



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:17 PM UTC

PDB ID : 2JES / pdb_00002jes
Title : Portal protein (gp6) 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

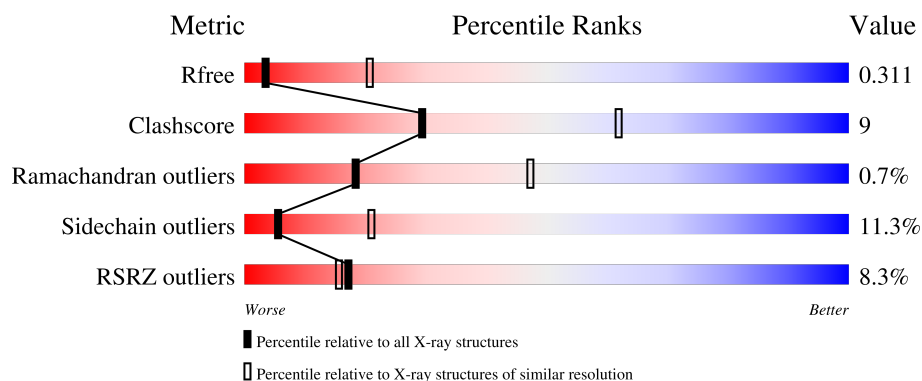
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
1	C	503	
1	E	503	
1	G	503	
1	I	503	

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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 (CCD ID: HG) (formula: Hg).

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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

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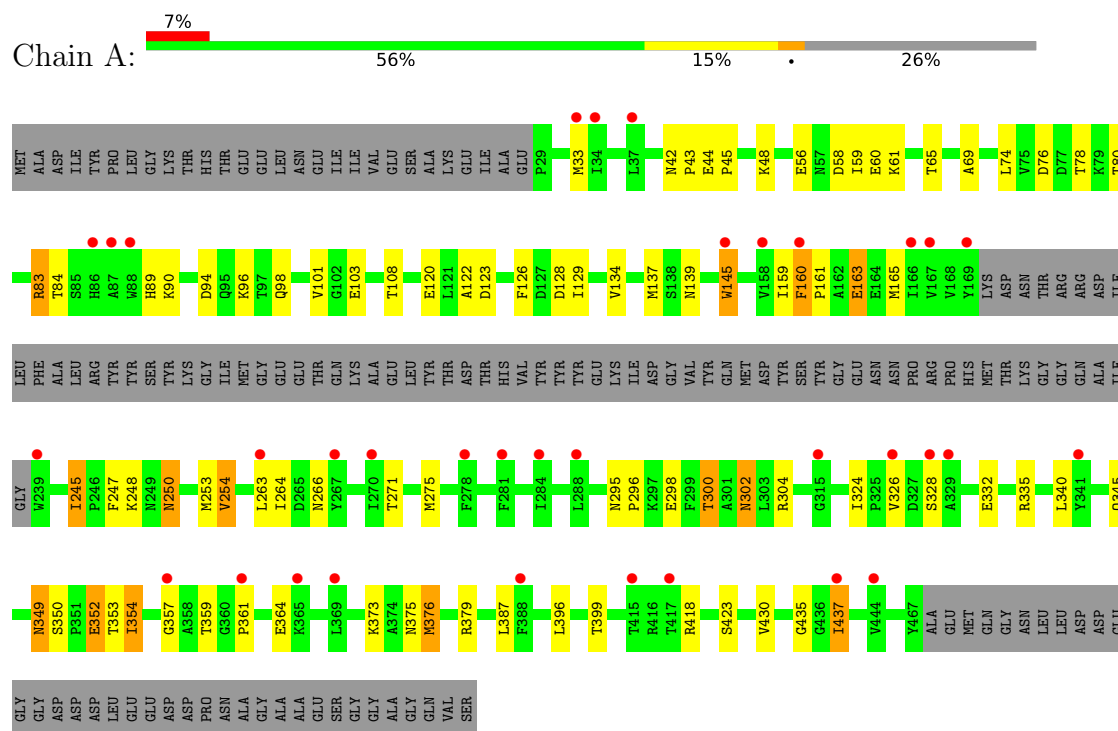
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	O	1	Total 1	Ca 1	0	0
4	Q	1	Total 1	Ca 1	0	0
4	S	1	Total 1	Ca 1	0	0
4	U	1	Total 1	Ca 1	0	0
4	W	1	Total 1	Ca 1	0	0
4	Y	1	Total 1	Ca 1	0	0

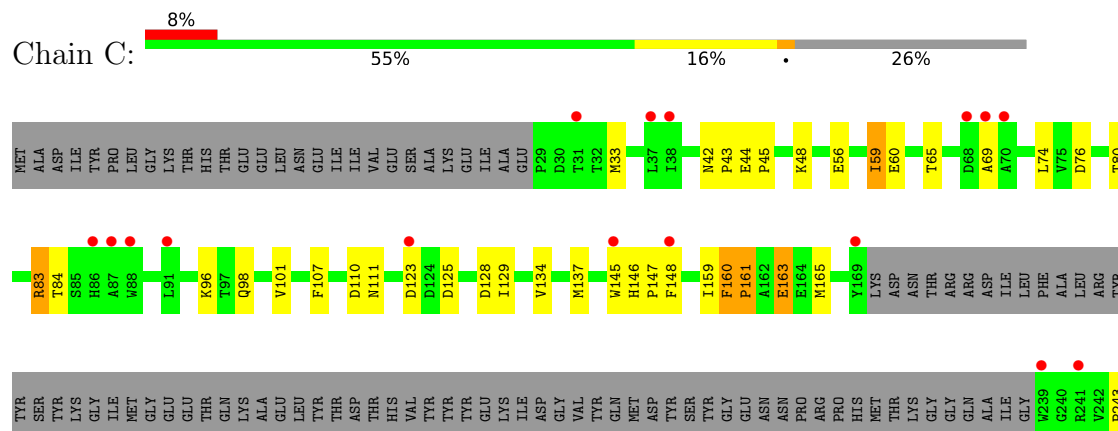
3 Residue-property plots [i](#)

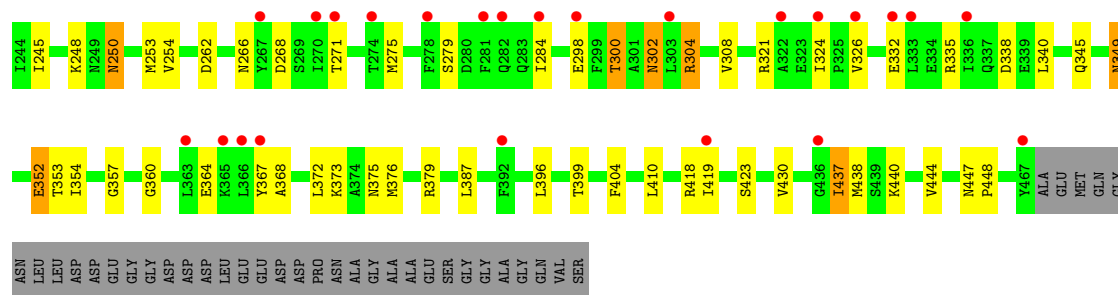
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: PORTAL PROTEIN

