



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:04 AM GMT

PDB ID : 2JES
Title : PORTAL PROTEIN FROM BACTERIOPHAGE SPP1
Authors : Lebedev, A.A.; Krause, M.H.; Isidro, A.L.; Vagin, A.A.; Orlova, E.V.; Turner, J.; Dodson, E.J.; Tavares, P.; Antson, A.A.
Deposited on : 2007-01-21
Resolution : 3.40 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

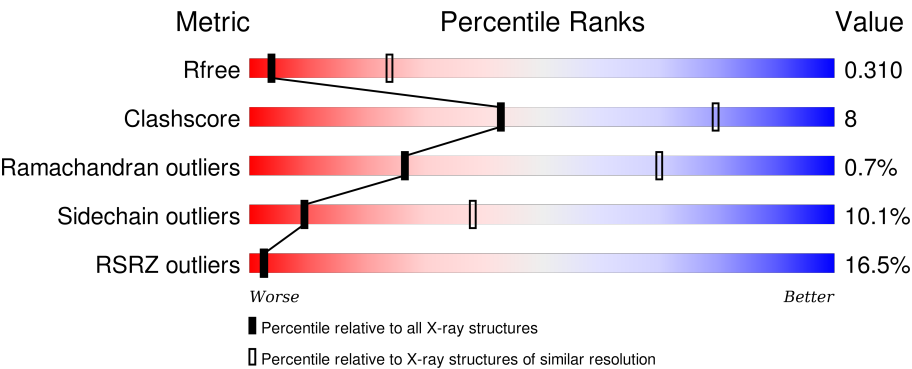
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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	503	<div><div>13%</div><div>58%</div><div>14%</div><div>•</div><div>26%</div></div>
1	C	503	<div><div>16%</div><div>56%</div><div>15%</div><div>•</div><div>26%</div></div>
1	E	503	<div><div>15%</div><div>58%</div><div>13%</div><div>•</div><div>26%</div></div>
1	G	503	<div><div>13%</div><div>55%</div><div>16%</div><div>•</div><div>26%</div></div>
1	I	503	<div><div>13%</div><div>55%</div><div>16%</div><div>•</div><div>26%</div></div>

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Mol	Chain	Length	Quality of chain
1	K	503	
1	M	503	
1	O	503	
1	Q	503	
1	S	503	
1	U	503	
1	W	503	
1	Y	503	
2	B	30	
2	D	30	
2	F	30	
2	H	30	
2	J	30	
2	L	30	
2	N	30	
2	P	30	
2	R	30	
2	T	30	
2	V	30	
2	X	30	
2	Z	30	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 39260 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 PORTAL PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	370	Total	C	N	O	S	0	0	0
			2868	1823	472	563	10			
1	C	370	Total	C	N	O	S	0	0	0
			2868	1823	472	563	10			
1	E	370	Total	C	N	O	S	0	0	0
			2868	1823	472	563	10			
1	G	370	Total	C	N	O	S	0	0	0
			2868	1823	472	563	10			
1	I	370	Total	C	N	O	S	0	0	0
			2868	1823	472	563	10			
1	K	370	Total	C	N	O	S	0	0	0
			2868	1823	472	563	10			
1	M	370	Total	C	N	O	S	0	0	0
			2868	1823	472	563	10			
1	O	370	Total	C	N	O	S	0	0	0
			2868	1823	472	563	10			
1	Q	370	Total	C	N	O	S	0	0	0
			2868	1823	472	563	10			
1	S	370	Total	C	N	O	S	0	0	0
			2868	1823	472	563	10			
1	U	370	Total	C	N	O	S	0	0	0
			2868	1823	472	563	10			
1	W	370	Total	C	N	O	S	0	0	0
			2868	1823	472	563	10			
1	Y	370	Total	C	N	O	S	0	0	0
			2868	1823	472	563	10			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	365	LYS	ASN	ENGINEERED MUTATION	UNP P54309
C	365	LYS	ASN	ENGINEERED MUTATION	UNP P54309
E	365	LYS	ASN	ENGINEERED MUTATION	UNP P54309

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Chain	Residue	Modelled	Actual	Comment	Reference
G	365	LYS	ASN	ENGINEERED MUTATION	UNP P54309
I	365	LYS	ASN	ENGINEERED MUTATION	UNP P54309
K	365	LYS	ASN	ENGINEERED MUTATION	UNP P54309
M	365	LYS	ASN	ENGINEERED MUTATION	UNP P54309
O	365	LYS	ASN	ENGINEERED MUTATION	UNP P54309
Q	365	LYS	ASN	ENGINEERED MUTATION	UNP P54309
S	365	LYS	ASN	ENGINEERED MUTATION	UNP P54309
U	365	LYS	ASN	ENGINEERED MUTATION	UNP P54309
W	365	LYS	ASN	ENGINEERED MUTATION	UNP P54309
Y	365	LYS	ASN	ENGINEERED MUTATION	UNP P54309

- Molecule 2 is a protein called UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	30	Total	C	N	O	0	0	0
			150	90	30	30			
2	D	30	Total	C	N	O	0	0	0
			150	90	30	30			
2	F	30	Total	C	N	O	0	0	0
			150	90	30	30			
2	H	30	Total	C	N	O	0	0	0
			150	90	30	30			
2	J	30	Total	C	N	O	0	0	0
			150	90	30	30			
2	L	30	Total	C	N	O	0	0	0
			150	90	30	30			
2	N	30	Total	C	N	O	0	0	0
			150	90	30	30			
2	P	30	Total	C	N	O	0	0	0
			150	90	30	30			
2	R	30	Total	C	N	O	0	0	0
			150	90	30	30			
2	T	30	Total	C	N	O	0	0	0
			150	90	30	30			
2	V	30	Total	C	N	O	0	0	0
			150	90	30	30			
2	X	30	Total	C	N	O	0	0	0
			150	90	30	30			
2	Z	30	Total	C	N	O	0	0	0
			150	90	30	30			

- Molecule 3 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Hg 1 1	0	0
3	Q	1	Total Hg 1 1	0	0
3	K	1	Total Hg 1 1	0	0
3	E	1	Total Hg 1 1	0	0
3	I	1	Total Hg 1 1	0	0
3	C	1	Total Hg 1 1	0	0
3	W	1	Total Hg 1 1	0	0
3	A	1	Total Hg 1 1	0	0
3	U	1	Total Hg 1 1	0	0
3	O	1	Total Hg 1 1	0	0
3	Y	1	Total Hg 1 1	0	0
3	S	1	Total Hg 1 1	0	0
3	M	1	Total Hg 1 1	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total Ca 1 1	0	0
4	Q	1	Total Ca 1 1	0	0
4	K	1	Total Ca 1 1	0	0
4	E	1	Total Ca 1 1	0	0
4	I	1	Total Ca 1 1	0	0
4	C	1	Total Ca 1 1	0	0
4	W	1	Total Ca 1 1	0	0

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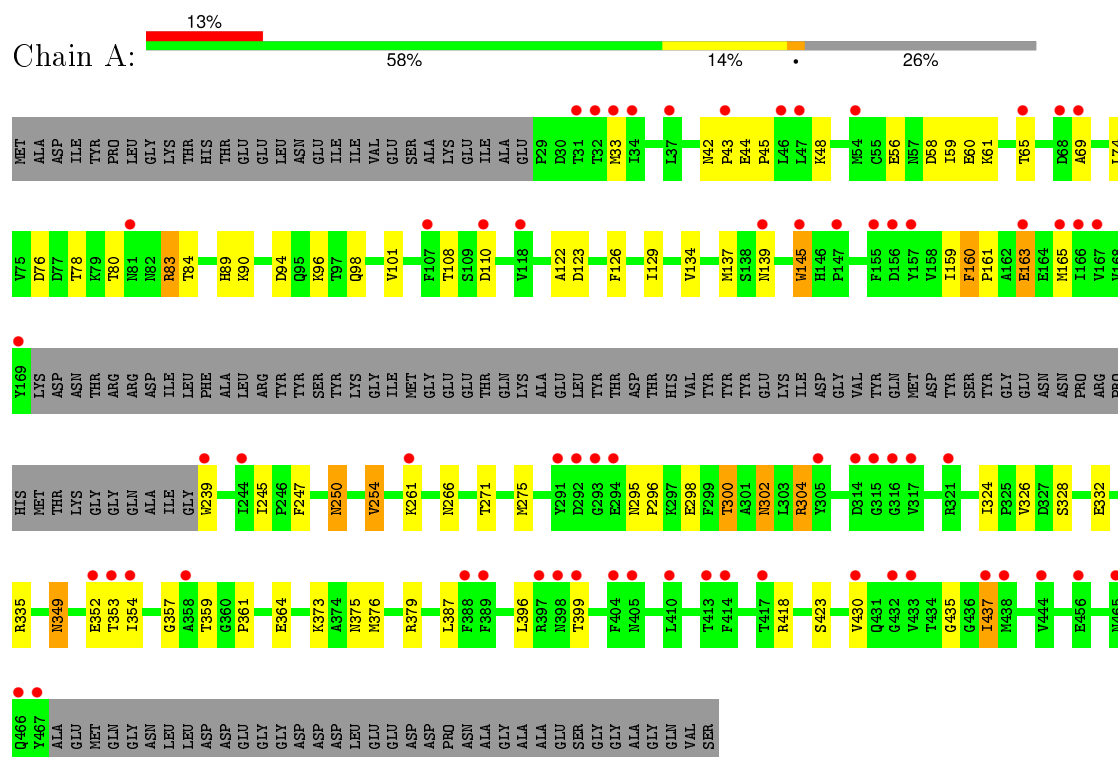
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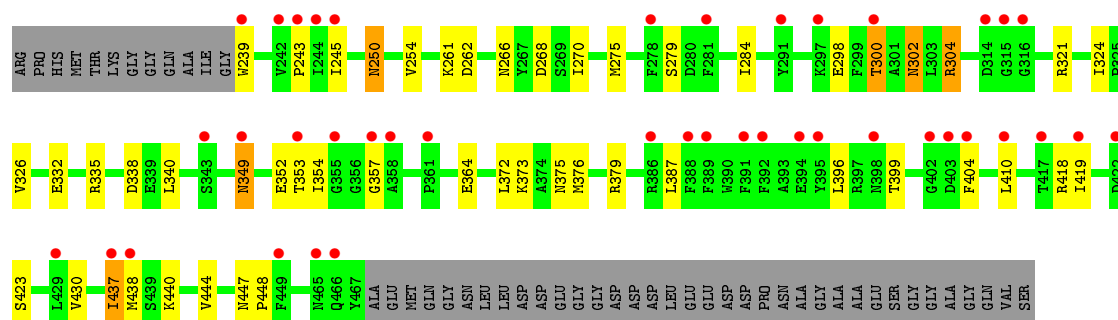
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Ca 1	0	0
4	U	1	Total 1	Ca 1	0	0
4	O	1	Total 1	Ca 1	0	0
4	Y	1	Total 1	Ca 1	0	0
4	S	1	Total 1	Ca 1	0	0
4	M	1	Total 1	Ca 1	0	0

3 Residue-property plots

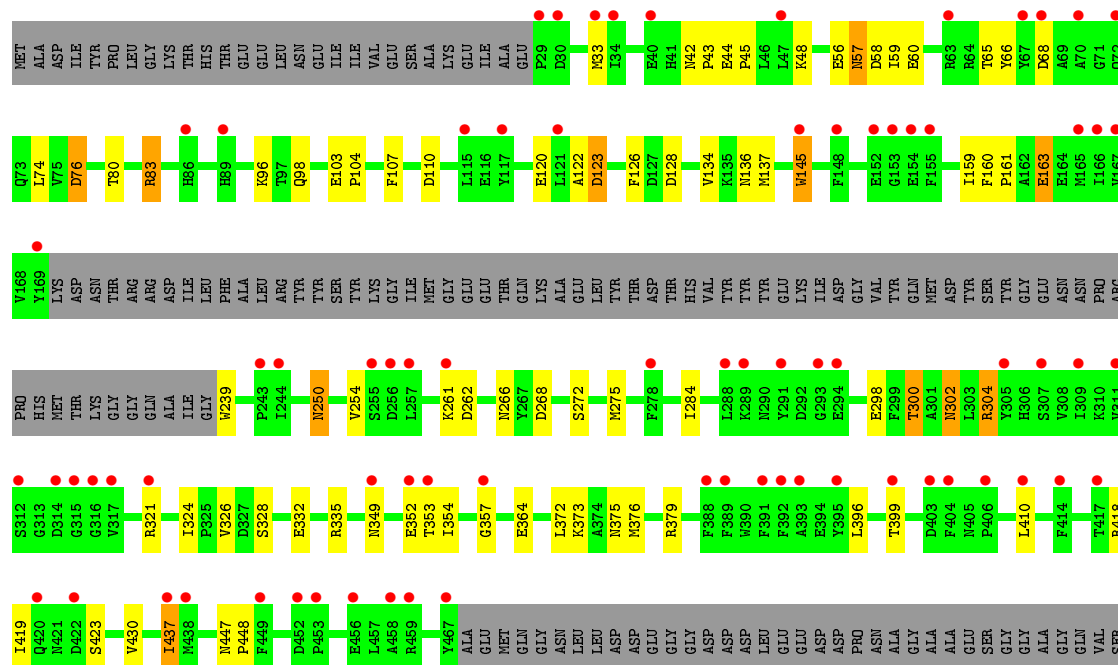
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

