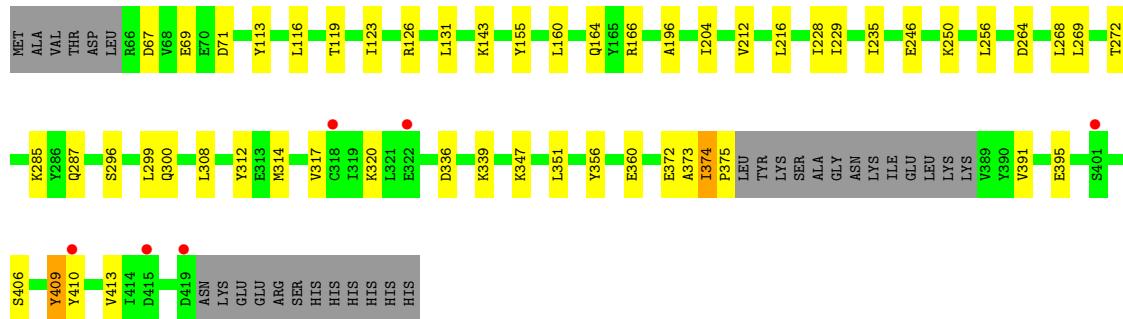


- Molecule 1: NprR

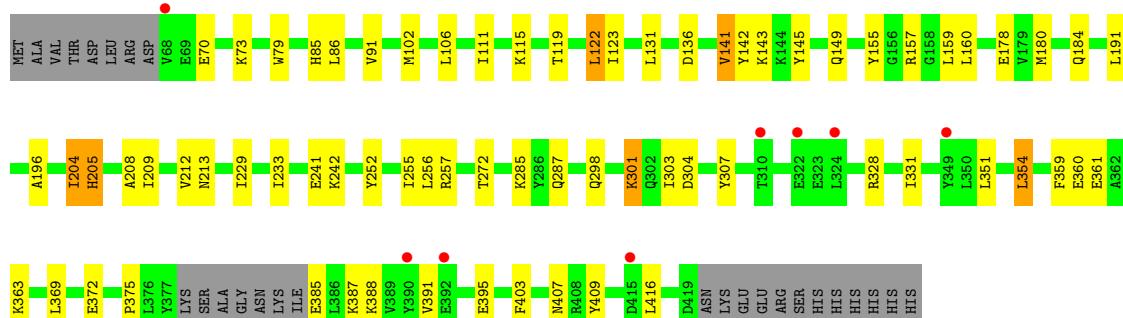
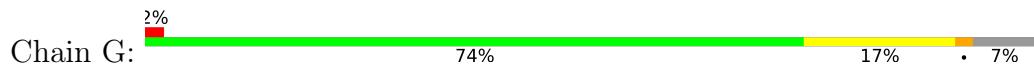


- Molecule 1: NprR

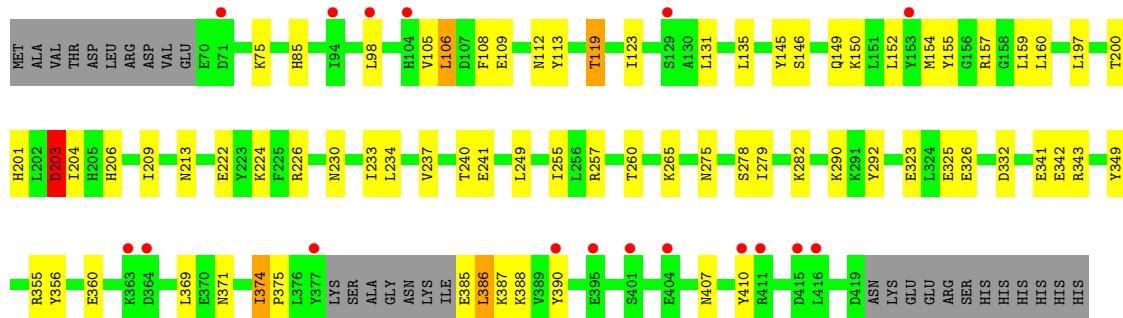




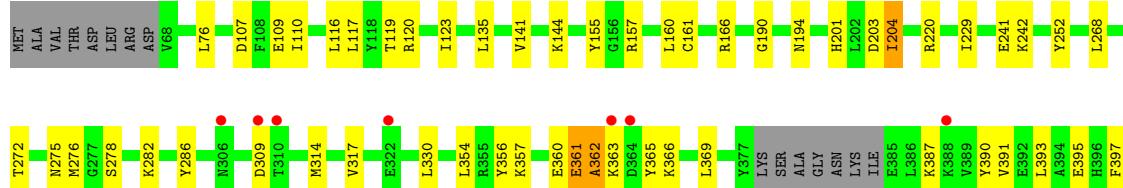
- Molecule 1: NprR



- Molecule 1: NprR

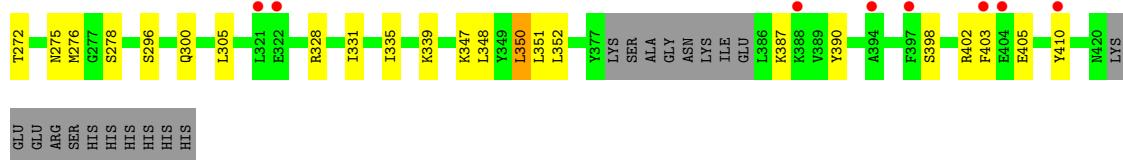
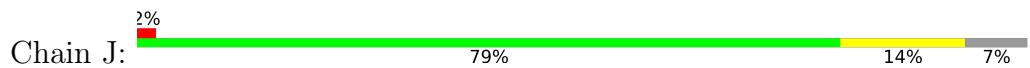


- Molecule 1: NprR

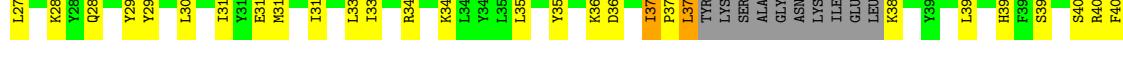
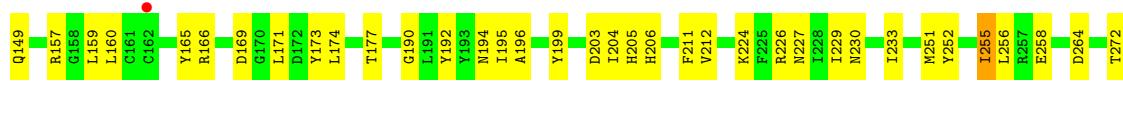




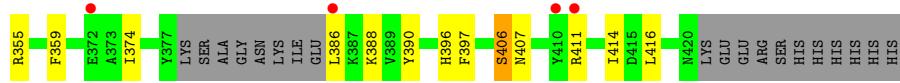
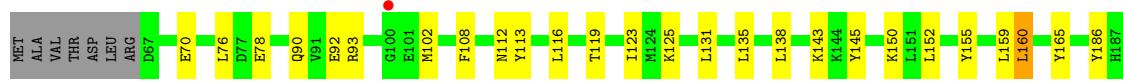
- Molecule 1: NprR