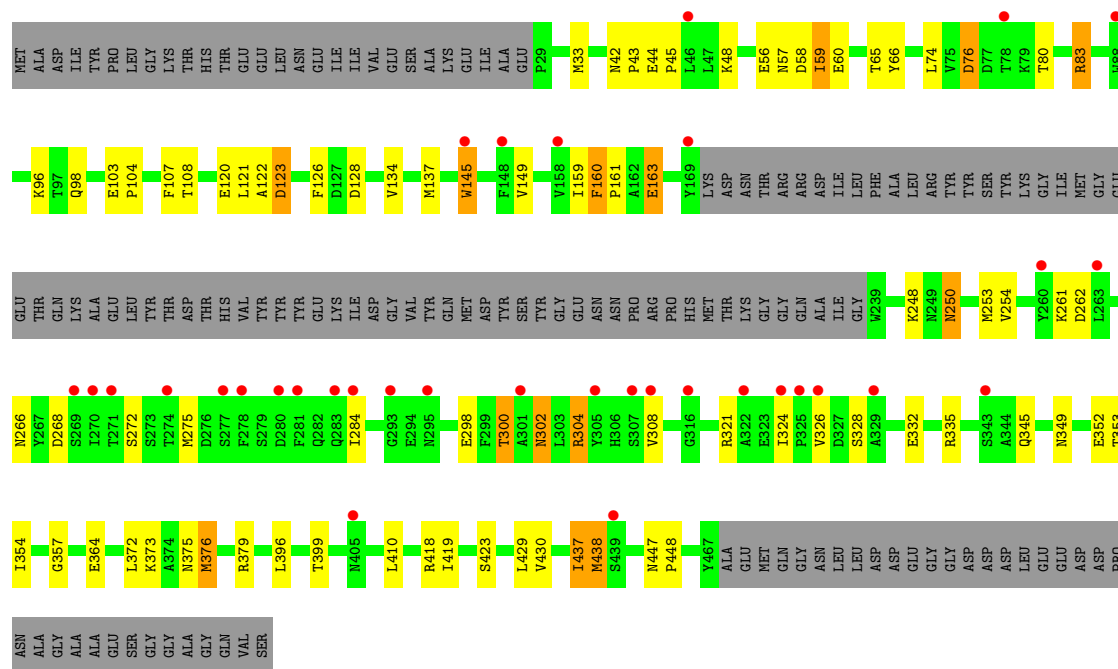


• Molecule 1: PORTAL PROTEIN

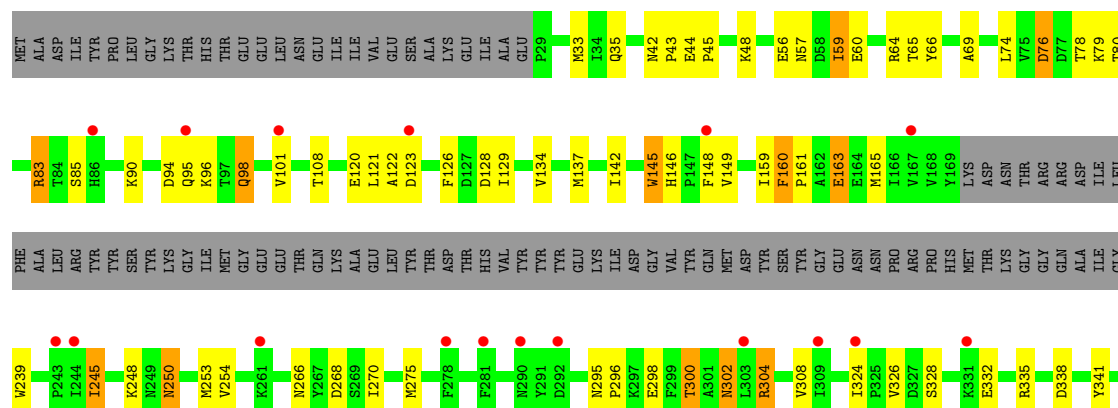


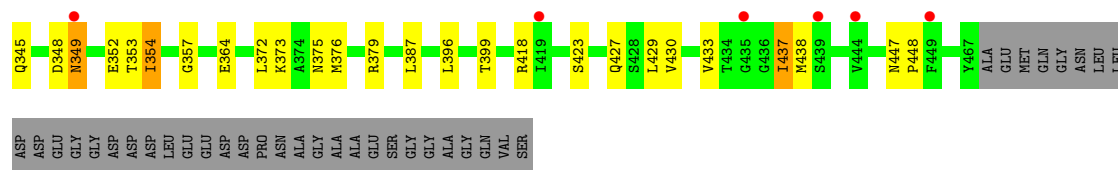


- Molecule 1: PORTAL PROTEIN

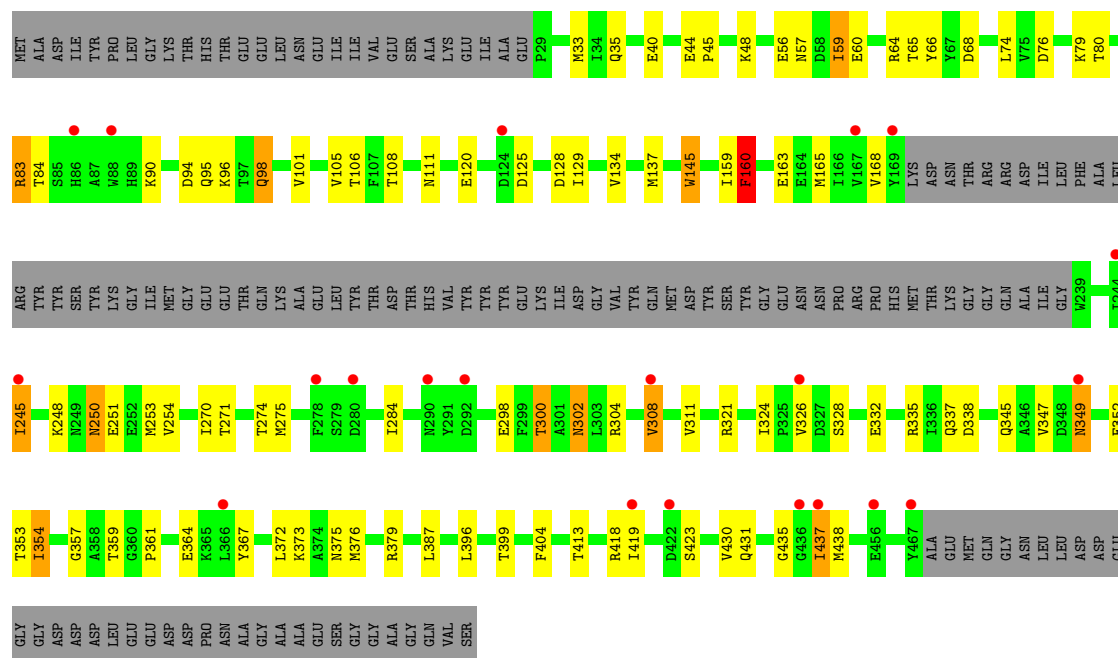


- Molecule 1: PORTAL PROTEIN

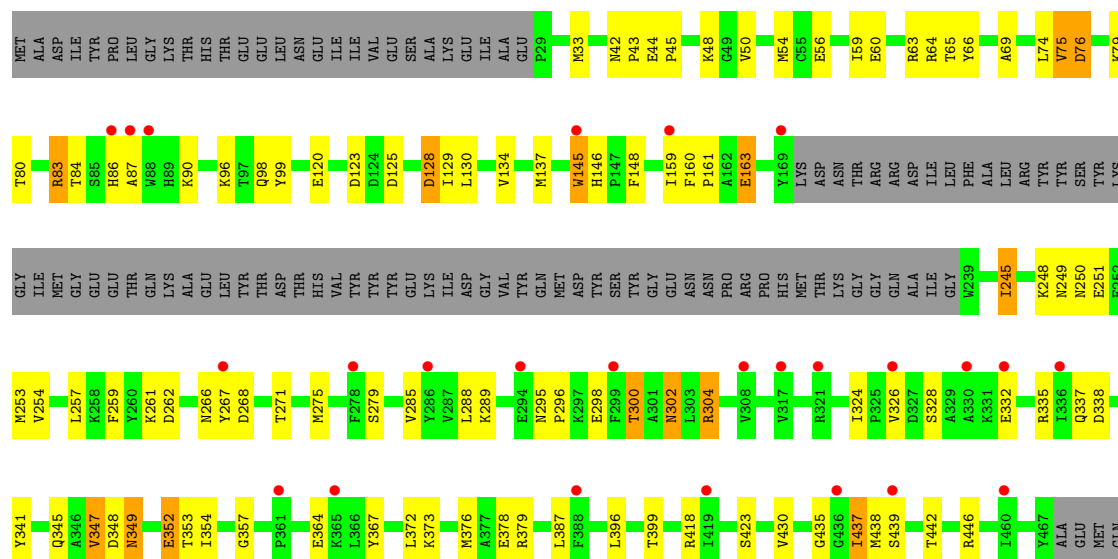




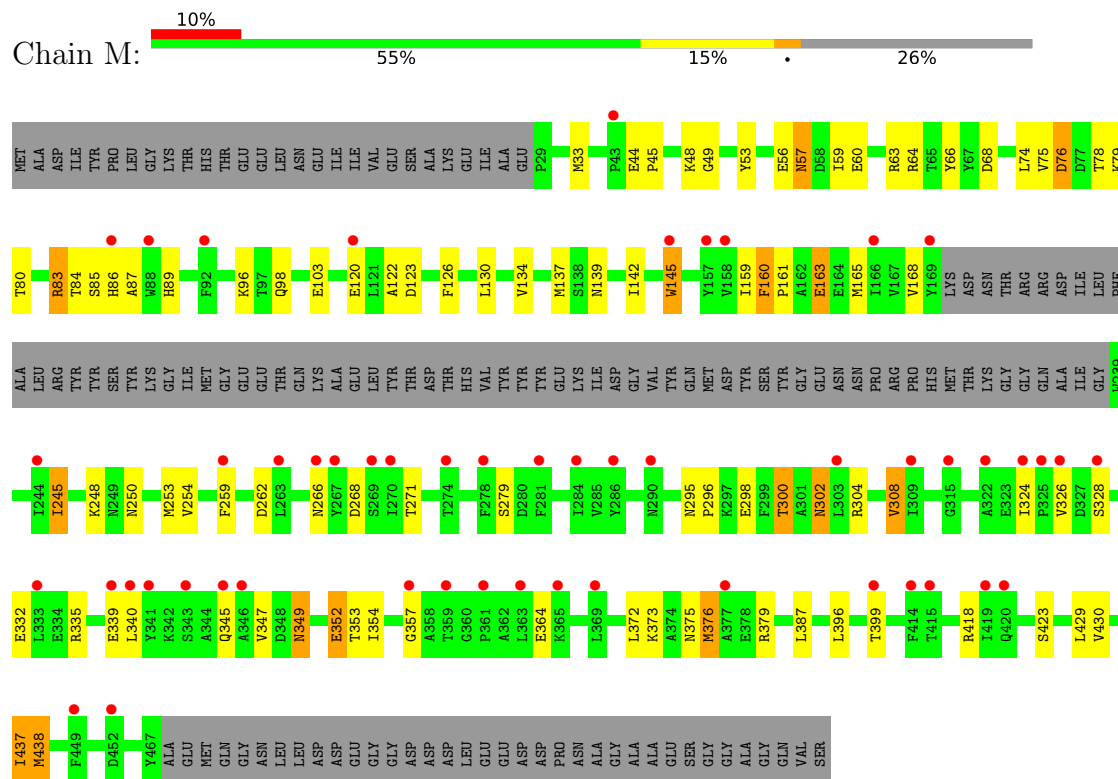
• Molecule 1: PORTAL PROTEIN



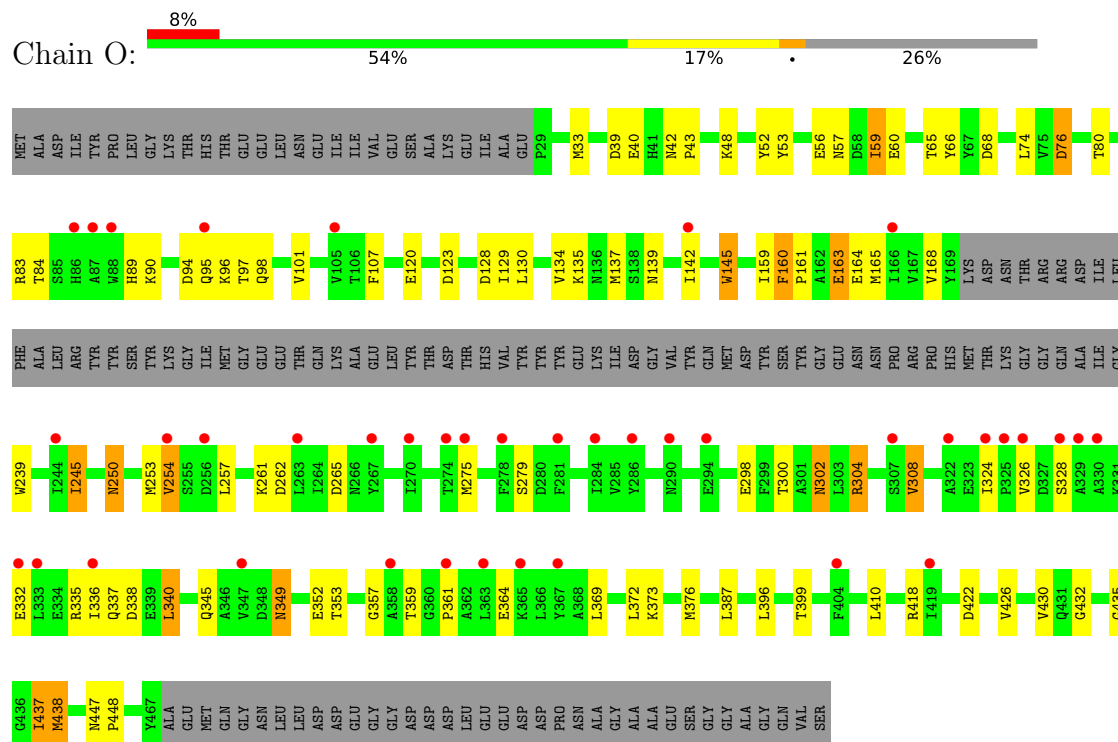
• Molecule 1: PORTAL PROTEIN



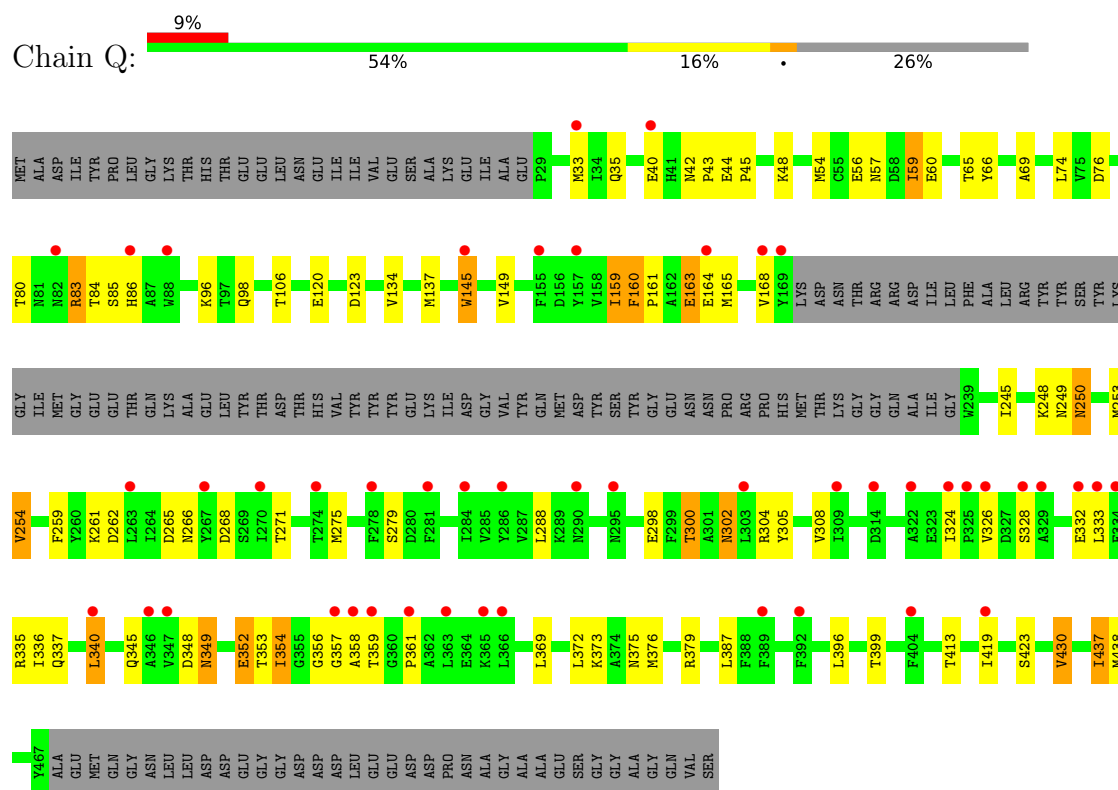
- Molecule 1: PORTAL PROTEIN



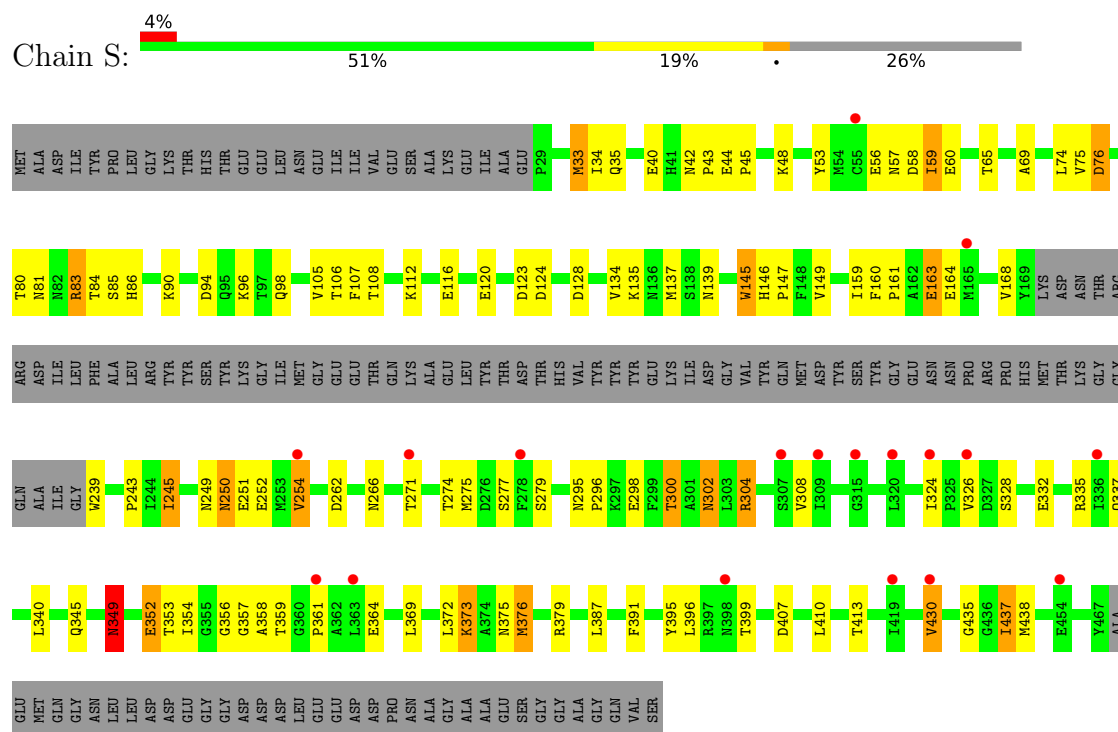
- Molecule 1: PORTAL PROTEIN



- Molecule 1: PORTAL PROTEIN

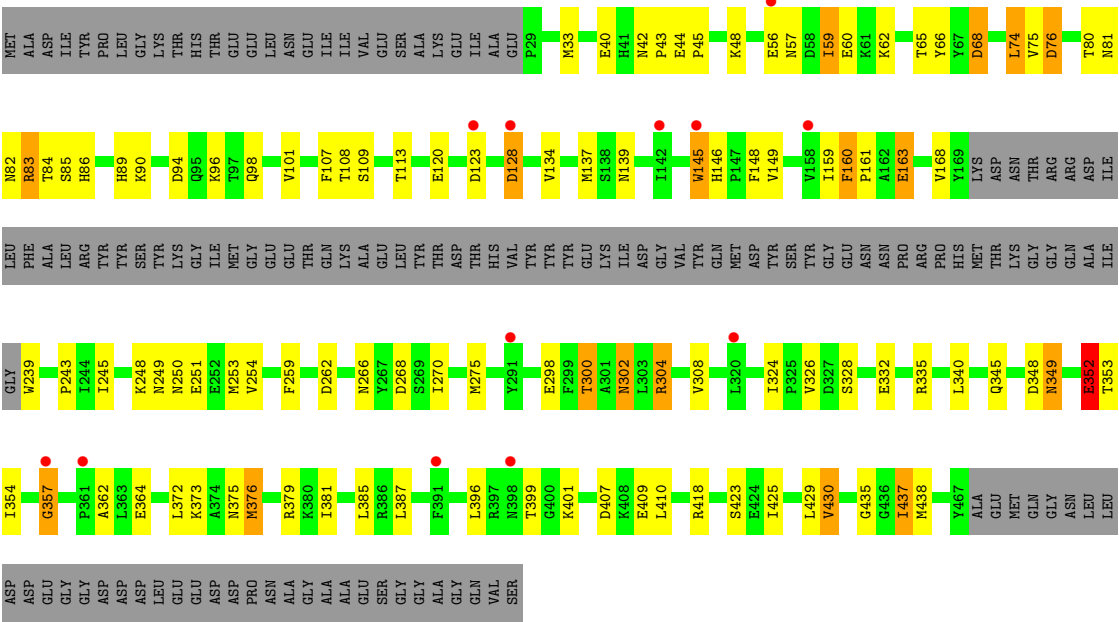


• Molecule 1: PORTAL PROTEIN

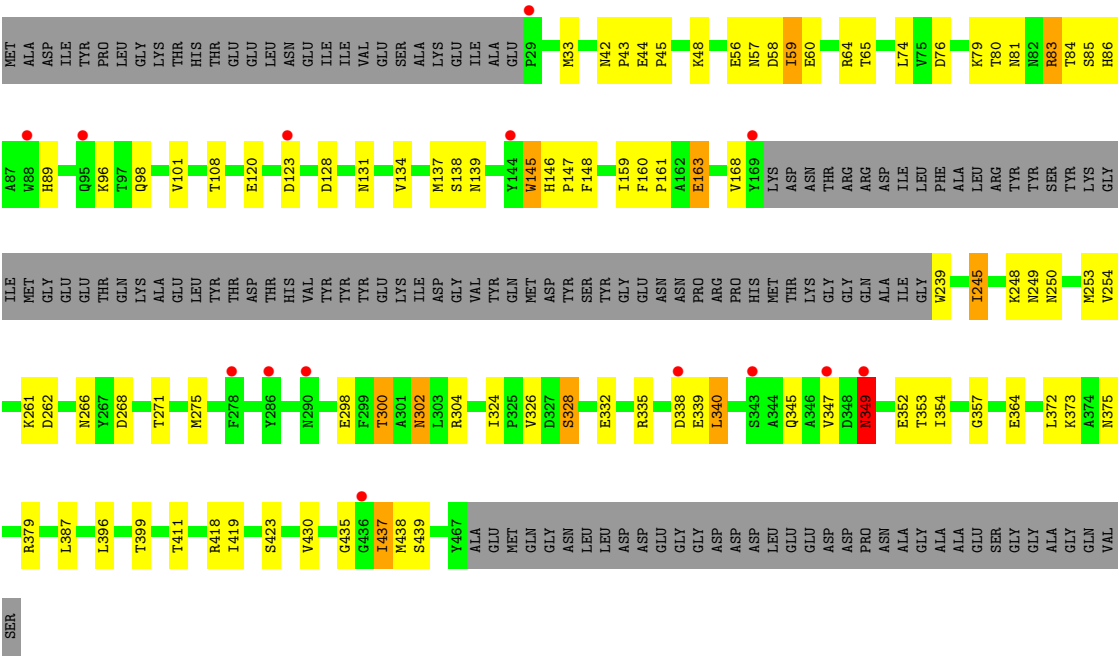


• Molecule 1: PORTAL PROTEIN

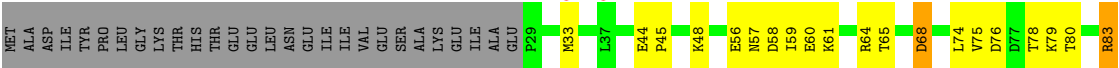


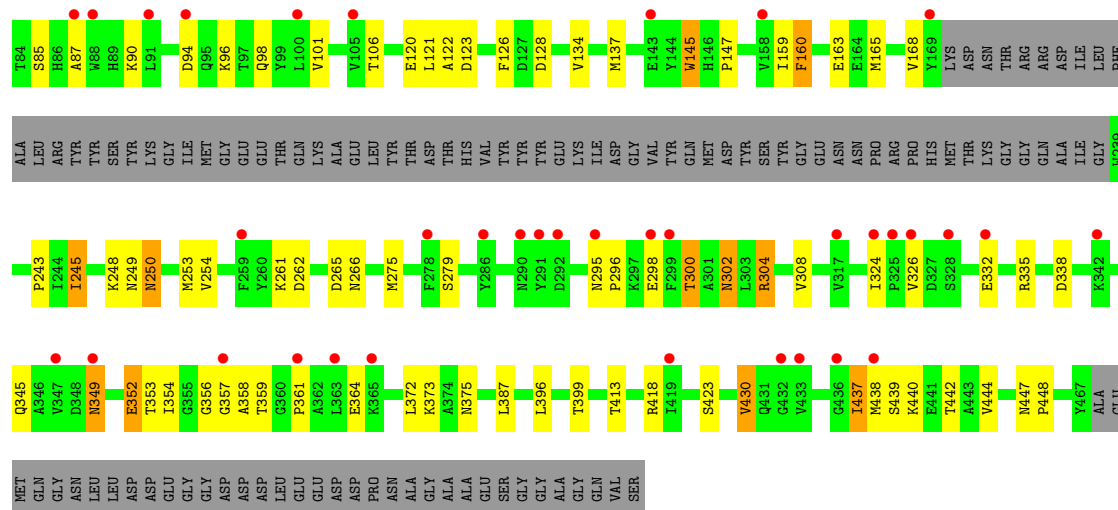


• Molecule 1: PORTAL PROTEIN



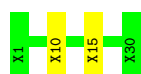
• Molecule 1: PORTAL PROTEIN





● Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN

Chain B: 93% 7%



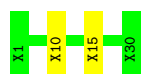
● Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN

Chain D: 93% 7%



● Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN

Chain F: 93% 7%



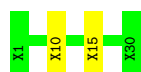
● Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN

Chain H: 93% 7%



● Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN

Chain J: 93% 7%

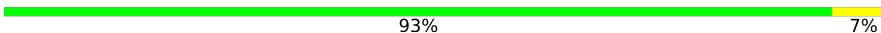


- Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN

Chain L:  93% 7%



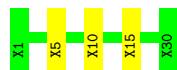
- Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN

Chain N:  93% 7%



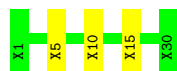
- Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN

Chain P:  90% 10%

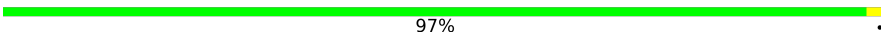


- Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN

Chain R:  90% 10%

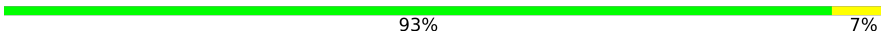


- Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN

Chain T:  97% .

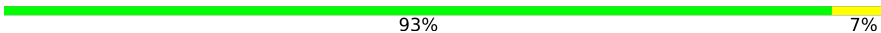


- Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN

Chain V:  93% 7%

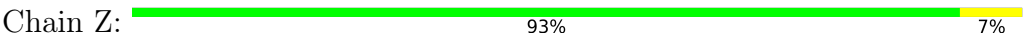


- Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN

Chain X:  93% 7%



- Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	174.31 Å 221.41 Å 421.87 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.81 – 3.40 39.81 – 3.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.81-3.40) 99.5 (39.81-3.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.05 (at 3.40 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.288 , 0.319 0.280 , 0.311	Depositor DCC
R_{free} test set	1121 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å ²)	107.2	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 168.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	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, 0.333 respectively for untwinned datasets, and 0.375, 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: HG, CA

