



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:59 PM GMT

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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

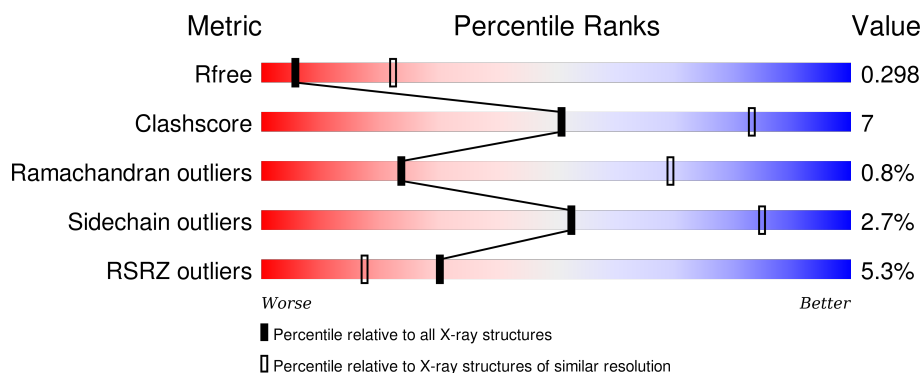
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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 ≥ 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	372	<div> <div>6%</div> <div>77%</div> <div>15%</div> <div>8%</div> </div>
1	B	372	<div> <div>10%</div> <div>69%</div> <div>21%</div> <div>8%</div> </div>
1	C	372	<div> <div>5%</div> <div>67%</div> <div>22%</div> <div>9%</div> </div>
1	D	372	<div> <div>4%</div> <div>67%</div> <div>24%</div> <div>8%</div> </div>
1	E	372	<div> <div>6%</div> <div>74%</div> <div>17%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	372	
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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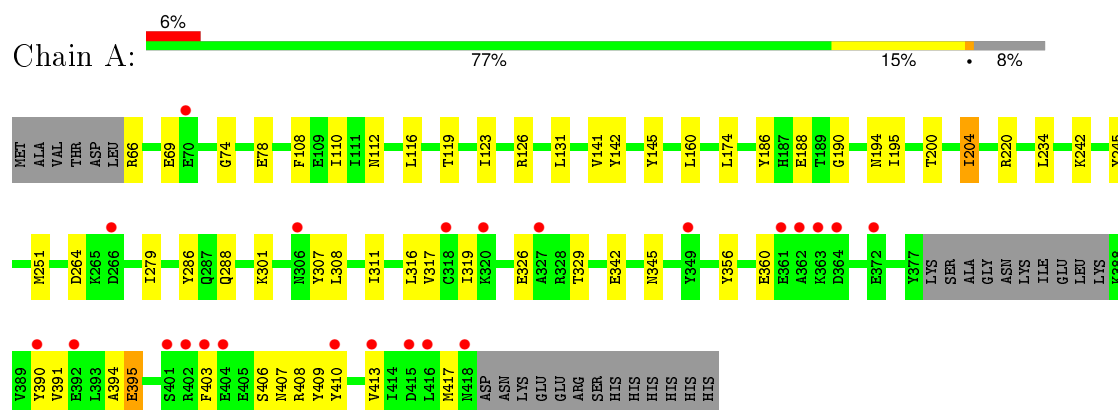
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	W	8	Total	C	N	O	0	0	0
			56	34	9	13			
2	X	8	Total	C	N	O	0	0	0
			56	34	9	13			

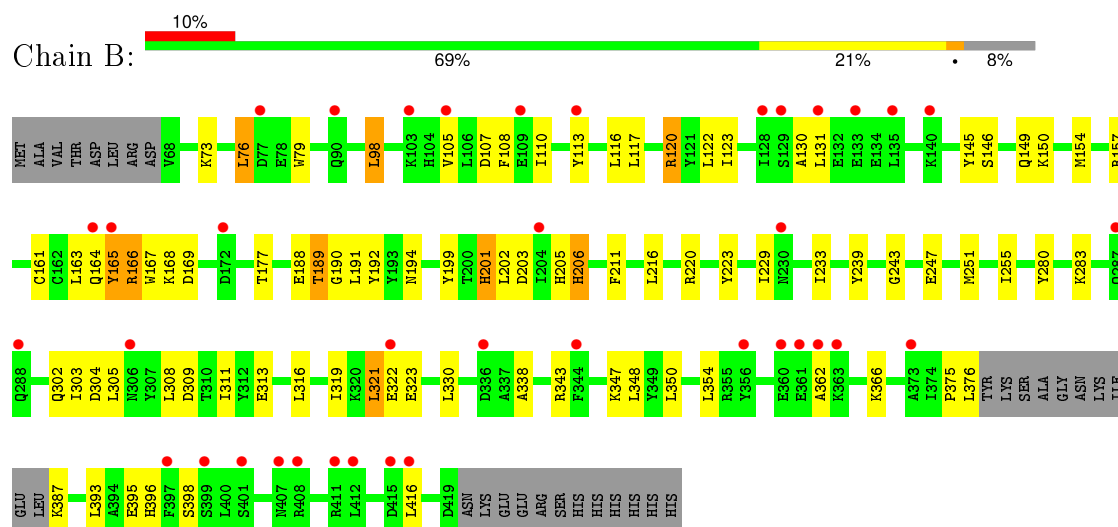
3 Residue-property plots

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 ($RSRZ > 2$). 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.

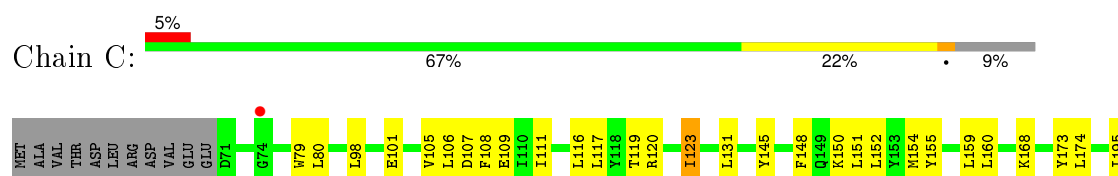
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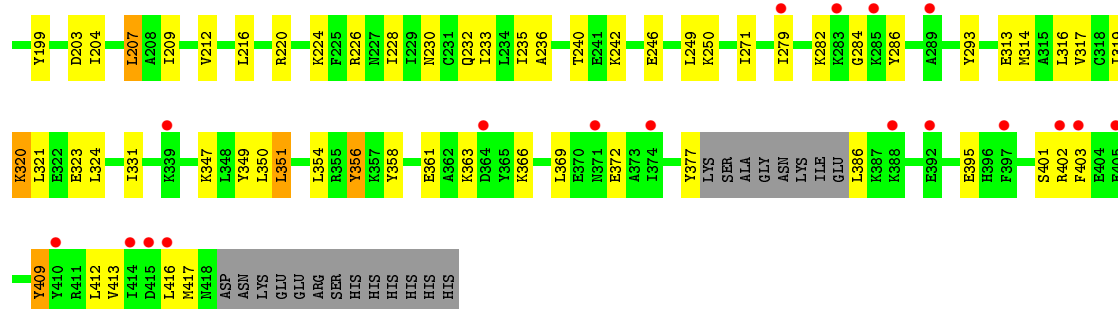