• Molecule 1: PORTAL PROTEIN

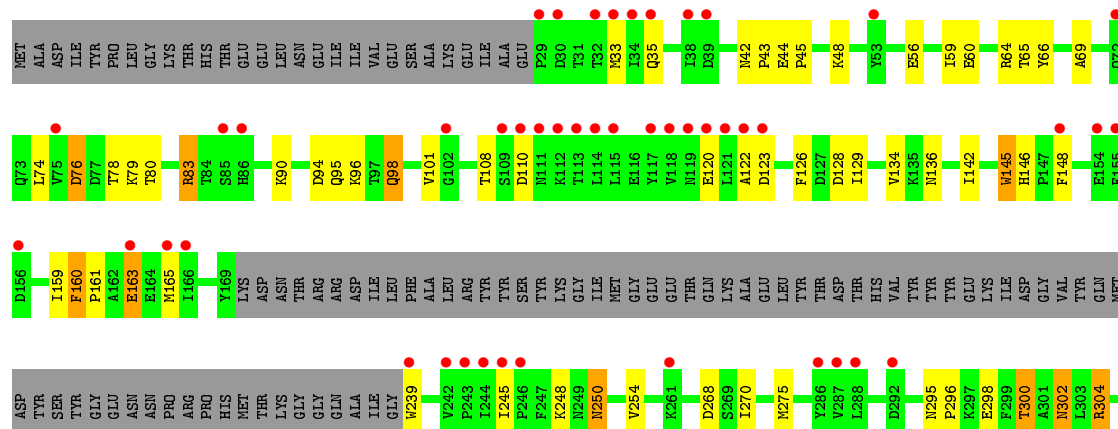


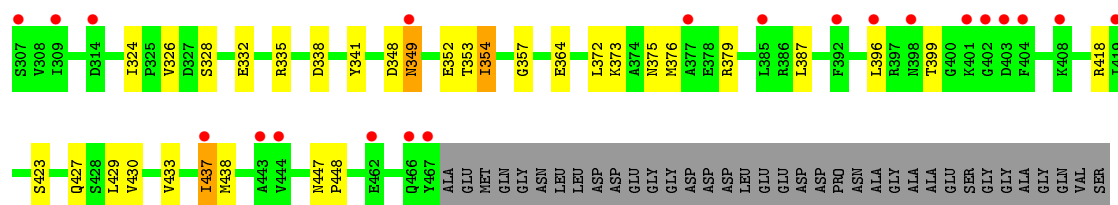


• Molecule 1: PORTAL PROTEIN

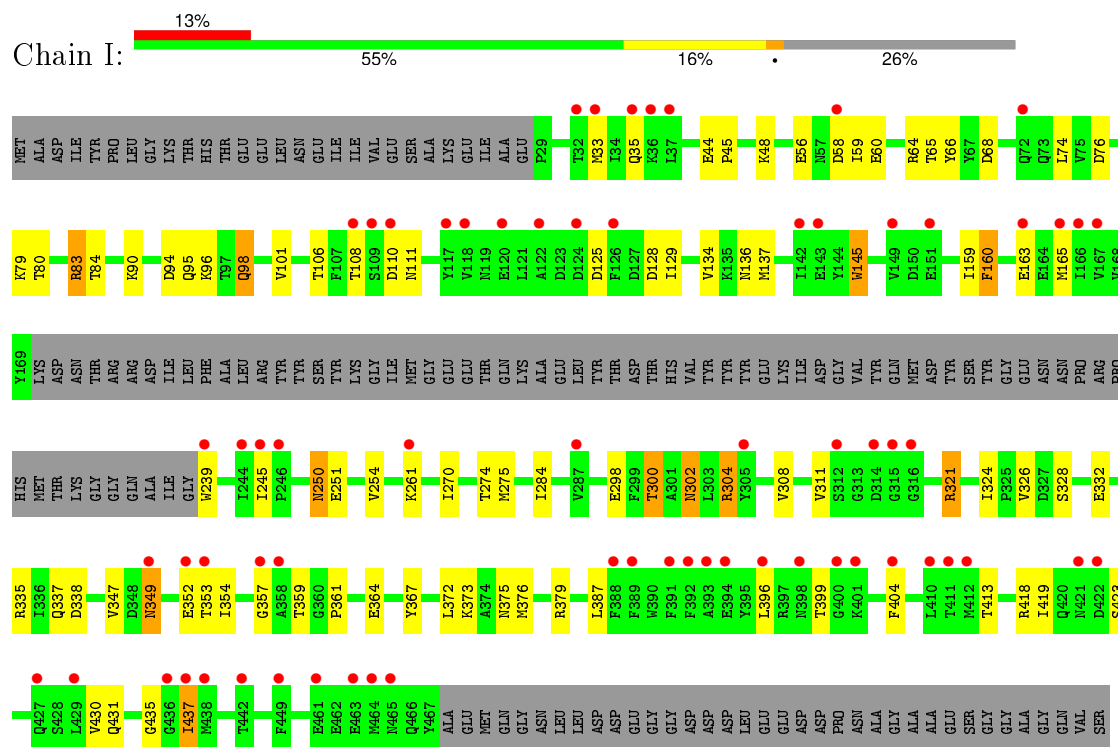


• Molecule 1: PORTAL PROTEIN

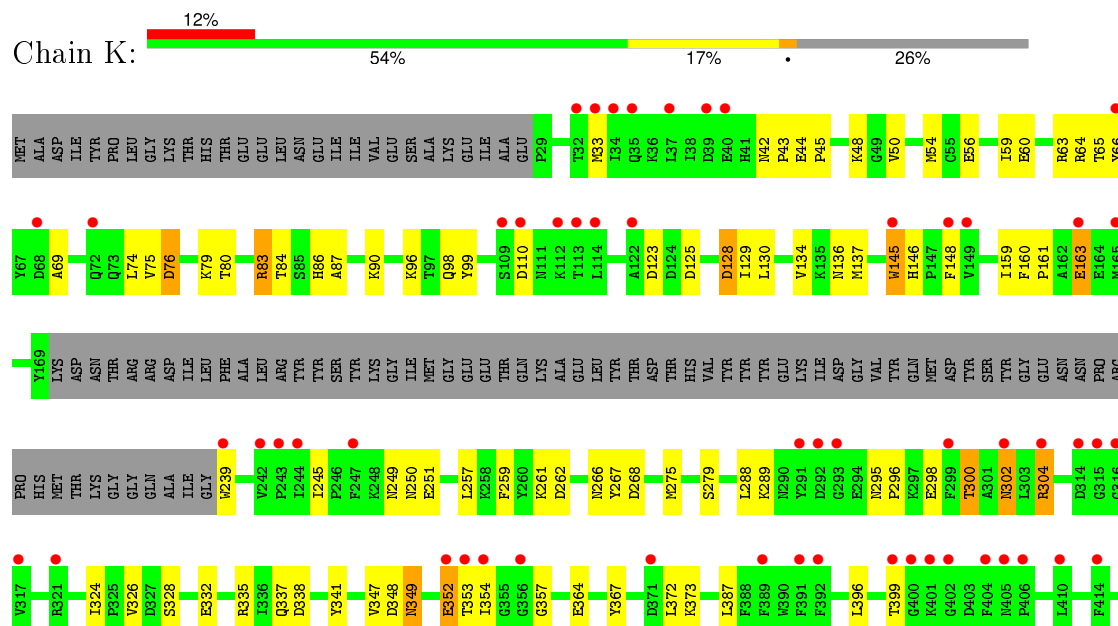




• Molecule 1: PORTAL PROTEIN

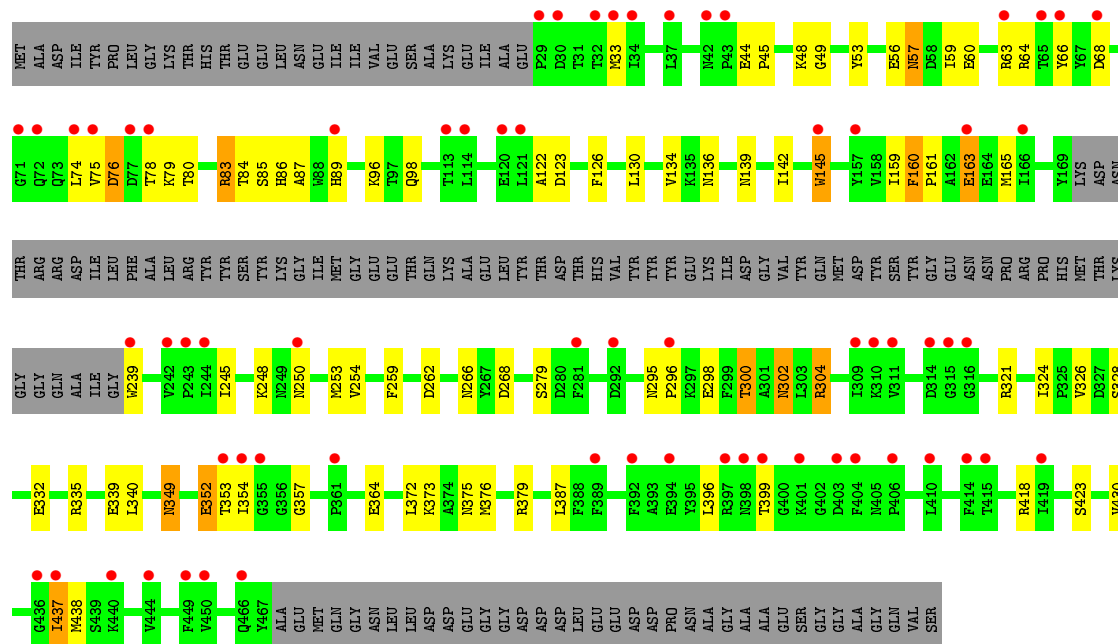


• Molecule 1: PORTAL PROTEIN

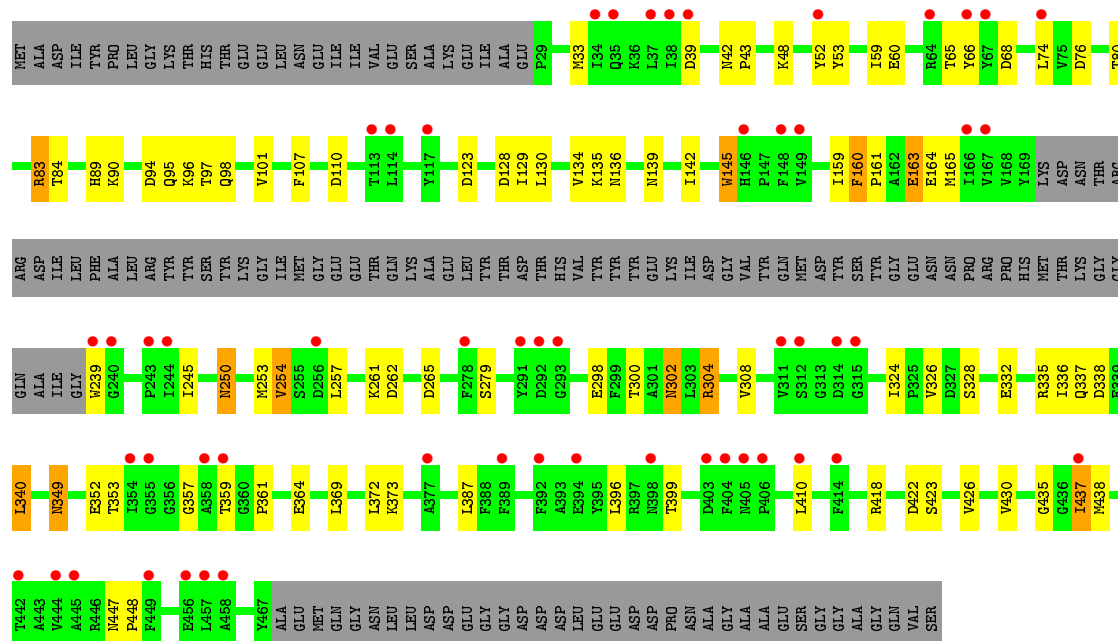




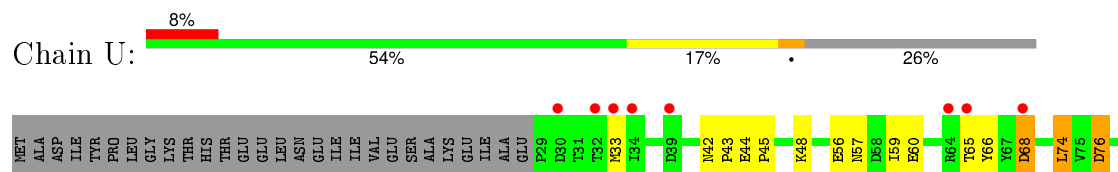
• Molecule 1: PORTAL PROTEIN

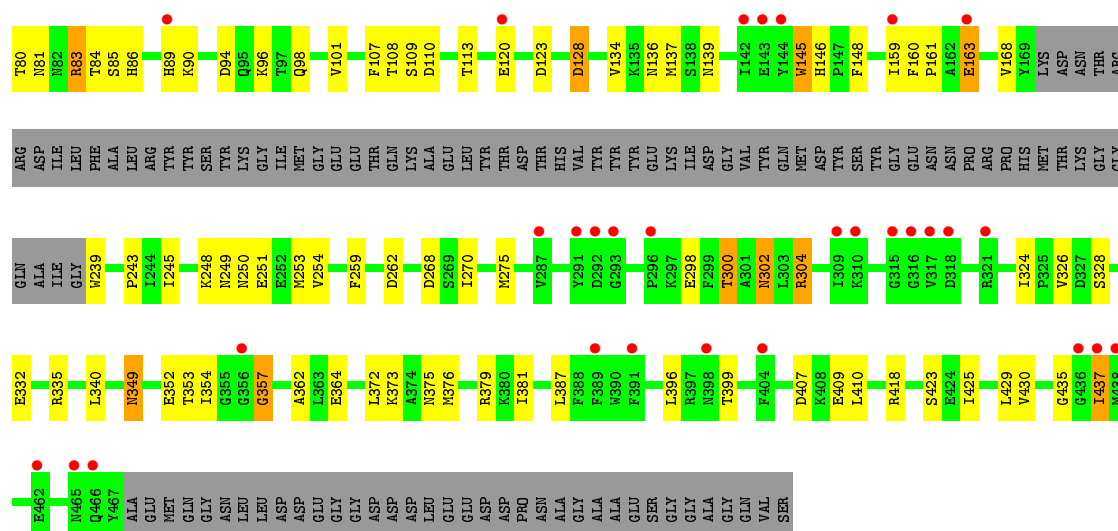


• Molecule 1: PORTAL PROTEIN

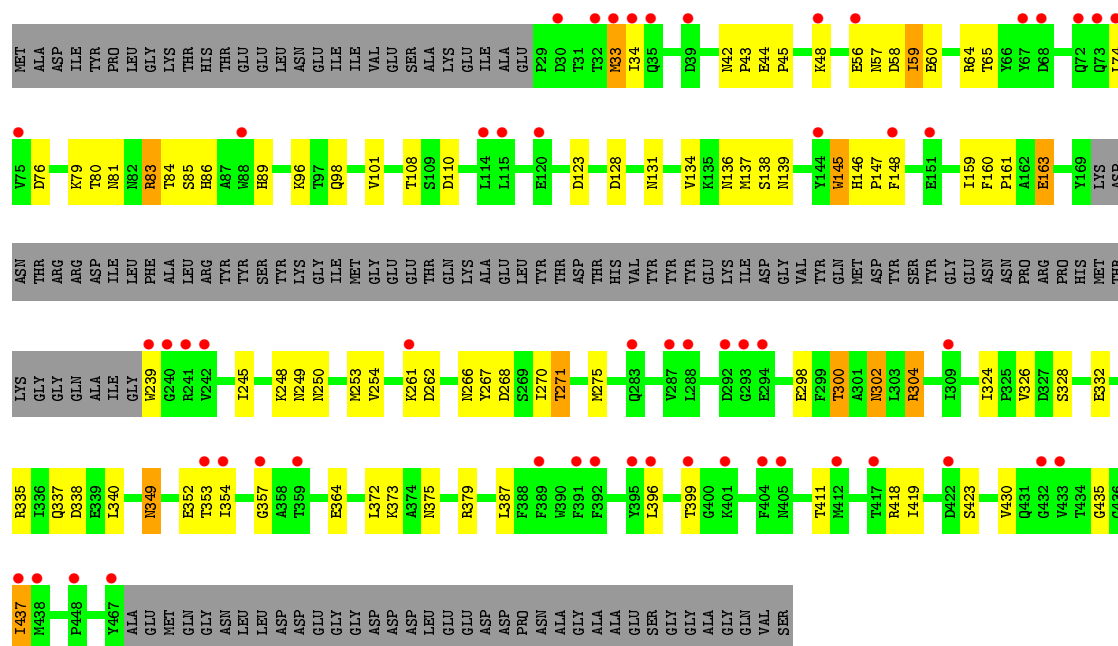


• Molecule 1: PORTAL PROTEIN

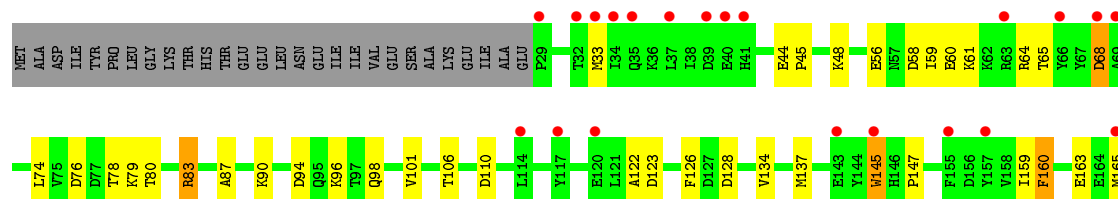


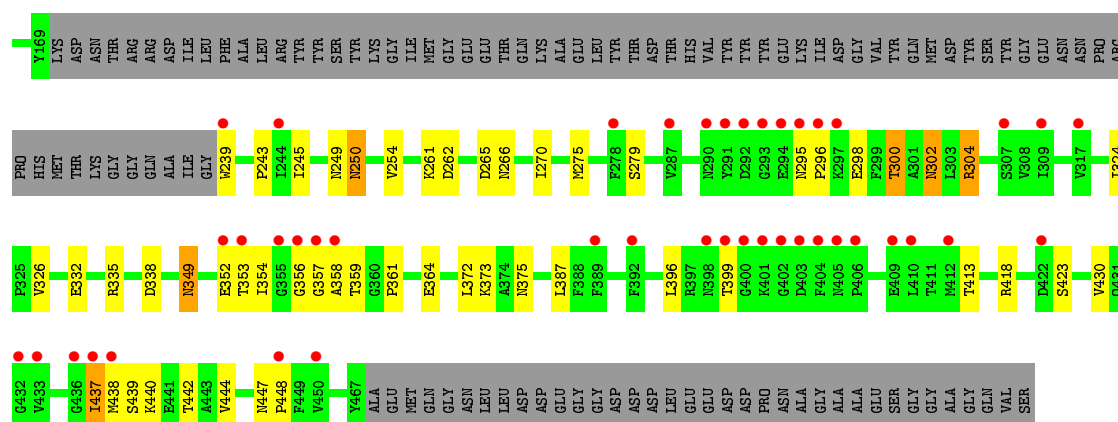


• Molecule 1: PORTAL PROTEIN



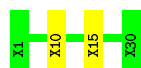
• Molecule 1: PORTAL PROTEIN





● Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN

Chain B: 93% 7%



● Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN

Chain D: 93% 7%



● Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN

Chain F: 93% 7%



● Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN

Chain H: 93% 7%



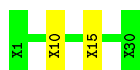
● Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN

Chain J: 93% 7%



● Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN

Chain L: 93% 7%




- Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN

Chain N:  93% 7%



- Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN

Chain P:  90% 10%



- Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN

Chain R:  90% 10%



- Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN

Chain T:  97% .



- Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN

Chain V:  93% 7%



- Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN

Chain X:  93% 7%



- Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN

Chain Z:  93% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	174.31Å 221.41Å 421.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.81 – 3.40 39.82 – 3.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.81-3.40) 99.6 (39.82-3.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.05 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.288 , 0.319 0.280 , 0.310	Depositor DCC
R_{free} test set	1121 reflections (1.02%)	DCC
Wilson B-factor (Å ²)	107.2	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 161.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	3 of 111409 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	39260	wwPDB-VP
Average B, all atoms (Å ²)	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% 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

Bond lengths and bond angles in the following residue types are not validated in this section: CA, HG

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	0.42	0/2928	0.55	0/3978
1	C	0.41	0/2928	0.54	0/3978
1	E	0.44	0/2928	0.55	0/3978
1	G	0.44	0/2928	0.57	0/3978
1	I	0.47	0/2928	0.58	0/3978
1	K	0.48	0/2928	0.58	0/3978
1	M	0.46	0/2928	0.58	0/3978
1	O	0.47	0/2928	0.57	0/3978
1	Q	0.53	0/2928	0.62	0/3978
1	S	0.60	0/2928	0.66	0/3978
1	U	0.58	0/2928	0.66	0/3978
1	W	0.49	0/2928	0.60	0/3978
1	Y	0.46	0/2928	0.57	0/3978
All	All	0.48	0/38064	0.59	0/51714

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	2868	0	2686	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2868	0	2686	53	1
1	E	2868	0	2686	46	0
1	G	2868	0	2686	58	0
1	I	2868	0	2686	61	0
1	K	2868	0	2686	57	0
1	M	2868	0	2686	50	0
1	O	2868	0	2685	53	1
1	Q	2868	0	2685	55	0
1	S	2868	0	2686	67	0
1	U	2868	0	2686	68	0
1	W	2868	0	2686	61	0
1	Y	2868	0	2686	51	0
2	B	150	0	36	1	0
2	D	150	0	37	1	0
2	F	150	0	37	1	0
2	H	150	0	38	1	0
2	J	150	0	37	1	0
2	L	150	0	38	1	0
2	N	150	0	36	1	0
2	P	150	0	36	2	0
2	R	150	0	37	2	0
2	T	150	0	37	1	0
2	V	150	0	37	1	0
2	X	150	0	37	1	0
2	Z	150	0	38	1	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
3	K	1	0	0	0	0
3	M	1	0	0	0	0
3	O	1	0	0	0	0
3	Q	1	0	0	0	0
3	S	1	0	0	0	0
3	U	1	0	0	0	0
3	W	1	0	0	0	0
3	Y	1	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	1	0	0	0	0
4	K	1	0	0	0	0
4	M	1	0	0	0	0
4	O	1	0	0	0	0
4	Q	1	0	0	0	0
4	S	1	0	0	0	0
4	U	1	0	0	0	0
4	W	1	0	0	0	0
4	Y	1	0	0	0	0
All	All	39260	0	35397	609	1

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 8.