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	0.54	0/2928	0.90	5/3978 (0.1%)
1	C	0.52	0/2928	0.91	3/3978 (0.1%)
1	E	0.54	0/2928	0.90	3/3978 (0.1%)
1	G	0.54	0/2928	0.93	2/3978 (0.1%)
1	I	0.58	0/2928	0.94	4/3978 (0.1%)
1	K	0.59	0/2928	0.94	1/3978 (0.0%)
1	M	0.58	0/2928	0.94	4/3978 (0.1%)
1	O	0.58	0/2928	0.94	3/3978 (0.1%)
1	Q	0.64	0/2928	0.97	2/3978 (0.1%)
1	S	0.72	0/2928	1.02	7/3978 (0.2%)
1	U	0.71	1/2928 (0.0%)	1.00	3/3978 (0.1%)
1	W	0.61	0/2928	0.96	2/3978 (0.1%)
1	Y	0.58	0/2928	0.93	2/3978 (0.1%)
All	All	0.60	1/38064 (0.0%)	0.95	41/51714 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	U	401	LYS	C-O	5.45	1.31	1.24

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	245	ILE	N-CA-C	6.21	114.25	107.60
1	W	245	ILE	N-CA-C	6.18	114.21	107.60
1	Y	245	ILE	N-CA-C	6.07	114.10	107.60
1	I	160	PHE	CA-C-N	6.00	127.33	119.84
1	I	160	PHE	C-N-CA	6.00	127.33	119.84
1	Q	86	HIS	N-CA-C	5.97	120.00	109.96
1	O	76	ASP	N-CA-C	5.82	118.21	108.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	349	ASN	N-CA-C	5.76	119.38	112.93
1	C	308	VAL	N-CA-C	5.72	117.24	108.71
1	S	308	VAL	N-CA-C	5.69	117.52	108.87
1	E	308	VAL	N-CA-C	5.69	117.19	108.71
1	U	308	VAL	N-CA-C	5.61	117.07	108.71
1	A	245	ILE	N-CA-C	5.47	113.46	107.60
1	S	86	HIS	N-CA-C	5.47	118.46	109.76
1	Y	308	VAL	N-CA-C	5.47	117.18	108.87
1	M	103	GLU	CA-C-N	5.46	125.39	119.76
1	M	103	GLU	C-N-CA	5.46	125.39	119.76
1	O	245	ILE	N-CA-C	5.40	113.37	107.60
1	U	352	GLU	N-CA-C	5.39	116.92	109.15
1	A	350	SER	CA-C-N	-5.37	114.19	119.99
1	A	350	SER	C-N-CA	-5.37	114.19	119.99
1	G	245	ILE	N-CA-C	5.35	113.33	107.60
1	I	308	VAL	N-CA-C	5.35	117.26	108.97
1	K	245	ILE	N-CA-C	5.34	113.32	107.60
1	Q	308	VAL	N-CA-C	5.32	116.64	108.71
1	G	308	VAL	N-CA-C	5.30	117.50	109.12
1	A	103	GLU	CA-C-N	5.23	125.14	119.76
1	A	103	GLU	C-N-CA	5.23	125.14	119.76
1	C	360	GLY	CA-C-N	5.21	124.83	119.05
1	C	360	GLY	C-N-CA	5.21	124.83	119.05
1	S	352	GLU	N-CA-C	5.17	116.69	108.67
1	S	251	GLU	N-CA-C	-5.16	104.61	112.04
1	S	76	ASP	N-CA-C	5.12	116.75	108.41
1	I	245	ILE	N-CA-C	5.10	113.06	107.60
1	U	401	LYS	CA-C-O	5.09	125.38	119.32
1	W	349	ASN	N-CA-C	5.07	118.30	112.57
1	M	308	VAL	N-CA-C	5.05	116.23	108.71
1	E	160	PHE	CA-C-N	5.04	126.14	119.84
1	E	160	PHE	C-N-CA	5.04	126.14	119.84
1	M	245	ILE	N-CA-C	5.01	112.96	107.60
1	O	308	VAL	N-CA-C	5.00	116.48	108.87

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
1	C	2868	0	2686	53	1
1	E	2868	0	2686	47	0
1	G	2868	0	2686	62	0
1	I	2868	0	2686	64	0
1	K	2868	0	2686	62	0
1	M	2868	0	2686	54	0
1	O	2868	0	2685	57	1
1	Q	2868	0	2685	58	0
1	S	2868	0	2686	73	0
1	U	2868	0	2686	75	0
1	W	2868	0	2686	60	0
1	Y	2868	0	2686	52	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	1	0	0	0	0
4	G	1	0	0	0	0
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	641	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 9.