• Molecule 1: NprR

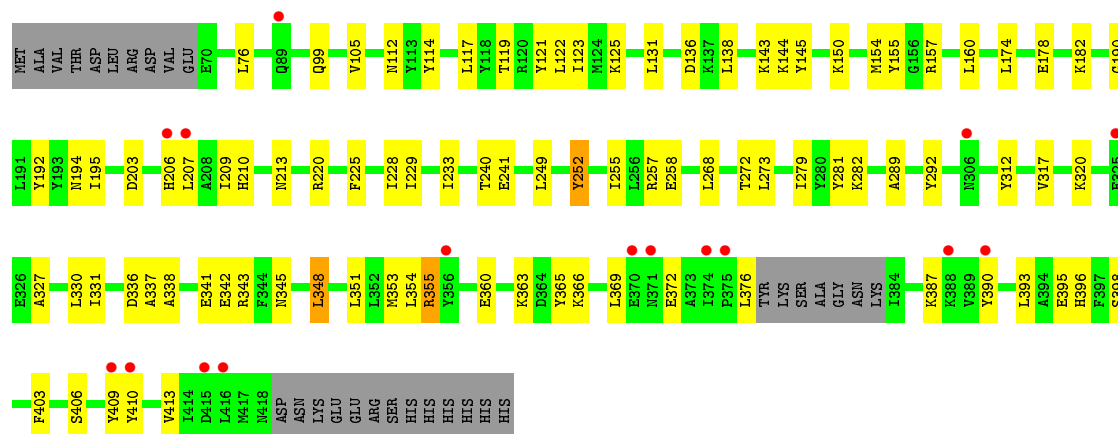


• Molecule 1: NprR

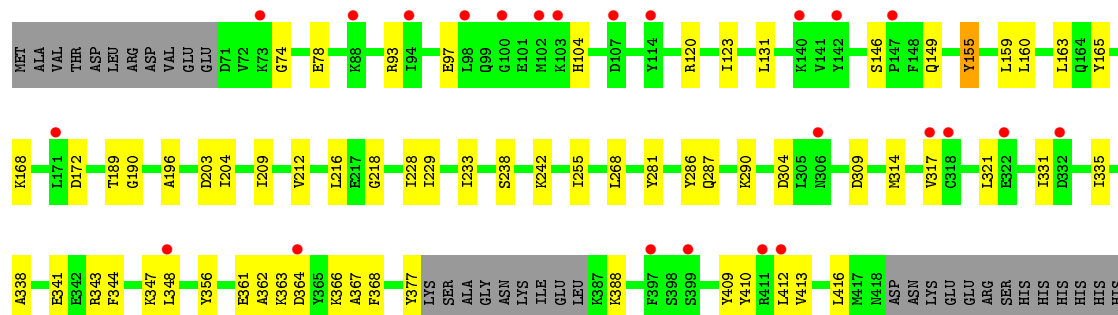
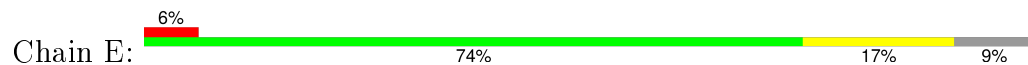




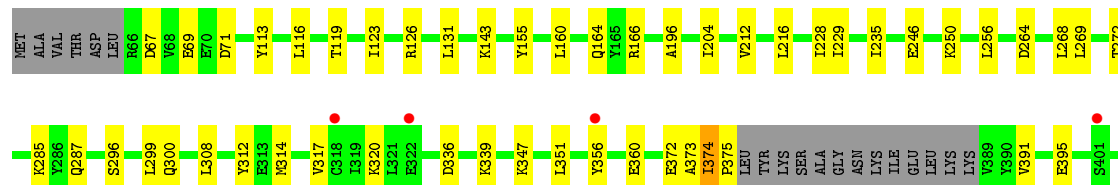
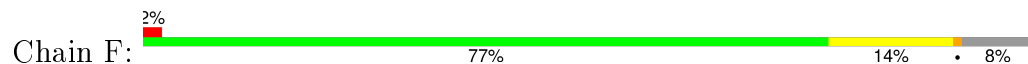
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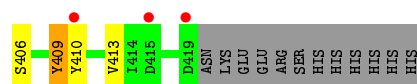


• Molecule 1: NprR

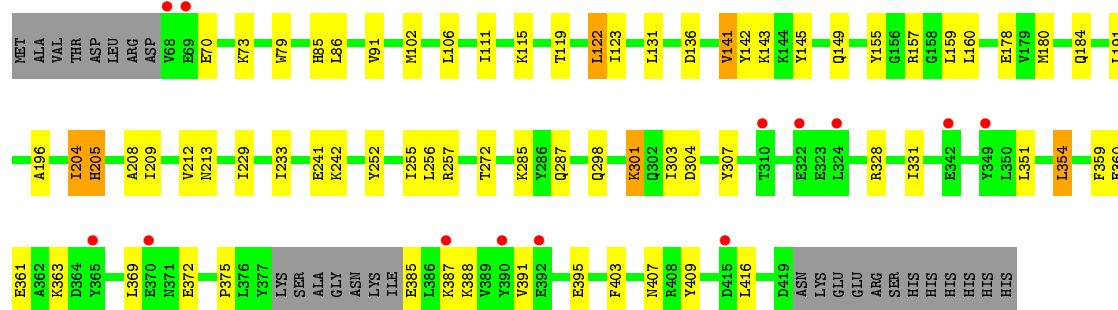
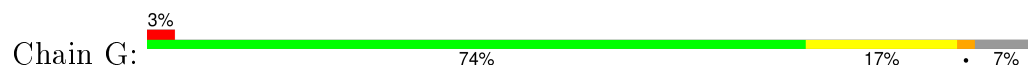


• Molecule 1: NprR

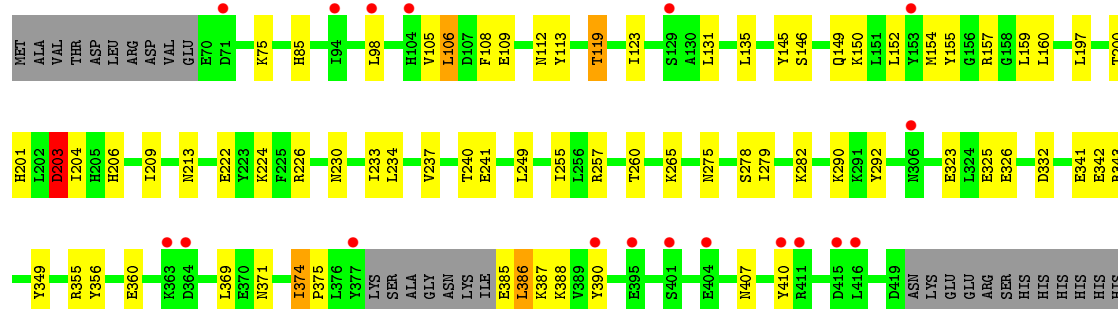
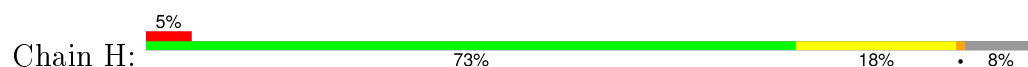