All (609) 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:M:96:LYS:HD3	1:M:373:LYS:HD3	1.34	1.06
1:S:430:VAL:HG23	1:U:437:ILE:HD11	1.37	1.03
1:C:96:LYS:HD3	1:C:373:LYS:HD3	1.42	1.00
1:Q:96:LYS:HD3	1:Q:373:LYS:HD3	1.46	0.96
1:E:96:LYS:HD3	1:E:373:LYS:HD3	1.48	0.96
1:G:96:LYS:HD3	1:G:373:LYS:HD3	1.48	0.95
1:I:96:LYS:HD3	1:I:373:LYS:HD3	1.48	0.95
1:M:430:VAL:HG23	1:O:437:ILE:HD11	1.45	0.94
1:A:437:ILE:HD11	1:Y:430:VAL:HG23	1.49	0.94
1:W:96:LYS:HD3	1:W:373:LYS:HD3	1.50	0.93
1:C:298:GLU:O	1:C:302:ASN:HB2	1.69	0.92
1:K:96:LYS:HD3	1:K:373:LYS:HD3	1.51	0.92
1:G:44:GLU:HG3	1:G:45:PRO:HD3	1.54	0.89
1:Q:430:VAL:HG23	1:S:437:ILE:HD11	1.55	0.89
1:I:298:GLU:O	1:I:302:ASN:HB2	1.76	0.86
1:I:304:ARG:HH21	1:K:76:ASP:HB2	1.38	0.86
1:Y:96:LYS:HD3	1:Y:373:LYS:HD3	1.56	0.85
1:S:96:LYS:HD3	1:S:373:LYS:HD3	1.57	0.85
1:A:96:LYS:HD3	1:A:373:LYS:HD3	1.57	0.85
1:U:44:GLU:HG3	1:U:45:PRO:HD3	1.57	0.84
1:Q:298:GLU:O	1:Q:302:ASN:HB2	1.79	0.82
1:A:298:GLU:O	1:A:302:ASN:HB2	1.80	0.82
1:I:44:GLU:HG3	1:I:45:PRO:HD3	1.60	0.81
1:Q:44:GLU:HG3	1:Q:45:PRO:HD3	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:298:GLU:O	1:O:302:ASN:HB2	1.83	0.79
1:Q:98:GLN:OE1	1:S:375:ASN:ND2	2.14	0.78
1:K:298:GLU:O	1:K:302:ASN:HB2	1.84	0.77
1:C:430:VAL:HG23	1:E:437:ILE:HD11	1.66	0.77
1:M:298:GLU:O	1:M:302:ASN:HB2	1.85	0.77
1:O:96:LYS:HD3	1:O:373:LYS:HD3	1.67	0.76
1:G:304:ARG:HH21	1:I:76:ASP:HB2	1.49	0.76
1:K:44:GLU:HG3	1:K:45:PRO:HD3	1.67	0.76
1:O:304:ARG:HH21	1:Q:76:ASP:HB2	1.50	0.76
1:U:96:LYS:HD3	1:U:373:LYS:HD3	1.68	0.76
1:Y:298:GLU:O	1:Y:302:ASN:HB2	1.86	0.75
1:W:298:GLU:O	1:W:302:ASN:HB2	1.85	0.75
1:S:298:GLU:O	1:S:302:ASN:HB2	1.86	0.74
1:W:430:VAL:HG23	1:Y:437:ILE:HD11	1.69	0.74
1:U:245:ILE:HG23	1:U:387:LEU:HD23	1.68	0.74
1:M:304:ARG:HH21	1:O:76:ASP:HB2	1.53	0.74
1:K:430:VAL:HG23	1:M:437:ILE:HD11	1.68	0.73
1:O:332:GLU:CD	1:O:335:ARG:HH21	1.91	0.73
1:A:430:VAL:HG23	1:C:437:ILE:HD11	1.70	0.73
1:Y:44:GLU:HG3	1:Y:45:PRO:HD3	1.70	0.72
1:G:430:VAL:HG23	1:I:437:ILE:HD11	1.72	0.72
1:S:275:MET:HE2	1:U:270:ILE:HD11	1.71	0.72
1:I:430:VAL:HG23	1:K:437:ILE:HD11	1.70	0.72
1:U:298:GLU:O	1:U:302:ASN:HB2	1.90	0.71
1:S:90:LYS:NZ	1:S:94:ASP:OD1	2.24	0.71
1:U:430:VAL:HG23	1:W:437:ILE:HD11	1.73	0.70
1:O:245:ILE:HG23	1:O:387:LEU:HD23	1.73	0.70
1:A:332:GLU:CD	1:A:335:ARG:HH21	1.94	0.70
1:M:44:GLU:HG3	1:M:45:PRO:HD3	1.73	0.69
1:K:304:ARG:HH21	1:M:76:ASP:HB2	1.56	0.69
1:E:44:GLU:HG3	1:E:45:PRO:HD3	1.73	0.69
1:M:430:VAL:CG2	1:O:437:ILE:HD11	2.23	0.69
1:S:304:ARG:HH21	1:U:76:ASP:HB2	1.58	0.68
1:Y:396:LEU:HA	1:Y:399:THR:HG22	1.76	0.68
1:W:304:ARG:HH21	1:Y:76:ASP:HB2	1.59	0.68
1:G:298:GLU:O	1:G:302:ASN:HB2	1.95	0.66
1:E:298:GLU:O	1:E:302:ASN:HB2	1.95	0.66
1:A:98:GLN:OE1	1:C:375:ASN:ND2	2.27	0.66
1:S:332:GLU:CD	1:S:335:ARG:HH21	1.99	0.66
1:E:430:VAL:HG23	1:G:437:ILE:HD11	1.76	0.66
1:Y:90:LYS:NZ	1:Y:94:ASP:OD1	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:44:GLU:HG3	1:W:45:PRO:HD3	1.78	0.65
1:A:304:ARG:HH21	1:C:76:ASP:HB2	1.61	0.65
1:Q:419:ILE:HG12	1:S:364:GLU:HG2	1.78	0.65
1:S:44:GLU:HG3	1:S:45:PRO:HD3	1.78	0.65
1:W:332:GLU:CD	1:W:335:ARG:HH21	2.00	0.64
1:S:98:GLN:OE1	1:U:375:ASN:ND2	2.30	0.64
1:I:250:ASN:ND2	1:I:254:VAL:O	2.30	0.64
1:I:332:GLU:CD	1:I:335:ARG:HH21	2.00	0.64
1:E:275:MET:CE	1:G:270:ILE:HD11	2.29	0.63
1:Y:250:ASN:ND2	1:Y:254:VAL:O	2.29	0.63
1:A:44:GLU:HG3	1:A:45:PRO:HD3	1.80	0.63
1:C:396:LEU:HA	1:C:399:THR:HG22	1.79	0.63
1:U:304:ARG:HH21	1:W:76:ASP:HB2	1.64	0.63
1:U:396:LEU:HA	1:U:399:THR:HG22	1.81	0.63
1:O:430:VAL:HG23	1:Q:437:ILE:HD11	1.81	0.62
1:I:300:THR:O	1:I:304:ARG:HB2	2.00	0.62
1:Y:332:GLU:CD	1:Y:335:ARG:HH21	2.02	0.62
1:A:396:LEU:HA	1:A:399:THR:HG22	1.82	0.62
1:S:145:TRP:HB2	1:S:159:ILE:HA	1.82	0.62
1:M:332:GLU:CD	1:M:335:ARG:HH21	2.03	0.62
1:S:245:ILE:HG23	1:S:387:LEU:HD23	1.81	0.61
1:W:98:GLN:HG2	1:Y:372:LEU:HD12	1.81	0.61
1:E:304:ARG:HH21	1:G:76:ASP:HB2	1.64	0.61
1:S:60:GLU:HA	1:S:83:ARG:HG3	1.82	0.61
1:Q:275:MET:HE3	1:S:266:ASN:HB3	1.82	0.61
1:W:60:GLU:HA	1:W:83:ARG:HG3	1.81	0.61
1:C:44:GLU:HG3	1:C:45:PRO:HD3	1.83	0.61
1:U:349:ASN:H	1:U:349:ASN:ND2	1.99	0.61
1:E:396:LEU:HA	1:E:399:THR:HG22	1.82	0.60
1:S:349:ASN:ND2	1:S:349:ASN:H	1.99	0.60
1:A:90:LYS:NZ	1:A:94:ASP:OD1	2.34	0.60
1:K:396:LEU:HA	1:K:399:THR:HG22	1.81	0.60
1:Q:275:MET:CE	1:S:266:ASN:HB3	2.31	0.60
1:S:300:THR:O	1:S:304:ARG:HB2	2.01	0.60
1:M:60:GLU:HA	1:M:83:ARG:HG3	1.84	0.60
1:A:275:MET:CE	1:C:266:ASN:HB3	2.32	0.59
1:G:332:GLU:CD	1:G:335:ARG:HH21	2.05	0.59
1:U:332:GLU:CD	1:U:335:ARG:HH21	2.05	0.59
1:Y:245:ILE:HG23	1:Y:387:LEU:HD23	1.83	0.59
1:U:109:SER:HB2	1:U:409:GLU:O	2.02	0.59
1:A:364:GLU:HG3	1:A:418:ARG:NH2	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:58:ASP:OD1	1:Y:261:LYS:NZ	2.35	0.59
2:B:10:UNK:HA	2:B:15:UNK:HA	1.85	0.59
1:U:326:VAL:HG21	1:W:328:SER:HB3	1.84	0.59
1:U:81:ASN:O	1:U:83:ARG:NH1	2.35	0.59
1:M:84:THR:HG23	1:O:262:ASP:HB3	1.85	0.59
1:M:245:ILE:HG23	1:M:387:LEU:HD23	1.85	0.58
1:S:395:TYR:O	1:S:399:THR:HG22	2.03	0.58
1:S:250:ASN:ND2	1:S:254:VAL:HG23	2.19	0.58
1:U:137:MET:O	1:U:249:ASN:HB2	2.03	0.58
1:C:60:GLU:HA	1:C:83:ARG:HG3	1.85	0.58
1:W:275:MET:CE	1:Y:266:ASN:HB3	2.33	0.58
1:Q:352:GLU:OE2	1:Q:354:ILE:HG12	2.04	0.58
1:A:375:ASN:ND2	1:Y:98:GLN:OE1	2.36	0.58
1:O:349:ASN:H	1:O:349:ASN:ND2	2.01	0.57
1:E:430:VAL:CG2	1:G:437:ILE:HD11	2.34	0.57
1:Q:332:GLU:CD	1:Q:335:ARG:HH21	2.08	0.57
1:Q:300:THR:O	1:Q:304:ARG:HB2	2.04	0.57
1:U:352:GLU:OE2	1:U:354:ILE:HG12	2.04	0.57
1:Q:430:VAL:CG2	1:S:437:ILE:HD11	2.32	0.57
1:A:76:ASP:HB2	1:Y:304:ARG:HH21	1.69	0.57
1:U:161:PRO:HB3	1:U:163:GLU:OE2	2.04	0.57
1:Q:349:ASN:ND2	1:Q:349:ASN:H	2.02	0.57
1:I:396:LEU:HA	1:I:399:THR:HG22	1.86	0.57
1:S:430:VAL:HG22	1:U:435:GLY:HA3	1.85	0.57
1:W:245:ILE:HG23	1:W:387:LEU:HD23	1.85	0.57
1:Q:60:GLU:HA	1:Q:83:ARG:HG3	1.85	0.57
1:A:250:ASN:ND2	1:A:254:VAL:O	2.36	0.56
1:Q:304:ARG:HH21	1:S:76:ASP:HB2	1.71	0.56
1:Q:161:PRO:HB3	1:Q:163:GLU:OE2	2.05	0.56
1:U:250:ASN:ND2	1:U:254:VAL:O	2.37	0.56
1:U:300:THR:O	1:U:304:ARG:HB2	2.05	0.56
1:O:101:VAL:O	1:O:101:VAL:HG12	2.06	0.56
1:I:324:ILE:HG22	1:I:326:VAL:HG23	1.87	0.56
1:U:98:GLN:OE1	1:W:375:ASN:ND2	2.39	0.56
1:O:324:ILE:HG22	1:O:326:VAL:HG23	1.86	0.56
1:E:275:MET:HE2	1:G:270:ILE:HD11	1.88	0.56
1:K:145:TRP:HB2	1:K:159:ILE:HA	1.88	0.56
1:W:352:GLU:OE2	1:W:354:ILE:HG12	2.06	0.56
1:U:134:VAL:HG22	1:U:381:ILE:HD11	1.87	0.55
1:C:364:GLU:HG3	1:C:418:ARG:NH2	2.21	0.55
1:K:275:MET:CE	1:M:266:ASN:HB3	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:396:LEU:HA	1:Q:399:THR:HG22	1.88	0.55
2:V:10:UNK:HA	2:V:15:UNK:HA	1.88	0.55
1:U:86:HIS:HD2	1:U:268:ASP:OD2	1.90	0.55
1:G:161:PRO:HB3	1:G:163:GLU:OE2	2.06	0.55
1:O:430:VAL:CG2	1:Q:437:ILE:HD11	2.36	0.55
1:E:98:GLN:HG2	1:G:372:LEU:HD12	1.88	0.55
1:A:275:MET:HE2	1:C:270:ILE:HD11	1.88	0.55
1:Y:60:GLU:HA	1:Y:83:ARG:HG3	1.88	0.55
1:W:275:MET:HE3	1:Y:266:ASN:HB3	1.89	0.55
1:Q:59:ILE:HD12	1:Q:268:ASP:HB3	1.89	0.55
1:S:35:GLN:OE1	1:S:35:GLN:HA	2.07	0.55
1:G:245:ILE:HG23	1:G:387:LEU:HD23	1.89	0.54
1:G:101:VAL:HG21	1:G:134:VAL:HG21	1.89	0.54
1:A:275:MET:HE3	1:C:266:ASN:HB3	1.87	0.54
1:U:107:PHE:HB3	1:U:410:LEU:HD11	1.89	0.54
1:C:300:THR:O	1:C:304:ARG:HB2	2.06	0.54
1:S:98:GLN:HG2	1:U:372:LEU:HD12	1.89	0.54
1:M:396:LEU:HA	1:M:399:THR:HG22	1.88	0.54
1:O:98:GLN:OE1	1:Q:375:ASN:ND2	2.41	0.54
1:C:332:GLU:CD	1:C:335:ARG:HH21	2.10	0.54
1:I:245:ILE:HG23	1:I:387:LEU:HD23	1.88	0.54
1:C:304:ARG:HH21	1:E:76:ASP:HB2	1.73	0.54
1:C:98:GLN:HG2	1:E:372:LEU:HD12	1.90	0.54
1:U:90:LYS:NZ	1:U:94:ASP:OD1	2.41	0.54
1:O:90:LYS:HD3	1:Q:259:PHE:CD2	2.42	0.54
1:K:275:MET:HE1	1:M:266:ASN:HB3	1.88	0.54
1:A:359:THR:HB	1:A:361:PRO:HD2	1.90	0.54
2:X:10:UNK:HA	2:X:15:UNK:HA	1.89	0.54
1:W:349:ASN:ND2	1:W:349:ASN:H	2.06	0.54
1:I:35:GLN:OE1	1:I:35:GLN:HA	2.07	0.54
1:Y:101:VAL:HG21	1:Y:134:VAL:HG21	1.88	0.53
1:I:376:MET:HG3	1:I:379:ARG:HH21	1.72	0.53
1:A:60:GLU:HA	1:A:83:ARG:HG3	1.90	0.53
1:Y:324:ILE:HG22	1:Y:326:VAL:HG23	1.90	0.53
1:M:96:LYS:HD3	1:M:373:LYS:CD	2.24	0.53
1:G:145:TRP:HB2	1:G:159:ILE:HA	1.90	0.53
1:C:161:PRO:HB3	1:C:163:GLU:OE2	2.08	0.53
1:S:396:LEU:HA	1:S:399:THR:HG22	1.89	0.53
1:C:98:GLN:OE1	1:E:375:ASN:ND2	2.41	0.53
1:G:324:ILE:HG22	1:G:326:VAL:HG23	1.91	0.53
1:Q:106:THR:HB	1:Q:413:THR:HB	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:84:THR:HG23	1:Y:262:ASP:HB3	1.91	0.53
1:C:250:ASN:ND2	1:C:254:VAL:O	2.34	0.53
1:S:164:GLU:O	2:T:5:UNK:HA	2.09	0.53
1:W:324:ILE:HG22	1:W:326:VAL:HG23	1.91	0.53
1:G:98:GLN:OE1	1:I:375:ASN:ND2	2.42	0.53
1:U:324:ILE:HG22	1:U:326:VAL:HG23	1.91	0.52
1:A:245:ILE:HG23	1:A:387:LEU:HD23	1.91	0.52
1:C:101:VAL:HG21	1:C:134:VAL:HG21	1.91	0.52
1:K:98:GLN:OE1	1:M:375:ASN:ND2	2.42	0.52
1:C:430:VAL:CG2	1:E:437:ILE:HD11	2.37	0.52
2:L:10:UNK:HA	2:L:15:UNK:HA	1.92	0.52
1:O:396:LEU:HA	1:O:399:THR:HG22	1.90	0.52
1:K:300:THR:O	1:K:304:ARG:HB2	2.09	0.52
1:I:352:GLU:OE2	1:I:354:ILE:HG12	2.09	0.52
1:K:332:GLU:CD	1:K:335:ARG:HH21	2.13	0.52
1:W:137:MET:O	1:W:249:ASN:HB2	2.10	0.52
1:W:161:PRO:HB3	1:W:163:GLU:OE2	2.09	0.52
1:Y:300:THR:O	1:Y:304:ARG:HB2	2.10	0.52
1:Y:364:GLU:HG3	1:Y:418:ARG:NH2	2.25	0.52
1:U:275:MET:CE	1:W:266:ASN:HB3	2.40	0.52
1:A:76:ASP:OD2	1:A:78:THR:HB	2.10	0.51
1:M:145:TRP:HB2	1:M:159:ILE:HA	1.92	0.51
1:U:84:THR:HG23	1:W:262:ASP:HB3	1.93	0.51
1:C:160:PHE:HD2	1:C:165:MET:SD	2.34	0.51
1:A:430:VAL:CG2	1:C:437:ILE:HD11	2.38	0.51
1:E:145:TRP:HB2	1:E:159:ILE:HA	1.92	0.51
1:M:430:VAL:HG22	1:O:435:GLY:HA3	1.92	0.51
1:C:84:THR:HG23	1:E:262:ASP:HB3	1.93	0.51
1:M:324:ILE:HG22	1:M:326:VAL:HG23	1.93	0.51
1:A:300:THR:O	1:A:304:ARG:HB2	2.09	0.51
1:Y:122:ALA:HB1	1:Y:126:PHE:CD2	2.46	0.51
1:M:122:ALA:HB1	1:M:126:PHE:CD2	2.45	0.51
1:K:324:ILE:HG22	1:K:326:VAL:HG23	1.93	0.51
1:Q:356:GLY:O	1:Q:358:ALA:N	2.44	0.51
1:Y:58:ASP:HA	1:Y:61:LYS:HE2	1.92	0.51
1:Y:352:GLU:OE2	1:Y:354:ILE:HG12	2.11	0.51
1:I:274:THR:HG21	1:K:332:GLU:OE1	2.10	0.51
1:W:145:TRP:HB2	1:W:159:ILE:HA	1.93	0.51
1:G:300:THR:O	1:G:304:ARG:HB2	2.10	0.50
1:U:60:GLU:HA	1:U:83:ARG:HG3	1.94	0.50
1:O:52:TYR:OH	1:O:265:ASP:OD1	2.23	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:349:ASN:H	1:I:349:ASN:ND2	2.09	0.50
1:G:396:LEU:HA	1:G:399:THR:HG22	1.92	0.50
1:I:364:GLU:HG3	1:I:418:ARG:NH2	2.27	0.50
1:U:101:VAL:HG12	1:U:101:VAL:O	2.12	0.50
2:P:10:UNK:HA	2:P:15:UNK:HA	1.94	0.50
1:O:60:GLU:HA	1:O:83:ARG:HG3	1.92	0.50
1:Y:349:ASN:ND2	1:Y:349:ASN:H	2.09	0.50
1:U:81:ASN:HD21	1:U:83:ARG:HD2	1.77	0.50
1:I:376:MET:HG3	1:I:379:ARG:NH2	2.27	0.50
1:U:275:MET:HE2	1:W:270:ILE:HD11	1.94	0.50
1:W:57:ASN:O	1:W:59:ILE:N	2.45	0.50
1:Q:324:ILE:HG22	1:Q:326:VAL:HG23	1.93	0.50
1:Q:250:ASN:ND2	1:Q:254:VAL:HG23	2.27	0.50
1:C:107:PHE:HB3	1:C:410:LEU:HD11	1.94	0.50
1:I:66:TYR:CD2	1:I:76:ASP:HB3	2.47	0.49
1:Y:160:PHE:HD2	1:Y:165:MET:SD	2.35	0.49
1:M:89:HIS:NE2	1:M:139:ASN:ND2	2.60	0.49
1:G:60:GLU:HA	1:G:83:ARG:HG3	1.93	0.49
1:Q:430:VAL:HG22	1:S:435:GLY:HA3	1.93	0.49
1:I:84:THR:HG23	1:K:262:ASP:HB3	1.93	0.49
1:M:376:MET:HG3	1:M:379:ARG:HH21	1.77	0.49
1:W:430:VAL:CG2	1:Y:437:ILE:HD11	2.39	0.49
1:E:59:ILE:HD11	1:E:272:SER:OG	2.12	0.49
1:O:422:ASP:O	1:O:426:VAL:HG23	2.12	0.49
1:I:101:VAL:HG21	1:I:134:VAL:HG21	1.93	0.49
1:I:134:VAL:HA	1:I:137:MET:CE	2.42	0.49
1:E:332:GLU:CD	1:E:335:ARG:HH21	2.15	0.49
1:I:98:GLN:HG2	1:K:372:LEU:HD12	1.94	0.49
1:S:161:PRO:HB3	1:S:163:GLU:OE2	2.12	0.49
1:Q:84:THR:HG23	1:S:262:ASP:HB3	1.95	0.49
1:Q:137:MET:O	1:Q:249:ASN:HB2	2.12	0.49
1:Y:76:ASP:OD2	1:Y:78:THR:HB	2.13	0.49
1:K:245:ILE:HG23	1:K:387:LEU:HD23	1.94	0.49
1:G:275:MET:HE2	1:I:270:ILE:HD11	1.94	0.49
1:S:124:ASP:O	1:S:128:ASP:OD2	2.31	0.49
1:S:96:LYS:HD3	1:S:373:LYS:CD	2.36	0.48
1:S:57:ASN:O	1:S:59:ILE:N	2.46	0.48
1:K:99:TYR:OH	1:K:418:ARG:HD2	2.13	0.48
1:W:396:LEU:HA	1:W:399:THR:HG22	1.95	0.48
1:E:60:GLU:HA	1:E:83:ARG:HG3	1.95	0.48
1:S:137:MET:O	1:S:249:ASN:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:TRP:HB2	1:C:159:ILE:HA	1.93	0.48
1:E:419:ILE:HG12	1:G:364:GLU:HG2	1.95	0.48
1:C:245:ILE:HG23	1:C:387:LEU:HD23	1.94	0.48
1:E:59:ILE:CD1	1:E:272:SER:OG	2.61	0.48
1:K:430:VAL:CG2	1:M:437:ILE:HD11	2.40	0.48
1:W:98:GLN:OE1	1:Y:375:ASN:ND2	2.46	0.48
1:C:59:ILE:HD12	1:C:268:ASP:HB3	1.95	0.48
1:S:90:LYS:HD3	1:U:259:PHE:CD2	2.48	0.48
1:Y:106:THR:HB	1:Y:413:THR:HB	1.95	0.48
1:I:430:VAL:HG22	1:K:435:GLY:HA3	1.95	0.48
1:K:341:TYR:CD2	1:K:348:ASP:HB2	2.49	0.48
1:A:58:ASP:OD1	1:A:261:LYS:NZ	2.46	0.48
1:W:101:VAL:HG12	1:W:131:ASN:ND2	2.29	0.48
1:K:128:ASP:HA	1:M:379:ARG:HD2	1.96	0.48
1:O:145:TRP:HB2	1:O:159:ILE:HA	1.96	0.48
1:U:349:ASN:N	1:U:349:ASN:ND2	2.62	0.47
1:Y:64:ARG:NH2	1:Y:79:LYS:HD3	2.29	0.47
1:A:101:VAL:HG21	1:A:134:VAL:HG21	1.95	0.47
1:W:86:HIS:HD2	1:W:268:ASP:OD2	1.97	0.47
1:S:349:ASN:N	1:S:349:ASN:ND2	2.62	0.47
1:U:275:MET:HE1	1:W:266:ASN:HB3	1.94	0.47
1:G:160:PHE:HD2	1:G:165:MET:SD	2.36	0.47
1:A:161:PRO:HB3	1:A:163:GLU:OE2	2.14	0.47
1:W:300:THR:O	1:W:304:ARG:HB2	2.15	0.47
1:I:349:ASN:H	1:I:349:ASN:HD22	1.63	0.47
1:Q:245:ILE:HG23	1:Q:387:LEU:HD23	1.96	0.47
1:K:50:VAL:O	1:K:54:MET:HG2	2.15	0.47
1:O:161:PRO:HB3	1:O:163:GLU:OE2	2.15	0.47
1:Y:137:MET:O	1:Y:249:ASN:HB2	2.14	0.47
1:I:364:GLU:HG3	1:I:418:ARG:HH22	1.79	0.47
1:K:267:TYR:OH	1:M:339:GLU:OE2	2.26	0.47
1:G:341:TYR:CD2	1:G:348:ASP:HB2	2.49	0.47
1:G:250:ASN:ND2	1:G:254:VAL:O	2.42	0.47