All (641) 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:A:275:MET:HE3	1:C:266:ASN:HB3	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:Q:275:MET:HE3	1:S:266:ASN:HB3	1.54	0.89
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:248:LYS:HD3	1:U:253:MET:HE2	1.57	0.83
1:E:275:MET:HE1	1:G:270:ILE:HD11	1.60	0.82
1:W:248:LYS:HD3	1:W:253:MET:HE2	1.61	0.82
1:W:275:MET:HE3	1:Y:266:ASN:HB3	1.61	0.82
1:Q:298:GLU:O	1:Q:302:ASN:HB2	1.79	0.82
1:E:134:VAL:HA	1:E:137:MET:HE3	1.59	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
1:A:134:VAL:HA	1:A:137:MET:HE3	1.64	0.79
1:C:134:VAL:HA	1:C:137:MET:HE3	1.63	0.79
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:O:332:GLU:CD	1:O:335:ARG:HH21	1.91	0.78
1:U:134:VAL:HA	1:U:137:MET:HE3	1.64	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:W:134:VAL:HA	1:W:137:MET:HE3	1.64	0.76
1:A:332:GLU:CD	1:A:335:ARG:HH21	1.94	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:A:248:LYS:HD3	1:A:253:MET:HE2	1.68	0.75
1:W:298:GLU:O	1:W:302:ASN:HB2	1.85	0.75
1:K:275:MET:HE3	1:M:266:ASN:HB3	1.68	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:A:430:VAL:HG23	1:C:437:ILE:HD11	1.70	0.73
1:K:134:VAL:HA	1:K:137:MET:HE3	1.70	0.73
1:S:134:VAL:HA	1:S:137:MET:HE3	1.70	0.73
1:Y:134:VAL:HA	1:Y:137:MET:HE3	1.70	0.72
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:I:430:VAL:HG23	1:K:437:ILE:HD11	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:S:332:GLU:CD	1:S:335:ARG:HH21	1.99	0.71
1:O:245:ILE:HG23	1:O:387:LEU:HD23	1.73	0.70
1:U:430:VAL:HG23	1:W:437:ILE:HD11	1.73	0.70
1:E:248:LYS:HD3	1:E:253:MET:HE2	1.72	0.70
1:M:134:VAL:HA	1:M:137:MET:HE3	1.73	0.70
1:I:134:VAL:HA	1:I:137:MET:HE3	1.74	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:U:275:MET:HE3	1:W:266:ASN:HB3	1.74	0.69
1:E:275:MET:HE1	1:G:270:ILE:CD1	2.22	0.69
1:E:44:GLU:HG3	1:E:45:PRO:HD3	1.73	0.69
1:W:332:GLU:CD	1:W:335:ARG:HH21	2.00	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:I:332:GLU:CD	1:I:335:ARG:HH21	2.00	0.68
1:S:275:MET:HE3	1:U:266:ASN:HB3	1.75	0.68
1:Y:396:LEU:HA	1:Y:399:THR:HG22	1.76	0.68
1:C:248:LYS:HD3	1:C:253:MET:HE2	1.75	0.68
1:W:304:ARG:HH21	1:Y:76:ASP:HB2	1.59	0.68
1:Y:248:LYS:HD3	1:Y:253:MET:HE2	1.76	0.67
1:Y:332:GLU:CD	1:Y:335:ARG:HH21	2.02	0.67
1:G:298:GLU:O	1:G:302:ASN:HB2	1.95	0.66
1:A:98:GLN:OE1	1:C:375:ASN:ND2	2.27	0.66
1:E:298:GLU:O	1:E:302:ASN:HB2	1.95	0.66
1:M:332:GLU:CD	1:M:335:ARG:HH21	2.03	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
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:G:332:GLU:CD	1:G:335:ARG:HH21	2.05	0.65
1:S:44:GLU:HG3	1:S:45:PRO:HD3	1.78	0.65
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:U:332:GLU:CD	1:U:335:ARG:HH21	2.05	0.64
1:G:134:VAL:HA	1:G:137:MET:HE3	1.80	0.64
1:M:248:LYS:HD3	1:M:253:MET:HE2	1.80	0.64
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:134:VAL:HA	1:O:137:MET:HE3	1.79	0.63
1:Y:250:ASN:ND2	1:Y:254:VAL:O	2.29	0.63
1:U:304:ARG:HH21	1:W:76:ASP:HB2	1.64	0.63
1:E:275:MET:CE	1:G:270:ILE:HD11	2.29	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:Q:332:GLU:CD	1:Q:335:ARG:HH21	2.08	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:S:245:ILE:HG23	1:S:387:LEU:HD23	1.81	0.61
1:A:266:ASN:HB3	1:Y:275:MET:HE3	1.80	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:G:248:LYS:HD3	1:G:253:MET:HE2	1.82	0.61
1:S:60:GLU:HA	1:S:83:ARG:HG3	1.82	0.61
1:C:44:GLU:HG3	1:C:45:PRO:HD3	1.83	0.61
1:W:60:GLU:HA	1:W:83:ARG:HG3	1.81	0.61
1:Q:248:LYS:HD3	1:Q:253:MET:HE2	1.83	0.61
1:U:349:ASN:ND2	1:U:349:ASN:H	1.99	0.61
1:A:90:LYS:NZ	1:A:94:ASP:OD1	2.34	0.60
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:K:396:LEU:HA	1:K:399:THR:HG22	1.81	0.60
1:C:275:MET:HE3	1:E:266:ASN:HB3	1.83	0.60
1:M:60:GLU:HA	1:M:83:ARG:HG3	1.84	0.60
1:S:300:THR:O	1:S:304:ARG:HB2	2.01	0.60
1:U:109:SER:HB2	1:U:409:GLU:O	2.02	0.59
1:Y:245:ILE:HG23	1:Y:387:LEU:HD23	1.83	0.59
1:A:364:GLU:HG3	1:A:418:ARG:NH2	2.18	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:C:332:GLU:CD	1:C:335:ARG:HH21	2.10	0.59
1:Q:275:MET:CE	1:S:266:ASN:HB3	2.31	0.59
1:I:275:MET:HE3	1:K:266:ASN: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:GLU:HA	1:C:83:ARG:HG3	1.85	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:E:430:VAL:CG2	1:G:437:ILE:HD11	2.34	0.57
1:Q:300:THR:O	1:Q:304:ARG:HB2	2.04	0.57
1:W:275:MET:CE	1:Y:266:ASN:HB3	2.33	0.57
1:U:352:GLU:OE2	1:U:354:ILE:HG12	2.04	0.57
1:A:76:ASP:HB2	1:Y:304:ARG:HH21	1.69	0.57
1:Q:349:ASN:H	1:Q:349:ASN:ND2	2.02	0.57
1:Q:430:VAL:CG2	1:S:437:ILE:HD11	2.32	0.57
1:U:161:PRO:HB3	1:U:163:GLU:OE2	2.04	0.57
1:I:396:LEU:HA	1:I:399:THR:HG22	1.86	0.57
1:Q:60:GLU:HA	1:Q:83:ARG:HG3	1.85	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:K:332:GLU:CD	1:K:335:ARG:HH21	2.13	0.57
1:A:250:ASN:ND2	1:A:254:VAL:O	2.36	0.56
1:I:248:LYS:HD3	1:I:253:MET:HE2	1.86	0.56
1:O:349:ASN:H	1:O:349:ASN:ND2	2.01	0.56
1:Q:134:VAL:HA	1:Q:137:MET:HE3	1.87	0.56
1:Q:161:PRO:HB3	1:Q:163:GLU:OE2	2.05	0.56
1:Q:304:ARG:HH21	1:S:76:ASP:HB2	1.71	0.56
1:U:250:ASN:ND2	1:U:254:VAL:O	2.37	0.56
1:O:101:VAL:O	1:O:101:VAL:HG12	2.06	0.56
1:U:300:THR:O	1:U:304:ARG:HB2	2.05	0.56
1:I:324:ILE:HG22	1:I:326:VAL:HG23	1.87	0.56
1:O:324:ILE:HG22	1:O:326:VAL:HG23	1.86	0.56
1:U:98:GLN:OE1	1:W:375:ASN:ND2	2.39	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:C:364:GLU:HG3	1:C:418:ARG:NH2	2.21	0.55
1:U:134:VAL:HG22	1:U:381:ILE:HD11	1.87	0.55
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:G:161:PRO:HB3	1:G:163:GLU:OE2	2.06	0.55
1:U:86:HIS:HD2	1:U:268:ASP:OD2	1.90	0.55
1:E:98:GLN:HG2	1:G:372:LEU:HD12	1.88	0.55
1:O:430:VAL:CG2	1:Q:437:ILE:HD11	2.36	0.55
1:Y:60:GLU:HA	1:Y:83:ARG:HG3	1.88	0.55
1:K:275:MET:CE	1:M:266:ASN:HB3	2.36	0.55
1:Q:59:ILE:HD12	1:Q:268:ASP:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:101:VAL:HG21	1:G:134:VAL:HG21	1.89	0.54
1:G:245:ILE:HG23	1:G:387:LEU:HD23	1.89	0.54
1:C:300:THR:O	1:C:304:ARG:HB2	2.06	0.54
1:U:107:PHE:HB3	1:U:410:LEU:HD11	1.89	0.54
1:A:275:MET:CE	1:C:266:ASN:HB3	2.32	0.54
1:M:396:LEU:HA	1:M:399:THR:HG22	1.88	0.54
1:S:98:GLN:HG2	1:U:372:LEU:HD12	1.89	0.54
1:I:245:ILE:HG23	1:I:387:LEU:HD23	1.88	0.54
1:O:98:GLN:OE1	1:Q:375:ASN:ND2	2.41	0.54
1:C:98:GLN:HG2	1:E:372:LEU:HD12	1.90	0.54
1:C:304:ARG:HH21	1:E:76:ASP:HB2	1.73	0.54
1:E:332:GLU:CD	1:E:335:ARG:HH21	2.15	0.54
1:O:90:LYS:HD3	1:Q:259:PHE:CD2	2.42	0.54
1:U:90:LYS:NZ	1:U:94:ASP:OD1	2.41	0.54
1:A:359:THR:HB	1:A:361:PRO:HD2	1.90	0.54
1:S:275:MET:HE1	1:U:270:ILE:CD1	2.37	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:A:60:GLU:HA	1:A:83:ARG:HG3	1.90	0.53
1:I:376:MET:HG3	1:I:379:ARG:HH21	1.72	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:C:161:PRO:HB3	1:C:163:GLU:OE2	2.08	0.53
1:G:145:TRP:HB2	1:G:159:ILE:HA	1.90	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
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:G:98:GLN:OE1	1:I:375:ASN:ND2	2.42	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: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
1:G:275:MET:HE1	1:I:270:ILE:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:10:UNK:HA	2:L:15:UNK:HA	1.92	0.52
1:S:35:GLN:HA	1:S:35:GLN:OE1	2.07	0.52
1:O:396:LEU:HA	1:O:399:THR:HG22	1.90	0.52
1:I:352:GLU:OE2	1:I:354:ILE:HG12	2.09	0.52
1:K:300:THR:O	1:K:304:ARG:HB2	2.09	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:A:76:ASP:OD2	1:A:78:THR:HB	2.10	0.51
1:E:275:MET:HE3	1:G:266:ASN:HB3	1.92	0.51
1:C:160:PHE:HD2	1:C:165:MET:SD	2.34	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:A:275:MET:HE3	1:C:266:ASN:CB	2.32	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: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:M:430:VAL:HG22	1:O:435:GLY:HA3	1.92	0.51
1:U:275:MET:HE3	1:W:266:ASN:CB	2.41	0.51
1:A:300:THR:O	1:A:304:ARG:HB2	2.09	0.51
1:G:275:MET:HE1	1:I:270:ILE:CD1	2.40	0.51
1:M:122:ALA:HB1	1:M:126:PHE:CD2	2.45	0.51
1:Q:275:MET:HE3	1:S:266:ASN:CB	2.33	0.51
1:Y:122:ALA:HB1	1:Y:126:PHE:CD2	2.46	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:W:57:ASN:C	1:W:59:ILE:N	2.68	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:O:52:TYR:OH	1:O:265:ASP:OD1	2.23	0.50
1:U:60:GLU:HA	1:U:83:ARG:HG3	1.94	0.50
1:U:275:MET:CE	1:W:266:ASN:HB3	2.40	0.50
1:I:349:ASN:ND2	1:I:349:ASN:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:Y:349:ASN:ND2	2.09	0.50
1:I:376:MET:HG3	1:I:379:ARG:NH2	2.27	0.50
1:U:81:ASN:HD21	1:U:83:ARG:HD2	1.77	0.50
1:Q:324:ILE:HG22	1:Q:326:VAL:HG23	1.93	0.50
1:W:57:ASN:O	1:W:59:ILE:N	2.45	0.50
1:C:107:PHE:HB3	1:C:410:LEU:HD11	1.94	0.50
1:Q:250:ASN:ND2	1:Q:254:VAL:HG23	2.27	0.50
1:I:66:TYR:CD2	1:I:76:ASP:HB3	2.47	0.49
1:G:60:GLU:HA	1:G:83:ARG:HG3	1.93	0.49
1:M:89:HIS:NE2	1:M:139:ASN:ND2	2.60	0.49
1:Y:160:PHE:HD2	1:Y:165:MET:SD	2.35	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:Q:430:VAL:HG22	1:S:435:GLY:HA3	1.93	0.49
1:S:57:ASN:C	1:S:59:ILE:N	2.70	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:W:430:VAL:CG2	1:Y:437:ILE:HD11	2.39	0.49
1:I:101:VAL:HG21	1:I:134:VAL:HG21	1.93	0.49
1:I:98:GLN:HG2	1:K:372:LEU:HD12	1.94	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:S:161:PRO:HB3	1:S:163:GLU:OE2	2.12	0.49
1:K:245:ILE:HG23	1:K:387:LEU:HD23	1.94	0.49
1:S:57:ASN:C	1:S:59:ILE:H	2.20	0.49
1:S:124:ASP:O	1:S:128:ASP:OD2	2.31	0.49
1:Y:76:ASP:OD2	1:Y:78:THR:HB	2.13	0.49
1:S:57:ASN:O	1:S:59:ILE:N	2.46	0.48
1:S:96:LYS:HD3	1:S:373:LYS:CD	2.36	0.48
1:K:99:TYR:OH	1:K:418:ARG:HD2	2.13	0.48
1:K:248:LYS:HD3	1:K:253:MET:HE2	1.94	0.48
1:W:57:ASN:C	1:W:59:ILE:H	2.21	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
1:W:396:LEU:HA	1:W:399:THR:HG22	1.95	0.48
1:C:145:TRP:HB2	1:C:159:ILE:HA	1.93	0.48
1:C:245:ILE:HG23	1:C:387:LEU:HD23	1.94	0.48
1:E:419:ILE:HG12	1:G:364:GLU:HG2	1.95	0.48
1:E:59:ILE:CD1	1:E:272:SER:OG	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:430:VAL:CG2	1:M:437:ILE:HD11	2.40	0.48
1:C:59:ILE:HD12	1:C:268:ASP:HB3	1.95	0.48
1:W:98:GLN:OE1	1:Y:375:ASN:ND2	2.46	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:U:57:ASN:CG	1:U:85:SER:HB2	2.39	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:W:101:VAL:HG12	1:W:131:ASN:ND2	2.29	0.48
1:U:349:ASN:ND2	1:U:349:ASN:N	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:I:134:VAL:HA	1:I:137:MET:CE	2.42	0.47
1:W:86:HIS:HD2	1:W:268:ASP:OD2	1.97	0.47
1:A:161:PRO:HB3	1:A:163:GLU:OE2	2.14	0.47
1:G:160:PHE:HD2	1:G:165:MET:SD	2.36	0.47
1:S:349:ASN:ND2	1:S:349:ASN:N	2.62	0.47
1:I:349:ASN:H	1:I:349:ASN:HD22	1.63	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:Q:245:ILE:HG23	1:Q:387:LEU:HD23	1.96	0.47
1:W:300:THR:O	1:W:304:ARG:HB2	2.15	0.47
1:G:250:ASN:ND2	1:G:254:VAL:O	2.42	0.47
1:G:341:TYR:CD2	1:G:348:ASP:HB2	2.49	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: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:S:275:MET:CE	1:U:270:ILE:HD11	2.45	0.47
1:Y:137:MET:O	1:Y:249:ASN:HB2	2.14	0.47
1:A:84:THR:HG23	1:C:262:ASP:HB3	1.96	0.47
1:M:76:ASP:OD2	1:M:78:THR:HB	2.15	0.47
1:O:275:MET:HE3	1:Q:266:ASN:HB3	1.96	0.47
1:U:128:ASP:HA	1:W:379:ARG:HD2	1.97	0.47
1:O:107:PHE:HB3	1:O:410:LEU:HD11	1.97	0.47
1:O:308:VAL:HG11	1:Q:288:LEU:HD12	1.96	0.47
1:Q:98:GLN:HG2	1:S:372:LEU:HD12	1.96	0.47
1:K:90:LYS:CD	1:M:259:PHE:CD2	2.98	0.47
2:N:10:UNK:HA	2:N:15:UNK:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:89:HIS:NE2	1:U:139:ASN:ND2	2.63	0.47
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:145:TRP:HD1	1:S:145:TRP:O	1.98	0.46
1:M:364:GLU:HG3	1:M:418:ARG:NH2	2.30	0.46
1:S:57:ASN:HB2	1:S:85:SER:HB2	1.96	0.46
1:S:146:HIS:HD2	1:S:243:PRO:O	1.97	0.46