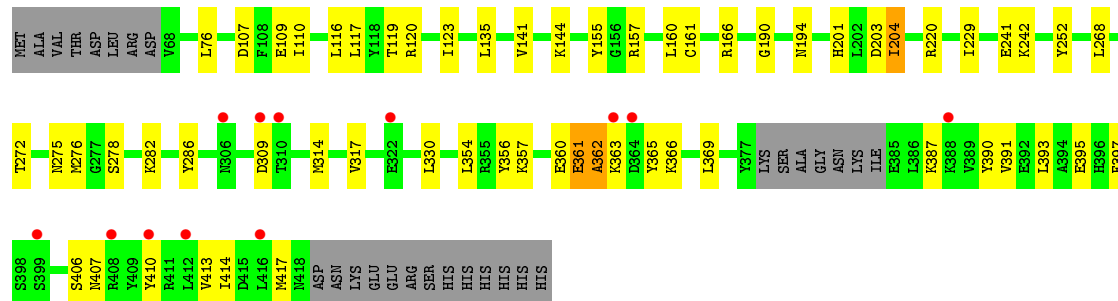
• Molecule 1: NprR



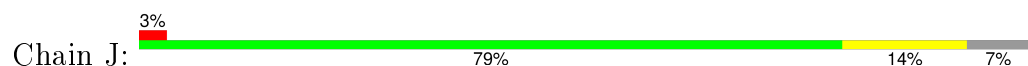
• Molecule 1: NprR

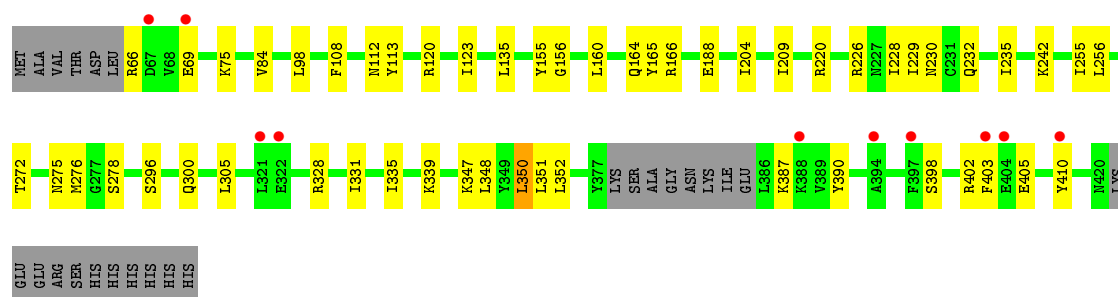


• Molecule 1: NprR

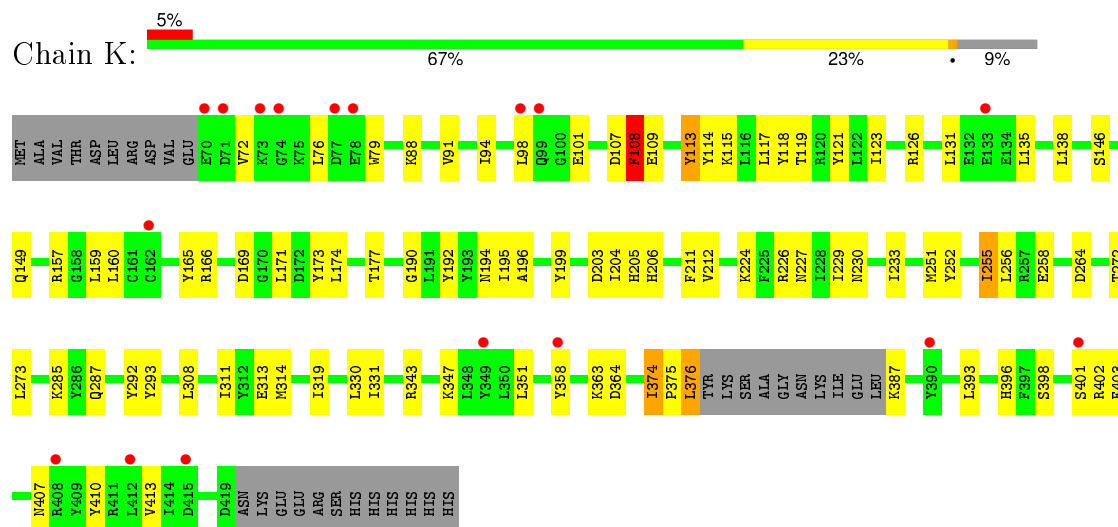


• Molecule 1: NprR

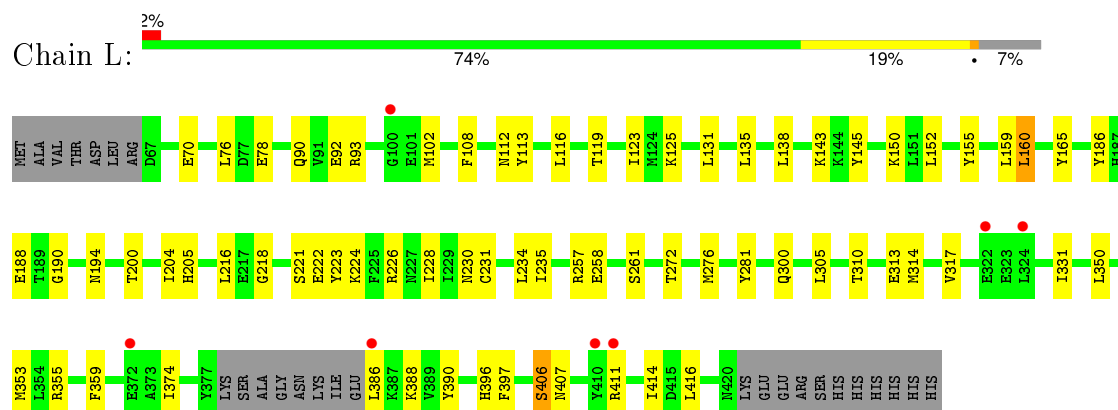




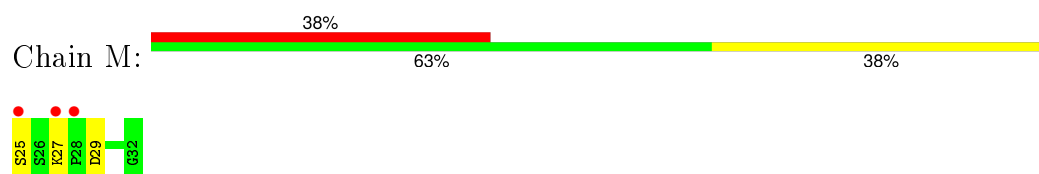
- Molecule 1: NprR



- Molecule 1: NprR

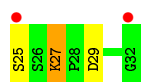


- Molecule 2: NprX peptide

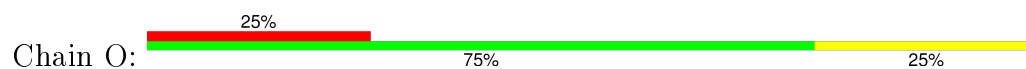


- Molecule 2: NprX peptide





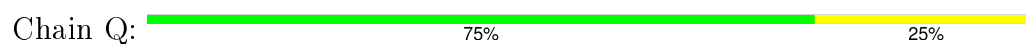
- Molecule 2: NprX peptide



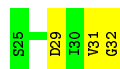
- Molecule 2: NprX peptide



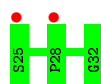
- Molecule 2: NprX peptide



- Molecule 2: NprX peptide



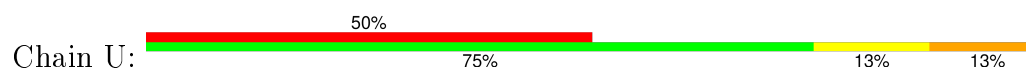
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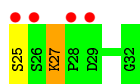