1:I:145:TRP:HB2	1:I:159:ILE:HA	1.95	0.47
1:I:347:VAL:HG21	1:I:367:TYR:CD2	2.50	0.47
1:M:76:ASP:OD2	1:M:78:THR:HB	2.15	0.47
1:U:128:ASP:HA	1:W:379:ARG:HD2	1.97	0.47
1:A:84:THR:HG23	1:C:262:ASP:HB3	1.96	0.47
1:Q:98:GLN:HG2	1:S:372:LEU:HD12	1.96	0.47
1:O:308:VAL:HG11	1:Q:288:LEU:HD12	1.96	0.47
1:O:107:PHE:HB3	1:O:410:LEU:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:90:LYS:CD	1:M:259:PHE:CD2	2.98	0.47
1:U:89:HIS:NE2	1:U:139:ASN:ND2	2.63	0.47
2:N:10:UNK:HA	2:N:15:UNK:HA	1.96	0.47
1:S:145:TRP:HD1	1:S:145:TRP:O	1.98	0.46
1:I:419:ILE:HG12	1:K:364:GLU:HG2	1.96	0.46
1:Q:369:LEU:O	1:Q:372:LEU:HB3	2.14	0.46
1:S:57:ASN:HB2	1:S:85:SER:HB2	1.96	0.46
1:U:248:LYS:HD3	1:U:253:MET:CE	2.45	0.46
1:S:146:HIS:HD2	1:S:243:PRO:O	1.97	0.46
1:M:364:GLU:HG3	1:M:418:ARG:NH2	2.30	0.46
1:I:101:VAL:HG12	1:I:101:VAL:O	2.15	0.46
1:I:58:ASP:OD1	1:I:261:LYS:NZ	2.45	0.46
1:K:257:LEU:O	1:K:261:LYS:HB2	2.15	0.46
1:G:341:TYR:CE2	1:G:348:ASP:HB2	2.50	0.46
1:E:364:GLU:HG3	1:E:418:ARG:NH2	2.30	0.46
1:K:66:TYR:CD2	1:K:76:ASP:HB3	2.51	0.46
1:M:300:THR:O	1:M:304:ARG:HB2	2.15	0.46
1:W:57:ASN:C	1:W:59:ILE:N	2.68	0.46
1:A:160:PHE:HD2	1:A:165:MET:SD	2.39	0.46
1:G:76:ASP:OD2	1:G:78:THR:HB	2.16	0.46
1:U:332:GLU:OE1	1:U:335:ARG:NH2	2.49	0.46
1:K:42:ASN:HA	1:K:43:PRO:HD3	1.82	0.46
1:M:142:ILE:HD12	1:M:253:MET:SD	2.55	0.46
1:U:145:TRP:HB2	1:U:159:ILE:HA	1.97	0.46
1:E:284:ILE:HG12	1:E:321:ARG:NH1	2.31	0.46
1:G:352:GLU:OE2	1:G:354:ILE:HG12	2.15	0.46
1:U:430:VAL:HG22	1:W:435:GLY:HA3	1.98	0.46
1:E:59:ILE:HD12	1:E:268:ASP:HB3	1.98	0.46
1:Q:164:GLU:O	2:R:5:UNK:HA	2.16	0.46
1:E:352:GLU:OE2	1:E:354:ILE:HG12	2.16	0.46
1:G:122:ALA:HB1	1:G:126:PHE:CD2	2.51	0.46
1:G:59:ILE:HD12	1:G:268:ASP:HB3	1.97	0.46
1:U:425:ILE:O	1:U:429:LEU:HG	2.16	0.46
1:C:419:ILE:HG12	1:E:364:GLU:HG2	1.98	0.46
1:K:347:VAL:HG21	1:K:367:TYR:CD2	2.51	0.46
1:M:349:ASN:ND2	1:M:349:ASN:H	2.14	0.46
1:O:164:GLU:O	2:P:5:UNK:HA	2.16	0.45
1:M:98:GLN:HG2	1:O:372:LEU:HD12	1.98	0.45
1:K:60:GLU:HA	1:K:83:ARG:HG3	1.99	0.45
1:S:324:ILE:HG22	1:S:326:VAL:HG23	1.98	0.45
1:W:332:GLU:OE1	1:W:335:ARG:NH2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:86:HIS:CD2	1:U:268:ASP:OD2	2.67	0.45
1:A:352:GLU:OE2	1:A:354:ILE:HG12	2.16	0.45
1:C:324:ILE:HG22	1:C:326:VAL:HG23	1.98	0.45
1:Q:66:TYR:CD2	1:Q:76:ASP:HB3	2.52	0.45
1:E:66:TYR:CD2	1:E:76:ASP:HB3	2.51	0.45
1:M:53:TYR:HB2	1:M:139:ASN:ND2	2.31	0.45
1:E:376:MET:HG3	1:E:379:ARG:HH21	1.82	0.45
1:C:440:LYS:O	1:C:444:VAL:HG23	2.17	0.45
1:I:134:VAL:HA	1:I:137:MET:HE2	1.98	0.45
1:E:275:MET:HE1	1:G:270:ILE:HD11	1.97	0.45
1:Q:349:ASN:HD22	1:Q:349:ASN:H	1.64	0.45
1:K:145:TRP:O	1:K:145:TRP:HD1	2.00	0.45
1:A:42:ASN:HA	1:A:43:PRO:HD3	1.86	0.45
1:M:64:ARG:NH2	1:M:79:LYS:HD3	2.32	0.45
1:E:161:PRO:HB3	1:E:163:GLU:OE2	2.17	0.45
1:S:106:THR:HB	1:S:413:THR:HB	1.98	0.45
1:S:84:THR:HG23	1:U:262:ASP:HB3	1.97	0.45
1:E:134:VAL:HA	1:E:137:MET:CE	2.46	0.45
2:D:10:UNK:HA	2:D:15:UNK:HA	1.99	0.45
1:A:435:GLY:HA3	1:Y:430:VAL:HG22	1.99	0.45
1:A:145:TRP:HB2	1:A:159:ILE:HA	1.96	0.45
1:A:266:ASN:HB3	1:Y:275:MET:CE	2.46	0.45
1:C:376:MET:HG3	1:C:379:ARG:HH21	1.82	0.45
1:W:146:HIS:HA	1:W:147:PRO:HD3	1.88	0.45
1:U:251:GLU:HA	1:U:251:GLU:OE1	2.17	0.45
1:S:57:ASN:C	1:S:59:ILE:N	2.70	0.45
1:I:160:PHE:HD2	1:I:165:MET:SD	2.40	0.45
1:K:86:HIS:HD2	1:K:268:ASP:OD2	2.00	0.45
1:S:53:TYR:HB2	1:S:139:ASN:ND2	2.32	0.45
1:O:95:GLN:HA	1:Q:372:LEU:HD11	1.99	0.45
1:W:248:LYS:HD3	1:W:253:MET:CE	2.47	0.45
1:W:419:ILE:HG12	1:Y:364:GLU:HG2	1.99	0.44
1:G:44:GLU:HG3	1:G:45:PRO:CD	2.35	0.44
1:A:98:GLN:HG2	1:C:372:LEU:HD12	1.97	0.44
2:F:10:UNK:HA	2:F:15:UNK:HA	1.98	0.44
1:W:58:ASP:OD1	1:W:261:LYS:NZ	2.44	0.44
1:U:364:GLU:HG3	1:U:418:ARG:NH2	2.32	0.44
1:S:274:THR:O	1:S:277:SER:HB2	2.17	0.44
1:W:89:HIS:NE2	1:W:139:ASN:ND2	2.66	0.44
1:O:364:GLU:HG3	1:O:418:ARG:NH2	2.32	0.44
1:K:349:ASN:H	1:K:349:ASN:ND2	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:250:ASN:ND2	1:U:254:VAL:HG23	2.33	0.44
1:S:57:ASN:C	1:S:59:ILE:H	2.20	0.44
1:A:266:ASN:HB3	1:Y:275:MET:HE3	1.98	0.44
1:U:146:HIS:HD2	1:U:243:PRO:O	2.00	0.44
2:R:10:UNK:HA	2:R:15:UNK:HA	1.98	0.44
1:A:275:MET:HE1	1:C:266:ASN:HB3	2.00	0.44
1:O:97:THR:HG23	1:O:134:VAL:HB	2.00	0.44
1:I:64:ARG:NH2	1:I:79:LYS:HD3	2.32	0.44
1:W:275:MET:HE2	1:Y:270:ILE:HD11	1.99	0.44
1:M:352:GLU:OE2	1:M:354:ILE:HG12	2.18	0.44
2:H:10:UNK:HA	2:H:15:UNK:HA	1.98	0.44
1:G:64:ARG:NH2	1:G:79:LYS:HD3	2.32	0.44
1:K:161:PRO:HB3	1:K:163:GLU:OE2	2.17	0.44
1:S:81:ASN:ND2	1:S:83:ARG:HD3	2.33	0.44
1:G:95:GLN:HA	1:I:372:LEU:HD11	2.00	0.44
1:Q:160:PHE:HD2	1:Q:165:MET:SD	2.40	0.44
1:C:447:ASN:HA	1:C:448:PRO:HD3	1.87	0.44
1:S:112:LYS:O	1:S:116:GLU:HG3	2.17	0.44
1:Q:145:TRP:HB2	1:Q:159:ILE:HA	1.99	0.44
1:W:96:LYS:HE3	1:W:138:SER:OG	2.18	0.44
1:U:326:VAL:CG2	1:W:328:SER:HB3	2.47	0.44
1:Q:349:ASN:N	1:Q:349:ASN:ND2	2.65	0.44
1:M:49:GLY:HA3	1:M:139:ASN:O	2.17	0.44
1:S:295:ASN:HA	1:S:296:PRO:HD3	1.90	0.44
1:G:295:ASN:HA	1:G:296:PRO:HD3	1.86	0.44
1:G:35:GLN:HA	1:G:35:GLN:OE1	2.18	0.44
1:W:57:ASN:C	1:W:59:ILE:H	2.21	0.44
1:K:125:ASP:O	1:K:129:ILE:HG12	2.18	0.44
1:G:42:ASN:HA	1:G:43:PRO:HD3	1.87	0.44
1:S:147:PRO:HG2	1:S:391:PHE:CD2	2.53	0.44
1:W:275:MET:HE1	1:Y:266:ASN:HB3	1.99	0.44
1:E:324:ILE:HG22	1:E:326:VAL:HG23	1.99	0.44
1:S:349:ASN:H	1:S:349:ASN:HD22	1.63	0.43
1:U:81:ASN:ND2	1:U:83:ARG:CD	2.81	0.43
1:G:275:MET:CE	1:I:270:ILE:HD11	2.48	0.43
1:A:145:TRP:CE2	1:A:247:PHE:HE1	2.36	0.43
1:S:352:GLU:OE2	1:S:354:ILE:HG12	2.18	0.43
1:C:58:ASP:OD1	1:C:261:LYS:NZ	2.51	0.43
1:U:134:VAL:HA	1:U:137:MET:CE	2.48	0.43
1:W:101:VAL:HG21	1:W:134:VAL:HG21	2.00	0.43
1:G:129:ILE:HG22	1:G:145:TRP:CZ3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:341:TYR:CE2	1:K:348:ASP:HB2	2.53	0.43
2:Z:10:UNK:HA	2:Z:15:UNK:HA	2.00	0.43
1:E:300:THR:O	1:E:304:ARG:HB2	2.17	0.43
1:W:163:GLU:H	1:W:163:GLU:HG3	1.62	0.43
1:I:90:LYS:HD3	1:K:259:PHE:CD2	2.53	0.43
1:A:96:LYS:HD3	1:A:373:LYS:CD	2.40	0.43
1:O:324:ILE:CG2	1:O:326:VAL:HG23	2.48	0.43
1:Y:134:VAL:HA	1:Y:137:MET:CE	2.48	0.43
1:A:122:ALA:HB1	1:A:126:PHE:CD2	2.53	0.43
1:G:59:ILE:O	1:G:59:ILE:HG12	2.18	0.43
1:Q:42:ASN:HA	1:Q:43:PRO:HD3	1.86	0.43
1:Q:348:ASP:C	1:Q:348:ASP:OD1	2.57	0.43
1:C:275:MET:HE3	1:E:266:ASN:HB3	2.00	0.43
1:G:66:TYR:CD2	1:G:76:ASP:HB3	2.53	0.43
1:O:101:VAL:O	1:O:101:VAL:CG1	2.67	0.43
1:W:146:HIS:CE1	1:W:148:PHE:HB3	2.54	0.43
1:G:427:GLN:HG2	1:I:431:GLN:OE1	2.19	0.43
1:U:57:ASN:CG	1:U:85:SER:HB2	2.39	0.43
1:Q:333:LEU:HA	1:Q:333:LEU:HD23	1.82	0.43
1:O:42:ASN:HA	1:O:43:PRO:HD3	1.90	0.43
1:O:332:GLU:OE1	1:O:335:ARG:NH2	2.51	0.43
1:U:376:MET:O	1:U:379:ARG:N	2.51	0.43
1:K:63:ARG:HH11	1:K:75:VAL:HG21	1.83	0.43
1:O:359:THR:HB	1:O:361:PRO:HD2	2.01	0.43
1:A:129:ILE:HG22	1:A:145:TRP:CZ3	2.54	0.43
1:E:42:ASN:HA	1:E:43:PRO:HD3	1.86	0.43
1:U:101:VAL:CG1	1:U:101:VAL:O	2.67	0.43
1:I:111:ASN:HD21	1:I:404:PHE:HD2	1.66	0.43
1:S:42:ASN:HA	1:S:43:PRO:HD3	1.85	0.43
1:Q:304:ARG:NH1	1:Q:305:TYR:CE1	2.87	0.42
1:K:98:GLN:HG2	1:M:372:LEU:HD12	2.01	0.42
1:M:248:LYS:HD3	1:M:253:MET:CE	2.49	0.42
1:A:324:ILE:HG22	1:A:326:VAL:HG23	2.01	0.42
1:I:60:GLU:HA	1:I:83:ARG:HG3	2.01	0.42
1:M:86:HIS:HD2	1:M:268:ASP:OD2	2.01	0.42
1:O:160:PHE:HD2	1:O:165:MET:SD	2.42	0.42
1:E:98:GLN:OE1	1:G:375:ASN:ND2	2.53	0.42
1:C:125:ASP:O	1:C:129:ILE:HG12	2.19	0.42
1:I:308:VAL:HG11	1:K:288:LEU:HD12	2.00	0.42
1:G:349:ASN:ND2	1:G:349:ASN:H	2.17	0.42
1:A:349:ASN:ND2	1:A:349:ASN:H	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:275:MET:CE	1:K:266:ASN:HB3	2.49	0.42
1:U:134:VAL:HA	1:U:137:MET:HE2	2.01	0.42
1:E:58:ASP:OD1	1:E:261:LYS:NZ	2.49	0.42
1:C:134:VAL:HA	1:C:137:MET:CE	2.49	0.42
1:O:369:LEU:O	1:O:372:LEU:HB3	2.20	0.42
1:Y:447:ASN:HA	1:Y:448:PRO:HD3	1.94	0.42
1:O:447:ASN:HA	1:O:448:PRO:HD3	1.89	0.42
2:J:10:UNK:HA	2:J:15:UNK:HA	2.00	0.42
1:S:107:PHE:HB3	1:S:410:LEU:HD11	2.01	0.42
1:S:437:ILE:HG13	1:S:437:ILE:H	1.69	0.42
1:I:95:GLN:HA	1:K:372:LEU:HD11	2.01	0.42
1:I:359:THR:HB	1:I:361:PRO:HD2	2.01	0.42
1:K:251:GLU:HA	1:K:251:GLU:OE1	2.19	0.42
1:G:429:LEU:O	1:G:433:VAL:HG23	2.20	0.42
1:C:364:GLU:HG3	1:C:418:ARG:HH22	1.85	0.42
1:G:364:GLU:HG3	1:G:418:ARG:NH2	2.35	0.42
1:U:146:HIS:CE1	1:U:148:PHE:HB3	2.54	0.42
1:O:250:ASN:ND2	1:O:254:VAL:HG23	2.34	0.42
1:K:137:MET:O	1:K:249:ASN:HB2	2.20	0.42
1:O:53:TYR:CZ	1:O:135:LYS:HE3	2.54	0.42
1:O:89:HIS:NE2	1:O:139:ASN:ND2	2.68	0.42
1:E:250:ASN:ND2	1:E:254:VAL:O	2.43	0.42
1:Q:35:GLN:OE1	1:Q:35:GLN:HA	2.19	0.42
1:M:130:LEU:O	1:M:134:VAL:HG23	2.19	0.42
1:U:437:ILE:HG13	1:U:437:ILE:H	1.65	0.42
1:A:134:VAL:HA	1:A:137:MET:CE	2.50	0.42
1:Y:439:SER:HG	1:Y:442:THR:HG1	1.66	0.42
1:I:311:VAL:O	1:K:289:LYS:HA	2.20	0.42
1:I:106:THR:HB	1:I:413:THR:HB	2.01	0.42
1:S:369:LEU:O	1:S:372:LEU:HB3	2.19	0.42
1:Y:145:TRP:HB2	1:Y:159:ILE:HA	2.02	0.42
1:C:284:ILE:HG12	1:C:321:ARG:NH1	2.34	0.42
1:W:64:ARG:NH2	1:W:79:LYS:HD3	2.34	0.42
1:S:376:MET:HG3	1:S:379:ARG:HH21	1.85	0.42
1:M:63:ARG:HH11	1:M:75:VAL:HG21	1.84	0.42
1:K:146:HIS:CE1	1:K:148:PHE:HB3	2.55	0.42
1:Y:440:LYS:O	1:Y:444:VAL:HG23	2.20	0.41
1:S:33:MET:HG2	1:S:34:ILE:N	2.34	0.41
1:C:147:PRO:HD2	1:C:243:PRO:O	2.20	0.41
1:A:376:MET:HG3	1:A:379:ARG:HH21	1.84	0.41
1:W:267:TYR:O	1:W:271:THR:OG1	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:147:PRO:HD2	1:Y:243:PRO:O	2.20	0.41
1:W:134:VAL:HA	1:W:137:MET:CE	2.51	0.41
1:W:57:ASN:CG	1:W:85:SER:HB2	2.40	0.41
1:Y:295:ASN:HA	1:Y:296:PRO:HD3	1.89	0.41
1:A:295:ASN:HA	1:A:296:PRO:HD3	1.87	0.41
1:G:430:VAL:CG2	1:I:437:ILE:HD11	2.47	0.41
1:W:81:ASN:O	1:W:83:ARG:NH1	2.53	0.41
1:C:275:MET:CE	1:E:266:ASN:HB3	2.50	0.41
1:E:103:GLU:HA	1:E:104:PRO:HD3	1.92	0.41
1:M:66:TYR:CD2	1:M:76:ASP:HB3	2.56	0.41
1:O:84:THR:HG23	1:Q:262:ASP:HB3	2.01	0.41
1:E:57:ASN:N	1:E:57:ASN:OD1	2.52	0.41
1:A:89:HIS:NE2	1:A:139:ASN:ND2	2.68	0.41
1:G:90:LYS:NZ	1:G:94:ASP:OD1	2.53	0.41
1:I:304:ARG:NH2	1:K:76:ASP:HB2	2.20	0.41
1:S:275:MET:CE	1:U:270:ILE:HD11	2.45	0.41
1:I:324:ILE:CG2	1:I:326:VAL:HG23	2.51	0.41
1:G:129:ILE:HG22	1:G:145:TRP:HZ3	1.85	0.41
1:K:295:ASN:HA	1:K:296:PRO:HD3	1.88	0.41
1:K:84:THR:HG23	1:M:262:ASP:HB3	2.01	0.41
1:O:336:ILE:O	1:O:340:LEU:HB2	2.21	0.41
1:M:57:ASN:OD1	1:M:57:ASN:N	2.54	0.41
1:C:352:GLU:OE2	1:C:354:ILE:HG12	2.20	0.41
1:E:107:PHE:HB3	1:E:410:LEU:HD11	2.02	0.41
1:Q:261:LYS:NZ	1:Q:265:ASP:OD2	2.51	0.41
1:G:98:GLN:HG2	1:I:372:LEU:HD12	2.02	0.41
1:C:101:VAL:O	1:C:101:VAL:HG12	2.21	0.41
1:M:53:TYR:HB2	1:M:139:ASN:HD21	1.85	0.41
1:I:129:ILE:HG22	1:I:145:TRP:CZ3	2.55	0.41
1:C:111:ASN:HD21	1:C:404:PHE:HD2	1.68	0.41
1:G:437:ILE:H	1:G:437:ILE:HG13	1.69	0.41
1:I:352:GLU:HG3	1:I:354:ILE:O	2.21	0.41
1:A:58:ASP:HA	1:A:61:LYS:HE2	2.01	0.41
1:O:308:VAL:CG1	1:Q:288:LEU:HD12	2.50	0.41
1:U:364:GLU:HG3	1:U:418:ARG:HH22	1.86	0.41
1:U:66:TYR:CE2	1:U:74:LEU:HB3	2.55	0.41
1:M:161:PRO:HB3	1:M:163:GLU:OE2	2.20	0.41
1:K:64:ARG:NH2	1:K:79:LYS:HD3	2.36	0.41
1:M:295:ASN:HA	1:M:296:PRO:HD3	1.85	0.41
1:K:130:LEU:O	1:K:134:VAL:HG23	2.21	0.41
1:K:352:GLU:OE2	1:K:354:ILE:HG12	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:430:VAL:HG22	1:I:435:GLY:HA3	2.02	0.41
1:I:125:ASP:O	1:I:129:ILE:HG12	2.20	0.41
1:O:130:LEU:O	1:O:134:VAL:HG23	2.20	0.41
1:I:284:ILE:HG12	1:I:321:ARG:NH1	2.36	0.41
1:Q:57:ASN:CG	1:Q:85:SER:HB2	2.41	0.41
1:G:146:HIS:CE1	1:G:148:PHE:HB3	2.56	0.41
1:S:128:ASP:HA	1:U:379:ARG:HD2	2.03	0.41
1:O:129:ILE:HG22	1:O:145:TRP:CZ3	2.56	0.41
1:I:90:LYS:NZ	1:I:94:ASP:OD1	2.53	0.41
1:G:142:ILE:HD12	1:G:248:LYS:HG2	2.03	0.41
1:E:122:ALA:HB1	1:E:126:PHE:CD2	2.55	0.41
1:O:257:LEU:HG	1:O:261:LYS:HB2	2.03	0.41
1:I:251:GLU:OE1	1:I:251:GLU:HA	2.21	0.41
1:U:42:ASN:HA	1:U:43:PRO:HD3	1.79	0.41
1:O:66:TYR:CD2	1:O:76:ASP:HB3	2.57	0.41
1:E:275:MET:HE1	1:G:270:ILE:CD1	2.51	0.41
1:Q:275:MET:HE1	1:S:266:ASN:HB3	2.03	0.41
1:S:250:ASN:HD21	1:S:254:VAL:HG23	1.86	0.41
1:U:250:ASN:HD22	1:U:254:VAL:H	1.67	0.41
1:U:98:GLN:HG2	1:W:372:LEU:HD12	2.03	0.41
1:O:90:LYS:NZ	1:O:94:ASP:OD1	2.54	0.41
1:O:128:ASP:HA	1:Q:379:ARG:HD2	2.03	0.41
1:M:160:PHE:HD2	1:M:165:MET:SD	2.44	0.41
1:G:447:ASN:HA	1:G:448:PRO:HD3	1.95	0.41
1:C:42:ASN:HA	1:C:43:PRO:HD3	1.91	0.41
1:Y:437:ILE:HG13	1:Y:437:ILE:H	1.76	0.40
1:K:437:ILE:HG13	1:K:437:ILE:H	1.70	0.40
1:Y:356:GLY:O	1:Y:358:ALA:N	2.54	0.40
1:C:349:ASN:H	1:C:349:ASN:ND2	2.19	0.40
1:W:364:GLU:HG3	1:W:418:ARG:HH22	1.87	0.40
1:W:33:MET:HG2	1:W:34:ILE:N	2.35	0.40
1:O:349:ASN:HD22	1:O:349:ASN:H	1.68	0.40
1:O:349:ASN:ND2	1:O:349:ASN:N	2.67	0.40
1:C:129:ILE:HG22	1:C:145:TRP:CZ3	2.56	0.40
1:M:57:ASN:CG	1:M:85:SER:HB2	2.42	0.40
1:O:142:ILE:HD12	1:O:253:MET:SD	2.61	0.40
1:G:376:MET:HG3	1:G:379:ARG:NH2	2.36	0.40
1:Q:336:ILE:O	1:Q:340:LEU:HB2	2.22	0.40
1:W:137:MET:HE2	1:W:137:MET:HB3	1.96	0.40
1:W:42:ASN:HA	1:W:43:PRO:HD3	1.91	0.40
1:Y:359:THR:HB	1:Y:361:PRO:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:356:GLY:O	1:S:358:ALA:N	2.54	0.40
1:S:359:THR:HB	1:S:361:PRO:HD2	2.03	0.40
1:K:446:ARG:HE	1:K:446:ARG:HB3	1.71	0.40
1:E:447:ASN:HA	1:E:448:PRO:HD3	1.91	0.40
1:Q:359:THR:HB	1:Q:361:PRO:HD2	2.04	0.40
1:W:349:ASN:H	1:W:349:ASN:HD22	1.67	0.40
1:C:146:HIS:CE1	1:C:148:PHE:HB3	2.56	0.40
1:Y:261:LYS:NZ	1:Y:265:ASP:OD2	2.54	0.40
1:C:250:ASN:ND2	1:C:254:VAL:HG23	2.36	0.40
1:Q:54:MET:SD	1:S:252:GLU:HG2	2.61	0.40
1:U:357:GLY:HA2	1:U:362:ALA:HB1	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:ASP:O	1:O:39:ASP:OD2[5_445]	2.08	0.12

