Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 10:26 pm BST

PDB ID	:	2JES
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 following versions of software and data (see references ⓘ) were used in the production of this report:

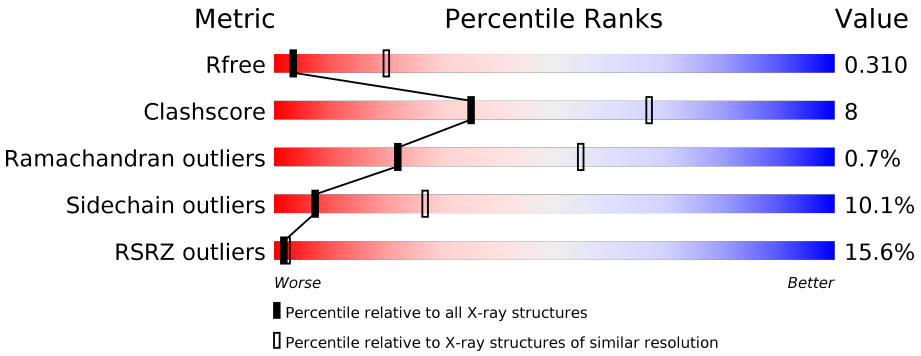
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (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}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	503	12% 58% 14% • 26%
1	C	503	14% 56% 15% • 26%
1	E	503	15% 58% 13% • 26%
1	G	503	13% 55% 16% • 26%
1	I	503	13% 55% 16% • 26%
1	K	503	11% 54% 17% • 26%

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Mol	Chain	Length	Quality of chain
1	M	503	12% 56% 15% 26%
1	O	503	11% 55% 16% 26%
1	Q	503	11% 56% 15% 26%
1	S	503	9% 53% 18% 26%
1	U	503	7% 54% 17% 26%
1	W	503	10% 55% 16% 26%
1	Y	503	13% 56% 16% 26%
2	B	30	93% 7%
2	D	30	93% 7%
2	F	30	93% 7%
2	H	30	93% 7%
2	J	30	93% 7%
2	L	30	93% 7%
2	N	30	93% 7%
2	P	30	90% 10%
2	R	30	90% 10%
2	T	30	97%
2	V	30	93% 7%
2	X	30	93% 7%
2	Z	30	93% 7%

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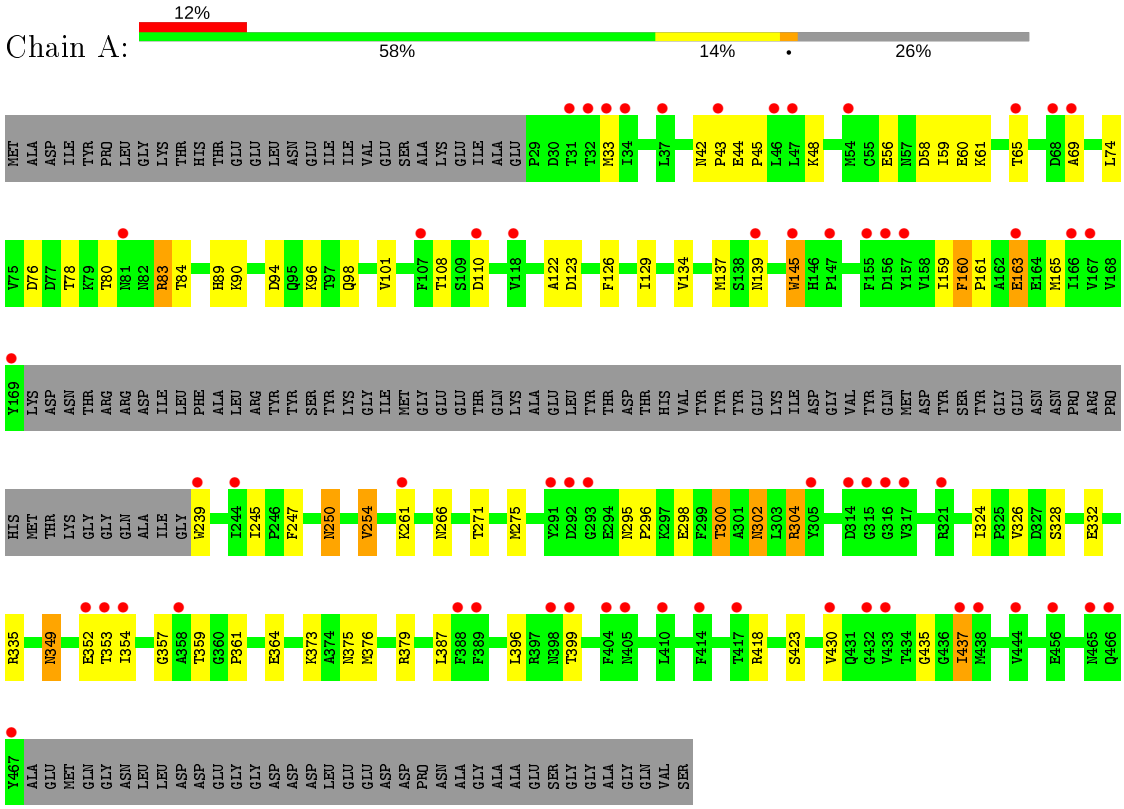
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ca 1 1	0	0
4	U	1	Total Ca 1 1	0	0
4	O	1	Total Ca 1 1	0	0
4	Y	1	Total Ca 1 1	0	0
4	S	1	Total Ca 1 1	0	0
4	M	1	Total Ca 1 1	0	0

3 Residue-property plots (i)

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

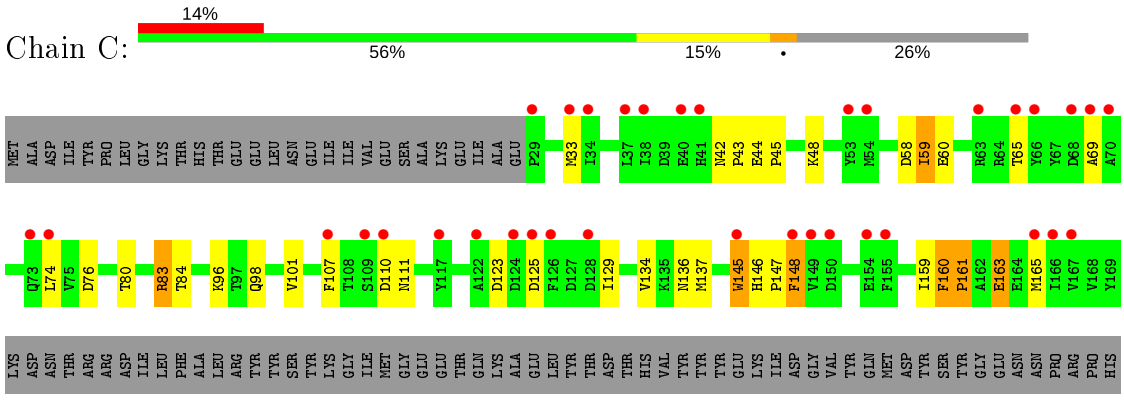
- Molecule 1: PORTAL PROTEIN

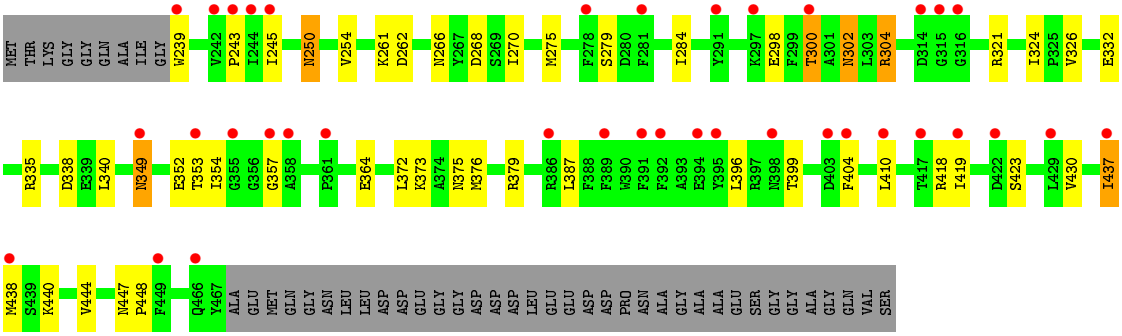
Chain A:



- Molecule 1: PORTAL PROTEIN

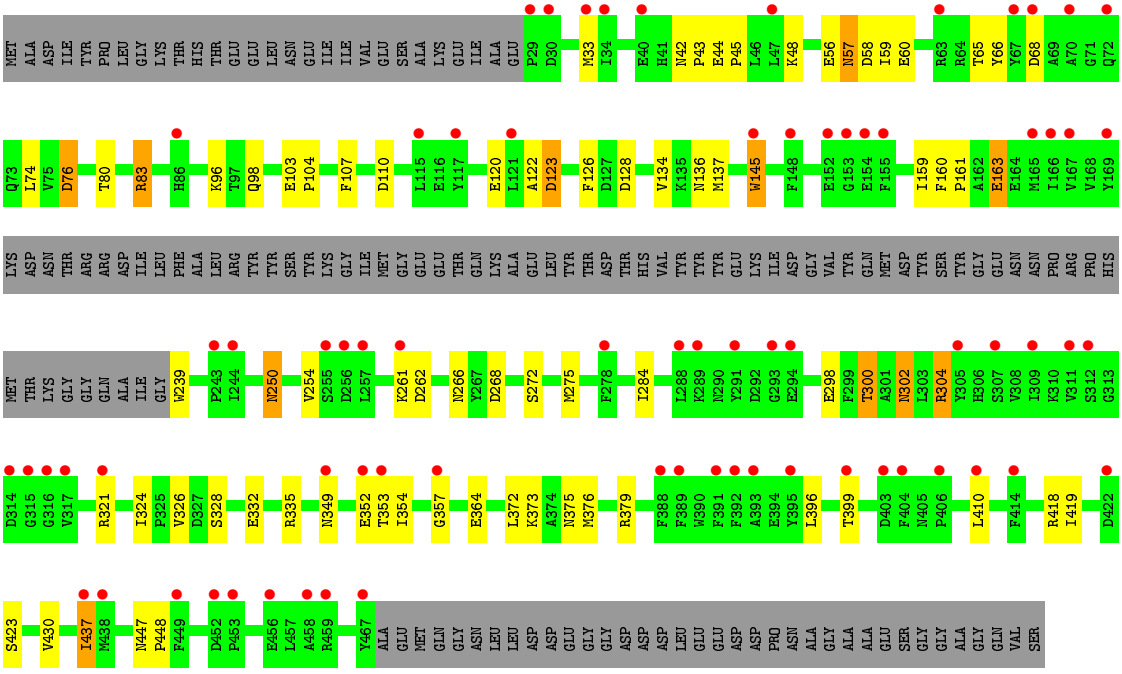
Chain C:





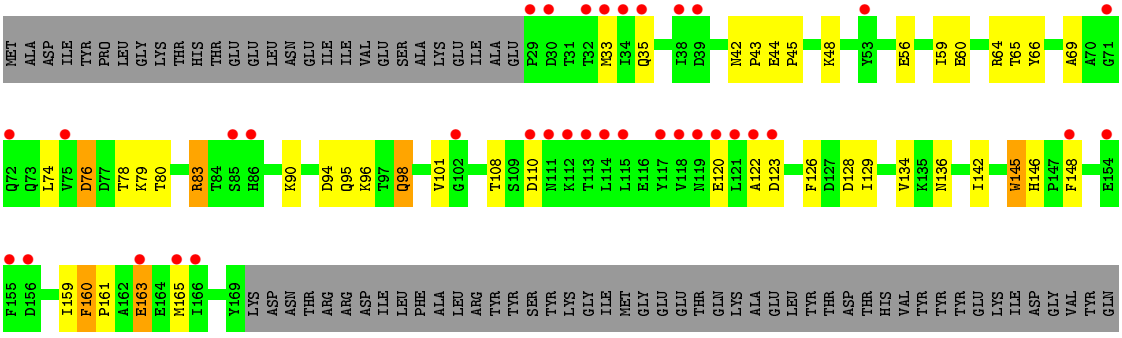
• Molecule 1: PORTAL PROTEIN

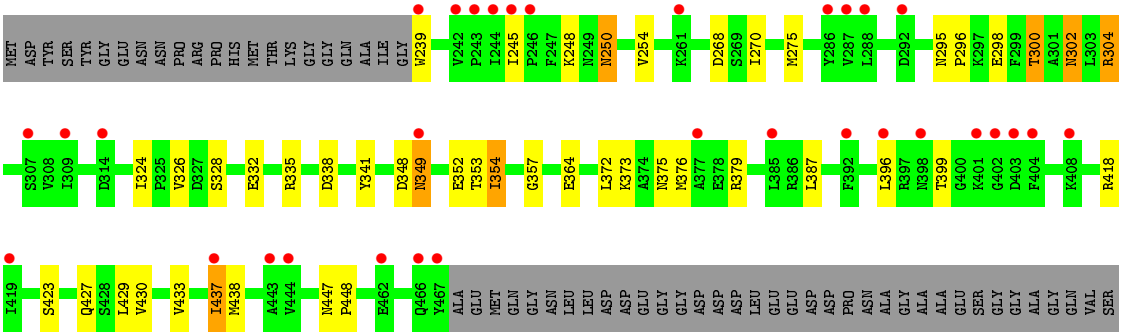
Chain E:



• Molecule 1: PORTAL PROTEIN

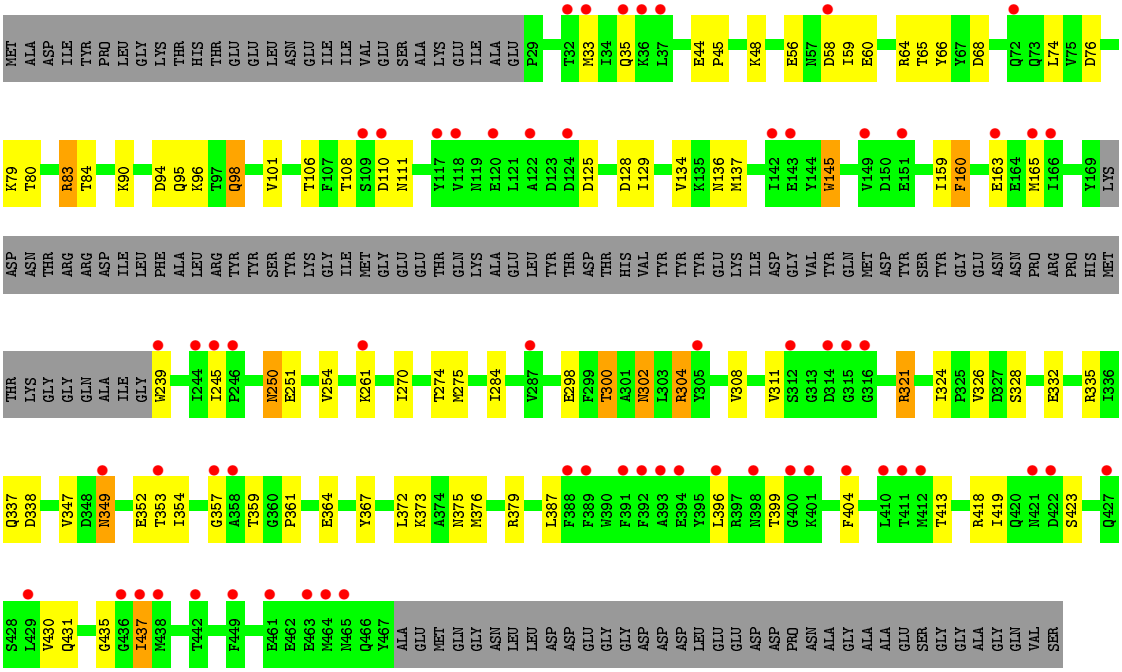
Chain G:





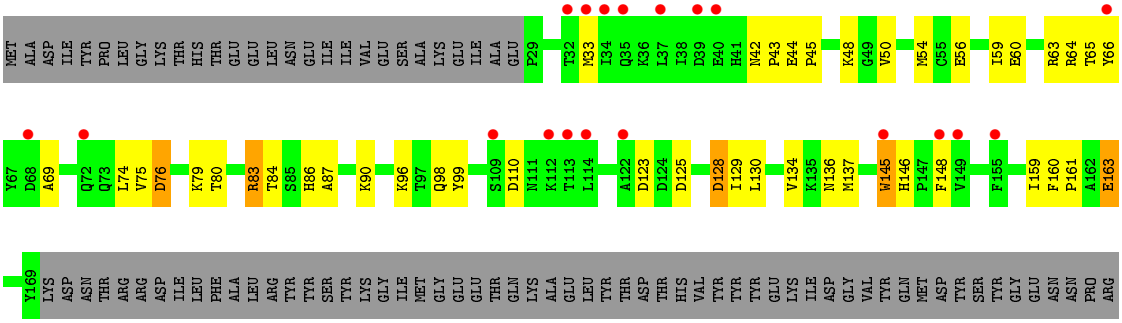
• Molecule 1: PORTAL PROTEIN

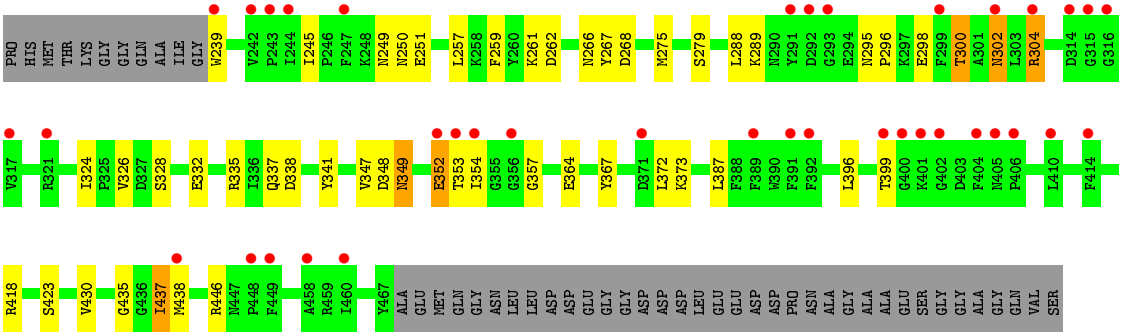
Chain I:



• Molecule 1: PORTAL PROTEIN

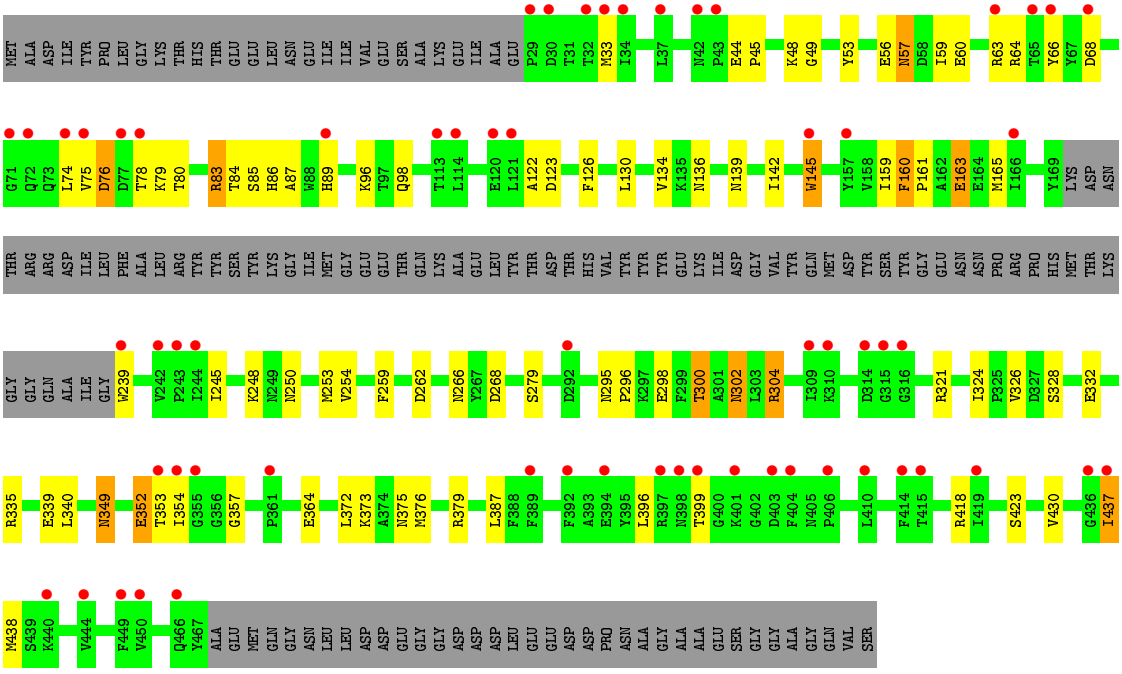
Chain K:





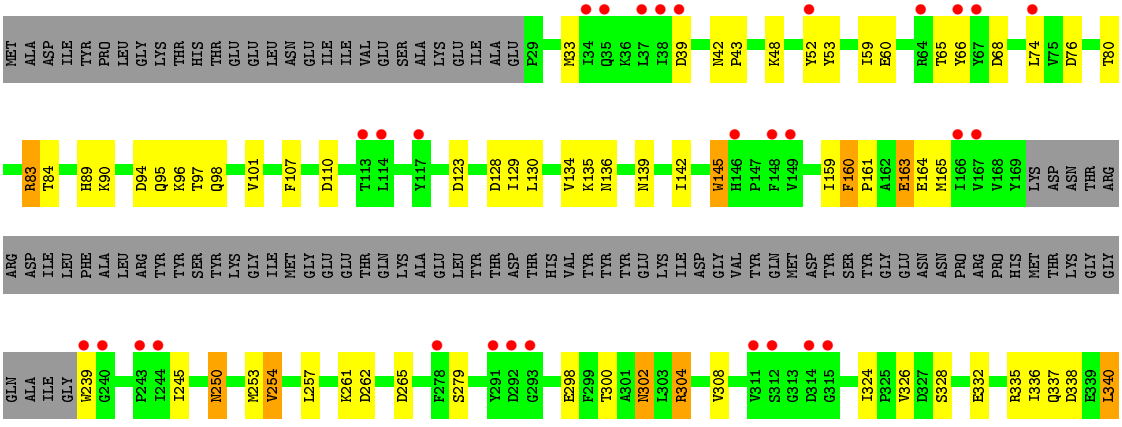
• Molecule 1: PORTAL PROTEIN

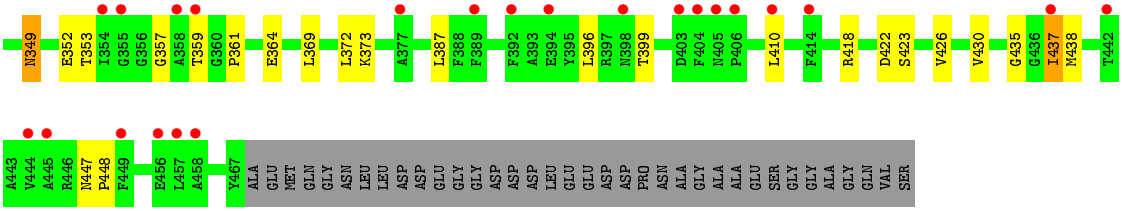
Chain M:



• Molecule 1: PORTAL PROTEIN

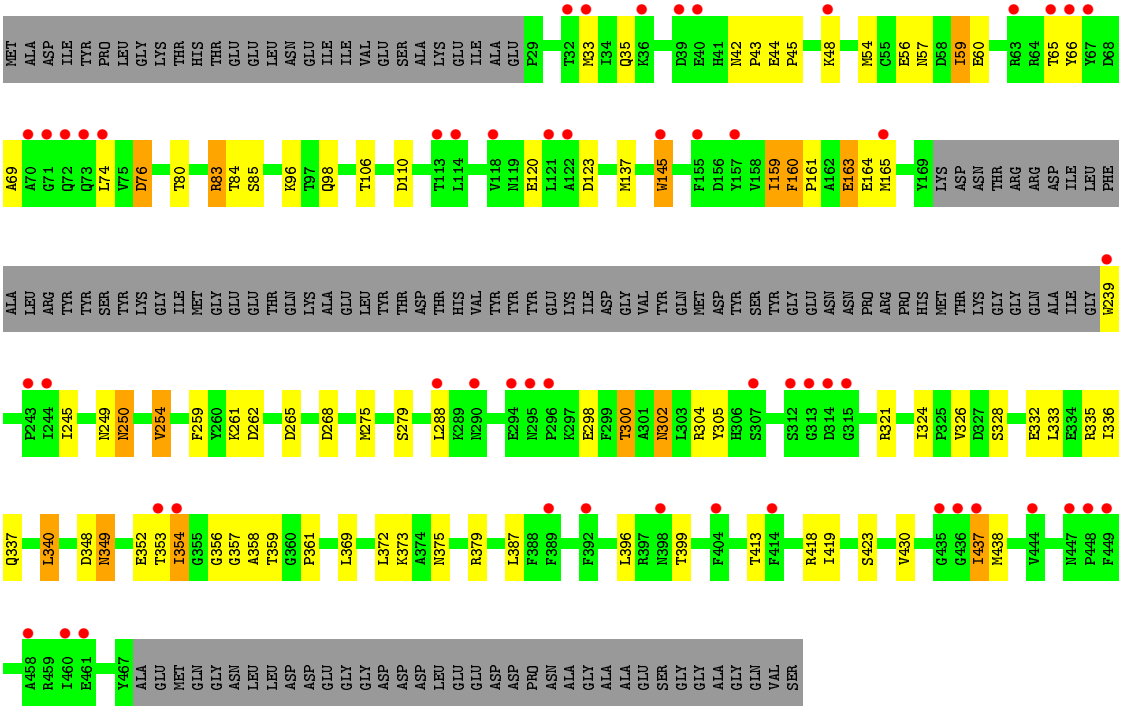
Chain O:





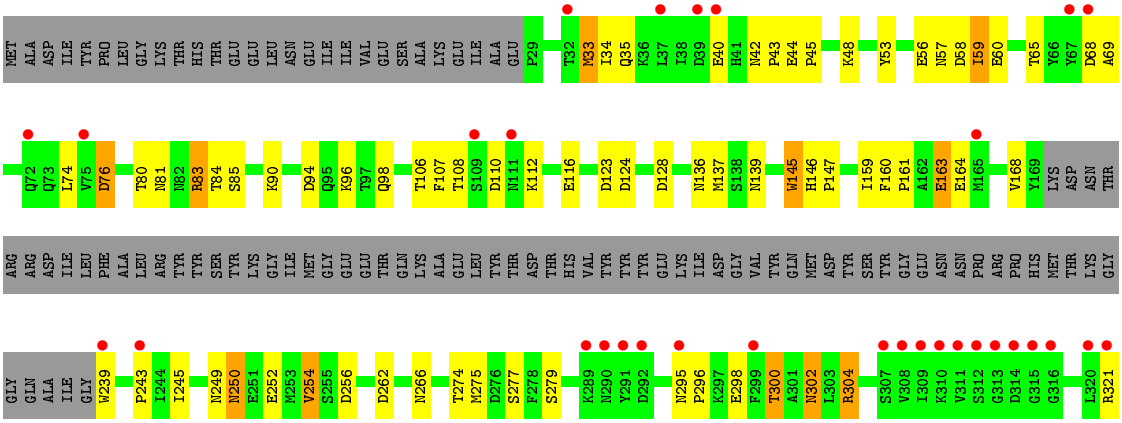
• Molecule 1: PORTAL PROTEIN

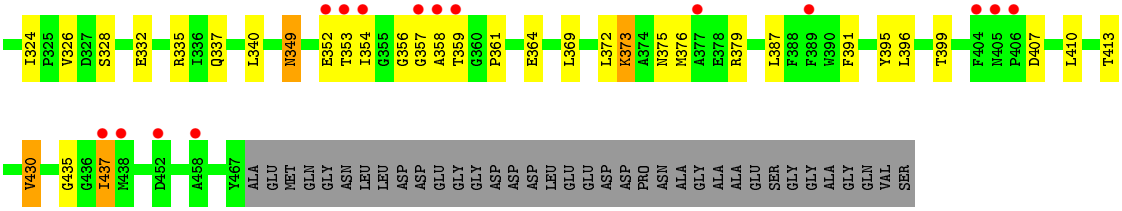
Chain Q:



• Molecule 1: PORTAL PROTEIN

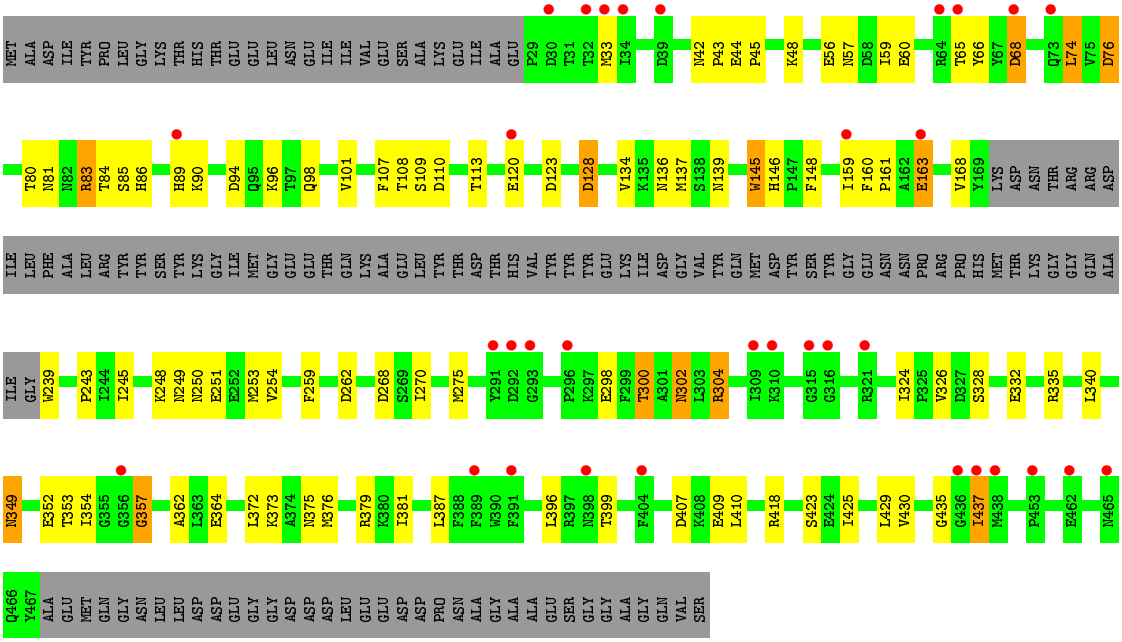
Chain S:





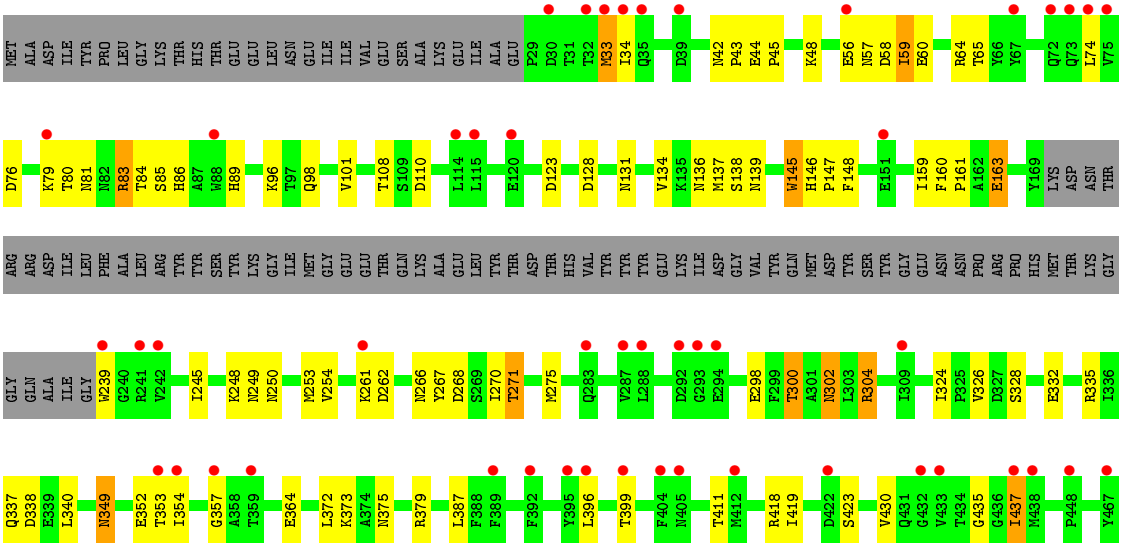
• Molecule 1: PORTAL PROTEIN

Chain U:



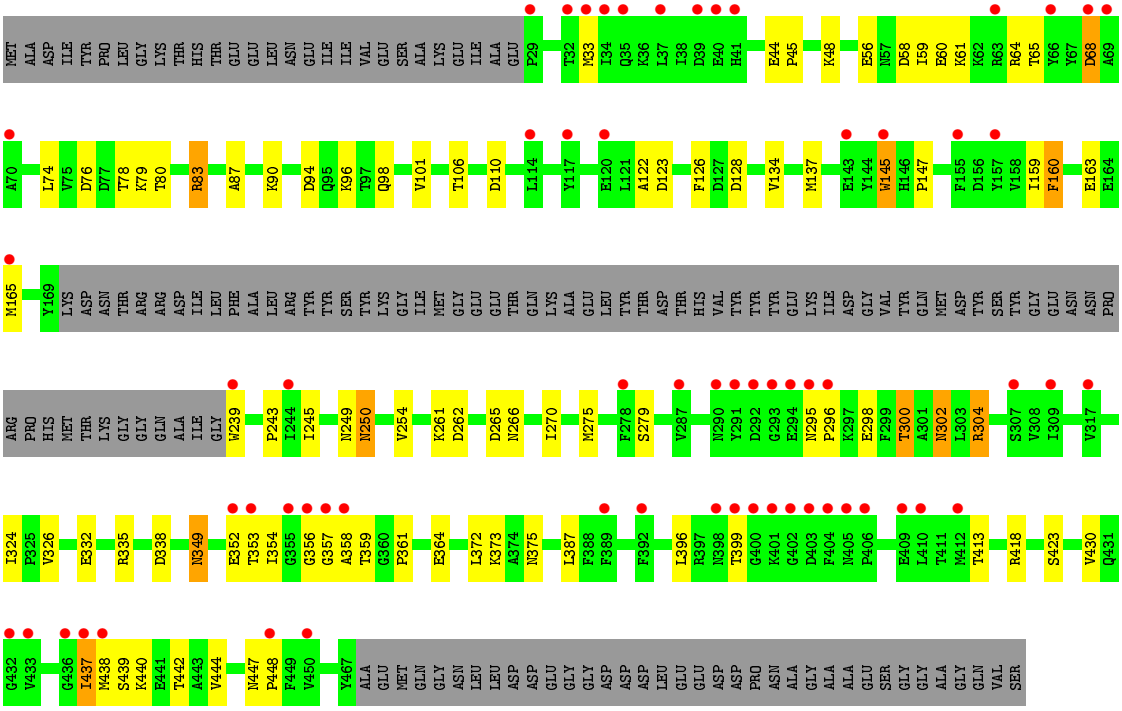
• Molecule 1: PORTAL PROTEIN

Chain W:



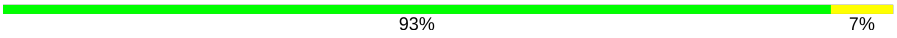
• Molecule 1: PORTAL PROTEIN

Chain Y:



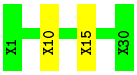
• Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN

Chain B:



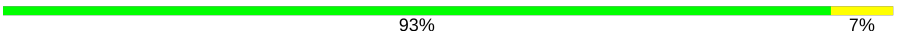
• Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN

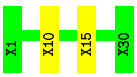
Chain D:



• Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN

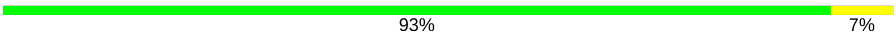
Chain F:

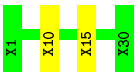




• Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN

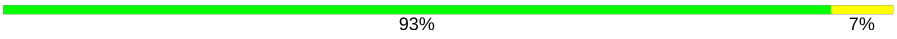
Chain H:

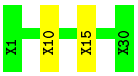




• Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN

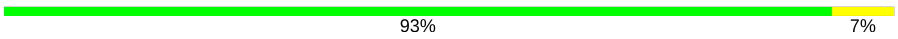
Chain J:

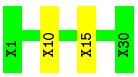




• Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN

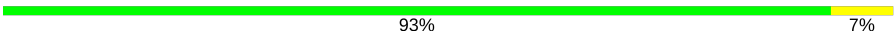
Chain L:

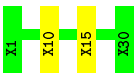




• Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN

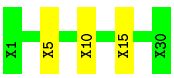
Chain N:





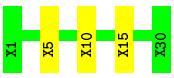
• Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN

Chain P:



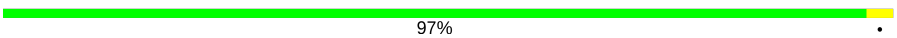
• Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN

Chain R:



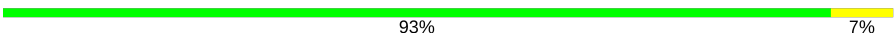
• Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN

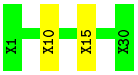
Chain T:



• Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN

Chain V:





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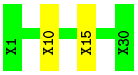
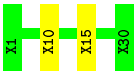
Chain X:



• Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN

Chain Z:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 (1.01%)	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)	0.27 , 161.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

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: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: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: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:E:430:VAL:HG23	1:G:437:ILE:HD11	1.76	0.66
1:S:332:GLU:CD	1:S:335:ARG:HH21	1.99	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:S:98:GLN:OE1	1:U:375:ASN:ND2	2.30	0.64
1:W:332:GLU:CD	1:W:335:ARG:HH21	2.00	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: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: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: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:C:44:GLU:HG3	1:C:45:PRO:HD3	1.83	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:U:349:ASN:H	1:U:349:ASN:ND2	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:Q:275:MET:CE	1:S:266:ASN:HB3	2.31	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:Y:58:ASP:OD1	1:Y:261:LYS:NZ	2.35	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:300:THR:O	1:Q:304:ARG:HB2	2.04	0.57
1:Q:332:GLU:CD	1:Q:335:ARG:HH21	2.08	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:ND2	1:Q:349:ASN:H	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:A:250:ASN:ND2	1:A:254:VAL:O	2.36	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: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: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: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: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: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: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:W:275:MET:HE3	1:Y:266:ASN:HB3	1.89	0.55
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:A:275:MET:HE3	1:C:266:ASN:HB3	1.87	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: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: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:O:98:GLN:OE1	1:Q:375:ASN:ND2	2.41	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: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:K:275:MET:HE1	1:M:266:ASN:HB3	1.88	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

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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: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
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: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: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:U:275:MET:CE	1:W:266:ASN:HB3	2.40	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: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: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:A:300:THR:O	1:A:304:ARG:HB2	2.09	0.51
1:M:122:ALA:HB1	1:M:126:PHE:CD2	2.45	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:Y:352:GLU:OE2	1:Y:354:ILE:HG12	2.11	0.51
1:Y:58:ASP:HA	1:Y:61:LYS:HE2	1.92	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

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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: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: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: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: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:E:332:GLU:CD	1:E:335:ARG:HH21	2.15	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:I:98:GLN:HG2	1:K:372:LEU:HD12	1.94	0.49
1:Q:137:MET:O	1:Q:249:ASN:HB2	2.12	0.49
1:Q:84:THR:HG23	1:S:262:ASP:HB3	1.95	0.49
1:S:161:PRO:HB3	1:S:163:GLU:OE2	2.12	0.49
1:G:275:MET:HE2	1:I:270:ILE:HD11	1.94	0.49
1:K:245:ILE:HG23	1:K:387:LEU:HD23	1.94	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: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