- Molecule 2: NprX peptide



- Molecule 2: NprX peptide





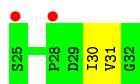
- Molecule 2: NprX peptide

Chain V: 88% 13%



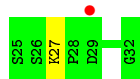
- Molecule 2: NprX peptide

Chain W: 25% 75% 25%



- Molecule 2: NprX peptide

Chain X: 13% 88% 13%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	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) 85.1 (29.74-3.20)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 3.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.270 , 0.299 0.267 , 0.298	Depositor DCC
R_{free} test set	24308 reflections (20.00%)	DCC
Wilson B-factor (Å ²)	116.6	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 62.8	EDS
Estimated twinning fraction	0.007 for -h,-l,-k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 121651 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	35360	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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.

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:K:190:GLY:O	1:K:194:ASN:ND2	2.25	0.70
1:H:341:GLU:O	1:H:343:ARG:N	2.23	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:H:75:LYS:HB3	1:H:98:LEU:HD11	1.78	0.64
1:B:161:CYS:SG	1:B:166:ARG:NH1	2.70	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:K:123:ILE:O	1:K:126:ARG:NH1	2.33	0.62
1:G:403:PHE:O	1:G:407:ASN:ND2	2.33	0.62
1:K:398:SER:HA	1:K:401:SER:HB2	1.81	0.61
1:B:189:THR:HA	1:B:192:TYR:HD2	1.65	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:E:131:LEU:HD23	1:E:160:LEU:HD23	1.86	0.58
1:A:108:PHE:O	1:A:112:ASN:ND2	2.37	0.58
1:B:123:ILE:HG13	1:B:163:LEU:HD11	1.86	0.57
1:A:69:GLU:HG3	1:A:110:ILE:HD11	1.85	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:K:72:VAL:O	1:K:76:LEU:HG	2.05	0.57
1:D:338:ALA:HB1	1:D:348:LEU:HB2	1.85	0.57
1:A:395:GLU:HG2	1:A:410:TYR:CZ	2.39	0.57
1:K:119:THR:HG23	1:K:131:LEU:HD11	1.85	0.57
1:D:336:ASP:OD1	1:D:337:ALA:N	2.38	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:K:376:LEU:O	1:K:387:LYS:NZ	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:LEU:O	1:B:396:HIS:ND1	2.32	0.56
1:D:182:LYS:NZ	1:D:192:TYR:OH	2.35	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:K:308:LEU:HA	1:K:311:ILE:HB	1.88	0.56
1:D:331:ILE:HD12	1:D:355:ARG:HB2	1.88	0.56
1:J:305:LEU:HB2	1:J:347:LYS:HZ2	1.71	0.55
1:A:116:LEU:O	1:A:119:THR:OG1	2.19	0.55
1:K:375:PRO:HB2	1:K:376:LEU:HD23	1.89	0.55
1:I:357:LYS:HE2	1:I:393:LEU:HD21	1.88	0.55
1:F:164:GLN:OE1	1:F:166:ARG:NH1	2.39	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:K:79:TRP:HZ2	1:K:121:TYR:HH	1.55	0.54
1:F:395:GLU:HG2	1:F:406:SER:HB2	1.89	0.54
1:L:204:ILE:O	1:L:205:HIS:ND1	2.40	0.54
1:J:350:LEU:HD23	1:J:351:LEU:HD22	1.90	0.54
1:H:278:SER:OG	1:H:282:LYS:NZ	2.40	0.54
1:F:216:LEU:HD11	1:F:228:ILE:HG23	1.90	0.54
1:F:196:ALA:HB1	1:F:212:VAL:HG23	1.90	0.54
1:A:316:LEU:HD12	1:A:319:ILE:HD11	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:G:252:TYR:HD1	1:G:255:ILE:HD11	1.74	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: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:410:TYR:HA	1:E:413:VAL:HG22	1.91	0.53
1:E:229:ILE:HD13	1:E:268:LEU:HD13	1.91	0.53
1:L:116:LEU:HD12	1:L:138:LEU:HD13	1.91	0.52
1:K:113:TYR:HD1	1:K:114:TYR:N	2.08	0.52
1:D:365:TYR:O	1:D:369:LEU:N	2.41	0.52
1:D:207:LEU:HA	1:D:210:HIS:HB3	1.90	0.52
1:H:260:THR:HA	1:H:265:LYS:HE2	1.90	0.52
1:D:257:ARG:HH11	1:D:258:GLU:HG2	1.74	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:K:196:ALA:HB1	1:K:212:VAL:HG23	1.92	0.51
1:H:385:GLU:HA	1:H:388:LYS:HE2	1.91	0.51
1:A:174:LEU:HB3	1:A:195:ILE:HG12	1.91	0.51
1:B:192:TYR:HD1	1:B:211:PHE:HD1	1.56	0.51
1:A:200:THR:HG21	1:A:234:LEU:HD22	1.91	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:393:LEU:HA	1:D:396:HIS:HD2	1.75	0.51
1:D:229:ILE:HD13	1:D:268:LEU:HD13	1.93	0.51
1:E:209:ILE:HA	1:E:212:VAL:HG22	1.93	0.50
1:C:233:ILE:HD13	1:C:271:ILE:HD11	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:H:203:ASP:HB3	1:H:204:ILE:HG13	1.93	0.50
1:G:145:TYR:HB3	1:G:149:GLN:HB2	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:J:229:ILE:HD11	1:J:255:ILE:HG23	1.93	0.49
1:C:230:ASN:HA	1:C:233:ILE:HD12	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:C:230:ASN:HD22	2:O:28:PRO:HB3	1.77	0.49
1:A:403:PHE:HB3	1:D:403:PHE:CE2	2.48	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:K:118:TYR:HA	1:K:121:TYR:CD2	2.48	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:D:353:MET:HE1	1:D:390:TYR:CE2	2.47	0.49
1:G:285:LYS:O	1:G:287:GLN:N	2.44	0.49
1:F:131:LEU:HD23	1:F:160:LEU:HD23	1.94	0.49
1:J:165:TYR:CZ	1:J:305:LEU:HD23	2.48	0.49
1:F:395:GLU:HG3	1:F:410:TYR:HB2	1.95	0.49
1:B:375:PRO:HG2	1:B:376:LEU:HD12	1.94	0.49
1:B:146:SER:H	1:B:149:GLN:HB2	1.77	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:B:280:TYR:HA	1:B:283:LYS:HB3	1.95	0.48
1:I:272:THR:HG22	1:I:276:MET:HE3	1.94	0.48
1:I:369:LEU:O	1:I:390:TYR:OH	2.30	0.48