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	366/503 (73%)	333 (91%)	31 (8%)	2 (0%)	34	75
1	C	366/503 (73%)	337 (92%)	26 (7%)	3 (1%)	24	67
1	E	366/503 (73%)	338 (92%)	26 (7%)	2 (0%)	34	75
1	G	366/503 (73%)	331 (90%)	33 (9%)	2 (0%)	34	75
1	I	366/503 (73%)	332 (91%)	32 (9%)	2 (0%)	34	75
1	K	366/503 (73%)	339 (93%)	24 (7%)	3 (1%)	24	67
1	M	366/503 (73%)	335 (92%)	29 (8%)	2 (0%)	34	75

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	366/503 (73%)	337 (92%)	27 (7%)	2 (0%)	34	75
1	Q	366/503 (73%)	343 (94%)	21 (6%)	2 (0%)	34	75
1	S	366/503 (73%)	333 (91%)	29 (8%)	4 (1%)	17	61
1	U	366/503 (73%)	337 (92%)	26 (7%)	3 (1%)	24	67
1	W	366/503 (73%)	338 (92%)	27 (7%)	1 (0%)	46	82
1	Y	366/503 (73%)	336 (92%)	27 (7%)	3 (1%)	24	67
All	All	4758/6539 (73%)	4369 (92%)	358 (8%)	31 (1%)	26	70

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Q	357	GLY
1	A	357	GLY
1	C	357	GLY
1	E	357	GLY
1	G	69	ALA
1	G	357	GLY
1	I	357	GLY
1	K	357	GLY
1	M	357	GLY
1	O	357	GLY
1	S	357	GLY
1	S	407	ASP
1	U	357	GLY
1	Y	357	GLY
1	I	68	ASP
1	K	69	ALA
1	Q	69	ALA
1	S	69	ALA
1	W	357	GLY
1	Y	87	ALA
1	C	69	ALA
1	E	123	ASP
1	K	87	ALA
1	M	87	ALA
1	S	58	ASP
1	U	68	ASP
1	Y	68	ASP
1	A	69	ALA
1	O	68	ASP

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Mol	Chain	Res	Type
1	U	407	ASP
1	C	161	PRO

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	296/436 (68%)	270 (91%)	26 (9%)	12	46
1	C	296/436 (68%)	270 (91%)	26 (9%)	12	46
1	E	296/436 (68%)	268 (90%)	28 (10%)	11	41
1	G	296/436 (68%)	265 (90%)	31 (10%)	8	36
1	I	296/436 (68%)	267 (90%)	29 (10%)	10	40
1	K	296/436 (68%)	265 (90%)	31 (10%)	8	36
1	M	296/436 (68%)	265 (90%)	31 (10%)	8	36
1	O	296/436 (68%)	266 (90%)	30 (10%)	9	38
1	Q	296/436 (68%)	263 (89%)	33 (11%)	8	33
1	S	296/436 (68%)	260 (88%)	36 (12%)	6	28
1	U	296/436 (68%)	265 (90%)	31 (10%)	8	36
1	W	296/436 (68%)	265 (90%)	31 (10%)	8	36
1	Y	296/436 (68%)	269 (91%)	27 (9%)	12	44
All	All	3848/5668 (68%)	3458 (90%)	390 (10%)	9	38

All (390) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	MET
1	A	48	LYS
1	A	56	GLU
1	A	59	ILE
1	A	65	THR
1	A	74	LEU

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Mol	Chain	Res	Type
1	A	80	THR
1	A	83	ARG
1	A	108	THR
1	A	110	ASP
1	A	123	ASP
1	A	145	TRP
1	A	160	PHE
1	A	163	GLU
1	A	239	TRP
1	A	250	ASN
1	A	254	VAL
1	A	271	THR
1	A	300	THR
1	A	302	ASN
1	A	304	ARG
1	A	328	SER
1	A	349	ASN
1	A	353	THR
1	A	423	SER
1	A	437	ILE
1	C	33	MET
1	C	48	LYS
1	C	59	ILE
1	C	65	THR
1	C	74	LEU
1	C	80	THR
1	C	83	ARG
1	C	123	ASP
1	C	136	ASN
1	C	145	TRP
1	C	148	PHE
1	C	160	PHE
1	C	163	GLU
1	C	239	TRP
1	C	250	ASN
1	C	279	SER
1	C	300	THR
1	C	302	ASN
1	C	304	ARG
1	C	338	ASP
1	C	340	LEU
1	C	349	ASN

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Mol	Chain	Res	Type
1	C	353	THR
1	C	423	SER
1	C	437	ILE
1	C	438	MET
1	E	33	MET
1	E	48	LYS
1	E	56	GLU
1	E	57	ASN
1	E	65	THR
1	E	68	ASP
1	E	74	LEU
1	E	76	ASP
1	E	80	THR
1	E	83	ARG
1	E	110	ASP
1	E	120	GLU
1	E	123	ASP
1	E	128	ASP
1	E	136	ASN
1	E	145	TRP
1	E	160	PHE
1	E	163	GLU
1	E	239	TRP
1	E	250	ASN
1	E	300	THR
1	E	302	ASN
1	E	304	ARG
1	E	328	SER
1	E	349	ASN
1	E	353	THR
1	E	423	SER
1	E	437	ILE
1	G	33	MET
1	G	48	LYS
1	G	56	GLU
1	G	65	THR
1	G	74	LEU
1	G	76	ASP
1	G	80	THR
1	G	83	ARG
1	G	98	GLN
1	G	108	THR

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Mol	Chain	Res	Type
1	G	110	ASP
1	G	120	GLU
1	G	123	ASP
1	G	128	ASP
1	G	136	ASN
1	G	145	TRP
1	G	160	PHE
1	G	163	GLU
1	G	239	TRP
1	G	250	ASN
1	G	300	THR
1	G	302	ASN
1	G	304	ARG
1	G	328	SER
1	G	338	ASP
1	G	349	ASN
1	G	353	THR
1	G	354	ILE
1	G	423	SER
1	G	437	ILE
1	G	438	MET
1	I	33	MET
1	I	48	LYS
1	I	56	GLU
1	I	59	ILE
1	I	65	THR
1	I	74	LEU
1	I	80	THR
1	I	83	ARG
1	I	98	GLN
1	I	108	THR
1	I	110	ASP
1	I	128	ASP
1	I	136	ASN
1	I	145	TRP
1	I	160	PHE
1	I	163	GLU
1	I	239	TRP
1	I	250	ASN
1	I	300	THR
1	I	302	ASN
1	I	304	ARG

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Mol	Chain	Res	Type
1	I	321	ARG
1	I	328	SER
1	I	337	GLN
1	I	338	ASP
1	I	349	ASN
1	I	353	THR
1	I	423	SER
1	I	437	ILE
1	K	33	MET
1	K	48	LYS
1	K	56	GLU
1	K	59	ILE
1	K	65	THR
1	K	74	LEU
1	K	76	ASP
1	K	80	THR
1	K	83	ARG
1	K	110	ASP
1	K	123	ASP
1	K	128	ASP
1	K	136	ASN
1	K	145	TRP
1	K	160	PHE
1	K	163	GLU
1	K	239	TRP
1	K	250	ASN
1	K	279	SER
1	K	300	THR
1	K	302	ASN
1	K	304	ARG
1	K	328	SER
1	K	337	GLN
1	K	338	ASP
1	K	349	ASN
1	K	352	GLU
1	K	353	THR
1	K	423	SER
1	K	437	ILE
1	K	438	MET
1	M	33	MET
1	M	48	LYS
1	M	56	GLU

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Mol	Chain	Res	Type
1	M	57	ASN
1	M	59	ILE
1	M	68	ASP
1	M	74	LEU
1	M	76	ASP
1	M	80	THR
1	M	83	ARG
1	M	123	ASP
1	M	136	ASN
1	M	145	TRP
1	M	160	PHE
1	M	163	GLU
1	M	239	TRP
1	M	250	ASN
1	M	254	VAL
1	M	279	SER
1	M	300	THR
1	M	302	ASN
1	M	304	ARG
1	M	321	ARG
1	M	328	SER
1	M	340	LEU
1	M	349	ASN
1	M	352	GLU
1	M	353	THR
1	M	423	SER
1	M	437	ILE
1	M	438	MET
1	O	33	MET
1	O	48	LYS
1	O	59	ILE
1	O	65	THR
1	O	74	LEU
1	O	80	THR
1	O	83	ARG
1	O	110	ASP
1	O	123	ASP
1	O	136	ASN
1	O	145	TRP
1	O	160	PHE
1	O	163	GLU
1	O	239	TRP

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Mol	Chain	Res	Type
1	O	250	ASN
1	O	254	VAL
1	O	279	SER
1	O	300	THR
1	O	302	ASN
1	O	304	ARG
1	O	328	SER
1	O	337	GLN
1	O	338	ASP
1	O	340	LEU
1	O	349	ASN
1	O	352	GLU
1	O	353	THR
1	O	423	SER
1	O	437	ILE
1	O	438	MET
1	Q	33	MET
1	Q	48	LYS
1	Q	56	GLU
1	Q	59	ILE
1	Q	65	THR
1	Q	74	LEU
1	Q	76	ASP
1	Q	80	THR
1	Q	83	ARG
1	Q	110	ASP
1	Q	120	GLU
1	Q	123	ASP
1	Q	145	TRP
1	Q	159	ILE
1	Q	160	PHE
1	Q	163	GLU
1	Q	239	TRP
1	Q	250	ASN
1	Q	254	VAL
1	Q	279	SER
1	Q	300	THR
1	Q	302	ASN
1	Q	321	ARG
1	Q	328	SER
1	Q	337	GLN
1	Q	340	LEU

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Mol	Chain	Res	Type
1	Q	349	ASN
1	Q	353	THR
1	Q	354	ILE
1	Q	418	ARG
1	Q	423	SER
1	Q	437	ILE
1	Q	438	MET
1	S	33	MET
1	S	40	GLU
1	S	48	LYS
1	S	56	GLU
1	S	59	ILE
1	S	65	THR
1	S	68	ASP
1	S	74	LEU
1	S	76	ASP
1	S	80	THR
1	S	83	ARG
1	S	108	THR
1	S	110	ASP
1	S	123	ASP
1	S	136	ASN
1	S	145	TRP
1	S	160	PHE
1	S	163	GLU
1	S	168	VAL
1	S	239	TRP
1	S	250	ASN
1	S	254	VAL
1	S	256	ASP
1	S	279	SER
1	S	300	THR
1	S	302	ASN
1	S	304	ARG
1	S	321	ARG
1	S	328	SER
1	S	337	GLN
1	S	340	LEU
1	S	349	ASN
1	S	353	THR
1	S	373	LYS
1	S	430	VAL

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Mol	Chain	Res	Type
1	S	437	ILE
1	U	33	MET
1	U	48	LYS
1	U	56	GLU
1	U	59	ILE
1	U	65	THR
1	U	68	ASP
1	U	74	LEU
1	U	76	ASP
1	U	80	THR
1	U	83	ARG
1	U	108	THR
1	U	110	ASP
1	U	113	THR
1	U	120	GLU
1	U	123	ASP
1	U	128	ASP
1	U	136	ASN
1	U	145	TRP
1	U	160	PHE
1	U	163	GLU
1	U	168	VAL
1	U	239	TRP
1	U	300	THR
1	U	302	ASN
1	U	304	ARG
1	U	328	SER
1	U	340	LEU
1	U	349	ASN
1	U	353	THR
1	U	423	SER
1	U	437	ILE
1	W	33	MET
1	W	48	LYS
1	W	56	GLU
1	W	59	ILE
1	W	65	THR
1	W	74	LEU
1	W	80	THR
1	W	83	ARG
1	W	108	THR
1	W	110	ASP

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Mol	Chain	Res	Type
1	W	123	ASP
1	W	128	ASP
1	W	136	ASN
1	W	145	TRP
1	W	160	PHE
1	W	163	GLU
1	W	239	TRP
1	W	250	ASN
1	W	254	VAL
1	W	271	THR
1	W	300	THR
1	W	302	ASN
1	W	304	ARG
1	W	337	GLN
1	W	338	ASP
1	W	340	LEU
1	W	349	ASN
1	W	353	THR
1	W	411	THR
1	W	423	SER
1	W	437	ILE
1	Y	33	MET
1	Y	48	LYS
1	Y	56	GLU
1	Y	59	ILE
1	Y	65	THR
1	Y	68	ASP
1	Y	74	LEU
1	Y	80	THR
1	Y	83	ARG
1	Y	110	ASP
1	Y	123	ASP
1	Y	128	ASP
1	Y	145	TRP
1	Y	160	PHE
1	Y	163	GLU
1	Y	239	TRP
1	Y	250	ASN
1	Y	279	SER
1	Y	300	THR
1	Y	302	ASN
1	Y	304	ARG