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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: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
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:A:58:ASP:OD1	1:A:261:LYS:NZ	2.46	0.48
1:K:341:TYR:CD2	1:K:348:ASP:HB2	2.49	0.48
1:I:430:VAL:HG22	1:K:435:GLY:HA3	1.95	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: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: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: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: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:K:267:TYR:OH	1:M:339:GLU:OE2	2.26	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: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:U:128:ASP:HA	1:W:379:ARG:HD2	1.97	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
1:Q:98:GLN:HG2	1:S:372:LEU:HD12	1.96	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
2:N:10:UNK:HA	2:N:15:UNK:HA	1.96	0.47
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:146:HIS:HD2	1:S:243:PRO:O	1.97	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: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: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: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:W:57:ASN:C	1:W:59:ILE:N	2.68	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: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: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: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:376:MET:HG3	1:E:379:ARG:HH21	1.82	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:Q:66:TYR:CD2	1:Q:76:ASP:HB3	2.52	0.45
1:I:134:VAL:HA	1:I:137:MET:HE2	1.98	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:E:275:MET:HE1	1:G:270:ILE:HD11	1.97	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:HD22	1:Q:349:ASN:H	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:E:134:VAL:HA	1:E:137:MET:CE	2.46	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: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: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: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:S:57:ASN:C	1:S:59:ILE:N	2.70	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: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:H	1:K:349:ASN:ND2	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:89:HIS:NE2	1:W:139:ASN:ND2	2.66	0.44
1:W:58:ASP:OD1	1:W:261:LYS:NZ	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:10:UNK:HA	2:R:15:UNK:HA	1.98	0.44
1:S:57:ASN:C	1:S:59:ILE:H	2.20	0.44
1:U:146:HIS:HD2	1:U:243:PRO:O	2.00	0.44
1:U:250:ASN:ND2	1:U:254:VAL:HG23	2.33	0.44
1:A:266:ASN:HB3	1:Y:275:MET:HE3	1.98	0.44
1:A:275:MET:HE1	1:C:266:ASN:HB3	2.00	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: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:W:275:MET:HE2	1:Y:270:ILE:HD11	1.99	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:112:LYS:O	1:S:116:GLU:HG3	2.17	0.44
1:S:81:ASN:ND2	1:S:83:ARG:HD3	2.33	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:M:49:GLY:HA3	1:M:139:ASN:O	2.17	0.44
1:Q:349:ASN:N	1:Q:349:ASN:ND2	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: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:W:57:ASN:C	1:W:59:ILE:H	2.21	0.44
1:E:324:ILE:HG22	1:E:326:VAL:HG23	1.99	0.44
1:W:275:MET:HE1	1:Y:266:ASN:HB3	1.99	0.44
1:A:145:TRP:CE2	1:A:247:PHE:HE1	2.36	0.43
1:C:58:ASP:OD1	1:C:261:LYS:NZ	2.51	0.43
1:G:275:MET:CE	1:I:270:ILE:HD11	2.48	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: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: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:122:ALA:HB1	1:A:126: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:C:275:MET:HE3	1:E:266:ASN:HB3	2.00	0.43
1:G:59:ILE:O	1:G:59:ILE:HG12	2.18	0.43
1:Q:348:ASP:C	1:Q:348:ASP:OD1	2.57	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:101:VAL:O	1:O:101:VAL:CG1	2.67	0.43
1:O:42:ASN:HA	1:O:43:PRO:HD3	1.90	0.43
1:Q:333:LEU:HD23	1:Q:333:LEU:HA	1.82	0.43
1:U:57:ASN:CG	1:U:85:SER:HB2	2.39	0.43
1:W:146:HIS:CE1	1:W:148:PHE:HB3	2.54	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: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:CG1	1:U:101:VAL:O	2.67	0.43
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: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: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: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:ND2	1:G:349:ASN:H	2.17	0.42
1:I:275:MET:CE	1:K:266:ASN:HB3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:308:VAL:HG11	1:K:288:LEU:HD12	2.00	0.42
1:E:58:ASP:OD1	1:E:261:LYS:NZ	2.49	0.42
1:U:134:VAL:HA	1:U:137:MET:HE2	2.01	0.42
1:C:134:VAL:HA	1:C:137:MET:CE	2.49	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:Y:447:ASN:HA	1:Y:448:PRO:HD3	1.94	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:I:95:GLN:HA	1:K:372:LEU:HD11	2.01	0.42
1:S:437:ILE:HG13	1:S:437:ILE:H	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: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:OE1	1:Q:35:GLN:HA	2.19	0.42
1:A:134:VAL:HA	1:A:137:MET:CE	2.50	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:U:437:ILE:HG13	1:U:437:ILE:H	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:W:267:TYR:O	1:W:271:THR:OG1	2.37	0.41
1:Y:147:PRO:HD2	1:Y:243:PRO:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
1:A:89:HIS:NE2	1:A:139:ASN:ND2	2.68	0.41
1:E:57:ASN:N	1:E:57:ASN:OD1	2.52	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:324:ILE:CG2	1:I:326:VAL:HG23	2.51	0.41
1:K:295:ASN:HA	1:K:296:PRO:HD3	1.88	0.41
1:I:304:ARG:NH2	1:K:76:ASP:HB2	2.20	0.41
1:K:84:THR:HG23	1:M:262:ASP:HB3	2.01	0.41
1:M:57:ASN:OD1	1:M:57:ASN:N	2.54	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:S:275:MET:CE	1:U:270:ILE:HD11	2.45	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:I:129:ILE:HG22	1:I:145:TRP:CZ3	2.55	0.41
1:G:98:GLN:HG2	1:I:372:LEU:HD12	2.02	0.41
1:M:53:TYR:HB2	1:M:139:ASN:HD21	1.85	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: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:K:64:ARG:NH2	1:K:79:LYS:HD3	2.36	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:146:HIS:CE1	1:G:148:PHE:HB3	2.56	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:G:430:VAL:HG22	1:I:435:GLY:HA3	2.02	0.41
1:O:130:LEU:O	1:O:134:VAL:HG23	2.20	0.41
1:Q:57:ASN:CG	1:Q:85:SER:HB2	2.41	0.41
1:E:122:ALA:HB1	1:E:126:PHE:CD2	2.55	0.41
1:G:142:ILE:HD12	1:G:248:LYS:HG2	2.03	0.41
1:I:251:GLU:OE1	1:I:251:GLU:HA	2.21	0.41
1:I:90:LYS:NZ	1:I:94:ASP:OD1	2.53	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: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:E:275:MET:HE1	1:G:270:ILE:CD1	2.51	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:Q:275:MET:HE1	1:S:266:ASN:HB3	2.03	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:C:349:ASN:H	1:C:349:ASN:ND2	2.19	0.40
1:K:437:ILE:HG13	1:K:437:ILE:H	1.70	0.40
1:W:33:MET:HG2	1:W:34:ILE:N	2.35	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: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: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: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

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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: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
1:C:146:HIS:CE1	1:C:148:PHE:HB3	2.56	0.40
1:W:349:ASN:HD22	1:W:349:ASN:H	1.67	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
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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	366/503 (73%)	333 (91%)	31 (8%)	2 (0%)	29	61
1	C	366/503 (73%)	337 (92%)	26 (7%)	3 (1%)	19	51
1	E	366/503 (73%)	338 (92%)	26 (7%)	2 (0%)	29	61
1	G	366/503 (73%)	331 (90%)	33 (9%)	2 (0%)	29	61
1	I	366/503 (73%)	332 (91%)	32 (9%)	2 (0%)	29	61
1	K	366/503 (73%)	339 (93%)	24 (7%)	3 (1%)	19	51
1	M	366/503 (73%)	335 (92%)	29 (8%)	2 (0%)	29	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	366/503 (73%)	337 (92%)	27 (7%)	2 (0%)	29	61
1	Q	366/503 (73%)	343 (94%)	21 (6%)	2 (0%)	29	61
1	S	366/503 (73%)	333 (91%)	29 (8%)	4 (1%)	14	44
1	U	366/503 (73%)	337 (92%)	26 (7%)	3 (1%)	19	51
1	W	366/503 (73%)	338 (92%)	27 (7%)	1 (0%)	41	72
1	Y	366/503 (73%)	336 (92%)	27 (7%)	3 (1%)	19	51
All	All	4758/6539 (73%)	4369 (92%)	358 (8%)	31 (1%)	22	55

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	296/436 (68%)	270 (91%)	26 (9%)	10 33
1	C	296/436 (68%)	270 (91%)	26 (9%)	10 33
1	E	296/436 (68%)	268 (90%)	28 (10%)	8 29
1	G	296/436 (68%)	265 (90%)	31 (10%)	7 25
1	I	296/436 (68%)	267 (90%)	29 (10%)	8 28
1	K	296/436 (68%)	265 (90%)	31 (10%)	7 25
1	M	296/436 (68%)	265 (90%)	31 (10%)	7 25
1	O	296/436 (68%)	266 (90%)	30 (10%)	7 27
1	Q	296/436 (68%)	263 (89%)	33 (11%)	6 22
1	S	296/436 (68%)	260 (88%)	36 (12%)	5 18
1	U	296/436 (68%)	265 (90%)	31 (10%)	7 25
1	W	296/436 (68%)	265 (90%)	31 (10%)	7 25
1	Y	296/436 (68%)	269 (91%)	27 (9%)	9 32
All	All	3848/5668 (68%)	3458 (90%)	390 (10%)	7 27

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, 95^{th} 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%)	0.96	61 (16%) 1 2	140, 140, 140, 140	0
1	C	370/503 (73%)	1.10	72 (19%) 1 1	140, 140, 140, 140	0
1	E	370/503 (73%)	1.14	73 (19%) 1 1	140, 140, 140, 140	0
1	G	370/503 (73%)	0.94	67 (18%) 1 1	140, 140, 140, 140	0
1	I	370/503 (73%)	0.95	63 (17%) 1 2	140, 140, 140, 140	0
1	K	370/503 (73%)	0.94	57 (15%) 2 2	140, 140, 140, 140	0
1	M	370/503 (73%)	0.97	61 (16%) 1 2	140, 140, 140, 140	0
1	O	370/503 (73%)	0.85	53 (14%) 2 3	140, 140, 140, 140	0
1	Q	370/503 (73%)	0.87	54 (14%) 2 3	140, 140, 140, 140	0
1	S	370/503 (73%)	0.80	46 (12%) 4 5	140, 140, 140, 140	0
1	U	370/503 (73%)	0.74	33 (8%) 9 11	140, 140, 140, 140	0
1	W	370/503 (73%)	0.74	48 (12%) 3 4	140, 140, 140, 140	0
1	Y	370/503 (73%)	0.96	63 (17%) 1 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%)	0.92	751 (15%) 2 2	140, 140, 140, 140	0