1:Y:58:ASP:OD1	1:Y:261:LYS:NZ	2.35	0.46
1:I:101:VAL:HG12	1:I:101:VAL:O	2.15	0.46
1:K:257:LEU:O	1:K:261:LYS:HB2	2.15	0.46
1:U:62:LYS:NZ	1:U:82:ASN:O	2.44	0.46
1:E:364:GLU:HG3	1:E:418:ARG:NH2	2.30	0.46
1:G:341:TYR:CE2	1:G:348:ASP:HB2	2.50	0.46
1:W:57:ASN:CG	1:W:85:SER:HB2	2.40	0.46
1:A:160:PHE:HD2	1:A:165:MET:SD	2.39	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:Q:348:ASP:OD1	1:Q:348:ASP:C	2.57	0.46
1:E:284:ILE:HG12	1:E:321:ARG:NH1	2.31	0.46
1:G:76:ASP:OD2	1:G:78:THR:HB	2.16	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:U:332:GLU:OE1	1:U:335:ARG:NH2	2.49	0.46
1:G:352:GLU:OE2	1:G:354:ILE:HG12	2.15	0.46
1:E:59:ILE:HD12	1:E:268:ASP:HB3	1.98	0.46
1:E:352:GLU:OE2	1:E:354:ILE:HG12	2.16	0.46
1:Q:164:GLU:O	2:R:5:UNK:HA	2.16	0.46
1:U:430:VAL:HG22	1:W:435:GLY:HA3	1.98	0.46
1:G:59:ILE:HD12	1:G:268:ASP:HB3	1.97	0.46
1:G:122:ALA:HB1	1:G:126:PHE:CD2	2.51	0.46
1:Q:57:ASN:CG	1:Q:85:SER:HB2	2.41	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:H	1:M:349:ASN:ND2	2.14	0.46
1:M:98:GLN:HG2	1:O:372:LEU:HD12	1.98	0.45
1:O:164:GLU:O	2:P:5:UNK:HA	2.16	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:A:352:GLU:OE2	1:A:354:ILE:HG12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:324:ILE:HG22	1:C:326:VAL:HG23	1.98	0.45
1:U:86:HIS:CD2	1:U:268:ASP:OD2	2.67	0.45
1:W:332:GLU:CD	1:W:335:ARG:NH2	2.73	0.45
1:W:332:GLU:OE1	1:W:335:ARG:NH2	2.49	0.45
1:C:440:LYS:O	1:C:444:VAL:HG23	2.17	0.45
1:E:66:TYR:CD2	1:E:76:ASP:HB3	2.51	0.45
1:E:376:MET:HG3	1:E:379:ARG:HH21	1.82	0.45
1:M:53:TYR:HB2	1:M:139:ASN:ND2	2.31	0.45
1:Q:66:TYR:CD2	1:Q:76:ASP:HB3	2.52	0.45
1:A:42:ASN:HA	1:A:43:PRO:HD3	1.86	0.45
1:E:161:PRO:HB3	1:E:163:GLU:OE2	2.17	0.45
1:K:145:TRP:HD1	1:K:145:TRP:O	2.00	0.45
1:M:64:ARG:NH2	1:M:79:LYS:HD3	2.32	0.45
1:Q:349:ASN:H	1:Q:349:ASN:HD22	1.64	0.45
1:S:106:THR:HB	1:S:413:THR:HB	1.98	0.45
2:D:10:UNK:HA	2:D:15:UNK:HA	1.99	0.45
1:S:84:THR:HG23	1:U:262:ASP:HB3	1.97	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:A:435:GLY:HA3	1:Y:430:VAL:HG22	1.99	0.45
1:C:376:MET:HG3	1:C:379:ARG:HH21	1.82	0.45
1:U:251:GLU:HA	1:U:251:GLU:OE1	2.17	0.45
1:W:146:HIS:HA	1:W:147:PRO:HD3	1.88	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:M:57:ASN:CG	1:M:85:SER:HB2	2.42	0.44
1:W:419:ILE:HG12	1:Y:364:GLU:HG2	1.99	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:G:44:GLU:HG3	1:G:45:PRO:CD	2.35	0.44
1:K:349:ASN:ND2	1:K:349:ASN:H	2.15	0.44
1:O:364:GLU:HG3	1:O:418:ARG:NH2	2.32	0.44
1:S:274:THR:O	1:S:277:SER:HB2	2.17	0.44
1:U:364:GLU:HG3	1:U:418:ARG:NH2	2.32	0.44
1:W:58:ASP:OD1	1:W:261:LYS:NZ	2.44	0.44
1:W:89:HIS:NE2	1:W:139:ASN:ND2	2.66	0.44
1:E:58:ASP:OD1	1:E:261:LYS:NZ	2.49	0.44
2:R:10:UNK:HA	2:R:15:UNK:HA	1.98	0.44
1:U:146:HIS:HD2	1:U:243:PRO:O	2.00	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:I:64:ARG:NH2	1:I:79:LYS:HD3	2.32	0.44
1:O:97:THR:HG23	1:O:134:VAL:HB	2.00	0.44
1:S:57:ASN:CG	1:S:85:SER:HB2	2.42	0.44
1:G:64:ARG:NH2	1:G:79:LYS:HD3	2.32	0.44
2:H:10:UNK:HA	2:H:15:UNK:HA	1.98	0.44
1:K:161:PRO:HB3	1:K:163:GLU:OE2	2.17	0.44
1:M:352:GLU:OE2	1:M:354:ILE:HG12	2.18	0.44
1:C:447:ASN:HA	1:C:448:PRO:HD3	1.87	0.44
1:G:95:GLN:HA	1:I:372:LEU:HD11	2.00	0.44
1:Q:145:TRP:HB2	1:Q:159:ILE:HA	1.99	0.44
1:Q:160:PHE:HD2	1:Q:165:MET:SD	2.40	0.44
1:S:81:ASN:ND2	1:S:83:ARG:HD3	2.33	0.44
1:S:112:LYS:O	1:S:116:GLU:HG3	2.17	0.44
1:G:35:GLN:HA	1:G:35:GLN:OE1	2.18	0.44
1:G:295:ASN:HA	1:G:296:PRO:HD3	1.86	0.44
1:M:49:GLY:HA3	1:M:139:ASN:O	2.17	0.44
1:Q:349:ASN:ND2	1:Q:349:ASN:N	2.65	0.44
1:S:295:ASN:HA	1:S:296:PRO:HD3	1.90	0.44
1:U:326:VAL:CG2	1:W:328:SER:HB3	2.47	0.44
1:W:96:LYS:HE3	1:W:138:SER:OG	2.18	0.44
1:G:42:ASN:HA	1:G:43:PRO:HD3	1.87	0.44
1:G:275:MET:CE	1:I:270:ILE:HD11	2.48	0.44
1:K:125:ASP:O	1:K:129:ILE:HG12	2.18	0.44
1:S:147:PRO:HG2	1:S:391:PHE:CD2	2.53	0.44
1:E:324:ILE:HG22	1:E:326:VAL:HG23	1.99	0.44
1:A:145:TRP:CE2	1:A:247:PHE:HE1	2.36	0.43
1:S:349:ASN:H	1:S:349:ASN:HD22	1.63	0.43
1:S:352:GLU:OE2	1:S:354:ILE:HG12	2.18	0.43
1:U:81:ASN:ND2	1:U:83:ARG:CD	2.81	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
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:C:367:TYR:O	1:C:368:ALA:C	2.61	0.43
1:E:300:THR:O	1:E:304:ARG:HB2	2.17	0.43
1:I:90:LYS:HD3	1:K:259:PHE:CD2	2.53	0.43
1:W:163:GLU:H	1:W:163:GLU:HG3	1.62	0.43
1:A:96:LYS:HD3	1:A:373:LYS:CD	2.40	0.43
1:A:122:ALA:HB1	1:A:126:PHE:CD2	2.53	0.43
1:O:324:ILE:CG2	1:O:326:VAL:HG23	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:59:ILE:HG12	1:G:59:ILE:O	2.18	0.43
1:K:275:MET:HE3	1:M:266:ASN:CB	2.42	0.43
1:Q:42:ASN:HA	1:Q:43:PRO:HD3	1.86	0.43
1:G:66:TYR:CD2	1:G:76:ASP:HB3	2.53	0.43
1:G:427:GLN:HG2	1:I:431:GLN:OE1	2.19	0.43
1:O:42:ASN:HA	1:O:43:PRO:HD3	1.90	0.43
1:O:101:VAL:O	1:O:101:VAL:CG1	2.67	0.43
1:Q:333:LEU:HA	1:Q:333:LEU:HD23	1.82	0.43
1:W:146:HIS:CE1	1:W:148:PHE:HB3	2.54	0.43
1:Y:57:ASN:CG	1:Y:85:SER:HB2	2.44	0.43
1:K:63:ARG:HH11	1:K:75:VAL:HG21	1.83	0.43
1:O:332:GLU:OE1	1:O:335:ARG:NH2	2.51	0.43
1:O:359:THR:HB	1:O:361:PRO:HD2	2.01	0.43
1:U:376:MET:O	1:U:379:ARG:N	2.51	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:K:378:GLU:O	1:K:379:ARG:C	2.62	0.43
1:W:339:GLU:O	1:W:340:LEU:C	2.62	0.43
1:G:57:ASN:CG	1:G:85:SER:HB2	2.44	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:U:101:VAL:O	1:U:101:VAL:CG1	2.67	0.43
1:A:324:ILE:HG22	1:A:326:VAL:HG23	2.01	0.42
1:I:57:ASN:C	1:I:59:ILE:H	2.27	0.42
1:I:60:GLU:HA	1:I:83:ARG:HG3	2.01	0.42
1:K:98:GLN:HG2	1:M:372:LEU:HD12	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:Q:304:ARG:NH1	1:Q:305:TYR:CE1	2.87	0.42
1:U:160:PHE:O	1:U:161:PRO:C	2.62	0.42
1:A:349:ASN:ND2	1:A:349:ASN:H	2.18	0.42
1:C:125:ASP:O	1:C:129:ILE:HG12	2.19	0.42
1:E:98:GLN:OE1	1:G:375:ASN:ND2	2.53	0.42
1:G:349:ASN:H	1:G:349:ASN:ND2	2.17	0.42
1:I:308:VAL:HG11	1:K:288:LEU:HD12	2.00	0.42
1:O:432:GLY:HA3	1:O:438:MET:HE3	2.00	0.42
2:J:10:UNK:HA	2:J:15:UNK:HA	2.00	0.42
1:O:369:LEU:O	1:O:372:LEU:HB3	2.20	0.42
1:O:447:ASN:HA	1:O:448:PRO:HD3	1.89	0.42
1:S:107:PHE:HB3	1:S:410:LEU:HD11	2.01	0.42
1:U:348:ASP:OD1	1:U:348:ASP:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:447:ASN:HA	1:Y:448:PRO:HD3	1.94	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:OE1	1:K:251:GLU:HA	2.19	0.42
1:S:437:ILE:H	1:S:437:ILE:HG13	1.69	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: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:250:ASN:ND2	1:O:254:VAL:HG23	2.34	0.42
1:U:146:HIS:CE1	1:U:148:PHE:HB3	2.54	0.42
1:A:263:LEU:O	1:A:264:ILE:C	2.63	0.42
1:E:250:ASN:ND2	1:E:254:VAL:O	2.43	0.42
1:M:130:LEU:O	1:M:134:VAL:HG23	2.19	0.42
1:O:89:HIS:NE2	1:O:139:ASN:ND2	2.68	0.42
1:Q:35:GLN:HA	1:Q:35:GLN:OE1	2.19	0.42
1:S:275:MET:HE3	1:U:266:ASN:CB	2.46	0.42
1:I:106:THR:HB	1:I:413:THR:HB	2.01	0.42
1:I:311:VAL:O	1:K:289:LYS:HA	2.20	0.42
1:U:437:ILE:H	1:U:437:ILE:HG13	1.65	0.42
1:Y:439:SER:HG	1:Y:442:THR:HG1	1.66	0.42
1:C:284:ILE:HG12	1:C:321:ARG:NH1	2.34	0.42
1:K:146:HIS:CE1	1:K:148:PHE:HB3	2.55	0.42
1:M:63:ARG:HH11	1:M:75:VAL:HG21	1.84	0.42
1:S:369:LEU:O	1:S:372:LEU:HB3	2.19	0.42
1:S:376:MET:HG3	1:S:379:ARG:HH21	1.85	0.42
1:W:64:ARG:NH2	1:W:79:LYS:HD3	2.34	0.42
1:Y:145:TRP:HB2	1:Y:159:ILE:HA	2.02	0.42
1:A:376:MET:HG3	1:A:379:ARG:HH21	1.84	0.41
1:C:147:PRO:HD2	1:C:243:PRO:O	2.20	0.41
1:S:33:MET:HG2	1:S:34:ILE:N	2.34	0.41
1:Y:147:PRO:HD2	1:Y:243:PRO:O	2.20	0.41
1:Y:440:LYS:O	1:Y:444:VAL:HG23	2.20	0.41
1:A:295:ASN:HA	1:A:296:PRO:HD3	1.87	0.41
1:U:275:MET:HE3	1:W:266:ASN:CG	2.45	0.41
1:Y:295:ASN:HA	1:Y:296:PRO:HD3	1.89	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:G:129:ILE:HG22	1:G:145:TRP:HZ3	1.85	0.41
1:I:304:ARG:NH2	1:K:76:ASP:HB2	2.20	0.41
1:I:324:ILE:CG2	1:I:326:VAL:HG23	2.51	0.41
1:K:84:THR:HG23	1:M:262:ASP:HB3	2.01	0.41
1:K:295:ASN:HA	1:K:296:PRO:HD3	1.88	0.41
1:K:439:SER:HG	1:K:442:THR:HG1	1.68	0.41
1:M:57:ASN:OD1	1:M:57:ASN:N	2.54	0.41
1:M:429:LEU:HA	1:M:438:MET:HE1	2.03	0.41
1:O:336:ILE:O	1:O:340:LEU:HB2	2.21	0.41
1:Q:261:LYS:NZ	1:Q:265:ASP:OD2	2.51	0.41
1:C:101:VAL:O	1:C:101:VAL:HG12	2.21	0.41
1:C:111:ASN:HD21	1:C:404:PHE:HD2	1.68	0.41
1:G:98:GLN:HG2	1:I:372:LEU:HD12	2.02	0.41
1:I:57:ASN:C	1:I:59:ILE:N	2.78	0.41
1:I:129:ILE:HG22	1:I:145:TRP:CZ3	2.55	0.41
1:M:53:TYR:HB2	1:M:139:ASN:HD21	1.85	0.41
1:O:57:ASN:C	1:O:59:ILE:N	2.79	0.41
1:A:58:ASP:HA	1:A:61:LYS:HE2	2.01	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:K:64:ARG:NH2	1:K:79:LYS:HD3	2.36	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
1:M:161:PRO:HB3	1:M:163:GLU:OE2	2.20	0.41
1:M:295:ASN:HA	1:M:296:PRO:HD3	1.85	0.41
1:O:308:VAL:CG1	1:Q:288:LEU:HD12	2.50	0.41
1:U:66:TYR:CE2	1:U:74:LEU:HB3	2.55	0.41
1:U:364:GLU:HG3	1:U:418:ARG:HH22	1.86	0.41
1:G:146:HIS:CE1	1:G:148:PHE:HB3	2.56	0.41
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:I:284:ILE:HG12	1:I:321:ARG:NH1	2.36	0.41
1:O:130:LEU:O	1:O:134:VAL:HG23	2.20	0.41
1:U:57:ASN:C	1:U:59:ILE:N	2.78	0.41
1:E:122:ALA:HB1	1:E:126:PHE:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:142:ILE:HD12	1:G:248:LYS:HG2	2.03	0.41
1:I:90:LYS:NZ	1:I:94:ASP:OD1	2.53	0.41
1:I:251:GLU:OE1	1:I:251:GLU:HA	2.21	0.41
1:M:248:LYS:HD3	1:M:253:MET:CE	2.49	0.41
1:O:129:ILE:HG22	1:O:145:TRP:CZ3	2.56	0.41
1:O:257:LEU:HG	1:O:261:LYS:HB2	2.03	0.41
1:S:128:ASP:HA	1:U:379:ARG:HD2	2.03	0.41
1:S:145:TRP:C	1:S:145:TRP:CD1	2.99	0.41
1:S:275:MET:HE1	1:U:270:ILE:HD11	2.03	0.41
1:U:42:ASN:HA	1:U:43:PRO:HD3	1.79	0.41
1:C:42:ASN:HA	1:C:43:PRO:HD3	1.91	0.41
1:G:447:ASN:HA	1:G:448:PRO:HD3	1.95	0.41
1:M:160:PHE:HD2	1:M:165:MET:SD	2.44	0.41
1:O:66:TYR:CD2	1:O:76:ASP:HB3	2.57	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:S:250:ASN:HD21	1:S:254:VAL:HG23	1.86	0.41
1:U:98:GLN:HG2	1:W:372:LEU:HD12	2.03	0.41
1:U:250:ASN:HD22	1:U:254:VAL:H	1.67	0.41
1:C:349:ASN:H	1:C:349:ASN:ND2	2.19	0.40
1:K:437:ILE:H	1:K:437:ILE:HG13	1.70	0.40
1:W:364:GLU:HG3	1:W:418:ARG:HH22	1.87	0.40
1:Y:356:GLY:O	1:Y:358:ALA:N	2.54	0.40
1:Y:437:ILE:H	1:Y:437:ILE:HG13	1.76	0.40
1:C:129:ILE:HG22	1:C:145:TRP:CZ3	2.56	0.40
1:G:376:MET:HG3	1:G:379:ARG:NH2	2.36	0.40
1:O:142:ILE:HD12	1:O:253:MET:SD	2.61	0.40
1:O:349:ASN:H	1:O:349:ASN:HD22	1.68	0.40
1:O:349:ASN:ND2	1:O:349:ASN:N	2.67	0.40
1:Q:336:ILE:O	1:Q:340:LEU:HB2	2.22	0.40
1:E:447:ASN:HA	1:E:448:PRO:HD3	1.91	0.40
1:K:446:ARG:HE	1:K:446:ARG:HB3	1.71	0.40
1:Q:359:THR:HB	1:Q:361:PRO:HD2	2.04	0.40
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:W:42:ASN:HA	1:W:43:PRO:HD3	1.91	0.40
1:W:275:MET:HE3	1:Y:266:ASN:CB	2.40	0.40
1:Y:359:THR:HB	1:Y:361:PRO:HD2	2.03	0.40
1:C:146:HIS:CE1	1:C:148:PHE:HB3	2.56	0.40
1:W:349:ASN:H	1:W:349:ASN:HD22	1.67	0.40
1:C:250:ASN:ND2	1:C:254:VAL:HG23	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:429:LEU:HA	1:E:438:MET:HE1	2.03	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
1:Y:261:LYS:NZ	1:Y:265:ASP:OD2	2.54	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%)	24	54
1	C	366/503 (73%)	337 (92%)	26 (7%)	3 (1%)	16	44
1	E	366/503 (73%)	338 (92%)	26 (7%)	2 (0%)	24	54
1	G	366/503 (73%)	331 (90%)	33 (9%)	2 (0%)	24	54
1	I	366/503 (73%)	332 (91%)	32 (9%)	2 (0%)	24	54
1	K	366/503 (73%)	339 (93%)	24 (7%)	3 (1%)	16	44
1	M	366/503 (73%)	335 (92%)	29 (8%)	2 (0%)	24	54
1	O	366/503 (73%)	337 (92%)	27 (7%)	2 (0%)	24	54
1	Q	366/503 (73%)	343 (94%)	21 (6%)	2 (0%)	24	54
1	S	366/503 (73%)	333 (91%)	29 (8%)	4 (1%)	11	38
1	U	366/503 (73%)	337 (92%)	26 (7%)	3 (1%)	16	44
1	W	366/503 (73%)	338 (92%)	27 (7%)	1 (0%)	36	65
1	Y	366/503 (73%)	336 (92%)	27 (7%)	3 (1%)	16	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	4758/6539 (73%)	4369 (92%)	358 (8%)	31 (1%)	18	47