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Mol	Chain	Res	Type
1	Y	338	ASP
1	Y	349	ASN
1	Y	353	THR
1	Y	423	SER
1	Y	437	ILE
1	Y	438	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (107) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	86	HIS
1	A	136	ASN
1	A	139	ASN
1	A	146	HIS
1	A	282	GLN
1	A	302	ASN
1	A	349	ASN
1	A	427	GLN
1	C	73	GLN
1	C	86	HIS
1	C	136	ASN
1	C	139	ASN
1	C	146	HIS
1	C	302	ASN
1	C	349	ASN
1	C	431	GLN
1	E	73	GLN
1	E	86	HIS
1	E	136	ASN
1	E	139	ASN
1	E	146	HIS
1	E	282	GLN
1	E	302	ASN
1	E	349	ASN
1	E	427	GLN
1	G	73	GLN
1	G	136	ASN
1	G	139	ASN
1	G	146	HIS
1	G	302	ASN
1	G	349	ASN

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Mol	Chain	Res	Type
1	G	431	GLN
1	I	73	GLN
1	I	86	HIS
1	I	136	ASN
1	I	139	ASN
1	I	146	HIS
1	I	302	ASN
1	I	345	GLN
1	I	349	ASN
1	K	73	GLN
1	K	86	HIS
1	K	136	ASN
1	K	139	ASN
1	K	146	HIS
1	K	302	ASN
1	K	349	ASN
1	M	73	GLN
1	M	86	HIS
1	M	136	ASN
1	M	139	ASN
1	M	146	HIS
1	M	302	ASN
1	M	349	ASN
1	M	427	GLN
1	O	86	HIS
1	O	136	ASN
1	O	139	ASN
1	O	146	HIS
1	O	282	GLN
1	O	302	ASN
1	O	349	ASN
1	O	431	GLN
1	Q	73	GLN
1	Q	86	HIS
1	Q	136	ASN
1	Q	139	ASN
1	Q	146	HIS
1	Q	302	ASN
1	Q	349	ASN
1	Q	427	GLN
1	S	73	GLN
1	S	136	ASN

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Mol	Chain	Res	Type
1	S	139	ASN
1	S	146	HIS
1	S	250	ASN
1	S	302	ASN
1	S	337	GLN
1	S	349	ASN
1	S	427	GLN
1	S	431	GLN
1	U	86	HIS
1	U	98	GLN
1	U	136	ASN
1	U	139	ASN
1	U	146	HIS
1	U	250	ASN
1	U	302	ASN
1	U	349	ASN
1	U	431	GLN
1	W	73	GLN
1	W	86	HIS
1	W	131	ASN
1	W	136	ASN
1	W	139	ASN
1	W	146	HIS
1	W	302	ASN
1	W	349	ASN
1	W	375	ASN
1	Y	73	GLN
1	Y	86	HIS
1	Y	136	ASN
1	Y	139	ASN
1	Y	146	HIS
1	Y	302	ASN
1	Y	349	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 26 ligands modelled in this entry, 26 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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	370/503 (73%)	0.99	65 (17%) 2 2	140, 140, 140, 140	0
1	C	370/503 (73%)	1.15	79 (21%) 1 1	140, 140, 140, 140	0
1	E	370/503 (73%)	1.17	76 (20%) 1 1	140, 140, 140, 140	0
1	G	370/503 (73%)	0.98	67 (18%) 2 2	140, 140, 140, 140	0
1	I	370/503 (73%)	0.99	67 (18%) 2 2	140, 140, 140, 140	0
1	K	370/503 (73%)	0.98	60 (16%) 3 2	140, 140, 140, 140	0
1	M	370/503 (73%)	1.01	66 (17%) 2 2	140, 140, 140, 140	0
1	O	370/503 (73%)	0.88	54 (14%) 3 3	140, 140, 140, 140	0
1	Q	370/503 (73%)	0.91	55 (14%) 3 3	140, 140, 140, 140	0
1	S	370/503 (73%)	0.83	48 (12%) 5 4	140, 140, 140, 140	0
1	U	370/503 (73%)	0.77	38 (10%) 9 8	140, 140, 140, 140	0
1	W	370/503 (73%)	0.78	55 (14%) 3 3	140, 140, 140, 140	0
1	Y	370/503 (73%)	0.99	64 (17%) 2 2	140, 140, 140, 140	0
2	B	0/30	-	-	-	-
2	D	0/30	-	-	-	-
2	F	0/30	-	-	-	-
2	H	0/30	-	-	-	-
2	J	0/30	-	-	-	-
2	L	0/30	-	-	-	-
2	N	0/30	-	-	-	-
2	P	0/30	-	-	-	-
2	R	0/30	-	-	-	-
2	T	0/30	-	-	-	-
2	V	0/30	-	-	-	-
2	X	0/30	-	-	-	-
2	Z	0/30	-	-	-	-
All	All	4810/6929 (69%)	0.95	794 (16%) 2 2	140, 140, 140, 140	0

All (794) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Y	292	ASP	10.6
1	I	315	GLY	10.1
1	Y	291	TYR	10.0
1	O	404	PHE	9.3
1	U	291	TYR	9.1
1	S	314	ASP	8.5
1	C	68	ASP	8.1
1	C	70	ALA	8.0
1	A	166	ILE	7.8
1	M	243	PRO	7.8
1	A	315	GLY	7.8
1	O	410	LEU	7.7
1	I	33	MET	7.3
1	W	33	MET	7.2
1	M	315	GLY	7.2
1	S	312	SER	7.1
1	M	316	GLY	7.1
1	I	314	ASP	7.0
1	C	69	ALA	7.0
1	K	406	PRO	7.0
1	E	316	GLY	6.7
1	E	33	MET	6.7
1	G	243	PRO	6.7
1	G	113	THR	6.7
1	S	315	GLY	6.6
1	C	244	ILE	6.5
1	Y	33	MET	6.4
1	G	117	TYR	6.4
1	E	148	PHE	6.4
1	C	124	ASP	6.4
1	A	417	THR	6.4
1	E	294	GLU	6.2
1	A	314	ASP	6.2
1	C	74	LEU	6.2
1	K	243	PRO	6.2
1	E	391	PHE	6.2
1	U	292	ASP	6.0
1	A	316	GLY	6.0
1	M	244	ILE	6.0
1	E	456	GLU	6.0
1	K	34	ILE	5.9
1	O	292	ASP	5.9

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Mol	Chain	Res	Type	RSRZ
1	Y	358	ALA	5.8
1	K	33	MET	5.8
1	M	404	PHE	5.8
1	S	292	ASP	5.8
1	I	151	GLU	5.8
1	S	437	ILE	5.7
1	A	34	ILE	5.7
1	C	438	MET	5.6
1	S	311	VAL	5.6
1	U	438	MET	5.6
1	G	30	ASP	5.6
1	Q	295	ASN	5.5
1	I	357	GLY	5.5
1	Y	450	VAL	5.5
1	E	34	ILE	5.4
1	K	314	ASP	5.4
1	E	154	GLU	5.4
1	Q	447	ASN	5.4
1	I	316	GLY	5.4
1	M	74	LEU	5.4
1	A	398	ASN	5.4
1	G	396	LEU	5.4
1	O	392	PHE	5.4
1	Q	392	PHE	5.4
1	M	113	THR	5.3
1	W	32	THR	5.3
1	Y	410	LEU	5.3
1	C	166	ILE	5.3
1	Y	357	GLY	5.2
1	G	244	ILE	5.2
1	I	349	ASN	5.2
1	E	392	PHE	5.2
1	A	239	TRP	5.2
1	M	314	ASP	5.2
1	G	166	ILE	5.1
1	C	154	GLU	5.1
1	I	437	ILE	5.1
1	I	464	MET	5.1
1	C	392	PHE	5.1
1	O	358	ALA	5.1
1	Q	404	PHE	5.1
1	A	33	MET	5.1