- Molecule 1: NprR



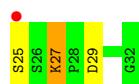
- Molecule 1: NprR



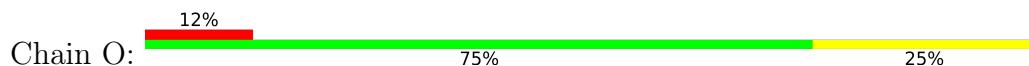
- Molecule 2: NprX peptide



- Molecule 2: NprX peptide



- Molecule 2: NprX peptide



- Molecule 2: NprX peptide



- Molecule 2: NprX peptide



- Molecule 2: NprX peptide



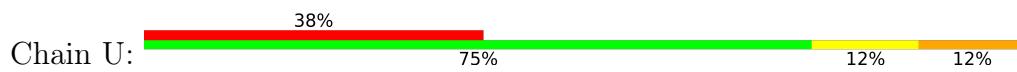
- Molecule 2: NprX peptide



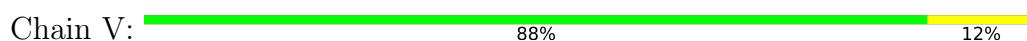
- Molecule 2: NprX peptide



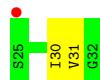
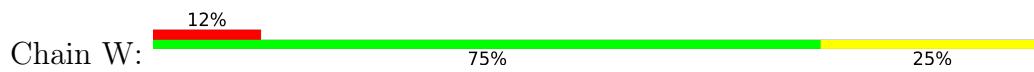
- Molecule 2: NprX peptide



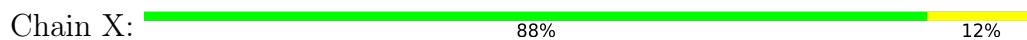
- Molecule 2: NprX peptide



- Molecule 2: NprX peptide



- Molecule 2: NprX peptide



## 4 Data and refinement statistics i

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
$< I/\sigma(I) >$ <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>	$<  L  > = 0.49$ , $< L^2 > = 0.32$	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  $< |L| >$ ,  $< L^2 >$  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 [\(i\)](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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.