All (751) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	315	GLY	10.6
1	Y	292	ASP	9.9
1	Y	291	TYR	9.6
1	O	404	PHE	9.0
1	U	291	TYR	8.7
1	S	314	ASP	8.3
1	C	70	ALA	7.9
1	C	68	ASP	7.8
1	A	315	GLY	7.6
1	A	166	ILE	7.6
1	M	243	PRO	7.5
1	O	410	LEU	7.4
1	M	315	GLY	7.4
1	I	33	MET	7.3
1	I	314	ASP	7.0
1	S	312	SER	7.0
1	W	33	MET	7.0
1	M	316	GLY	6.9
1	K	406	PRO	6.8
1	S	315	GLY	6.7
1	E	148	PHE	6.7
1	G	113	THR	6.6
1	C	69	ALA	6.4
1	E	316	GLY	6.4
1	E	33	MET	6.3
1	A	314	ASP	6.3
1	G	243	PRO	6.3
1	G	117	TYR	6.3
1	K	243	PRO	6.2
1	C	124	ASP	6.2
1	Y	33	MET	6.2
1	E	391	PHE	6.1
1	C	244	ILE	6.1
1	C	74	LEU	6.1
1	O	292	ASP	6.0
1	S	292	ASP	6.0
1	U	292	ASP	6.0
1	A	417	THR	6.0
1	E	456	GLU	6.0
1	E	294	GLU	5.9
1	K	34	ILE	5.8
1	Y	358	ALA	5.8

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Mol	Chain	Res	Type	RSRZ
1	M	404	PHE	5.7
1	A	316	GLY	5.7
1	S	437	ILE	5.7
1	M	244	ILE	5.6
1	E	154	GLU	5.6
1	G	30	ASP	5.6
1	S	311	VAL	5.5
1	U	438	MET	5.5
1	K	314	ASP	5.5
1	I	151	GLU	5.4
1	Q	447	ASN	5.4
1	A	34	ILE	5.4
1	M	74	LEU	5.4
1	K	33	MET	5.4
1	I	316	GLY	5.4
1	C	438	MET	5.3
1	E	34	ILE	5.3
1	E	392	PHE	5.3
1	G	396	LEU	5.3
1	Q	295	ASN	5.3
1	A	398	ASN	5.3
1	I	357	GLY	5.3
1	O	392	PHE	5.2
1	Y	450	VAL	5.2
1	Q	392	PHE	5.2
1	C	166	ILE	5.2
1	G	244	ILE	5.1
1	A	239	TRP	5.1
1	M	113	THR	5.1
1	I	437	ILE	5.1
1	Y	410	LEU	5.1
1	A	33	MET	5.0
1	W	32	THR	5.0
1	Q	404	PHE	5.0
1	I	349	ASN	5.0
1	Y	357	GLY	5.0
1	M	314	ASP	5.0
1	C	149	VAL	5.0
1	C	392	PHE	4.9
1	W	353	THR	4.9
1	O	314	ASP	4.9
1	O	166	ILE	4.9

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Mol	Chain	Res	Type	RSRZ
1	G	166	ILE	4.9
1	O	358	ALA	4.9
1	C	154	GLU	4.8
1	I	110	ASP	4.8
1	I	394	GLU	4.8
1	I	464	MET	4.8
1	C	449	PHE	4.8
1	A	305	TYR	4.8
1	C	155	PHE	4.7
1	E	353	THR	4.7
1	S	68	ASP	4.7
1	G	155	PHE	4.7
1	Y	432	GLY	4.7
1	Y	401	LYS	4.7
1	Y	143	GLU	4.7
1	Y	402	GLY	4.7
1	M	72	GLN	4.7
1	C	395	TYR	4.7
1	C	37	LEU	4.7
1	E	438	MET	4.7
1	U	309	ILE	4.6
1	M	33	MET	4.6
1	M	410	LEU	4.6
1	A	388	PHE	4.6
1	C	117	TYR	4.6
1	K	353	THR	4.6
1	O	244	ILE	4.6
1	E	155	PHE	4.6
1	Y	404	PHE	4.6
1	G	120	GLU	4.6
1	Q	74	LEU	4.6
1	A	405	ASN	4.6
1	Q	113	THR	4.5
1	I	422	ASP	4.5
1	Y	438	MET	4.5
1	E	68	ASP	4.5
1	Q	40	GLU	4.5
1	A	353	THR	4.5
1	M	30	ASP	4.5
1	C	417	THR	4.5
1	E	145	TRP	4.5
1	E	352	GLU	4.5