1:E:281:TYR:HD1	1:E:317:VAL:HG23	1.78	0.48
1:E:286:TYR:HB3	1:E:317:VAL:HG22	1.95	0.48
1:B:309:ASP:HA	1:B:347:LYS:HE2	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:J:328:ARG:HA	1:J:331:ILE:HG22	1.96	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:G:369:LEU:HA	1:G:372:GLU:HB2	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: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:B:107:ASP:OD1	1:B:108:PHE:N	2.47	0.48
1:I:314:MET:HE3	1:I:330:LEU:HD13	1.96	0.48
1:I:252:TYR:OH	1:I:275:ASN:ND2	2.46	0.48
1:H:197:LEU:HD23	2:T:30:ILE:HG22	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:K:229:ILE:O	1:K:233:ILE:HG12	2.14	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:E:146:SER:OG	1:E:149:GLN:NE2	2.47	0.47
1:J:275:ASN:O	1:J:278:SER:OG	2.24	0.47
1:D:369:LEU:O	1:D:372:GLU:HG3	2.14	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:K:113:TYR:C	1:K:113:TYR:HD1	2.17	0.47
1:G:204:ILE:HD12	1:G:241:GLU:HB3	1.96	0.47
1:E:93:ARG:O	1:E:97:GLU:HG2	2.13	0.47
1:D:229:ILE:HD11	1:D:255:ILE:HG23	1.96	0.47
1:A:307:TYR:HD2	1:A:308:LEU:HD12	1.80	0.47
1:L:218:GLY:O	1:L:221:SER:OG	2.24	0.47
1:C:107:ASP:O	1:C:109:GLU:N	2.46	0.47
1:B:73:LYS:HA	1:B:76:LEU:HB2	1.97	0.47
1:J:331:ILE:O	1:J:335:ILE:HG12	2.15	0.47
1:I:278:SER:OG	1:I:282:LYS:NZ	2.41	0.47
1:A:264:ASP:OD1	1:A:264:ASP:N	2.48	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:I:354:LEU:HA	1:I:357:LYS:HB3	1.97	0.46
1:H:386:LEU:HD22	1:H:387:LYS:HG2	1.97	0.46
1:K:331:ILE:HG13	1:K:351:LEU:HD22	1.96	0.46
1:D:119:THR:O	1:D:123:ILE:HG13	2.15	0.46
1:C:286:TYR:CG	1:C:320:LYS:HD2	2.50	0.46
1:G:385:GLU:HB3	1:G:388:LYS:HE2	1.97	0.46
1:E:338:ALA:HB3	1:E:348:LEU:HD13	1.96	0.46
1:K:113:TYR:C	1:K:113:TYR:CD1	2.89	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:F:409:TYR:O	1:F:413:VAL:HG13	2.15	0.46
1:I:410:TYR:HE1	1:L:414:ILE:HB	1.80	0.46
1:C:98:LEU:HA	1:C:101:GLU:HB2	1.96	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: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:391:VAL:HG13	1:G:409:TYR:HB3	1.97	0.46
1:K:285:LYS:O	1:K:287:GLN:N	2.48	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:G:209:ILE:O	1:G:213:ASN:ND2	2.47	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:D:240:THR:HG23	1:D:279:ILE:HG12	1.98	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:362:ALA:O	1:B:366:LYS:NZ	2.50	0.45
1:K:108:PHE:CD2	1:K:108:PHE:N	2.84	0.45
1:B:201:HIS:CE1	2:N:27:LYS:HD3	2.50	0.45
1:C:79:TRP:CZ3	1:C:117:LEU:HB3	2.51	0.45
1:B:188:GLU:HG2	1:B:191:LEU:H	1.81	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:HA	1:I:242:LYS:HD2	1.73	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:G:359:PHE:N	1:G:360:GLU:HA	2.31	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:I:410:TYR:CE1	1:L:414:ILE:HB	2.52	0.45
1:E:287:GLN:HA	1:E:290:LYS:HE2	1.98	0.45
1:H:109:GLU:HA	1:H:112:ASN:HD22	1.82	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:B:168:LYS:HG2	1:B:202:LEU:HD21	1.98	0.44
1:L:108:PHE:O	1:L:112:ASN:ND2	2.50	0.44
1:E:361:GLU:HA	1:E:362:ALA:HA	1.70	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: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: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:B:165:TYR:O	1:B:167:TRP:N	2.51	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:E:331:ILE:O	1:E:335:ILE:HG12	2.18	0.44
1:D:273:LEU:HD22	1:D:292:TYR:HD1	1.82	0.44
1:C:331:ILE:HD12	1:C:354:LEU:HD22	2.00	0.44
1:C:116:LEU:O	1:C:119:THR:HB	2.18	0.44
1:L:258:GLU:O	1:L:261:SER:OG	2.30	0.44
1:F:256:LEU:HB2	1:F:272:THR:HG21	1.99	0.44
1:D:76:LEU:HD22	1:D:117:LEU:HD12	1.99	0.44
1:C:154:MET:HE3	1:C:173:TYR:HD1	1.82	0.44
1:L:143:LYS:HB2	1:L:143:LYS:HE3	1.90	0.44
1:A:409:TYR:O	1:A:413:VAL:HG23	2.18	0.44
1:I:76:LEU:HD12	1:I:117:LEU:HD12	2.00	0.44
1:I:410:TYR:O	1:I:413:VAL:HG12	2.18	0.44
1:I:119:THR:O	1:I:123:ILE:HG13	2.18	0.44
1:E:216:LEU:HD11	1:E:228:ILE:HG23	1.99	0.44
1:I:201:HIS:CE1	2:U:27:LYS:HG3	2.52	0.44
1:E:168:LYS:NZ	1:E:172:ASP:OD2	2.50	0.44
1:D:252:TYR:CD1	1:D:272:THR:HG23	2.53	0.44
1:K:227:ASN:HA	1:K:230:ASN:HD22	1.83	0.44
1:H:369:LEU:HD21	1:H:390:TYR:HB2	2.00	0.44
1:L:145:TYR:O	1:L:150:LYS:NZ	2.51	0.44
1:E:388:LYS:HG3	1:E:416:LEU:HD22	1.99	0.44
1:J:135:LEU:HD12	1:J:160:LEU:HD22	1.99	0.44
1:C:356:TYR:HE2	1:C:363:LYS:HB3	1.82	0.44
1:F:67:ASP:OD1	1:F:67:ASP:N	2.51	0.44
1:B:150:LYS:O	1:B:154:MET:HG2	2.18	0.44
1:A:308:LEU:O	1:A:311:ILE:HG13	2.18	0.44
1:H:325:GLU:HG2	1:H:326:GLU:H	1.83	0.44
1:C:313:GLU:HA	1:C:316:LEU:HD12	2.00	0.44
1:I:161:CYS:SG	1:I:166:ARG:NH1	2.88	0.44
1:D:241:GLU:OE1	1:D:282:LYS:NZ	2.51	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:L:116:LEU:O	1:L:119:THR:HB	2.18	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:369:LEU:HD22	1:I:390:TYR:HE1	1.82	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:107:ASP:HB3	1:I:110:ILE:HG12	2.00	0.43
1:A:326:GLU:O	1:A:329:THR:OG1	2.24	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:I:354:LEU:H	1:I:354:LEU:HD23	1.83	0.43