All (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
1:D:395:GLU:HG3	1:D:410:TYR:HB2	1.72	0.71
1:L:300:GLN:HE22	1:L:310:THR:HG21	1.56	0.70
1:I:356:TYR:HA	1:I:360:GLU:HB3	1.71	0.70
1:H:341:GLU:O	1:H:343:ARG:N	2.23	0.70
1:K:190:GLY:O	1:K:194:ASN:ND2	2.25	0.70
1:E:120:ARG:HA	1:E:123:ILE:HD12	1.75	0.69
1:J:331:ILE:HG13	1:J:351:LEU:HD12	1.74	0.69
1:L:119:THR:HG23	1:L:131:LEU:HD11	1.75	0.69
1:G:85:HIS:HB3	1:H:257:ARG:HD3	1.74	0.68
1:E:364:ASP:HB3	1:E:367:ALA:HB3	1.75	0.68
1:I:190:GLY:O	1:I:194:ASN:ND2	2.27	0.68
1:I:220:ARG:HH11	1:J:220:ARG:HH11	1.42	0.67
1:L:226:ARG:O	1:L:230:ASN:ND2	2.28	0.67
1:D:190:GLY:O	1:D:194:ASN:ND2	2.28	0.66
1:K:123:ILE:HG12	1:K:159:LEU:HD13	1.77	0.66
1:C:220:ARG:HH11	1:D:220:ARG:HH11	1.44	0.66
1:C:123:ILE:HD13	1:C:159:LEU:HD23	1.77	0.65
1:D:398:SER:HB2	1:D:406:SER:HB3	1.78	0.65
1:K:374:ILE:HG23	1:K:375:PRO:HD3	1.77	0.65
1:H:204:ILE:HG12	1:H:241:GLU:HB3	1.79	0.65
1:B:161:CYS:SG	1:B:166:ARG:NH1	2.70	0.64
1:H:75:LYS:HB3	1:H:98:LEU:HD11	1.78	0.64
1:H:108:PHE:O	1:H:112:ASN:ND2	2.31	0.64
1:C:369:LEU:HD12	1:C:372:GLU:HB3	1.80	0.64
1:J:275:ASN:OD1	2:V:25:SER:N	2.31	0.64
1:I:135:LEU:HD13	1:I:157:ARG:HD2	1.80	0.64
1:L:190:GLY:O	1:L:194:ASN:ND2	2.30	0.63
1:B:190:GLY:O	1:B:194:ASN:ND2	2.31	0.63
1:J:164:GLN:OE1	1:J:166:ARG:NH2	2.32	0.62
1:C:402:ARG:HB3	1:C:403:PHE:HB3	1.81	0.62
1:G:331:ILE:HG13	1:G:351:LEU:HD12	1.80	0.62
1:C:366:LYS:HA	1:C:369:LEU:HB3	1.81	0.62
1:G:403:PHE:O	1:G:407:ASN:ND2	2.33	0.62
1:K:123:ILE:O	1:K:126:ARG:NH1	2.33	0.62
1:B:189:THR:HA	1:B:192:TYR:HD2	1.65	0.61
1:K:398:SER:HA	1:K:401:SER:HB2	1.81	0.61
1:C:331:ILE:HG13	1:C:351:LEU:HD12	1.83	0.61
1:F:126:ARG:NH2	2:R:29:ASP:OD2	2.34	0.61
1:A:251:MET:SD	1:B:223:TYR:OH	2.58	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:341:GLU:HG3	1:E:343:ARG:H	1.65	0.61
1:B:146:SER:O	1:B:150:LYS:N	2.28	0.60
1:B:229:ILE:HD11	1:B:255:ILE:HG23	1.84	0.60
1:B:113:TYR:HA	1:B:116:LEU:HB2	1.84	0.60
1:D:341:GLU:O	1:D:343:ARG:N	2.32	0.60
1:A:190:GLY:O	1:A:194:ASN:ND2	2.34	0.60
1:C:145:TYR:O	1:C:150:LYS:NZ	2.35	0.60
1:F:356:TYR:HA	1:F:360:GLU:HB2	1.82	0.60
1:K:224:LYS:HE2	1:L:257:ARG:HH22	1.67	0.59
1:G:79:TRP:HE1	1:G:91:VAL:HB	1.67	0.59
1:A:245:TYR:HB3	1:A:279:ILE:HG23	1.84	0.59
1:F:372:GLU:O	1:F:374:ILE:N	2.35	0.59
1:G:141:VAL:O	1:G:143:LYS:N	2.35	0.59
1:K:98:LEU:HA	1:K:101:GLU:HB2	1.84	0.59
1:E:123:ILE:HD13	1:E:159:LEU:HD11	1.84	0.59
1:K:226:ARG:O	1:K:230:ASN:ND2	2.35	0.59
1:C:347:LYS:HD2	1:C:350:LEU:HD21	1.85	0.59
1:L:350:LEU:HD11	1:L:386:LEU:HD11	1.85	0.58
1:F:126:ARG:NH1	2:R:32:GLY:O	2.36	0.58
1:H:290:LYS:NZ	1:H:323:GLU:OE1	2.36	0.58
1:D:363:LYS:HB3	1:D:366:LYS:HE2	1.84	0.58
1:G:257:ARG:HD2	1:H:85:HIS:HB3	1.85	0.58
1:B:216:LEU:HD21	1:B:220:ARG:HE	1.68	0.58
1:H:123:ILE:HG21	1:H:159:LEU:HD23	1.84	0.58
1:K:229:ILE:HD11	1:K:255:ILE:HB	1.85	0.58
1:H:209:ILE:O	1:H:213:ASN:ND2	2.35	0.58
1:H:374:ILE:HG13	1:H:375:PRO:HD3	1.85	0.58
1:A:108:PHE:O	1:A:112:ASN:ND2	2.37	0.58
1:E:131:LEU:HD23	1:E:160:LEU:HD23	1.86	0.58
1:A:69:GLU:HG3	1:A:110:ILE:HD11	1.85	0.57
1:B:123:ILE:HG13	1:B:163:LEU:HD11	1.86	0.57
1:J:75:LYS:HG2	1:J:98:LEU:HD21	1.85	0.57
1:F:336:ASP:HA	1:F:339:LYS:HE3	1.87	0.57
1:A:395:GLU:HG2	1:A:410:TYR:CZ	2.39	0.57
1:D:338:ALA:HB1	1:D:348:LEU:HB2	1.85	0.57
1:K:72:VAL:O	1:K:76:LEU:HG	2.05	0.57
1:D:336:ASP:OD1	1:D:337:ALA:N	2.38	0.57
1:K:119:THR:HG23	1:K:131:LEU:HD11	1.85	0.57
1:J:339:LYS:HD2	1:J:348:LEU:HD11	1.87	0.57
1:K:166:ARG:NH1	1:K:169:ASP:OD2	2.38	0.57
1:B:393:LEU:O	1:B:396:HIS:ND1	2.32	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:LYS:NZ	1:D:192:TYR:OH	2.35	0.56
1:K:376:LEU:O	1:K:387:LYS:NZ	2.38	0.56
1:F:212:VAL:HG11	1:F:235:ILE:HG23	1.86	0.56
1:B:105:VAL:HG11	1:B:110:ILE:HG21	1.87	0.56
1:D:331:ILE:HD12	1:D:355:ARG:HB2	1.88	0.56
1:K:308:LEU:HA	1:K:311:ILE:HB	1.88	0.56
1:A:116:LEU:O	1:A:119:THR:OG1	2.19	0.55
1:J:305:LEU:HB2	1:J:347:LYS:HZ2	1.71	0.55
1:K:375:PRO:HB2	1:K:376:LEU:HD23	1.89	0.55
1:F:164:GLN:OE1	1:F:166:ARG:NH1	2.39	0.55
1:I:357:LYS:HE2	1:I:393:LEU:HD21	1.88	0.55
1:H:145:TYR:O	1:H:150:LYS:NZ	2.32	0.55
1:L:135:LEU:HD12	1:L:160:LEU:HD12	1.87	0.55
1:F:395:GLU:HG2	1:F:406:SER:HB2	1.89	0.54
1:K:79:TRP:HZ2	1:K:121:TYR:HH	1.55	0.54
1:L:204:ILE:O	1:L:205:HIS:ND1	2.40	0.54
1:F:216:LEU:HD11	1:F:228:ILE:HG23	1.90	0.54
1:H:278:SER:OG	1:H:282:LYS:NZ	2.40	0.54
1:J:350:LEU:HD23	1:J:351:LEU:HD22	1.90	0.54
1:A:316:LEU:HD12	1:A:319:ILE:HD11	1.90	0.54
1:F:196:ALA:HB1	1:F:212:VAL:HG23	1.90	0.54
1:D:327:ALA:HA	1:D:330:LEU:HD12	1.90	0.54
1:K:393:LEU:HA	1:K:396:HIS:HB3	1.89	0.54
1:J:387:LYS:HA	1:J:390:TYR:CE2	2.43	0.54
1:B:199:TYR:HB3	1:B:205:HIS:HB2	1.90	0.53
1:I:361:GLU:HG3	1:I:362:ALA:N	2.24	0.53
1:D:99:GLN:OE1	1:D:114:TYR:OH	2.27	0.53
1:G:70:GLU:HB2	1:G:73:LYS:HG3	1.90	0.53
1:G:252:TYR:HD1	1:G:255:ILE:HD11	1.74	0.53
1:F:246:GLU:HG2	1:F:250:LYS:HE3	1.91	0.53
1:C:116:LEU:HD23	1:C:152:LEU:HB2	1.90	0.53
1:E:165:TYR:OH	1:E:304:ASP:OD1	2.25	0.53
1:E:229:ILE:HD13	1:E:268:LEU:HD13	1.91	0.53
1:E:410:TYR:HA	1:E:413:VAL:HG22	1.91	0.53
1:D:207:LEU:HA	1:D:210:HIS:HB3	1.90	0.52
1:D:257:ARG:HH11	1:D:258:GLU:HG2	1.74	0.52
1:D:365:TYR:O	1:D:369:LEU:N	2.41	0.52
1:H:260:THR:HA	1:H:265:LYS:HE2	1.90	0.52
1:K:113:TYR:HD1	1:K:114:TYR:N	2.08	0.52
1:L:116:LEU:HD12	1:L:138:LEU:HD13	1.91	0.52