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
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%)	266 (90%)	30 (10%)	7	25
1	C	296/436 (68%)	269 (91%)	27 (9%)	9	30
1	E	296/436 (68%)	265 (90%)	31 (10%)	6	23
1	G	296/436 (68%)	263 (89%)	33 (11%)	6	21
1	I	296/436 (68%)	264 (89%)	32 (11%)	6	22
1	K	296/436 (68%)	260 (88%)	36 (12%)	5	19
1	M	296/436 (68%)	262 (88%)	34 (12%)	5	20
1	O	296/436 (68%)	264 (89%)	32 (11%)	6	22
1	Q	296/436 (68%)	260 (88%)	36 (12%)	5	19
1	S	296/436 (68%)	257 (87%)	39 (13%)	4	16
1	U	296/436 (68%)	258 (87%)	38 (13%)	4	17
1	W	296/436 (68%)	262 (88%)	34 (12%)	5	20
1	Y	296/436 (68%)	264 (89%)	32 (11%)	6	22
All	All	3848/5668 (68%)	3414 (89%)	434 (11%)	5	21

All (434) 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
1	A	80	THR
1	A	83	ARG
1	A	108	THR
1	A	120	GLU
1	A	123	ASP
1	A	128	ASP
1	A	145	TRP
1	A	160	PHE
1	A	163	GLU
1	A	250	ASN
1	A	254	VAL
1	A	271	THR