1:J:84:VAL:HG22	1:J:120:ARG:HH12	1.84	0.43
1:G:111:ILE:HG22	1:G:115:LYS:NZ	2.33	0.43
1:G:328:ARG:HA	1:G:331:ILE:HG22	2.00	0.43
1:C:80:LEU:HD13	1:C:117:LEU:HD11	2.01	0.43
1:I:116:LEU:O	1:I:119:THR:HB	2.18	0.43
1:C:209:ILE:HG23	1:C:235:ILE:HD13	1.99	0.43
1:K:115:LYS:HD3	1:K:138:LEU:HD21	2.01	0.43
1:D:229:ILE:O	1:D:233:ILE:HG13	2.18	0.43
1:C:413:VAL:O	1:C:417:MET:HG2	2.19	0.43
1:L:76:LEU:HD23	1:L:102:MET:HE1	2.00	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:E:74:GLY:O	1:E:78:GLU:HG2	2.18	0.43
1:J:296:SER:O	1:J:300:GLN:HG3	2.18	0.43
1:I:135:LEU:HD12	1:I:160:LEU:HD22	2.00	0.43
1:C:401:SER:OG	1:C:402:ARG:N	2.52	0.43
1:F:374:ILE:H	1:F:375:PRO:HD3	1.84	0.43
1:D:345:ASN:O	1:D:348:LEU:HB3	2.18	0.43
1:A:406:SER:O	1:A:408:ARG:N	2.52	0.43
1:A:126:ARG:HD3	1:A:126:ARG:HA	1.87	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:C:236:ALA:O	1:C:240:THR:HG23	2.19	0.43
1:C:131:LEU:HD23	1:C:160:LEU:HD23	1.99	0.43
1:G:229:ILE:O	1:G:233:ILE:HG13	2.18	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:E:314:MET:HA	1:E:317:VAL:HG12	2.00	0.42
1:H:222:GLU:HG3	1:H:224:LYS:HG2	2.00	0.42
1:F:269:LEU:HB3	1:F:299:LEU:HD13	2.00	0.42
1:K:146:SER:HB2	1:K:149:GLN:HG3	2.00	0.42
1:F:264:ASP:N	1:F:264:ASP:OD1	2.51	0.42
1:D:281:TYR:HE1	1:D:320:LYS:HG3	1.85	0.42
1:F:308:LEU:HD23	1:F:347:LYS:HB3	2.01	0.42
1:I:356:TYR:HB3	1:I:365:TYR:HD2	1.84	0.42
1:L:218:GLY:O	1:L:222:GLU:HG2	2.20	0.42
1:A:186:TYR:CE2	1:A:188:GLU:HG3	2.55	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:K:174:LEU:HB3	1:K:195:ILE:HG12	2.01	0.42
1:I:387:LYS:O	1:I:391:VAL:HG22	2.20	0.42
1:H:407:ASN:HA	1:H:410:TYR:HD2	1.83	0.42
1:L:272:THR:O	1:L:276:MET:HG3	2.19	0.42
1:L:224:LYS:O	1:L:228:ILE:HG13	2.20	0.42
1:B:120:ARG:HB2	1:B:120:ARG:HE	1.69	0.42
1:E:155:TYR:O	1:E:159:LEU:HG	2.19	0.42
1:L:331:ILE:HD12	1:L:359:PHE:HE2	1.84	0.42
1:H:237:VAL:O	1:H:240:THR:OG1	2.29	0.42
1:J:66:ARG:HD2	1:J:69:GLU:HG3	2.01	0.42
1:I:309:ASP:OD2	2:U:25:SER:N	2.52	0.42
1:K:123:ILE:HD11	2:W:30:ILE:HD11	2.00	0.42
1:D:355:ARG:NH2	1:D:360:GLU:OE2	2.53	0.42
1:J:226:ARG:O	1:J:229:ILE:HG22	2.19	0.42
1:E:286:TYR:HB2	1:E:321:LEU:HD21	2.02	0.42
1:B:347:LYS:HD2	1:B:350:LEU:HD21	2.02	0.42
1:A:413:VAL:O	1:A:417:MET:HG2	2.19	0.42
1:L:200:THR:HG21	1:L:234:LEU:HD22	2.01	0.42
1:L:165:TYR:CZ	1:L:305:LEU:HB2	2.54	0.42
1:I:229:ILE:HD13	1:I:268:LEU:HD13	2.01	0.42
1:L:92:GLU:OE2	1:L:125:LYS:NZ	2.51	0.42
1:K:273:LEU:HD22	1:K:292:TYR:HD1	1.84	0.42
1:L:116:LEU:HD23	1:L:152:LEU:HB2	2.01	0.42
1:E:341:GLU:HG2	1:E:343:ARG:HH11	1.85	0.42
1:B:177:THR:HG22	1:B:191:LEU:HD11	2.01	0.42
1:J:398:SER:HB3	1:J:405:GLU:HB2	2.02	0.42
1:A:286:TYR:HB3	1:A:317:VAL:HG13	2.02	0.42
1:G:205:HIS:HB3	1:G:208:ALA:H	1.85	0.42
1:F:229:ILE:HD13	1:F:268:LEU:HD13	2.00	0.42
1:K:398:SER:OG	1:K:402:ARG:O	2.24	0.42
1:C:293:TYR:OH	1:C:313:GLU:HB3	2.19	0.42
1:B:316:LEU:HA	1:B:319:ILE:HG12	2.02	0.42
1:H:226:ARG:NH1	1:H:230:ASN:OD1	2.50	0.42
1:D:121:TYR:CZ	1:D:125:LYS:HD2	2.55	0.42
1:B:308:LEU:HA	1:B:311:ILE:HG22	2.01	0.41
1:A:74:GLY:O	1:A:78:GLU:HG2	2.19	0.41
1:H:146:SER:HB3	1:H:149:GLN:HG3	2.02	0.41
1:A:342:GLU:O	1:A:345:ASN:ND2	2.53	0.41
1:K:98:LEU:HD13	1:K:114:TYR:CE1	2.55	0.41
1:H:150:LYS:O	1:H:154:MET:HG2	2.20	0.41
1:K:79:TRP:HE1	1:K:117:LEU:HD23	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:LEU:HD22	1:D:131:LEU:HB2	2.02	0.41
1:C:106:LEU:HA	1:C:111:ILE:HD11	2.02	0.41
1:B:229:ILE:O	1:B:233:ILE:HG13	2.19	0.41
1:G:360:GLU:HG2	1:G:363:LYS:HD3	2.01	0.41
1:E:168:LYS:HD3	1:E:377:TYR:HD1	1.85	0.41
1:I:141:VAL:HG22	1:I:144:LYS:HB3	2.02	0.41
1:C:366:LYS:HG2	1:C:366:LYS:H	1.62	0.41
1:K:192:TYR:HD1	1:K:211:PHE:HD1	1.68	0.41
1:G:178:GLU:HA	1:G:191:LEU:HD21	2.02	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:L:411:ARG:HA	1:L:414:ILE:HG22	2.03	0.41
1:L:314:MET:O	1:L:317:VAL:HG22	2.19	0.41
1:H:249:LEU:HG	1:H:279:ILE:HG21	2.01	0.41
1:F:69:GLU:O	1:F:71:ASP:N	2.52	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:B:302:GLN:HB3	1:B:303:ILE:H	1.56	0.41
1:L:231:CYS:O	1:L:235:ILE:HG12	2.21	0.41
1:D:225:PHE:HA	1:D:228:ILE:HD12	2.01	0.41
1:A:406:SER:HB2	1:D:403:PHE:CZ	2.56	0.41
1:H:135:LEU:HD13	1:H:157:ARG:HD2	2.02	0.41
1:C:412:LEU:HD13	1:C:416:LEU:HD23	2.03	0.41
1:B:206:HIS:CD2	1:C:242:LYS:HD3	2.56	0.41
1:L:78:GLU:OE2	1:L:90:GLN:NE2	2.53	0.41
1:J:242:LYS:HD3	1:J:242:LYS:HA	1.88	0.41
1:E:242:LYS:HG2	1:H:206:HIS:CE1	2.56	0.41
1:K:171:LEU:HD11	1:K:199:TYR:CZ	2.55	0.41
1:A:142:TYR:HA	1:A:145:TYR:CD2	2.56	0.41
1:L:119:THR:O	1:L:123:ILE:HG13	2.21	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:A:408:ARG:HG3	1:E:366:LYS:HZ3	1.85	0.41
1:C:228:ILE:O	1:C:232:GLN:HG2	2.21	0.41
1:H:157:ARG:NH1	1:H:160:LEU:HD23	2.36	0.41
1:L:216:LEU:HD11	1:L:228:ILE:HG23	2.02	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:B:338:ALA:HB3	1:B:348:LEU:HD13	2.02	0.41
1:G:122:LEU:HD13	1:G:131:LEU:HA	2.03	0.41
1:I:395:GLU:HG2	1:I:406:SER:HB3	2.03	0.41