1:C:395:GLU:HG2	1:C:409:TYR:HD2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:ILE:HG13	1:B:330:LEU:HD12	1.91	0.52
1:G:136:ASP:OD1	1:G:157:ARG:NH2	2.42	0.52
1:G:196:ALA:HB1	1:G:212:VAL:HG23	1.91	0.52
1:B:387:LYS:HD3	1:B:416:LEU:HD23	1.91	0.52
1:J:108:PHE:O	1:J:112:ASN:ND2	2.37	0.52
1:J:226:ARG:O	1:J:230:ASN:ND2	2.42	0.52
1:B:321:LEU:HD23	1:B:322:GLU:H	1.75	0.52
1:J:402:ARG:HB3	1:J:403:PHE:HA	1.91	0.52
1:E:229:ILE:HD11	1:E:255:ILE:HG23	1.92	0.51
1:H:385:GLU:HA	1:H:388:LYS:HE2	1.91	0.51
1:K:196:ALA:HB1	1:K:212:VAL:HG23	1.92	0.51
1:A:174:LEU:HB3	1:A:195:ILE:HG12	1.91	0.51
1:A:200:THR:HG21	1:A:234:LEU:HD22	1.91	0.51
1:B:192:TYR:HD1	1:B:211:PHE:HD1	1.56	0.51
1:K:194:ASN:HD21	2:W:31:VAL:HG22	1.74	0.51
1:I:366:LYS:HD3	1:I:369:LEU:HD12	1.91	0.51
1:H:233:ILE:HG12	1:H:255:ILE:HD13	1.93	0.51
1:J:410:TYR:HE2	1:K:407:ASN:HD22	1.57	0.51
1:G:351:LEU:HD13	1:G:354:LEU:HD21	1.92	0.51
1:D:229:ILE:HD13	1:D:268:LEU:HD13	1.93	0.51
1:D:393:LEU:HA	1:D:396:HIS:HD2	1.75	0.51
1:C:233:ILE:HD13	1:C:271:ILE:HD11	1.93	0.50
1:E:209:ILE:HA	1:E:212:VAL:HG22	1.93	0.50
1:B:145:TYR:HB3	1:B:146:SER:HB2	1.94	0.50
1:C:216:LEU:HG	1:C:220:ARG:HE	1.77	0.50
1:D:209:ILE:O	1:D:213:ASN:ND2	2.36	0.50
1:A:131:LEU:HD23	1:A:160:LEU:HD23	1.93	0.50
1:D:376:LEU:HD13	1:D:387:LYS:HB2	1.92	0.50
1:G:145:TYR:HB3	1:G:149:GLN:HB2	1.93	0.50
1:H:203:ASP:HB3	1:H:204:ILE:HG13	1.93	0.50
1:B:247:GLU:N	1:B:247:GLU:OE1	2.43	0.50
1:E:309:ASP:HB2	1:E:347:LYS:HE2	1.94	0.50
1:B:120:ARG:HA	1:B:123:ILE:HG22	1.93	0.49
1:B:202:LEU:HB3	1:B:205:HIS:HE1	1.77	0.49
1:C:230:ASN:HA	1:C:233:ILE:HD12	1.93	0.49
1:J:229:ILE:HD11	1:J:255:ILE:HG23	1.93	0.49
1:B:122:LEU:HD21	1:B:130:ALA:HB3	1.94	0.49
1:G:298:GLN:O	1:G:301:LYS:NZ	2.42	0.49
1:A:403:PHE:HB3	1:D:403:PHE:CE2	2.48	0.49
1:C:230:ASN:HD22	2:O:28:PRO:HB3	1.77	0.49
1:K:363:LYS:HG2	1:K:364:ASP:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:LEU:HB3	1:C:195:ILE:HG12	1.93	0.49
1:D:353:MET:HE1	1:D:390:TYR:CE2	2.47	0.49
1:F:285:LYS:O	1:F:287:GLN:N	2.44	0.49
1:G:180:MET:HG2	1:G:184:GLN:HE21	1.77	0.49
1:K:118:TYR:HA	1:K:121:TYR:CD2	2.48	0.49
1:F:131:LEU:HD23	1:F:160:LEU:HD23	1.94	0.49
1:G:285:LYS:O	1:G:287:GLN:N	2.44	0.49
1:B:375:PRO:HG2	1:B:376:LEU:HD12	1.94	0.49
1:F:395:GLU:HG3	1:F:410:TYR:HB2	1.95	0.49
1:J:165:TYR:CZ	1:J:305:LEU:HD23	2.48	0.49
1:B:146:SER:H	1:B:149:GLN:HB2	1.77	0.48
1:B:280:TYR:HA	1:B:283:LYS:HB3	1.95	0.48
1:D:131:LEU:HD23	1:D:160:LEU:HD23	1.95	0.48
1:G:372:GLU:HA	1:G:375:PRO:HD2	1.95	0.48
1:I:272:THR:HG22	1:I:276:MET:HE3	1.94	0.48
1:E:281:TYR:HD1	1:E:317:VAL:HG23	1.78	0.48
1:I:369:LEU:O	1:I:390:TYR:OH	2.30	0.48
1:B:309:ASP:HA	1:B:347:LYS:HE2	1.95	0.48
1:E:286:TYR:HB3	1:E:317:VAL:HG22	1.95	0.48
1:K:410:TYR:HA	1:K:413:VAL:HG22	1.95	0.48
1:I:407:ASN:OD1	1:L:406:SER:OG	2.28	0.48
1:C:279:ILE:HA	1:C:282:LYS:HB2	1.95	0.48
1:F:116:LEU:O	1:F:119:THR:OG1	2.25	0.48
1:C:246:GLU:O	1:C:250:LYS:HG2	2.14	0.48
1:H:200:THR:HG21	1:H:234:LEU:HD22	1.94	0.48
1:J:328:ARG:HA	1:J:331:ILE:HG22	1.96	0.48
1:G:369:LEU:HA	1:G:372:GLU:HB2	1.96	0.48
1:D:289:ALA:HB3	1:D:317:VAL:HG21	1.95	0.48
1:G:387:LYS:HG3	1:G:416:LEU:HG	1.96	0.48
1:I:366:LYS:HE3	1:I:397:PHE:HB2	1.96	0.48
1:L:388:LYS:HE3	1:L:416:LEU:HD11	1.95	0.48
1:B:107:ASP:OD1	1:B:108:PHE:N	2.47	0.48
1:H:197:LEU:HD23	2:T:30:ILE:HG22	1.96	0.48
1:I:252:TYR:OH	1:I:275:ASN:ND2	2.46	0.48
1:I:314:MET:HE3	1:I:330:LEU:HD13	1.96	0.48
1:K:135:LEU:HD21	1:K:157:ARG:HD2	1.96	0.48
1:C:226:ARG:NH1	1:C:230:ASN:OD1	2.47	0.47
1:D:143:LYS:HG3	1:D:144:LYS:HG3	1.95	0.47
1:K:258:GLU:HG2	1:L:223:TYR:O	2.14	0.47
1:E:146:SER:OG	1:E:149:GLN:NE2	2.47	0.47
1:E:309:ASP:OD1	2:Q:25:SER:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:229:ILE:O	1:K:233:ILE:HG12	2.14	0.47
1:D:369:LEU:O	1:D:372:GLU:HG3	2.14	0.47
1:J:275:ASN:O	1:J:278:SER:OG	2.24	0.47
1:A:220:ARG:HH11	1:B:220:ARG:HD3	1.78	0.47
1:C:199:TYR:CZ	1:C:207:LEU:HD23	2.49	0.47
1:E:356:TYR:HD2	1:E:368:PHE:HZ	1.61	0.47
1:E:189:THR:HG21	1:E:218:GLY:HA3	1.96	0.47
1:E:93:ARG:O	1:E:97:GLU:HG2	2.13	0.47
1:G:204:ILE:HD12	1:G:241:GLU:HB3	1.96	0.47
1:K:113:TYR:HD1	1:K:113:TYR:C	2.17	0.47
1:A:307:TYR:HD2	1:A:308:LEU:HD12	1.80	0.47
1:C:107:ASP:O	1:C:109:GLU:N	2.46	0.47
1:D:229:ILE:HD11	1:D:255:ILE:HG23	1.96	0.47
1:L:218:GLY:O	1:L:221:SER:OG	2.24	0.47
1:B:73:LYS:HA	1:B:76:LEU:HB2	1.97	0.47
1:A:264:ASP:OD1	1:A:264:ASP:N	2.48	0.47
1:I:278:SER:OG	1:I:282:LYS:NZ	2.41	0.47
1:J:331:ILE:O	1:J:335:ILE:HG12	2.15	0.47
1:B:304:ASP:OD1	1:B:305:LEU:N	2.45	0.47
1:D:174:LEU:HB3	1:D:195:ILE:HG12	1.96	0.47
1:H:386:LEU:HD22	1:H:387:LYS:HG2	1.97	0.46
1:I:354:LEU:HA	1:I:357:LYS:HB3	1.97	0.46
1:C:286:TYR:CG	1:C:320:LYS:HD2	2.50	0.46
1:D:119:THR:O	1:D:123:ILE:HG13	2.15	0.46
1:K:331:ILE:HG13	1:K:351:LEU:HD22	1.96	0.46
1:E:338:ALA:HB3	1:E:348:LEU:HD13	1.96	0.46
1:G:385:GLU:HB3	1:G:388:LYS:HE2	1.97	0.46
1:F:409:TYR:O	1:F:413:VAL:HG13	2.15	0.46
1:G:256:LEU:HB2	1:G:272:THR:HG21	1.97	0.46
1:H:275:ASN:OD1	2:T:25:SER:N	2.49	0.46
1:K:113:TYR:C	1:K:113:TYR:CD1	2.89	0.46
1:C:98:LEU:HA	1:C:101:GLU:HB2	1.96	0.46
1:I:410:TYR:HE1	1:L:414:ILE:HB	1.80	0.46
1:A:356:TYR:HA	1:A:360:GLU:HB2	1.98	0.46
1:B:239:TYR:HD1	1:B:251:MET:HE1	1.81	0.46
1:D:345:ASN:HA	1:D:348:LEU:HB3	1.98	0.46
1:G:391:VAL:HG13	1:G:409:TYR:HB3	1.97	0.46
1:H:332:ASP:OD1	1:H:355:ARG:NH1	2.49	0.46
1:H:356:TYR:HA	1:H:360:GLU:HB2	1.96	0.46
1:G:209:ILE:O	1:G:213:ASN:ND2	2.47	0.46