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Mol	Chain	Res	Type	RSRZ
1	Y	143	GLU	5.1
1	O	314	ASP	5.0
1	Q	40	GLU	5.0
1	Y	432	GLY	5.0
1	C	449	PHE	5.0
1	C	149	VAL	4.9
1	W	353	THR	4.9
1	C	395	TYR	4.9
1	U	309	ILE	4.9
1	Y	404	PHE	4.9
1	Y	401	LYS	4.9
1	O	166	ILE	4.9
1	A	388	PHE	4.9
1	I	394	GLU	4.9
1	A	305	TYR	4.8
1	K	353	THR	4.8
1	M	33	MET	4.8
1	S	68	ASP	4.8
1	E	438	MET	4.8
1	I	110	ASP	4.8
1	C	155	PHE	4.8
1	Q	74	LEU	4.7
1	E	353	THR	4.7
1	G	155	PHE	4.7
1	O	244	ILE	4.7
1	Q	314	ASP	4.7
1	M	410	LEU	4.7
1	C	117	TYR	4.7
1	M	72	GLN	4.7
1	K	316	GLY	4.6
1	M	30	ASP	4.6
1	E	145	TRP	4.6
1	Y	438	MET	4.6
1	C	291	TYR	4.6
1	C	37	LEU	4.6
1	A	405	ASN	4.6
1	I	358	ALA	4.6
1	U	30	ASP	4.6
1	Y	402	GLY	4.6
1	G	121	LEU	4.6
1	I	422	ASP	4.5
1	E	155	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
1	O	243	PRO	4.5
1	U	465	ASN	4.5
1	C	417	THR	4.5
1	K	37	LEU	4.5
1	C	410	LEU	4.5
1	M	239	TRP	4.5
1	G	120	GLU	4.5
1	M	399	THR	4.5
1	E	404	PHE	4.5
1	U	404	PHE	4.5
1	Q	113	THR	4.4
1	E	68	ASP	4.4
1	I	245	ILE	4.4
1	K	239	TRP	4.4
1	U	398	ASN	4.4
1	I	117	TYR	4.4
1	E	422	ASP	4.4
1	A	353	THR	4.4
1	W	357	GLY	4.3
1	W	241	ARG	4.3
1	I	122	ALA	4.3
1	O	291	TYR	4.3
1	E	40	GLU	4.3
1	I	37	LEU	4.3
1	K	32	THR	4.3
1	E	352	GLU	4.3
1	M	242	VAL	4.3
1	W	67	TYR	4.2
1	W	261	LYS	4.2
1	E	70	ALA	4.2
1	U	120	GLU	4.2
1	E	243	PRO	4.2
1	E	458	ALA	4.2
1	E	166	ILE	4.2
1	S	358	ALA	4.2
1	Q	71	GLY	4.2
1	W	287	VAL	4.2
1	O	359	THR	4.2
1	M	71	GLY	4.2
1	K	410	LEU	4.2
1	A	54	MET	4.2
1	Q	67	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
1	I	438	MET	4.2
1	I	149	VAL	4.2
1	U	310	LYS	4.2
1	K	148	PHE	4.1
1	Q	312	SER	4.1
1	E	467	TYR	4.1
1	C	38	ILE	4.1
1	A	317	VAL	4.1
1	G	401	LYS	4.1
1	O	398	ASN	4.1
1	A	155	PHE	4.1
1	W	288	LEU	4.1
1	C	239	TRP	4.1
1	O	394	GLU	4.0
1	G	53	TYR	4.0
1	G	118	VAL	4.0
1	Q	66	TYR	4.0
1	W	73	GLN	4.0
1	I	393	ALA	4.0
1	K	401	LYS	4.0
1	Y	287	VAL	4.0
1	S	239	TRP	3.9
1	I	142	ILE	3.9
1	W	30	ASP	3.9
1	E	311	VAL	3.9
1	E	47	LEU	3.9
1	Y	34	ILE	3.9
1	S	377	ALA	3.9
1	I	239	TRP	3.8
1	A	438	MET	3.8
1	C	243	PRO	3.8
1	I	442	THR	3.8
1	S	109	SER	3.8
1	K	315	GLY	3.8
1	Y	400	GLY	3.8
1	G	444	VAL	3.8
1	Q	398	ASN	3.8
1	K	352	GLU	3.8
1	M	437	ILE	3.8
1	W	239	TRP	3.8
1	A	169	TYR	3.8
1	C	316	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	G	122	ALA	3.8
1	K	460	ILE	3.8
1	M	63	ARG	3.7
1	S	309	ILE	3.7
1	G	437	ILE	3.7
1	Y	436	GLY	3.7
1	C	66	TYR	3.7
1	C	391	PHE	3.7
1	K	247	PHE	3.7
1	A	167	VAL	3.7
1	C	167	VAL	3.7
1	G	39	ASP	3.7
1	I	401	LYS	3.7
1	A	43	PRO	3.7
1	W	404	PHE	3.7
1	G	239	TRP	3.7
1	Y	239	TRP	3.7
1	U	65	THR	3.7
1	O	312	SER	3.7
1	K	402	GLY	3.7
1	M	43	PRO	3.7
1	E	389	PHE	3.7
1	A	467	TYR	3.7
1	C	386	ARG	3.7
1	M	403	ASP	3.7
1	Q	437	ILE	3.6
1	G	292	ASP	3.6
1	E	291	TYR	3.6
1	K	405	ASN	3.6
1	C	40	GLU	3.6
1	C	314	ASP	3.6
1	Y	37	LEU	3.6
1	C	125	ASP	3.6
1	G	34	ILE	3.6
1	G	165	MET	3.6
1	W	292	ASP	3.6
1	A	261	LYS	3.6
1	O	311	VAL	3.6
1	K	145	TRP	3.6
1	Q	39	ASP	3.6
1	Y	353	THR	3.6
1	A	465	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	G	32	THR	3.6
1	C	315	GLY	3.6
1	U	293	GLY	3.6
1	G	466	GLN	3.5
1	M	120	GLU	3.5
1	W	114	LEU	3.5
1	A	156	ASP	3.5
1	A	292	ASP	3.5
1	Y	63	ARG	3.5
1	E	244	ILE	3.5
1	Q	73	GLN	3.5
1	G	114	LEU	3.5
1	K	354	ILE	3.5
1	U	437	ILE	3.5
1	A	444	VAL	3.5
1	G	398	ASN	3.5
1	C	278	PHE	3.5
1	I	166	ILE	3.5
1	I	436	GLY	3.5
1	M	145	TRP	3.5
1	S	389	PHE	3.5
1	S	406	PRO	3.5
1	W	294	GLU	3.5
1	I	72	GLN	3.5
1	C	429	LEU	3.5
1	O	114	LEU	3.5
1	O	456	GLU	3.5
1	Q	458	ALA	3.4
1	G	115	LEU	3.4
1	G	242	VAL	3.4
1	A	145	TRP	3.4
1	O	148	PHE	3.4
1	U	33	MET	3.4
1	Q	243	PRO	3.4
1	C	358	ALA	3.4
1	M	398	ASN	3.4
1	C	165	MET	3.4
1	C	404	PHE	3.4
1	S	452	ASP	3.4
1	G	111	ASN	3.4
1	M	34	ILE	3.4
1	S	72	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	317	VAL	3.4
1	O	406	PRO	3.4
1	W	448	PRO	3.4
1	G	419	ILE	3.4
1	E	117	TYR	3.4
1	E	167	VAL	3.4
1	G	287	VAL	3.4
1	K	109	SER	3.4
1	Q	353	THR	3.4
1	I	305	TYR	3.4
1	Q	239	TRP	3.4
1	Q	461	GLU	3.3
1	Q	460	ILE	3.3
1	M	450	VAL	3.3
1	K	392	PHE	3.3
1	M	389	PHE	3.3
1	Y	39	ASP	3.3
1	M	78	THR	3.3
1	C	353	THR	3.3
1	C	398	ASN	3.3
1	M	419	ILE	3.3
1	Q	33	MET	3.3
1	W	293	GLY	3.3
1	G	309	ILE	3.3
1	A	163	GLU	3.3
1	E	453	PRO	3.3
1	O	149	VAL	3.3
1	A	389	PHE	3.3
1	C	437	ILE	3.3
1	E	293	GLY	3.3
1	G	154	GLU	3.3
1	O	38	ILE	3.3
1	Q	444	VAL	3.3
1	K	321	ARG	3.3
1	W	34	ILE	3.3
1	K	458	ALA	3.2
1	O	442	THR	3.2
1	G	72	GLN	3.2
1	M	392	PHE	3.2
1	O	239	TRP	3.2
1	O	444	VAL	3.2
1	Q	435	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	S	243	PRO	3.2
1	K	448	PRO	3.2
1	K	399	THR	3.2
1	K	449	PHE	3.2
1	K	68	ASP	3.2
1	I	143	GLU	3.2
1	I	463	GLU	3.2
1	S	307	SER	3.2
1	C	357	GLY	3.2
1	M	121	LEU	3.2
1	E	314	ASP	3.2
1	E	165	MET	3.2
1	E	410	LEU	3.2
1	G	385	LEU	3.2
1	W	395	TYR	3.2
1	M	292	ASP	3.2
1	O	293	GLY	3.2
1	A	456	GLU	3.2
1	C	65	THR	3.2
1	U	462	GLU	3.2
1	M	449	PHE	3.2
1	A	293	GLY	3.1
1	O	34	ILE	3.1
1	Y	155	PHE	3.1
1	S	313	GLY	3.1
1	A	466	GLN	3.1
1	E	449	PHE	3.1
1	G	403	ASP	3.1
1	W	399	THR	3.1
1	Q	436	GLY	3.1
1	K	35	GLN	3.1
1	G	38	ILE	3.1
1	C	41	HIS	3.1
1	K	112	LYS	3.1
1	Q	389	PHE	3.1
1	O	66	TYR	3.1
1	C	150	ASP	3.1
1	M	77	ASP	3.1
1	I	244	ILE	3.1
1	Q	354	ILE	3.1
1	M	444	VAL	3.1
1	Y	120	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	I	36	LYS	3.0
1	M	414	PHE	3.0
1	Y	293	GLY	3.0
1	A	69	ALA	3.0
1	S	299	PHE	3.0
1	G	112	LYS	3.0
1	E	406	PRO	3.0
1	U	39	ASP	3.0
1	W	35	GLN	3.0
1	Q	296	PRO	3.0
1	I	404	PHE	3.0
1	E	399	THR	3.0
1	K	389	PHE	3.0
1	Y	69	ALA	3.0
1	Y	295	ASN	3.0
1	A	244	ILE	3.0
1	C	29	PRO	3.0
1	K	404	PHE	3.0
1	M	354	ILE	3.0
1	S	310	LYS	3.0
1	M	37	LEU	3.0
1	A	352	GLU	3.0
1	Q	290	ASN	3.0
1	M	32	THR	3.0
1	Q	414	PHE	3.0
1	G	33	MET	3.0
1	K	39	ASP	3.0
1	C	107	PHE	3.0
1	S	458	ALA	3.0
1	U	315	GLY	3.0
1	A	68	ASP	3.0
1	O	146	HIS	3.0
1	Y	392	PHE	3.0
1	Q	145	TRP	3.0
1	M	75	VAL	2.9
1	C	126	PHE	2.9
1	Q	72	GLN	2.9
1	K	114	LEU	2.9
1	C	73	GLN	2.9
1	I	388	PHE	2.9
1	Y	40	GLU	2.9
1	U	89	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	246	PRO	2.9
1	K	292	ASP	2.9
1	M	440	LYS	2.9
1	A	354	ILE	2.9
1	K	72	GLN	2.9
1	M	309	ILE	2.9
1	A	107	PHE	2.9
1	A	414	PHE	2.9
1	K	414	PHE	2.9
1	Q	63	ARG	2.9
1	Y	317	VAL	2.9
1	S	438	MET	2.9
1	C	145	TRP	2.9
1	O	437	ILE	2.9
1	Q	165	MET	2.9
1	I	246	PRO	2.9
1	S	165	MET	2.9
1	G	307	SER	2.9
1	O	445	ALA	2.9
1	C	110	ASP	2.9
1	G	123	ASP	2.9
1	E	315	GLY	2.9
1	A	47	LEU	2.8
1	Y	296	PRO	2.8
1	S	316	GLY	2.8
1	O	278	PHE	2.8
1	E	67	TYR	2.8
1	U	64	ARG	2.8
1	C	466	GLN	2.8
1	I	412	MET	2.8
1	Q	448	PRO	2.8
1	C	389	PHE	2.8
1	I	389	PHE	2.8
1	Y	406	PRO	2.8
1	Y	448	PRO	2.8
1	Y	66	TYR	2.8
1	C	122	ALA	2.8
1	Y	433	VAL	2.8
1	Y	356	GLY	2.8
1	Q	70	ALA	2.8
1	A	31	THR	2.8
1	I	449	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	O	37	LEU	2.8
1	Y	68	ASP	2.8
1	O	315	GLY	2.8
1	I	429	LEU	2.8
1	W	74	LEU	2.7
1	G	288	LEU	2.7
1	A	404	PHE	2.7
1	E	121	LEU	2.7
1	K	356	GLY	2.7
1	I	124	ASP	2.7
1	U	296	PRO	2.7
1	G	261	LYS	2.7
1	W	412	MET	2.7
1	I	392	PHE	2.7
1	G	163	GLU	2.7
1	S	40	GLU	2.7
1	I	353	THR	2.7
1	I	411	THR	2.7
1	Y	307	SER	2.7
1	C	33	MET	2.7
1	C	34	ILE	2.7
1	Q	307	SER	2.7
1	A	139	ASN	2.7
1	U	34	ILE	2.7
1	W	309	ILE	2.7
1	O	354	ILE	2.7
1	U	436	GLY	2.7
1	C	361	PRO	2.7
1	G	110	ASP	2.7
1	E	395	TYR	2.7
1	E	393	ALA	2.7
1	K	244	ILE	2.7
1	E	452	ASP	2.7
1	I	32	THR	2.7
1	Q	118	VAL	2.7
1	W	120	GLU	2.6
1	O	35	GLN	2.6
1	U	159	ILE	2.6
1	E	289	LYS	2.6
1	Y	290	ASN	2.6
1	G	245	ILE	2.6
1	M	397	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	M	157	TYR	2.6
1	A	65	THR	2.6
1	Q	65	THR	2.6
1	A	46	LEU	2.6
1	A	410	LEU	2.6
1	E	72	GLN	2.6
1	G	29	PRO	2.6
1	K	291	TYR	2.6
1	M	355	GLY	2.6
1	S	39	ASP	2.6
1	U	316	GLY	2.6
1	A	433	VAL	2.6
1	K	293	GLY	2.6
1	Q	157	TYR	2.6
1	Y	309	ILE	2.6
1	M	353	THR	2.6
1	O	113	THR	2.6
1	S	404	PHE	2.6
1	U	32	THR	2.6
1	I	261	LYS	2.6
1	S	308	VAL	2.6
1	O	52	TYR	2.6
1	E	257	LEU	2.6
1	M	68	ASP	2.6
1	C	242	VAL	2.6
1	E	152	GLU	2.6
1	U	356	GLY	2.6
1	M	65	THR	2.6
1	W	151	GLU	2.6
1	I	465	ASN	2.5
1	U	68	ASP	2.5
1	E	305	TYR	2.5
1	O	414	PHE	2.5
1	M	436	GLY	2.5
1	I	312	SER	2.5
1	M	29	PRO	2.5
1	A	110	ASP	2.5
1	Q	122	ALA	2.5
1	M	114	LEU	2.5
1	E	63	ARG	2.5
1	E	388	PHE	2.5
1	G	462	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	M	89	HIS	2.5
1	M	310	LYS	2.5
1	Y	35	GLN	2.5
1	A	321	ARG	2.5
1	E	307	SER	2.5
1	C	148	PHE	2.5
1	Y	352	GLU	2.5
1	G	86	HIS	2.5
1	M	42	ASN	2.5
1	Q	36	LYS	2.5
1	E	256	ASP	2.5
1	Q	48	LYS	2.5
1	Q	114	LEU	2.5
1	U	321	ARG	2.5
1	S	291	TYR	2.5
1	K	317	VAL	2.5
1	M	401	LYS	2.5
1	Y	32	THR	2.5
1	E	437	ILE	2.5
1	W	422	ASP	2.5
1	C	394	GLU	2.5
1	I	396	LEU	2.5
1	Q	315	GLY	2.4
1	E	309	ILE	2.4
1	I	165	MET	2.4
1	Y	409	GLU	2.4
1	S	354	ILE	2.4
1	I	410	LEU	2.4
1	O	240	GLY	2.4
1	I	120	GLU	2.4
1	I	461	GLU	2.4
1	U	391	PHE	2.4
1	G	314	ASP	2.4
1	A	157	TYR	2.4
1	C	53	TYR	2.4
1	Y	157	TYR	2.4
1	W	437	ILE	2.4
1	K	299	PHE	2.4
1	C	422	ASP	2.4
1	I	58	ASP	2.4
1	E	153	GLY	2.4
1	M	66	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	288	LEU	2.4
1	K	242	VAL	2.4
1	Y	399	THR	2.4
1	O	355	GLY	2.4
1	C	297	LYS	2.4
1	A	32	THR	2.4
1	C	300	THR	2.4
1	C	355	GLY	2.4
1	G	402	GLY	2.4
1	E	169	TYR	2.4
1	W	242	VAL	2.4
1	E	261	LYS	2.4
1	Y	244	ILE	2.4
1	S	289	LYS	2.4
1	A	358	ALA	2.4
1	G	392	PHE	2.4
1	W	75	VAL	2.4
1	W	389	PHE	2.4
1	A	81	ASN	2.4
1	O	64	ARG	2.4
1	G	75	VAL	2.4
1	O	117	TYR	2.4
1	S	353	THR	2.4
1	W	438	MET	2.4
1	Q	294	GLU	2.4
1	I	391	PHE	2.4
1	M	361	PRO	2.3
1	G	156	ASP	2.3
1	K	371	ASP	2.3
1	O	389	PHE	2.3
1	Y	437	ILE	2.3
1	A	430	VAL	2.3
1	O	377	ALA	2.3
1	O	457	LEU	2.3
1	Q	121	LEU	2.3
1	W	467	TYR	2.3
1	E	30	ASP	2.3
1	U	389	PHE	2.3
1	G	286	TYR	2.3
1	W	432	GLY	2.3
1	E	278	PHE	2.3
1	Y	278	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	245	ILE	2.3
1	K	66	TYR	2.3
1	G	102	GLY	2.3
1	I	427	GLN	2.3
1	Y	398	ASN	2.3
1	S	320	LEU	2.3
1	W	88	TRP	2.3
1	W	396	LEU	2.3
1	A	437	ILE	2.3
1	K	391	PHE	2.3
1	Y	145	TRP	2.3
1	K	122	ALA	2.3
1	C	128	ASP	2.3
1	K	400	GLY	2.3
1	G	349	ASN	2.2
1	I	163	GLU	2.2
1	K	302	ASN	2.2
1	A	291	TYR	2.2
1	W	39	ASP	2.2
1	Y	355	GLY	2.2
1	C	419	ILE	2.2
1	G	119	ASN	2.2
1	A	147	PRO	2.2
1	M	406	PRO	2.2
1	S	37	LEU	2.2
1	K	438	MET	2.2
1	M	163	GLU	2.2
1	Y	405	ASN	2.2
1	Q	449	PHE	2.2
1	E	312	SER	2.2
1	W	359	THR	2.2
1	I	398	ASN	2.2
1	Y	114	LEU	2.2
1	Y	165	MET	2.2
1	S	352	GLU	2.2
1	G	148	PHE	2.2
1	S	67	TYR	2.2
1	S	359	THR	2.2
1	U	287	VAL	2.2
1	E	255	SER	2.2
1	G	85	SER	2.2
1	Y	389	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	413	THR	2.2
1	M	415	THR	2.2
1	Q	32	THR	2.2
1	C	349	ASN	2.2
1	S	321	ARG	2.2
1	C	403	ASP	2.2
1	E	403	ASP	2.2
1	O	403	ASP	2.2
1	C	281	PHE	2.2
1	S	75	VAL	2.2
1	U	142	ILE	2.2
1	W	283	GLN	2.2
1	E	29	PRO	2.2
1	C	30	ASP	2.2
1	O	39	ASP	2.2
1	Q	155	PHE	2.2
1	M	166	ILE	2.2
1	C	343	SER	2.2
1	G	109	SER	2.2
1	I	108	THR	2.2
1	I	400	GLY	2.2
1	Y	41	HIS	2.2
1	W	433	VAL	2.2
1	G	467	TYR	2.2
1	W	144	TYR	2.2
1	I	109	SER	2.2
1	K	149	VAL	2.2
1	U	318	ASP	2.2
1	U	144	TYR	2.1
1	A	37	LEU	2.1
1	E	414	PHE	2.1
1	G	35	GLN	2.1
1	G	404	PHE	2.1
1	G	443	ALA	2.1
1	M	466	GLN	2.1
1	K	40	GLU	2.1
1	U	163	GLU	2.1
1	A	165	MET	2.1
1	C	54	MET	2.1
1	K	304	ARG	2.1
1	W	72	GLN	2.1
1	W	115	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	S	357	GLY	2.1
1	A	294	GLU	2.1
1	M	394	GLU	2.1
1	E	86	HIS	2.1
1	C	157	TYR	2.1
1	C	63	ARG	2.1
1	K	113	THR	2.1
1	W	392	PHE	2.1
1	W	56	GLU	2.1
1	W	417	THR	2.1
1	I	126	PHE	2.1
1	O	458	ALA	2.1
1	I	167	VAL	2.1
1	Q	244	ILE	2.1
1	E	459	ARG	2.1
1	S	32	THR	2.1
1	Y	117	TYR	2.1
1	Y	297	LYS	2.1
1	Y	403	ASP	2.1
1	A	118	VAL	2.1
1	E	115	LEU	2.1
1	O	256	ASP	2.1
1	S	111	ASN	2.1
1	K	453	PRO	2.1
1	O	449	PHE	2.1
1	W	148	PHE	2.1
1	A	397	ARG	2.1
1	Q	313	GLY	2.1
1	I	287	VAL	2.1
1	K	110	ASP	2.1
1	Q	317	VAL	2.1
1	U	143	GLU	2.1
1	S	405	ASN	2.1
1	U	317	VAL	2.1
1	G	377	ALA	2.1
1	I	421	ASN	2.1
1	C	388	PHE	2.1
1	W	391	PHE	2.1
1	W	240	GLY	2.1
1	Y	412	MET	2.1
1	M	311	VAL	2.1
1	O	167	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	420	GLN	2.1
1	W	354	ILE	2.1
1	E	417	THR	2.1
1	S	295	ASN	2.1
1	Y	422	ASP	2.1
1	M	281	PHE	2.1
1	O	74	LEU	2.1
1	Q	148	PHE	2.1
1	K	163	GLU	2.1
1	I	35	GLN	2.0
1	W	405	ASN	2.0
1	A	432	GLY	2.0
1	Y	294	GLU	2.0
1	Y	29	PRO	2.0
1	E	89	HIS	2.0
1	W	48	LYS	2.0
1	C	465	ASN	2.0
1	I	352	GLU	2.0
1	O	67	TYR	2.0
1	M	296	PRO	2.0
1	C	109	SER	2.0
1	O	405	ASN	2.0
1	E	321	ARG	2.0
1	K	165	MET	2.0
1	S	430	VAL	2.0
1	S	451	GLN	2.0
1	E	357	GLY	2.0
1	A	399	THR	2.0
1	E	349	ASN	2.0
1	W	401	LYS	2.0
1	C	147	PRO	2.0
1	U	466	GLN	2.0
1	C	402	GLY	2.0
1	G	408	LYS	2.0
1	I	118	VAL	2.0
1	S	305	TYR	2.0
1	W	68	ASP	2.0
1	M	250	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	HG	E	701	1/1	0.95	0.28	-0.63	140,140,140,140	1
3	HG	C	701	1/1	0.87	0.20	-1.15	140,140,140,140	1
3	HG	U	701	1/1	0.96	0.10	-1.21	140,140,140,140	1
3	HG	Y	701	1/1	0.95	0.13	-1.26	140,140,140,140	1
3	HG	G	701	1/1	0.96	0.11	-1.95	140,140,140,140	1
3	HG	A	701	1/1	0.93	0.16	-2.04	140,140,140,140	1
3	HG	I	701	1/1	0.87	0.11	-2.13	140,140,140,140	1
3	HG	Q	701	1/1	0.88	0.12	-2.48	140,140,140,140	1
3	HG	W	701	1/1	0.95	0.09	-2.53	140,140,140,140	1
3	HG	O	701	1/1	0.73	0.14	-2.94	140,140,140,140	1
3	HG	S	701	1/1	0.71	0.13	-2.98	140,140,140,140	1
3	HG	M	701	1/1	0.82	0.14	-3.46	140,140,140,140	1
3	HG	K	701	1/1	0.96	0.09	-3.73	140,140,140,140	1
4	CA	I	801	1/1	0.94	0.05	-	140,140,140,140	0
4	CA	U	801	1/1	0.91	0.07	-	140,140,140,140	0
4	CA	O	801	1/1	0.73	0.11	-	140,140,140,140	0
4	CA	A	801	1/1	0.79	0.09	-	140,140,140,140	0
4	CA	Y	801	1/1	0.92	0.06	-	140,140,140,140	0
4	CA	K	801	1/1	0.90	0.13	-	140,140,140,140	0
4	CA	C	801	1/1	0.88	0.08	-	140,140,140,140	0
4	CA	M	801	1/1	0.83	0.15	-	140,140,140,140	0
4	CA	W	801	1/1	0.92	0.17	-	140,140,140,140	0
4	CA	Q	801	1/1	0.95	0.08	-	140,140,140,140	0
4	CA	S	801	1/1	0.87	0.13	-	140,140,140,140	0
4	CA	E	801	1/1	0.97	0.07	-	140,140,140,140	0
4	CA	G	801	1/1	0.95	0.12	-	140,140,140,140	0

6.5 Other polymers [i](#)

There are no such residues in this entry.