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

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	21	67
1	B	338/372 (91%)	313 (93%)	21 (6%)	4 (1%)	16	60
1	C	336/372 (90%)	314 (94%)	19 (6%)	3 (1%)	21	67
1	D	338/372 (91%)	316 (94%)	20 (6%)	2 (1%)	30	75
1	E	335/372 (90%)	312 (93%)	20 (6%)	3 (1%)	21	67
1	F	337/372 (91%)	315 (94%)	20 (6%)	2 (1%)	30	75
1	G	341/372 (92%)	323 (95%)	14 (4%)	4 (1%)	16	60
1	H	339/372 (91%)	322 (95%)	13 (4%)	4 (1%)	16	60
1	I	340/372 (91%)	325 (96%)	13 (4%)	2 (1%)	30	75
1	J	343/372 (92%)	326 (95%)	16 (5%)	1 (0%)	46	85
1	K	336/372 (90%)	308 (92%)	24 (7%)	4 (1%)	16	60
1	L	342/372 (92%)	326 (95%)	14 (4%)	2 (1%)	30	75
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%)	24	69

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 ⓘ

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%)	70	91
1	B	308/335 (92%)	298 (97%)	10 (3%)	46	81
1	C	306/335 (91%)	288 (94%)	18 (6%)	24	65
1	D	308/335 (92%)	299 (97%)	9 (3%)	50	83
1	E	305/335 (91%)	303 (99%)	2 (1%)	88	97
1	F	307/335 (92%)	301 (98%)	6 (2%)	63	88
1	G	311/335 (93%)	300 (96%)	11 (4%)	43	80
1	H	309/335 (92%)	298 (96%)	11 (4%)	42	79
1	I	310/335 (92%)	306 (99%)	4 (1%)	76	92
1	J	313/335 (93%)	309 (99%)	4 (1%)	76	92
1	K	306/335 (91%)	297 (97%)	9 (3%)	50	83
1	L	312/335 (93%)	305 (98%)	7 (2%)	60	87
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%)	4	19
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%)	4	19
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%)	4	19
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%)	4	19
All	All	3788/4104 (92%)	3684 (97%)	104 (3%)	52	85

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

Some 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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	343/372 (92%)	0.36	23 (6%) 21 12	27, 72, 144, 152	0
1	B	342/372 (91%)	0.65	38 (11%) 7 4	36, 90, 143, 162	0
1	C	340/372 (91%)	0.23	19 (5%) 28 16	28, 69, 151, 163	0
1	D	342/372 (91%)	0.22	16 (4%) 35 22	31, 67, 147, 157	0
1	E	339/372 (91%)	0.39	24 (7%) 19 10	18, 76, 149, 159	0
1	F	341/372 (91%)	0.08	7 (2%) 67 52	15, 52, 131, 155	0
1	G	345/372 (92%)	0.20	13 (3%) 44 29	16, 62, 135, 152	0
1	H	343/372 (92%)	0.32	18 (5%) 31 18	19, 79, 147, 157	0
1	I	344/372 (92%)	0.07	12 (3%) 48 32	9, 44, 128, 145	0
1	J	347/372 (93%)	0.13	10 (2%) 55 41	11, 51, 135, 146	0
1	K	340/372 (91%)	0.35	17 (5%) 32 19	13, 72, 134, 146	0
1	L	346/372 (93%)	0.08	7 (2%) 68 54	18, 52, 135, 147	0
2	M	8/8 (100%)	1.68	3 (37%) 0 0	46, 54, 66, 68	0
2	N	8/8 (100%)	1.81	2 (25%) 1 1	57, 61, 65, 72	0
2	O	8/8 (100%)	1.50	2 (25%) 1 1	43, 46, 73, 81	0
2	P	8/8 (100%)	1.63	2 (25%) 1 1	39, 42, 52, 69	0
2	Q	8/8 (100%)	1.22	0 100 100	40, 44, 63, 63	0
2	R	8/8 (100%)	0.97	0 100 100	17, 23, 42, 45	0
2	S	8/8 (100%)	1.57	2 (25%) 1 1	23, 32, 47, 52	0
2	T	8/8 (100%)	1.38	1 (12%) 5 3	36, 47, 53, 74	0
2	U	8/8 (100%)	1.80	4 (50%) 0 0	19, 27, 31, 36	0
2	V	8/8 (100%)	0.99	0 100 100	22, 28, 40, 47	0
2	W	8/8 (100%)	1.51	2 (25%) 1 1	31, 40, 47, 54	0
2	X	8/8 (100%)	1.02	1 (12%) 5 3	21, 25, 36, 38	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
All	All	4208/4560 (92%)	0.28	223 (5%)	30	17	9, 66, 141, 163	0