1:H:201:HIS:HA	2:T:27:LYS:HE2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:285:LYS:O	1:K:287:GLN:N	2.48	0.46
1:D:240:THR:HG23	1:D:279:ILE:HG12	1.98	0.46
1:J:123:ILE:HD11	1:J:156:GLY:HA2	1.98	0.46
1:J:209:ILE:HD13	1:J:235:ILE:HG22	1.97	0.46
1:A:126:ARG:NH1	2:M:29:ASP:OD2	2.43	0.45
1:D:136:ASP:OD1	1:D:157:ARG:NH2	2.47	0.45
1:A:406:SER:HB2	1:D:403:PHE:HZ	1.82	0.45
1:B:201:HIS:CE1	2:N:27:LYS:HD3	2.50	0.45
1:B:362:ALA:O	1:B:366:LYS:NZ	2.50	0.45
1:K:108:PHE:N	1:K:108:PHE:CD2	2.84	0.45
1:B:188:GLU:HG2	1:B:191:LEU:H	1.81	0.45
1:C:79:TRP:CZ3	1:C:117:LEU:HB3	2.51	0.45
1:B:117:LEU:O	1:B:120:ARG:HG3	2.17	0.45
1:G:204:ILE:HG21	1:G:242:LYS:HD3	1.99	0.45
1:C:224:LYS:O	1:C:228:ILE:HG13	2.16	0.45
1:I:242:LYS:HD2	1:I:242:LYS:HA	1.73	0.45
1:G:359:PHE:N	1:G:360:GLU:HA	2.31	0.45
1:H:203:ASP:HA	1:H:204:ILE:HA	1.60	0.45
1:K:131:LEU:HD23	1:K:160:LEU:HD23	1.97	0.45
1:K:165:TYR:CD2	1:K:343:ARG:HB3	2.52	0.45
1:E:196:ALA:HB1	1:E:212:VAL:HG13	1.99	0.45
1:K:293:TYR:CZ	1:K:313:GLU:HB3	2.52	0.45
1:D:366:LYS:O	1:D:369:LEU:HB2	2.17	0.45
1:E:287:GLN:HA	1:E:290:LYS:HE2	1.98	0.45
1:I:410:TYR:CE1	1:L:414:ILE:HB	2.52	0.45
1:F:119:THR:O	1:F:123:ILE:HG13	2.17	0.45
1:F:314:MET:HA	1:F:317:VAL:HG12	1.99	0.45
1:H:109:GLU:HA	1:H:112:ASN:HD22	1.82	0.45
1:B:168:LYS:HG2	1:B:202:LEU:HD21	1.98	0.44
1:E:361:GLU:HA	1:E:362:ALA:HA	1.70	0.44
1:L:108:PHE:O	1:L:112:ASN:ND2	2.50	0.44
1:A:204:ILE:HG13	1:A:242:LYS:HE3	1.99	0.44
1:B:79:TRP:CH2	1:B:98:LEU:HD13	2.52	0.44
1:B:154:MET:HA	1:B:157:ARG:HG2	1.98	0.44
1:B:347:LYS:HD2	1:B:347:LYS:HA	1.86	0.44
1:C:203:ASP:OD2	1:C:386:LEU:N	2.50	0.44
1:L:313:GLU:O	1:L:317:VAL:HG13	2.17	0.44
1:B:165:TYR:O	1:B:167:TRP:N	2.51	0.44
1:D:273:LEU:HD22	1:D:292:TYR:HD1	1.82	0.44
1:E:331:ILE:O	1:E:335:ILE:HG12	2.18	0.44
1:F:296:SER:O	1:F:300:GLN:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:94:ILE:O	1:K:98:LEU:HG	2.17	0.44
1:L:281:TYR:CD1	1:L:317:VAL:HG12	2.52	0.44
1:C:116:LEU:O	1:C:119:THR:HB	2.18	0.44
1:C:331:ILE:HD12	1:C:354:LEU:HD22	2.00	0.44
1:F:256:LEU:HB2	1:F:272:THR:HG21	1.99	0.44
1:L:258:GLU:O	1:L:261:SER:OG	2.30	0.44
1:A:409:TYR:O	1:A:413:VAL:HG23	2.18	0.44
1:C:154:MET:HE3	1:C:173:TYR:HD1	1.82	0.44
1:D:76:LEU:HD22	1:D:117:LEU:HD12	1.99	0.44
1:I:76:LEU:HD12	1:I:117:LEU:HD12	2.00	0.44
1:L:143:LYS:HE3	1:L:143:LYS:HB2	1.90	0.44
1:D:252:TYR:CD1	1:D:272:THR:HG23	2.53	0.44
1:E:168:LYS:NZ	1:E:172:ASP:OD2	2.50	0.44
1:E:216:LEU:HD11	1:E:228:ILE:HG23	1.99	0.44
1:I:119:THR:O	1:I:123:ILE:HG13	2.18	0.44
1:I:201:HIS:CE1	2:U:27:LYS:HG3	2.52	0.44
1:I:410:TYR:O	1:I:413:VAL:HG12	2.18	0.44
1:C:356:TYR:HE2	1:C:363:LYS:HB3	1.82	0.44
1:E:388:LYS:HG3	1:E:416:LEU:HD22	1.99	0.44
1:F:67:ASP:N	1:F:67:ASP:OD1	2.51	0.44
1:H:369:LEU:HD21	1:H:390:TYR:HB2	2.00	0.44
1:J:135:LEU:HD12	1:J:160:LEU:HD22	1.99	0.44
1:K:227:ASN:HA	1:K:230:ASN:HD22	1.83	0.44
1:L:145:TYR:O	1:L:150:LYS:NZ	2.51	0.44
1:A:308:LEU:O	1:A:311:ILE:HG13	2.18	0.44
1:B:150:LYS:O	1:B:154:MET:HG2	2.18	0.44
1:C:313:GLU:HA	1:C:316:LEU:HD12	2.00	0.44
1:D:241:GLU:OE1	1:D:282:LYS:NZ	2.51	0.44
1:H:325:GLU:HG2	1:H:326:GLU:H	1.83	0.44
1:I:161:CYS:SG	1:I:166:ARG:NH1	2.88	0.44
1:K:98:LEU:HD13	1:K:114:TYR:HE1	1.83	0.43
1:K:173:TYR:O	1:K:177:THR:HG23	2.18	0.43
1:A:326:GLU:O	1:A:329:THR:OG1	2.24	0.43
1:B:164:GLN:HA	1:B:343:ARG:HG2	2.00	0.43
1:C:369:LEU:HA	1:C:372:GLU:HB3	1.99	0.43
1:I:107:ASP:HB3	1:I:110:ILE:HG12	2.00	0.43
1:I:120:ARG:HA	1:I:123:ILE:HD12	2.00	0.43
1:I:286:TYR:HD1	1:I:317:VAL:HG23	1.83	0.43
1:I:369:LEU:HD22	1:I:390:TYR:HE1	1.82	0.43
1:L:116:LEU:O	1:L:119:THR:HB	2.18	0.43
1:J:272:THR:O	1:J:276:MET:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:THR:O	1:A:123:ILE:HG13	2.18	0.43
1:G:111:ILE:HG22	1:G:115:LYS:NZ	2.33	0.43
1:I:354:LEU:HD23	1:I:354:LEU:H	1.83	0.43
1:J:84:VAL:HG22	1:J:120:ARG:HH12	1.84	0.43
1:C:80:LEU:HD13	1:C:117:LEU:HD11	2.01	0.43
1:C:209:ILE:HG23	1:C:235:ILE:HD13	1.99	0.43
1:G:328:ARG:HA	1:G:331:ILE:HG22	2.00	0.43
1:I:116:LEU:O	1:I:119:THR:HB	2.18	0.43
1:K:115:LYS:HD3	1:K:138:LEU:HD21	2.01	0.43
1:C:413:VAL:O	1:C:417:MET:HG2	2.19	0.43
1:D:229:ILE:O	1:D:233:ILE:HG13	2.18	0.43
1:L:76:LEU:HD23	1:L:102:MET:HE1	2.00	0.43
1:E:74:GLY:O	1:E:78:GLU:HG2	2.18	0.43
1:E:409:TYR:O	1:E:413:VAL:HG13	2.19	0.43
1:G:106:LEU:HA	1:G:111:ILE:HD11	2.00	0.43
1:J:296:SER:O	1:J:300:GLN:HG3	2.18	0.43
1:A:126:ARG:HA	1:A:126:ARG:HD3	1.87	0.43
1:A:406:SER:O	1:A:408:ARG:N	2.52	0.43
1:C:131:LEU:HD23	1:C:160:LEU:HD23	1.99	0.43
1:C:236:ALA:O	1:C:240:THR:HG23	2.19	0.43
1:C:401:SER:OG	1:C:402:ARG:N	2.52	0.43
1:D:345:ASN:O	1:D:348:LEU:HB3	2.18	0.43
1:F:374:ILE:H	1:F:375:PRO:HD3	1.84	0.43
1:G:229:ILE:O	1:G:233:ILE:HG13	2.18	0.43
1:I:135:LEU:HD12	1:I:160:LEU:HD22	2.00	0.43
1:J:256:LEU:HD13	1:J:276:MET:HE3	2.01	0.43
1:L:186:TYR:OH	1:L:188:GLU:OE2	2.29	0.43
1:B:113:TYR:O	1:B:117:LEU:HG	2.18	0.43
1:D:178:GLU:O	1:D:182:LYS:HG2	2.18	0.43
1:H:131:LEU:HD23	1:H:160:LEU:HD13	2.01	0.43
1:D:281:TYR:HE1	1:D:320:LYS:HG3	1.85	0.42
1:E:314:MET:HA	1:E:317:VAL:HG12	2.00	0.42
1:F:264:ASP:OD1	1:F:264:ASP:N	2.51	0.42
1:F:269:LEU:HB3	1:F:299:LEU:HD13	2.00	0.42
1:F:308:LEU:HD23	1:F:347:LYS:HB3	2.01	0.42
1:H:222:GLU:HG3	1:H:224:LYS:HG2	2.00	0.42
1:K:146:SER:HB2	1:K:149:GLN:HG3	2.00	0.42
1:I:356:TYR:HB3	1:I:365:TYR:HD2	1.84	0.42
1:A:186:TYR:CE2	1:A:188:GLU:HG3	2.55	0.42