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Mol	Chain	Res	Type
1	A	300	THR
1	A	302	ASN
1	A	328	SER
1	A	340	LEU
1	A	345	GLN
1	A	349	ASN
1	A	352	GLU
1	A	353	THR
1	A	354	ILE
1	A	376	MET
1	A	423	SER
1	A	437	ILE
1	C	33	MET
1	C	48	LYS
1	C	56	GLU
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	128	ASP
1	C	160	PHE
1	C	163	GLU
1	C	250	ASN
1	C	271	THR
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	345	GLN
1	C	349	ASN
1	C	352	GLU
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

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Mol	Chain	Res	Type
1	E	57	ASN
1	E	59	ILE
1	E	65	THR
1	E	74	LEU
1	E	76	ASP
1	E	80	THR
1	E	83	ARG
1	E	108	THR
1	E	120	GLU
1	E	121	LEU
1	E	123	ASP
1	E	128	ASP
1	E	145	TRP
1	E	149	VAL
1	E	160	PHE
1	E	163	GLU
1	E	250	ASN
1	E	300	THR
1	E	302	ASN
1	E	304	ARG
1	E	328	SER
1	E	345	GLN
1	E	349	ASN
1	E	353	THR
1	E	376	MET
1	E	423	SER
1	E	437	ILE
1	E	438	MET
1	G	33	MET
1	G	48	LYS
1	G	56	GLU
1	G	59	ILE
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
1	G	120	GLU
1	G	121	LEU
1	G	123	ASP

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Mol	Chain	Res	Type
1	G	128	ASP
1	G	145	TRP
1	G	149	VAL
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	345	GLN
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	40	GLU
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	105	VAL
1	I	108	THR
1	I	120	GLU
1	I	128	ASP
1	I	145	TRP
1	I	160	PHE
1	I	163	GLU
1	I	168	VAL
1	I	250	ASN
1	I	271	THR
1	I	300	THR
1	I	302	ASN
1	I	328	SER

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Mol	Chain	Res	Type
1	I	337	GLN
1	I	338	ASP
1	I	345	GLN
1	I	349	ASN
1	I	353	THR
1	I	354	ILE
1	I	423	SER
1	I	437	ILE
1	I	438	MET
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	75	VAL
1	K	76	ASP
1	K	80	THR
1	K	83	ARG
1	K	120	GLU
1	K	123	ASP
1	K	128	ASP
1	K	145	TRP
1	K	160	PHE
1	K	163	GLU
1	K	250	ASN
1	K	254	VAL
1	K	271	THR
1	K	279	SER
1	K	285	VAL
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	345	GLN
1	K	347	VAL
1	K	349	ASN
1	K	352	GLU
1	K	353	THR
1	K	376	MET

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Mol	Chain	Res	Type
1	K	423	SER
1	K	437	ILE
1	K	438	MET
1	M	33	MET
1	M	48	LYS
1	M	56	GLU
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	120	GLU
1	M	123	ASP
1	M	145	TRP
1	M	160	PHE
1	M	163	GLU
1	M	168	VAL
1	M	250	ASN
1	M	254	VAL
1	M	271	THR
1	M	279	SER
1	M	300	THR
1	M	302	ASN
1	M	308	VAL
1	M	328	SER
1	M	340	LEU
1	M	345	GLN
1	M	347	VAL
1	M	349	ASN
1	M	352	GLU
1	M	353	THR
1	M	376	MET
1	M	423	SER
1	M	437	ILE
1	M	438	MET
1	O	33	MET
1	O	40	GLU
1	O	48	LYS
1	O	56	GLU
1	O	59	ILE

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Mol	Chain	Res	Type
1	O	65	THR
1	O	74	LEU
1	O	80	THR
1	O	120	GLU
1	O	123	ASP
1	O	145	TRP
1	O	160	PHE
1	O	163	GLU
1	O	168	VAL
1	O	239	TRP
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	345	GLN
1	O	349	ASN
1	O	352	GLU
1	O	353	THR
1	O	376	MET
1	O	437	ILE
1	O	438	MET
1	Q	33	MET
1	Q	40	GLU
1	Q	48	LYS
1	Q	56	GLU
1	Q	59	ILE
1	Q	65	THR
1	Q	74	LEU
1	Q	80	THR
1	Q	83	ARG
1	Q	120	GLU
1	Q	123	ASP
1	Q	145	TRP
1	Q	149	VAL
1	Q	159	ILE
1	Q	160	PHE

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Mol	Chain	Res	Type
1	Q	163	GLU
1	Q	168	VAL
1	Q	250	ASN
1	Q	254	VAL
1	Q	271	THR
1	Q	279	SER
1	Q	300	THR
1	Q	302	ASN
1	Q	328	SER
1	Q	337	GLN
1	Q	340	LEU
1	Q	345	GLN
1	Q	349	ASN
1	Q	352	GLU
1	Q	353	THR
1	Q	354	ILE
1	Q	376	MET
1	Q	423	SER
1	Q	430	VAL
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	74	LEU
1	S	75	VAL
1	S	80	THR
1	S	83	ARG
1	S	105	VAL
1	S	108	THR
1	S	120	GLU
1	S	123	ASP
1	S	135	LYS
1	S	145	TRP
1	S	149	VAL
1	S	160	PHE
1	S	163	GLU
1	S	168	VAL
1	S	239	TRP

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Mol	Chain	Res	Type
1	S	250	ASN
1	S	254	VAL
1	S	271	THR
1	S	279	SER
1	S	300	THR
1	S	302	ASN
1	S	304	ARG
1	S	328	SER
1	S	337	GLN
1	S	340	LEU
1	S	345	GLN
1	S	349	ASN
1	S	353	THR
1	S	373	LYS
1	S	376	MET
1	S	430	VAL
1	S	437	ILE
1	S	438	MET
1	U	33	MET
1	U	40	GLU
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	75	VAL
1	U	76	ASP
1	U	80	THR
1	U	83	ARG
1	U	108	THR
1	U	113	THR
1	U	120	GLU
1	U	123	ASP
1	U	128	ASP
1	U	145	TRP
1	U	149	VAL
1	U	160	PHE
1	U	163	GLU
1	U	168	VAL
1	U	239	TRP
1	U	300	THR

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Mol	Chain	Res	Type
1	U	302	ASN
1	U	304	ARG
1	U	328	SER
1	U	340	LEU
1	U	345	GLN
1	U	349	ASN
1	U	352	GLU
1	U	353	THR
1	U	376	MET
1	U	385	LEU
1	U	423	SER
1	U	430	VAL
1	U	437	ILE
1	U	438	MET
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	120	GLU
1	W	123	ASP
1	W	128	ASP
1	W	145	TRP
1	W	160	PHE
1	W	163	GLU
1	W	168	VAL
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	328	SER
1	W	338	ASP
1	W	340	LEU
1	W	345	GLN
1	W	347	VAL
1	W	349	ASN

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Mol	Chain	Res	Type
1	W	353	THR
1	W	411	THR
1	W	423	SER
1	W	437	ILE
1	W	438	MET
1	W	439	SER
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	75	VAL
1	Y	80	THR
1	Y	83	ARG
1	Y	120	GLU
1	Y	121	LEU
1	Y	123	ASP
1	Y	128	ASP
1	Y	145	TRP
1	Y	160	PHE
1	Y	163	GLU
1	Y	168	VAL
1	Y	250	ASN
1	Y	279	SER
1	Y	300	THR
1	Y	302	ASN
1	Y	304	ARG
1	Y	338	ASP
1	Y	345	GLN
1	Y	349	ASN
1	Y	352	GLU
1	Y	353	THR
1	Y	423	SER
1	Y	430	VAL
1	Y	437	ILE
1	Y	438	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (105) 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	282	GLN
1	A	349	ASN
1	A	427	GLN
1	C	73	GLN
1	C	136	ASN
1	C	139	ASN
1	C	146	HIS
1	C	250	ASN
1	C	349	ASN
1	E	73	GLN
1	E	86	HIS
1	E	136	ASN
1	E	139	ASN
1	E	146	HIS
1	E	250	ASN
1	E	282	GLN
1	E	345	GLN
1	E	349	ASN
1	G	73	GLN
1	G	136	ASN
1	G	139	ASN
1	G	146	HIS
1	G	349	ASN
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	41	HIS
1	K	73	GLN
1	K	86	HIS
1	K	136	ASN
1	K	139	ASN
1	K	146	HIS
1	K	250	ASN
1	K	302	ASN

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Mol	Chain	Res	Type
1	K	349	ASN
1	K	398	ASN
1	M	73	GLN
1	M	86	HIS
1	M	136	ASN
1	M	139	ASN
1	M	146	HIS
1	M	282	GLN
1	M	302	ASN
1	M	345	GLN
1	M	349	ASN
1	M	427	GLN
1	O	73	GLN
1	O	136	ASN
1	O	139	ASN
1	O	146	HIS
1	O	250	ASN
1	O	302	ASN
1	O	349	ASN
1	O	431	GLN
1	Q	73	GLN
1	Q	136	ASN
1	Q	139	ASN
1	Q	146	HIS
1	Q	302	ASN
1	Q	349	ASN
1	Q	398	ASN
1	S	73	GLN
1	S	136	ASN
1	S	139	ASN
1	S	146	HIS
1	S	250	ASN
1	S	337	GLN
1	S	349	ASN
1	U	86	HIS
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	W	73	GLN

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Mol	Chain	Res	Type
1	W	82	ASN
1	W	86	HIS
1	W	131	ASN
1	W	136	ASN
1	W	139	ASN
1	W	146	HIS
1	W	250	ASN
1	W	302	ASN
1	W	345	GLN
1	W	349	ASN
1	Y	73	GLN
1	Y	82	ASN
1	Y	86	HIS
1	Y	131	ASN
1	Y	136	ASN
1	Y	139	ASN
1	Y	146	HIS
1	Y	282	GLN
1	Y	302	ASN
1	Y	349	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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%)	0.73	34 (9%) 14 14	140, 140, 140, 140	0
1	C	370/503 (73%)	0.84	40 (10%) 11 11	140, 140, 140, 140	0
1	E	370/503 (73%)	0.77	34 (9%) 14 14	140, 140, 140, 140	0
1	G	370/503 (73%)	0.65	23 (6%) 26 21	140, 140, 140, 140	0
1	I	370/503 (73%)	0.63	21 (5%) 29 22	140, 140, 140, 140	0
1	K	370/503 (73%)	0.68	25 (6%) 23 19	140, 140, 140, 140	0
1	M	370/503 (73%)	0.92	52 (14%) 6 8	140, 140, 140, 140	0
1	O	370/503 (73%)	0.86	40 (10%) 11 11	140, 140, 140, 140	0
1	Q	370/503 (73%)	0.87	47 (12%) 8 9	140, 140, 140, 140	0
1	S	370/503 (73%)	0.59	18 (4%) 35 26	140, 140, 140, 140	0
1	U	370/503 (73%)	0.48	12 (3%) 50 37	140, 140, 140, 140	0
1	W	370/503 (73%)	0.57	14 (3%) 44 31	140, 140, 140, 140	0
1	Y	370/503 (73%)	0.74	38 (10%) 12 12	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%)	0.72	398 (8%) 17 15	140, 140, 140, 140	0