All (223) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	410	TYR	7.2
1	J	388	LYS	6.9
1	A	418	ASN	6.3
1	H	390	TYR	5.4
1	H	415	ASP	5.3
1	E	102	MET	5.2
1	E	98	LEU	4.9
1	D	416	LEU	4.9
1	C	415	ASP	4.7
1	K	77	ASP	4.7
1	A	402	ARG	4.7
1	A	361	GLU	4.6
1	K	98	LEU	4.5
1	K	390	TYR	4.4
1	F	419	ASP	4.4
1	H	410	TYR	4.4
1	B	356	TYR	4.3
1	J	67	ASP	4.2
1	D	415	ASP	4.1
1	B	401	SER	4.1
1	C	388	LYS	4.0
2	P	25	SER	4.0
1	A	327	ALA	4.0
1	C	414	ILE	4.0
1	K	73	LYS	4.0
1	G	390	TYR	3.9
1	I	410	TYR	3.9
1	C	392	GLU	3.9
1	B	336	ASP	3.8
1	A	401	SER	3.8
1	L	100	GLY	3.8
1	B	77	ASP	3.8
1	K	415	ASP	3.8
1	A	415	ASP	3.8
2	O	25	SER	3.7
1	E	103	LYS	3.7
1	B	416	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	E	411	ARG	3.7
1	E	332	ASP	3.6
1	L	411	ARG	3.6
2	N	25	SER	3.6
1	J	403	PHE	3.6
1	G	415	ASP	3.6
1	G	392	GLU	3.5
1	J	394	ALA	3.5
2	W	25	SER	3.5
1	A	390	TYR	3.5
1	I	306	ASN	3.5
1	E	94	ILE	3.4
1	H	363	LYS	3.4
2	S	25	SER	3.4
1	K	408	ARG	3.4
1	F	318	CYS	3.4
1	A	392	GLU	3.4
1	B	397	PHE	3.3
1	I	322	GLU	3.3
1	L	410	TYR	3.3
1	B	128	ILE	3.3
1	E	100	GLY	3.3
1	A	363	LYS	3.2
1	D	390	TYR	3.2
1	B	360	GLU	3.2
1	B	408	ARG	3.2
1	C	283	LYS	3.2
1	I	388	LYS	3.2
1	B	411	ARG	3.2
1	I	399	SER	3.1
1	D	410	TYR	3.1
1	B	399	SER	3.1
1	B	129	SER	3.1
1	F	401	SER	3.1
1	A	70	GLU	3.1
1	C	410	TYR	3.1
1	B	287	GLN	3.1
1	I	309	ASP	3.1
1	K	349	TYR	3.0
2	M	28	PRO	3.0
1	A	364	ASP	3.0
1	C	364	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	K	358	TYR	3.0
1	E	322	GLU	3.0
1	B	164	GLN	3.0
1	H	401	SER	3.0
1	C	289	ALA	3.0
1	A	416	LEU	2.9
1	E	140	LYS	2.9
1	D	206	HIS	2.9
2	U	26	SER	2.9
1	B	407	ASN	2.9
1	E	364	ASP	2.9
1	G	68	VAL	2.9
1	K	71	ASP	2.8
1	B	103	LYS	2.8
1	B	373	ALA	2.8
1	K	412	LEU	2.8
1	B	415	ASP	2.8
1	K	78	GLU	2.8
1	E	317	VAL	2.8
1	E	306	ASN	2.8
1	G	349	TYR	2.8
1	C	374	ILE	2.7
1	L	372	GLU	2.7
1	C	416	LEU	2.7
1	H	395	GLU	2.7
1	E	88	LYS	2.7
1	H	411	ARG	2.7
1	E	171	LEU	2.7
1	F	415	ASP	2.7
1	H	94	ILE	2.7
1	A	320	LYS	2.7
1	C	402	ARG	2.7
1	D	356	TYR	2.7
1	B	344	PHE	2.7
1	C	405	GLU	2.7
1	E	397	PHE	2.7
1	B	113	TYR	2.6
1	B	133	GLU	2.6
1	I	412	LEU	2.6
2	T	25	SER	2.6
1	E	318	CYS	2.6
1	H	71	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	363	LYS	2.6
1	H	104	HIS	2.6
1	G	322	GLU	2.6
1	D	375	PRO	2.6
1	J	321	LEU	2.6
1	I	310	THR	2.6
1	K	99	GLN	2.6
1	E	107	ASP	2.6
1	G	324	LEU	2.5
1	D	89	GLN	2.5
1	B	361	GLU	2.5
1	E	147	PRO	2.5
2	U	25	SER	2.5
1	D	207	LEU	2.5
1	D	374	ILE	2.5
1	D	409	TYR	2.5
1	J	410	TYR	2.5
1	I	408	ARG	2.5
1	A	413	VAL	2.5
1	H	98	LEU	2.5
1	B	288	GLN	2.4
1	H	129	SER	2.4
1	B	412	LEU	2.4
1	B	165	TYR	2.4
1	A	306	ASN	2.4
1	A	410	TYR	2.4
1	B	204	ILE	2.4
1	B	135	LEU	2.4
1	G	310	THR	2.4
1	I	364	ASP	2.4
2	U	28	PRO	2.4
1	A	349	TYR	2.4
1	B	109	GLU	2.3
1	C	371	ASN	2.3
1	A	372	GLU	2.3
1	K	133	GLU	2.3
2	M	25	SER	2.3
2	M	27	LYS	2.3
1	B	172	ASP	2.3
1	H	364	ASP	2.3
1	A	362	ALA	2.3
1	D	370	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	J	322	GLU	2.3
1	J	404	GLU	2.3
1	I	363	LYS	2.3
1	E	412	LEU	2.3
2	N	32	GLY	2.3
1	C	285	LYS	2.3
1	L	322	GLU	2.3
1	H	416	LEU	2.3
1	K	74	GLY	2.3
1	A	318	CYS	2.3
1	C	74	GLY	2.2
1	H	153	TYR	2.2
1	E	73	LYS	2.2
1	B	362	ALA	2.2
1	E	399	SER	2.2
1	F	322	GLU	2.2
1	K	70	GLU	2.2
1	K	162	CYS	2.2
1	L	386	LEU	2.2
1	A	404	GLU	2.2
1	B	306	ASN	2.2
1	I	416	LEU	2.2
1	D	325	GLU	2.2
1	D	388	LYS	2.2
1	A	266	ASP	2.2
1	E	142	TYR	2.2
1	G	342	GLU	2.2
1	G	387	LYS	2.2
1	A	403	PHE	2.2
1	C	403	PHE	2.2
2	U	29	ASP	2.2
1	D	371	ASN	2.1
2	X	29	ASP	2.1
1	B	230	ASN	2.1
2	P	32	GLY	2.1
1	H	306	ASN	2.1
1	J	397	PHE	2.1
1	L	324	LEU	2.1
1	C	397	PHE	2.1
1	E	114	TYR	2.1
1	C	339	LYS	2.1
1	B	131	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	306	ASN	2.1
1	H	377	TYR	2.1
1	B	105	VAL	2.1
1	B	140	LYS	2.1
1	K	401	SER	2.1
1	E	348	LEU	2.1
1	B	322	GLU	2.1
2	W	28	PRO	2.1
1	C	279	ILE	2.0
1	F	356	TYR	2.0
2	S	28	PRO	2.0
1	G	69	GLU	2.0
1	J	69	GLU	2.0
1	H	404	GLU	2.0
1	G	365	TYR	2.0
1	B	90	GLN	2.0
1	G	370	GLU	2.0
2	O	26	SER	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 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.