1:L:218:GLY:O	1:L:222:GLU:HG2	2.20	0.42
1:C:349:TYR:HB3	1:C:372:GLU:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:407:ASN:HA	1:H:410:TYR:HD2	1.83	0.42
1:I:387:LYS:O	1:I:391:VAL:HG22	2.20	0.42
1:K:174:LEU:HB3	1:K:195:ILE:HG12	2.01	0.42
1:L:224:LYS:O	1:L:228:ILE:HG13	2.20	0.42
1:L:272:THR:O	1:L:276:MET:HG3	2.19	0.42
1:B:120:ARG:HE	1:B:120:ARG:HB2	1.69	0.42
1:E:155:TYR:O	1:E:159:LEU:HG	2.19	0.42
1:H:237:VAL:O	1:H:240:THR:OG1	2.29	0.42
1:I:309:ASP:OD2	2:U:25:SER:N	2.52	0.42
1:J:66:ARG:HD2	1:J:69:GLU:HG3	2.01	0.42
1:L:331:ILE:HD12	1:L:359:PHE:HE2	1.84	0.42
1:A:413:VAL:O	1:A:417:MET:HG2	2.19	0.42
1:B:347:LYS:HD2	1:B:350:LEU:HD21	2.02	0.42
1:D:355:ARG:NH2	1:D:360:GLU:OE2	2.53	0.42
1:E:286:TYR:HB2	1:E:321:LEU:HD21	2.02	0.42
1:J:226:ARG:O	1:J:229:ILE:HG22	2.19	0.42
1:K:123:ILE:HD11	2:W:30:ILE:HD11	2.00	0.42
1:L:165:TYR:CZ	1:L:305:LEU:HB2	2.54	0.42
1:L:200:THR:HG21	1:L:234:LEU:HD22	2.01	0.42
1:I:229:ILE:HD13	1:I:268:LEU:HD13	2.01	0.42
1:K:273:LEU:HD22	1:K:292:TYR:HD1	1.84	0.42
1:L:92:GLU:OE2	1:L:125:LYS:NZ	2.51	0.42
1:A:286:TYR:HB3	1:A:317:VAL:HG13	2.02	0.42
1:B:177:THR:HG22	1:B:191:LEU:HD11	2.01	0.42
1:E:341:GLU:HG2	1:E:343:ARG:HH11	1.85	0.42
1:F:229:ILE:HD13	1:F:268:LEU:HD13	2.00	0.42
1:G:205:HIS:HB3	1:G:208:ALA:H	1.85	0.42
1:J:398:SER:HB3	1:J:405:GLU:HB2	2.02	0.42
1:L:116:LEU:HD23	1:L:152:LEU:HB2	2.01	0.42
1:B:316:LEU:HA	1:B:319:ILE:HG12	2.02	0.42
1:C:293:TYR:OH	1:C:313:GLU:HB3	2.19	0.42
1:D:121:TYR:CZ	1:D:125:LYS:HD2	2.55	0.42
1:H:226:ARG:NH1	1:H:230:ASN:OD1	2.50	0.42
1:K:398:SER:OG	1:K:402:ARG:O	2.24	0.42
1:A:74:GLY:O	1:A:78:GLU:HG2	2.19	0.41
1:A:342:GLU:O	1:A:345:ASN:ND2	2.53	0.41
1:B:308:LEU:HA	1:B:311:ILE:HG22	2.01	0.41
1:H:146:SER:HB3	1:H:149:GLN:HG3	2.02	0.41
1:C:106:LEU:HA	1:C:111:ILE:HD11	2.02	0.41
1:D:122:LEU:HD22	1:D:131:LEU:HB2	2.02	0.41
1:H:150:LYS:O	1:H:154:MET:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:79:TRP:HE1	1:K:117:LEU:HD23	1.85	0.41
1:K:98:LEU:HD13	1:K:114:TYR:CE1	2.55	0.41
1:B:229:ILE:O	1:B:233:ILE:HG13	2.19	0.41
1:E:168:LYS:HD3	1:E:377:TYR:HD1	1.85	0.41
1:G:360:GLU:HG2	1:G:363:LYS:HD3	2.01	0.41
1:I:141:VAL:HG22	1:I:144:LYS:HB3	2.02	0.41
1:C:366:LYS:H	1:C:366:LYS:HG2	1.62	0.41
1:G:178:GLU:HA	1:G:191:LEU:HD21	2.02	0.41
1:K:192:TYR:HD1	1:K:211:PHE:HD1	1.68	0.41
1:K:314:MET:HG2	1:K:330:LEU:HD13	2.03	0.41
1:E:341:GLU:HB3	1:E:344:PHE:CE2	2.56	0.41
1:F:69:GLU:O	1:F:71:ASP:N	2.52	0.41
1:H:249:LEU:HG	1:H:279:ILE:HG21	2.01	0.41
1:L:314:MET:O	1:L:317:VAL:HG22	2.19	0.41
1:L:411:ARG:HA	1:L:414:ILE:HG22	2.03	0.41
1:B:302:GLN:HB3	1:B:303:ILE:H	1.56	0.41
1:C:120:ARG:O	1:C:123:ILE:HG13	2.21	0.41
1:E:209:ILE:HD11	1:E:238:SER:HB3	2.02	0.41
1:D:225:PHE:HA	1:D:228:ILE:HD12	2.01	0.41
1:L:231:CYS:O	1:L:235:ILE:HG12	2.21	0.41
1:A:142:TYR:HA	1:A:145:TYR:CD2	2.56	0.41
1:A:406:SER:HB2	1:D:403:PHE:CZ	2.56	0.41
1:B:206:HIS:CD2	1:C:242:LYS:HD3	2.56	0.41
1:C:412:LEU:HD13	1:C:416:LEU:HD23	2.03	0.41
1:E:242:LYS:HG2	1:H:206:HIS:CE1	2.56	0.41
1:H:135:LEU:HD13	1:H:157:ARG:HD2	2.02	0.41
1:J:242:LYS:HA	1:J:242:LYS:HD3	1.88	0.41
1:K:171:LEU:HD11	1:K:199:TYR:CZ	2.55	0.41
1:L:78:GLU:OE2	1:L:90:GLN:NE2	2.53	0.41
1:A:408:ARG:HG3	1:E:366:LYS:HZ3	1.85	0.41
1:B:161:CYS:SG	1:B:169:ASP:HB3	2.61	0.41
1:B:192:TYR:HD1	1:B:211:PHE:CD1	2.36	0.41
1:B:338:ALA:HB3	1:B:348:LEU:HD13	2.02	0.41
1:C:228:ILE:O	1:C:232:GLN:HG2	2.21	0.41
1:G:122:LEU:HD13	1:G:131:LEU:HA	2.03	0.41
1:H:157:ARG:NH1	1:H:160:LEU:HD23	2.36	0.41
1:I:395:GLU:HG2	1:I:406:SER:HB3	2.03	0.41
1:K:319:ILE:HG23	1:K:358:TYR:HE1	1.86	0.41
1:K:319:ILE:HD13	1:K:319:ILE:HA	1.95	0.41
1:L:119:THR:O	1:L:123:ILE:HG13	2.21	0.41
1:L:216:LEU:HD11	1:L:228:ILE:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286:TYR:HB3	1:C:317:VAL:HG23	2.03	0.41
1:C:319:ILE:HD12	1:C:358:TYR:CE2	2.56	0.41
1:E:409:TYR:O	1:E:412:LEU:HB3	2.21	0.41
1:F:312:TYR:HD1	1:F:351:LEU:HD23	1.86	0.41
1:G:123:ILE:HD13	1:G:159:LEU:HD12	2.02	0.41
1:K:226:ARG:O	1:K:229:ILE:HG22	2.21	0.41
1:B:164:GLN:O	1:B:166:ARG:N	2.54	0.40
1:F:143:LYS:HD3	1:F:143:LYS:HA	1.92	0.40
1:G:304:ASP:H	1:G:307:TYR:HB3	1.85	0.40
1:C:284:GLY:HA2	1:C:286:TYR:CZ	2.57	0.40
1:D:409:TYR:O	1:D:413:VAL:HG23	2.21	0.40
1:F:216:LEU:HD12	1:F:216:LEU:HA	1.90	0.40
1:H:119:THR:O	1:H:123:ILE:HG13	2.21	0.40
1:K:252:TYR:O	1:K:256:LEU:HB2	2.20	0.40
1:K:255:ILE:HD11	1:K:272:THR:OG1	2.22	0.40
1:K:264:ASP:OD1	1:K:264:ASP:N	2.54	0.40
1:L:90:GLN:HG3	1:L:93:ARG:HH21	1.87	0.40
1:L:123:ILE:HD13	1:L:159:LEU:HD12	2.03	0.40
1:D:150:LYS:O	1:D:154:MET:HG2	2.21	0.40
1:E:146:SER:O	1:E:149:GLN:N	2.49	0.40
1:E:229:ILE:O	1:E:233:ILE:HG13	2.21	0.40
1:I:203:ASP:HB3	1:I:204:ILE:HD12	2.04	0.40
1:I:204:ILE:HG13	1:I:241:GLU:HB3	2.02	0.40
1:J:120:ARG:HH22	1:J:188:GLU:CD	2.25	0.40
1:K:88:LYS:HA	1:K:91:VAL:HG22	2.02	0.40
1:K:251:MET:O	1:K:255:ILE:HG23	2.21	0.40
1:L:353:MET:HG3	1:L:390:TYR:CE1	2.56	0.40
1:L:355:ARG:HD2	1:L:359:PHE:HB2	2.03	0.40
1:E:363:LYS:HB3	1:E:364:ASP:OD1	2.21	0.40
1:I:414:ILE:HA	1:I:417:MET:HG2	2.03	0.40
1:K:233:ILE:HD11	1:K:255:ILE:HD13	2.03	0.40
1:A:390:TYR:CE1	1:A:394:ALA:HB2	2.57	0.40
1:D:312:TYR:CE1	1:D:354:LEU:HD22	2.57	0.40
1:E:190:GLY:HA2	2:Q:31:VAL:HG11	2.03	0.40
1:J:228:ILE:O	1:J:232:GLN:HG2	2.21	0.40
1:K:347:LYS:O	1:K:351:LEU:HG	2.22	0.40
2:T:27:LYS:HA	2:T:28:PRO:HD3	1.97	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [\(i\)](#)