All (398) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	349	ASN	5.8
1	O	326	VAL	5.1
1	Y	436	GLY	4.8
1	C	278	PHE	4.7
1	Y	33	MET	4.4
1	Q	157	TYR	4.2
1	O	278	PHE	4.2
1	C	169	TYR	4.0
1	M	419	ILE	4.0
1	A	37	LEU	4.0
1	K	419	ILE	3.9
1	W	347	VAL	3.9
1	Q	392	PHE	3.8
1	Y	158	VAL	3.8
1	K	145	TRP	3.7
1	Y	88	TRP	3.7
1	C	324	ILE	3.7
1	W	144	TYR	3.7
1	Y	326	VAL	3.7
1	C	419	ILE	3.7
1	E	325	PRO	3.7
1	O	281	PHE	3.6
1	Q	325	PRO	3.6
1	M	345	GLN	3.6
1	Q	324	ILE	3.6
1	S	307	SER	3.6
1	C	365	LYS	3.5
1	U	291	TYR	3.5
1	A	328	SER	3.5
1	Y	37	LEU	3.4
1	Q	419	ILE	3.4
1	Q	278	PHE	3.4
1	C	303	LEU	3.4
1	S	320	LEU	3.4
1	M	365	LYS	3.4
1	M	267	TYR	3.4
1	G	95	GLN	3.4
1	O	325	PRO	3.4
1	A	357	GLY	3.3
1	M	357	GLY	3.3
1	M	86	HIS	3.3
1	I	436	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	O	254	VAL	3.3
1	M	324	ILE	3.3
1	E	269	SER	3.3
1	Q	281	PHE	3.3
1	Q	267	TYR	3.2
1	O	361	PRO	3.2
1	M	333	LEU	3.2
1	C	148	PHE	3.2
1	M	322	ALA	3.2
1	W	169	TYR	3.2
1	I	308	VAL	3.2
1	A	166	ILE	3.2
1	A	145	TRP	3.2
1	C	37	LEU	3.2
1	O	419	ILE	3.2
1	C	281	PHE	3.2
1	C	284	ILE	3.2
1	Q	270	ILE	3.2
1	Q	332	GLU	3.1
1	E	278	PHE	3.1
1	M	281	PHE	3.1
1	A	361	PRO	3.1
1	A	415	THR	3.1
1	M	88	TRP	3.1
1	E	284	ILE	3.1
1	E	274	THR	3.1
1	A	169	TYR	3.1
1	M	169	TYR	3.1
1	Q	88	TRP	3.1
1	O	324	ILE	3.1
1	G	419	ILE	3.1
1	O	322	ALA	3.0
1	A	417	THR	3.0
1	A	158	VAL	3.0
1	O	365	LYS	3.0
1	E	343	SER	3.0
1	A	33	MET	3.0
1	Q	286	TYR	3.0
1	M	92	PHE	3.0
1	A	88	TRP	3.0
1	Q	334	GLU	3.0
1	M	343	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	243	PRO	3.0
1	G	123	ASP	3.0
1	O	290	ASN	3.0
1	Y	365	LYS	3.0
1	M	326	VAL	3.0
1	E	324	ILE	3.0
1	I	245	ILE	3.0
1	K	336	ILE	3.0
1	Q	333	LEU	3.0
1	G	167	VAL	3.0
1	M	309	ILE	3.0
1	Y	325	PRO	2.9
1	A	267	TYR	2.9
1	E	295	ASN	2.9
1	K	169	TYR	2.9
1	Y	347	VAL	2.9
1	K	299	PHE	2.9
1	S	278	PHE	2.9
1	C	86	HIS	2.9
1	G	278	PHE	2.9
1	I	86	HIS	2.9
1	K	86	HIS	2.9
1	W	88	TRP	2.9
1	O	105	VAL	2.9
1	K	460	ILE	2.9
1	Y	87	ALA	2.9
1	C	392	PHE	2.9
1	W	343	SER	2.8
1	Q	263	LEU	2.8
1	Y	361	PRO	2.8
1	I	124	ASP	2.8
1	C	241	ARG	2.8
1	Y	298	GLU	2.8
1	G	349	ASN	2.8
1	C	270	ILE	2.8
1	C	267	TYR	2.8
1	C	363	LEU	2.8
1	M	145	TRP	2.8
1	M	284	ILE	2.8
1	C	38	ILE	2.8
1	G	244	ILE	2.8
1	Y	357	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	Q	346	ALA	2.8
1	U	142	ILE	2.8
1	Y	278	PHE	2.7
1	Q	357	GLY	2.7
1	M	414	PHE	2.7
1	O	294	GLU	2.7
1	W	123	ASP	2.7
1	W	290	ASN	2.7
1	C	322	ALA	2.7
1	Q	322	ALA	2.7
1	E	326	VAL	2.7
1	M	369	LEU	2.7
1	G	444	VAL	2.7
1	Q	363	LEU	2.7
1	K	388	PHE	2.7
1	O	88	TRP	2.7
1	A	87	ALA	2.7
1	M	377	ALA	2.7
1	I	366	LEU	2.7
1	K	326	VAL	2.7
1	M	278	PHE	2.7
1	C	239	TRP	2.7
1	M	328	SER	2.7
1	E	329	ALA	2.7
1	C	367	TYR	2.7
1	Q	169	TYR	2.7
1	Y	91	LEU	2.7
1	O	86	HIS	2.7
1	Q	361	PRO	2.6
1	E	145	TRP	2.6
1	E	308	VAL	2.6
1	A	86	HIS	2.6
1	S	398	ASN	2.6
1	M	339	GLU	2.6
1	Y	169	TYR	2.6
1	A	388	PHE	2.6
1	M	361	PRO	2.6
1	Y	438	MET	2.6
1	O	307	SER	2.6
1	M	43	PRO	2.6
1	Y	299	PHE	2.6
1	E	158	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	34	ILE	2.6
1	E	270	ILE	2.6
1	A	329	ALA	2.6
1	K	87	ALA	2.6
1	K	317	VAL	2.6
1	C	88	TRP	2.5
1	E	78	THR	2.6
1	G	309	ILE	2.5
1	Q	155	PHE	2.5
1	I	169	TYR	2.5
1	K	365	LYS	2.5
1	O	347	VAL	2.5
1	M	157	TYR	2.5
1	S	315	GLY	2.5
1	Q	365	LYS	2.5
1	M	399	THR	2.5
1	I	278	PHE	2.5
1	C	333	LEU	2.5
1	O	363	LEU	2.5
1	G	435	GLY	2.5
1	K	436	GLY	2.5
1	U	357	GLY	2.5
1	M	244	ILE	2.5
1	G	86	HIS	2.5
1	S	363	LEU	2.5
1	W	436	GLY	2.5
1	C	326	VAL	2.5
1	C	70	ALA	2.5
1	M	346	ALA	2.5
1	O	330	ALA	2.5
1	Q	40	GLU	2.5
1	Y	324	ILE	2.5
1	U	145	TRP	2.5
1	U	320	LEU	2.5
1	O	87	ALA	2.4
1	Q	329	ALA	2.4
1	M	270	ILE	2.4
1	O	328	SER	2.4
1	Q	164	GLU	2.4
1	E	280	ASP	2.4
1	G	290	ASN	2.4
1	G	292	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	Q	290	ASN	2.4
1	Y	286	TYR	2.4
1	Q	326	VAL	2.4
1	O	244	ILE	2.4
1	O	333	LEU	2.4
1	K	88	TRP	2.4
1	O	256	ASP	2.4
1	A	315	GLY	2.4
1	M	158	VAL	2.4
1	U	158	VAL	2.4
1	Y	419	ILE	2.4
1	K	278	PHE	2.4
1	K	332	GLU	2.4
1	S	361	PRO	2.4
1	K	321	ARG	2.4
1	G	281	PHE	2.4
1	C	91	LEU	2.4
1	Q	366	LEU	2.4
1	Y	332	GLU	2.4
1	A	326	VAL	2.4
1	C	69	ALA	2.4
1	E	283	GLN	2.4
1	G	148	PHE	2.4
1	U	391	PHE	2.4
1	C	145	TRP	2.4
1	O	142	ILE	2.3
1	I	292	ASP	2.3
1	M	363	LEU	2.3
1	A	167	VAL	2.3
1	A	239	TRP	2.3
1	G	439	SER	2.3
1	M	325	PRO	2.3
1	S	419	ILE	2.3
1	C	366	LEU	2.3
1	Q	389	PHE	2.3
1	U	56	GLU	2.3
1	C	271	THR	2.3
1	M	415	THR	2.3
1	E	169	TYR	2.3
1	Y	291	TYR	2.3
1	M	290	ASN	2.3
1	M	340	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	W	349	ASN	2.3
1	Y	292	ASP	2.3
1	M	120	GLU	2.3
1	O	332	GLU	2.3
1	S	309	ILE	2.3
1	U	361	PRO	2.3
1	Y	432	GLY	2.3
1	E	277	SER	2.3
1	Y	259	PHE	2.3
1	K	159	ILE	2.3
1	K	361	PRO	2.3
1	M	166	ILE	2.3
1	O	166	ILE	2.3
1	O	284	ILE	2.3
1	M	303	LEU	2.3
1	Q	274	THR	2.3
1	Q	359	THR	2.3
1	K	267	TYR	2.3
1	A	365	LYS	2.3
1	Q	295	ASN	2.3
1	I	326	VAL	2.3
1	U	123	ASP	2.3
1	Y	94	ASP	2.3
1	Y	317	VAL	2.3
1	Y	433	VAL	2.3
1	C	298	GLU	2.2
1	Q	284	ILE	2.2
1	W	29	PRO	2.2
1	Q	33	MET	2.2
1	E	263	LEU	2.2
1	Q	145	TRP	2.2
1	Y	105	VAL	2.2
1	K	294	GLU	2.2
1	Y	143	GLU	2.2
1	M	263	LEU	2.2
1	C	31	THR	2.2
1	W	286	TYR	2.2
1	Q	168	VAL	2.2
1	S	254	VAL	2.2
1	C	282	GLN	2.2
1	O	270	ILE	2.2
1	E	322	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	Q	340	LEU	2.2
1	Y	100	LEU	2.2
1	O	274	THR	2.2
1	Q	86	HIS	2.2
1	S	271	THR	2.2
1	A	341	TYR	2.2
1	M	341	TYR	2.2
1	A	444	VAL	2.2
1	W	95	GLN	2.2
1	I	419	ILE	2.2
1	M	266	ASN	2.2
1	Y	295	ASN	2.2
1	K	330	ALA	2.2
1	C	68	ASP	2.2
1	Y	342	LYS	2.2
1	A	281	PHE	2.2
1	W	278	PHE	2.2
1	E	88	TRP	2.2
1	M	274	THR	2.2
1	G	101	VAL	2.2
1	O	267	TYR	2.2
1	O	286	TYR	2.2
1	S	430	VAL	2.2
1	O	336	ILE	2.2
1	G	331	LYS	2.2
1	Y	349	ASN	2.2
1	I	422	ASP	2.2
1	M	452	ASP	2.2
1	S	55	CYS	2.2
1	E	271	THR	2.1
1	M	359	THR	2.1
1	Q	347	VAL	2.1
1	C	467	TYR	2.1
1	O	263	LEU	2.1
1	E	307	SER	2.1
1	O	329	ALA	2.1
1	O	358	ALA	2.1
1	Y	290	ASN	2.1
1	U	128	ASP	2.1
1	W	338	ASP	2.1
1	A	270	ILE	2.1
1	C	336	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	260	TYR	2.1
1	G	324	ILE	2.1
1	O	275	MET	2.1
1	S	165	MET	2.1
1	E	316	GLY	2.1
1	I	456	GLU	2.1
1	S	454	GLU	2.1
1	E	281	PHE	2.1
1	I	167	VAL	2.1
1	S	336	ILE	2.1
1	O	95	GLN	2.1
1	Q	358	ALA	2.1
1	E	439	SER	2.1
1	G	449	PHE	2.1
1	K	439	SER	2.1
1	M	269	SER	2.1
1	G	261	LYS	2.1
1	A	284	ILE	2.1
1	Q	303	LEU	2.1
1	Q	309	ILE	2.1
1	Q	314	ASP	2.1
1	E	305	TYR	2.1
1	I	467	TYR	2.1
1	C	87	ALA	2.1
1	M	315	GLY	2.1
1	E	148	PHE	2.1
1	M	259	PHE	2.1
1	Q	404	PHE	2.1
1	Q	328	SER	2.1
1	E	405	ASN	2.1
1	I	290	ASN	2.1
1	Q	82	ASN	2.1
1	A	288	LEU	2.1
1	A	369	LEU	2.1
1	G	303	LEU	2.1
1	S	324	ILE	2.1
1	C	123	ASP	2.1
1	K	286	TYR	2.1
1	M	286	TYR	2.1
1	O	367	TYR	2.1
1	M	420	GLN	2.1
1	O	404	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	S	326	VAL	2.0
1	Y	328	SER	2.0
1	A	263	LEU	2.0
1	I	244	ILE	2.0
1	U	398	ASN	2.0
1	I	88	TRP	2.0
1	I	280	ASP	2.0
1	C	436	GLY	2.0
1	E	293	GLY	2.0
1	M	449	PHE	2.0
1	C	332	GLU	2.0
1	E	46	LEU	2.0
1	Y	363	LEU	2.0
1	C	274	THR	2.0
1	E	301	ALA	2.0
1	A	160	PHE	2.0
1	A	278	PHE	2.0
1	K	308	VAL	2.0
1	A	437	ILE	2.0
1	I	437	ILE	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 oligosaccharides 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. 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	B-factors(Å ²)	Q<0.9
3	HG	Q	701	1/1	0.86	0.14	140,140,140,140	1
3	HG	C	701	1/1	0.92	0.15	140,140,140,140	1
3	HG	O	701	1/1	0.93	0.11	140,140,140,140	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	HG	S	701	1/1	0.93	0.15	140,140,140,140	1
3	HG	M	701	1/1	0.94	0.11	140,140,140,140	1
4	CA	K	801	1/1	0.94	0.08	140,140,140,140	0
3	HG	G	701	1/1	0.95	0.12	140,140,140,140	1
3	HG	A	701	1/1	0.95	0.11	140,140,140,140	1
4	CA	Q	801	1/1	0.95	0.07	140,140,140,140	0
4	CA	S	801	1/1	0.95	0.07	140,140,140,140	0
4	CA	I	801	1/1	0.96	0.10	140,140,140,140	0
3	HG	K	701	1/1	0.96	0.09	140,140,140,140	1
3	HG	Y	701	1/1	0.97	0.11	140,140,140,140	1
4	CA	A	801	1/1	0.97	0.08	140,140,140,140	0
4	CA	G	801	1/1	0.97	0.07	140,140,140,140	0
3	HG	I	701	1/1	0.97	0.09	140,140,140,140	1
3	HG	E	701	1/1	0.97	0.14	140,140,140,140	1
4	CA	M	801	1/1	0.97	0.08	140,140,140,140	0
3	HG	U	701	1/1	0.97	0.12	140,140,140,140	1
3	HG	W	701	1/1	0.97	0.08	140,140,140,140	1
4	CA	W	801	1/1	0.97	0.07	140,140,140,140	0
4	CA	C	801	1/1	0.98	0.07	140,140,140,140	0
4	CA	E	801	1/1	0.98	0.07	140,140,140,140	0
4	CA	U	801	1/1	0.98	0.06	140,140,140,140	0
4	CA	O	801	1/1	0.98	0.07	140,140,140,140	0
4	CA	Y	801	1/1	0.98	0.08	140,140,140,140	0

6.5 Other polymers [i](#)

There are no such residues in this entry.