### 5.3.1 Protein backbone [\(i\)](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	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
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

All (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
1	H	342	GLU
1	A	407	ASN
1	B	165	TYR
1	C	361	GLU
1	E	104	HIS
1	J	204	ILE
1	A	301	LYS
1	C	323	GLU
1	D	203	ASP
1	H	106	LEU
1	H	203	ASP
1	I	204	ILE
1	C	108	PHE
1	D	342	GLU
1	E	203	ASP
1	F	374	ILE
1	G	361	GLU
1	K	108	PHE
1	K	203	ASP
1	K	205	HIS
1	L	70	GLU
1	G	301	LYS
1	G	395	GLU
1	I	362	ALA
1	B	203	ASP
1	L	374	ILE
1	K	204	ILE
1	E	204	ILE
1	B	243	GLY

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

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	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
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

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ARG
1	A	141	VAL
1	A	288	GLN
1	A	391	VAL

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Mol	Chain	Res	Type
1	A	395	GLU
1	B	76	LEU
1	B	98	LEU
1	B	120	ARG
1	B	131	LEU
1	B	189	THR
1	B	201	HIS
1	B	206	HIS
1	B	321	LEU
1	B	323	GLU
1	B	354	LEU
1	C	105	VAL
1	C	123	ILE
1	C	148	PHE
1	C	151	LEU
1	C	155	TYR
1	C	168	LYS
1	C	204	ILE
1	C	207	LEU
1	C	212	VAL
1	C	249	LEU
1	C	314	MET
1	C	320	LYS
1	C	321	LEU
1	C	324	LEU
1	C	351	LEU
1	C	356	TYR
1	C	377	TYR
1	C	409	TYR
1	D	105	VAL
1	D	138	LEU
1	D	155	TYR
1	D	206	HIS
1	D	249	LEU
1	D	252	TYR
1	D	348	LEU
1	D	351	LEU
1	D	355	ARG
1	E	155	TYR
1	E	163	LEU
1	F	113	TYR
1	F	155	TYR

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Mol	Chain	Res	Type
1	F	204	ILE
1	F	320	LYS
1	F	391	VAL
1	F	409	TYR
1	G	86	LEU
1	G	102	MET
1	G	119	THR
1	G	122	LEU
1	G	141	VAL
1	G	155	TYR
1	G	160	LEU
1	G	204	ILE
1	G	205	HIS
1	G	303	ILE
1	G	354	LEU
1	H	106	LEU
1	H	113	TYR
1	H	119	THR
1	H	152	LEU
1	H	155	TYR
1	H	203	ASP
1	H	292	TYR
1	H	349	TYR
1	H	371	ASN
1	H	374	ILE
1	H	386	LEU
1	I	109	GLU
1	I	155	TYR
1	I	361	GLU
1	I	363	LYS
1	J	113	TYR
1	J	155	TYR
1	J	350	LEU
1	J	352	LEU
1	K	107	ASP
1	K	108	PHE
1	K	109	GLU
1	K	113	TYR
1	K	206	HIS
1	K	255	ILE
1	K	374	ILE
1	K	376	LEU

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Mol	Chain	Res	Type
1	K	403	PHE
1	L	113	TYR
1	L	155	TYR
1	L	160	LEU
1	L	396	HIS
1	L	397	PHE
1	L	406	SER
1	L	407	ASN
2	M	25	SER
2	M	27	LYS
2	N	27	LYS
2	N	29	ASP
2	O	30	ILE
2	R	31	VAL
2	U	27	LYS
2	X	27	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	HIS
1	A	194	ASN
1	D	396	HIS
1	E	149	GLN
1	K	194	ASN
1	L	300	GLN

### 5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [\(i\)](#)

There are no ligands in this entry.

## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

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

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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

All (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
1	E	102	MET	4.9
1	E	98	LEU	4.8
1	K	77	ASP	4.7
1	D	416	LEU	4.6
1	C	415	ASP	4.5
1	K	390	TYR	4.4
1	K	98	LEU	4.2
1	A	361	GLU	4.2
1	J	67	ASP	4.2
1	F	419	ASP	4.1
1	D	415	ASP	4.1
1	H	410	TYR	4.1
1	B	356	TYR	4.1
1	A	402	ARG	4.0
1	I	410	TYR	3.9
1	C	414	ILE	3.9
1	K	73	LYS	3.9
2	P	25	SER	3.9
1	C	388	LYS	3.9
1	C	392	GLU	3.8
1	A	401	SER	3.8
1	A	327	ALA	3.8
1	G	390	TYR	3.8
1	B	401	SER	3.8
1	L	100	GLY	3.7
1	J	403	PHE	3.7
1	B	77	ASP	3.6
2	O	25	SER	3.5
1	B	336	ASP	3.5
1	L	411	ARG	3.5
1	G	392	GLU	3.5
1	E	411	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	103	LYS	3.5
1	G	415	ASP	3.4
1	K	415	ASP	3.4
1	A	415	ASP	3.4
1	E	332	ASP	3.4
1	A	392	GLU	3.4
2	N	25	SER	3.4
1	H	363	LYS	3.4
1	B	416	LEU	3.4
1	J	394	ALA	3.4
1	A	390	TYR	3.4
1	B	397	PHE	3.3
1	E	94	ILE	3.3
1	K	408	ARG	3.3
2	S	25	SER	3.2
1	I	306	ASN	3.2
2	W	25	SER	3.2
1	I	322	GLU	3.2
1	D	410	TYR	3.2
1	I	399	SER	3.2
1	C	283	LYS	3.1
1	L	410	TYR	3.1
1	F	318	CYS	3.0
1	F	401	SER	3.0
1	A	363	LYS	3.0
1	B	399	SER	3.0
1	C	364	ASP	3.0
1	C	410	TYR	2.9
1	A	70	GLU	2.9
1	B	128	ILE	2.9
1	I	388	LYS	2.9
1	B	360	GLU	2.9
1	B	411	ARG	2.9
1	E	322	GLU	2.9
1	B	129	SER	2.9
1	K	78	GLU	2.9
2	M	28	PRO	2.9
1	K	358	TYR	2.9
1	E	100	GLY	2.9
1	B	287	GLN	2.9
1	I	309	ASP	2.9
1	K	349	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	408	ARG	2.9
1	D	390	TYR	2.9
1	A	364	ASP	2.9
1	C	289	ALA	2.8
1	K	71	ASP	2.8
1	B	407	ASN	2.8
1	H	401	SER	2.8
1	E	364	ASP	2.8
1	B	164	GLN	2.8
1	D	356	TYR	2.8
1	E	140	LYS	2.8
1	G	68	VAL	2.8
1	D	206	HIS	2.8
1	H	104	HIS	2.8
1	K	412	LEU	2.7
2	U	26	SER	2.7
1	B	415	ASP	2.7
1	A	416	LEU	2.7
1	E	171	LEU	2.7
1	B	344	PHE	2.7
1	H	94	ILE	2.7
1	C	416	LEU	2.7
1	L	372	GLU	2.7
1	H	395	GLU	2.7
1	C	374	ILE	2.7
1	E	88	LYS	2.6
1	G	349	TYR	2.6
1	E	318	CYS	2.6
1	H	411	ARG	2.6
1	B	373	ALA	2.6
1	C	402	ARG	2.6
1	E	306	ASN	2.6
1	A	320	LYS	2.6
1	C	405	GLU	2.5
1	E	317	VAL	2.5
1	F	415	ASP	2.5
1	G	324	LEU	2.5
1	B	133	GLU	2.5
1	B	103	LYS	2.5
1	E	397	PHE	2.5
1	D	375	PRO	2.5
1	B	113	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	K	99	GLN	2.5
1	A	349	TYR	2.5
1	H	71	ASP	2.5
1	I	408	ARG	2.5
1	B	135	LEU	2.5
1	I	310	THR	2.5
1	G	322	GLU	2.5
1	D	207	LEU	2.4
1	D	374	ILE	2.4
1	I	412	LEU	2.4
1	B	165	TYR	2.4
1	E	107	ASP	2.4
2	U	25	SER	2.4
1	J	321	LEU	2.4
1	B	363	LYS	2.4
1	J	410	TYR	2.4
1	B	204	ILE	2.4
1	C	371	ASN	2.4
1	B	412	LEU	2.4
1	D	89	GLN	2.3
1	B	109	GLU	2.3
1	H	129	SER	2.3
1	B	361	GLU	2.3
1	D	409	TYR	2.3
1	E	147	PRO	2.3
2	T	25	SER	2.3
1	L	322	GLU	2.3
1	H	364	ASP	2.3
1	A	410	TYR	2.3
1	K	133	GLU	2.3
1	A	413	VAL	2.3
1	A	372	GLU	2.3
1	I	364	ASP	2.3
1	I	363	LYS	2.3
1	B	288	GLN	2.3
1	A	306	ASN	2.2
1	H	416	LEU	2.2
2	U	28	PRO	2.2
1	A	318	CYS	2.2
1	H	98	LEU	2.2
1	D	371	ASN	2.2
1	G	310	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	397	PHE	2.2
2	M	25	SER	2.2
1	C	74	GLY	2.2
1	L	386	LEU	2.2
2	M	27	LYS	2.2
1	C	285	LYS	2.2
1	E	73	LYS	2.2
1	E	412	LEU	2.2
1	C	397	PHE	2.2
1	J	322	GLU	2.2
1	H	153	TYR	2.1
1	D	370	GLU	2.1
1	F	322	GLU	2.1
1	I	416	LEU	2.1
1	B	172	ASP	2.1
1	A	403	PHE	2.1
1	A	404	GLU	2.1
1	K	70	GLU	2.1
1	K	162	CYS	2.1
1	E	142	TYR	2.1
1	D	325	GLU	2.1
1	B	131	LEU	2.1
1	K	74	GLY	2.1
1	B	306	ASN	2.1
1	D	306	ASN	2.1
1	A	362	ALA	2.1
1	B	362	ALA	2.1
1	B	140	LYS	2.0
1	B	322	GLU	2.0
1	H	404	GLU	2.0
1	H	377	TYR	2.0
1	B	230	ASN	2.0
1	J	404	GLU	2.0
1	D	388	LYS	2.0
1	E	114	TYR	2.0

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

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

### 6.3 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [\(i\)](#)

There are no ligands in this entry.

### 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.