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Mol	Chain	Res	Type	RSRZ
1	K	239	TRP	4.5
1	Q	314	ASP	4.4
1	C	410	LEU	4.4
1	G	121	LEU	4.4
1	K	37	LEU	4.4
1	U	30	ASP	4.4
1	U	465	ASN	4.4
1	M	399	THR	4.4
1	I	358	ALA	4.3
1	E	422	ASP	4.3
1	E	166	ILE	4.3
1	I	117	TYR	4.3
1	C	291	TYR	4.3
1	E	404	PHE	4.3
1	U	404	PHE	4.3
1	K	316	GLY	4.3
1	E	40	GLU	4.3
1	K	148	PHE	4.3
1	O	243	PRO	4.3
1	O	398	ASN	4.3
1	I	245	ILE	4.3
1	I	37	LEU	4.2
1	U	398	ASN	4.2
1	W	261	LYS	4.2
1	Q	71	GLY	4.2
1	Q	312	SER	4.2
1	A	155	PHE	4.2
1	E	458	ALA	4.2
1	W	67	TYR	4.2
1	W	241	ARG	4.2
1	O	291	TYR	4.2
1	M	239	TRP	4.2
1	G	401	LYS	4.1
1	K	32	THR	4.1
1	W	357	GLY	4.1
1	E	243	PRO	4.1
1	U	120	GLU	4.1
1	W	73	GLN	4.1
1	O	359	THR	4.1
1	M	242	VAL	4.1
1	S	358	ALA	4.1
1	E	70	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	38	ILE	4.0
1	I	122	ALA	4.0
1	A	54	MET	4.0
1	M	71	GLY	4.0
1	A	317	VAL	4.0
1	G	118	VAL	4.0
1	O	394	GLU	3.9
1	K	410	LEU	3.9
1	I	393	ALA	3.9
1	W	288	LEU	3.9
1	U	310	LYS	3.9
1	I	149	VAL	3.9
1	S	377	ALA	3.9
1	W	30	ASP	3.9
1	I	438	MET	3.9
1	E	467	TYR	3.9
1	S	239	TRP	3.9
1	Y	34	ILE	3.9
1	G	53	TYR	3.9
1	E	47	LEU	3.9
1	K	460	ILE	3.9
1	K	401	LYS	3.8
1	C	239	TRP	3.8
1	U	65	THR	3.8
1	W	287	VAL	3.8
1	K	315	GLY	3.8
1	M	120	GLU	3.8
1	Q	66	TYR	3.8
1	Y	287	VAL	3.8
1	Y	400	GLY	3.8
1	W	292	ASP	3.8
1	I	401	LYS	3.8
1	Q	398	ASN	3.8
1	C	243	PRO	3.7
1	K	402	GLY	3.7
1	M	437	ILE	3.7
1	A	261	LYS	3.7
1	Q	67	TYR	3.7
1	G	39	ASP	3.7
1	K	405	ASN	3.7
1	U	293	GLY	3.7
1	I	442	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	467	TYR	3.7
1	I	142	ILE	3.7
1	K	352	GLU	3.7
1	E	389	PHE	3.7
1	G	444	VAL	3.7
1	O	312	SER	3.7
1	G	34	ILE	3.7
1	A	169	TYR	3.7
1	C	40	GLU	3.6
1	I	239	TRP	3.6
1	C	66	TYR	3.6
1	E	311	VAL	3.6
1	Q	437	ILE	3.6
1	G	239	TRP	3.6
1	W	404	PHE	3.6
1	G	437	ILE	3.6
1	O	456	GLU	3.6
1	S	109	SER	3.6
1	K	247	PHE	3.6
1	A	438	MET	3.6
1	A	43	PRO	3.6
1	Y	37	LEU	3.6
1	K	354	ILE	3.6
1	Y	353	THR	3.6
1	G	122	ALA	3.6
1	M	63	ARG	3.6
1	G	398	ASN	3.6
1	A	156	ASP	3.6
1	O	311	VAL	3.5
1	S	309	ILE	3.5
1	C	316	GLY	3.5
1	C	429	LEU	3.5
1	A	167	VAL	3.5
1	C	167	VAL	3.5
1	Y	436	GLY	3.5
1	C	314	ASP	3.5
1	M	43	PRO	3.5
1	C	386	ARG	3.5
1	U	437	ILE	3.5
1	W	239	TRP	3.5
1	E	167	VAL	3.5
1	W	114	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	G	32	THR	3.5
1	C	125	ASP	3.5
1	E	117	TYR	3.5
1	O	114	LEU	3.5
1	C	315	GLY	3.4
1	G	165	MET	3.4
1	Y	239	TRP	3.4
1	G	466	GLN	3.4
1	A	444	VAL	3.4
1	G	111	ASN	3.4
1	K	145	TRP	3.4
1	S	72	GLN	3.4
1	Q	458	ALA	3.4
1	Y	39	ASP	3.4
1	I	72	GLN	3.4
1	C	391	PHE	3.4
1	M	34	ILE	3.4
1	Q	39	ASP	3.4
1	Q	461	GLU	3.4
1	M	398	ASN	3.4
1	Q	243	PRO	3.4
1	M	392	PHE	3.4
1	C	353	THR	3.4
1	I	436	GLY	3.4
1	Q	353	THR	3.4
1	S	389	PHE	3.3
1	M	78	THR	3.3
1	O	149	VAL	3.3
1	C	278	PHE	3.3
1	S	406	PRO	3.3
1	C	437	ILE	3.3
1	M	403	ASP	3.3
1	A	465	ASN	3.3
1	C	398	ASN	3.3
1	C	358	ALA	3.3
1	C	404	PHE	3.3
1	O	148	PHE	3.3
1	G	115	LEU	3.3
1	U	33	MET	3.3
1	E	244	ILE	3.3
1	O	406	PRO	3.3
1	G	242	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	G	292	ASP	3.3
1	Q	444	VAL	3.3
1	K	392	PHE	3.3
1	I	166	ILE	3.3
1	Y	120	GLU	3.3
1	C	165	MET	3.3
1	G	114	LEU	3.3
1	M	145	TRP	3.3
1	G	309	ILE	3.3
1	E	291	TYR	3.3
1	M	389	PHE	3.3
1	O	239	TRP	3.3
1	Q	73	GLN	3.3
1	W	294	GLU	3.3
1	W	34	ILE	3.3
1	A	292	ASP	3.3
1	G	72	GLN	3.2
1	K	109	SER	3.2
1	Q	460	ILE	3.2
1	E	314	ASP	3.2
1	W	448	PRO	3.2
1	K	458	ALA	3.2
1	A	389	PHE	3.2
1	G	403	ASP	3.2
1	K	448	PRO	3.2
1	Y	63	ARG	3.2
1	C	150	ASP	3.2
1	K	68	ASP	3.2
1	U	39	ASP	3.2
1	S	458	ALA	3.2
1	M	419	ILE	3.2
1	C	65	THR	3.2
1	O	34	ILE	3.2
1	O	293	GLY	3.2
1	W	293	GLY	3.2
1	O	38	ILE	3.2
1	G	385	LEU	3.2
1	O	444	VAL	3.2
1	E	317	VAL	3.2
1	G	287	VAL	3.2
1	M	354	ILE	3.1
1	M	450	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	419	ILE	3.1
1	U	315	GLY	3.1
1	K	389	PHE	3.1
1	E	410	LEU	3.1
1	S	313	GLY	3.1
1	A	145	TRP	3.1
1	E	449	PHE	3.1
1	M	292	ASP	3.1
1	Y	155	PHE	3.1
1	W	395	TYR	3.1
1	Q	354	ILE	3.1
1	S	307	SER	3.1
1	E	165	MET	3.1
1	U	462	GLU	3.1
1	W	35	GLN	3.1
1	O	442	THR	3.1
1	W	399	THR	3.1
1	A	69	ALA	3.1
1	I	305	TYR	3.1
1	E	293	GLY	3.1
1	M	121	LEU	3.1
1	Q	239	TRP	3.1
1	K	35	GLN	3.1
1	A	163	GLU	3.1
1	S	452	ASP	3.1
1	E	399	THR	3.1
1	K	399	THR	3.1
1	I	463	GLU	3.1
1	Y	40	GLU	3.1
1	Q	33	MET	3.1
1	S	243	PRO	3.1
1	G	154	GLU	3.1
1	Q	435	GLY	3.0
1	M	32	THR	3.0
1	A	293	GLY	3.0
1	S	40	GLU	3.0
1	C	357	GLY	3.0
1	M	77	ASP	3.0
1	M	440	LYS	3.0
1	A	456	GLU	3.0
1	Q	389	PHE	3.0
1	K	321	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	Q	436	GLY	3.0
1	E	406	PRO	3.0
1	A	68	ASP	3.0
1	K	292	ASP	3.0
1	O	315	GLY	3.0
1	O	146	HIS	3.0
1	I	404	PHE	3.0
1	M	414	PHE	3.0
1	M	37	LEU	3.0
1	E	453	PRO	3.0
1	I	143	GLU	3.0
1	I	36	LYS	3.0
1	K	112	LYS	2.9
1	C	41	HIS	2.9
1	G	112	LYS	2.9
1	Y	66	TYR	2.9
1	Y	69	ALA	2.9
1	K	404	PHE	2.9
1	Q	72	GLN	2.9
1	A	466	GLN	2.9
1	Q	290	ASN	2.9
1	K	449	PHE	2.9
1	A	414	PHE	2.9
1	Q	414	PHE	2.9
1	Y	295	ASN	2.9
1	Y	392	PHE	2.9
1	Y	356	GLY	2.9
1	M	449	PHE	2.9
1	Y	406	PRO	2.9
1	E	121	LEU	2.9
1	I	388	PHE	2.9
1	Y	68	ASP	2.9
1	A	352	GLU	2.9
1	Q	296	PRO	2.9
1	A	354	ILE	2.9
1	K	114	LEU	2.9
1	O	37	LEU	2.9
1	K	72	GLN	2.9
1	S	310	LYS	2.9
1	G	38	ILE	2.9
1	M	444	VAL	2.9
1	C	73	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	244	ILE	2.8
1	O	66	TYR	2.8
1	K	39	ASP	2.8
1	C	34	ILE	2.8
1	G	29	PRO	2.8
1	M	75	VAL	2.8
1	U	89	HIS	2.8
1	A	47	LEU	2.8
1	O	437	ILE	2.8
1	A	107	PHE	2.8
1	S	299	PHE	2.8
1	E	395	TYR	2.8
1	Y	433	VAL	2.8
1	S	438	MET	2.8
1	O	445	ALA	2.8
1	E	315	GLY	2.8
1	G	288	LEU	2.8
1	W	74	LEU	2.8
1	G	246	PRO	2.8
1	U	64	ARG	2.8
1	A	404	PHE	2.8
1	Q	118	VAL	2.8
1	S	316	GLY	2.8
1	O	354	ILE	2.8
1	G	307	SER	2.8
1	I	389	PHE	2.8
1	G	33	MET	2.8
1	E	72	GLN	2.8
1	S	165	MET	2.8
1	A	139	ASN	2.8
1	E	67	TYR	2.8
1	C	466	GLN	2.7
1	Y	307	SER	2.7
1	C	126	PHE	2.7
1	C	110	ASP	2.7
1	C	389	PHE	2.7
1	C	29	PRO	2.7
1	M	42	ASN	2.7
1	Y	448	PRO	2.7
1	Q	145	TRP	2.7
1	I	449	PHE	2.7
1	M	355	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	123	ASP	2.7
1	I	353	THR	2.7
1	C	107	PHE	2.7
1	E	152	GLU	2.7
1	I	312	SER	2.7
1	M	353	THR	2.7
1	Q	165	MET	2.7
1	W	412	MET	2.7
1	A	31	THR	2.7
1	I	392	PHE	2.7
1	O	278	PHE	2.7
1	M	309	ILE	2.7
1	Y	290	ASN	2.7
1	I	411	THR	2.7
1	Y	317	VAL	2.7
1	Q	448	PRO	2.7
1	Q	63	ARG	2.7
1	U	436	GLY	2.7
1	Y	293	GLY	2.7
1	G	163	GLU	2.7
1	W	120	GLU	2.7
1	Q	65	THR	2.7
1	I	412	MET	2.7
1	Q	70	ALA	2.7
1	A	65	THR	2.7
1	K	414	PHE	2.6
1	E	153	GLY	2.6
1	O	35	GLN	2.6
1	W	151	GLU	2.6
1	C	145	TRP	2.6
1	S	39	ASP	2.6
1	U	316	GLY	2.6
1	I	246	PRO	2.6
1	W	309	ILE	2.6
1	G	261	LYS	2.6
1	I	124	ASP	2.6
1	U	34	ILE	2.6
1	G	314	ASP	2.6
1	I	32	THR	2.6
1	A	46	LEU	2.6
1	Y	35	GLN	2.6
1	E	289	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	M	65	THR	2.6
1	O	113	THR	2.6
1	G	245	ILE	2.6
1	Q	307	SER	2.6
1	M	397	ARG	2.6
1	I	429	LEU	2.6
1	E	393	ALA	2.6
1	A	433	VAL	2.6
1	C	361	PRO	2.6
1	K	244	ILE	2.6
1	A	410	LEU	2.6
1	C	33	MET	2.6
1	M	89	HIS	2.6
1	E	388	PHE	2.5
1	U	356	GLY	2.5
1	M	68	ASP	2.5
1	I	244	ILE	2.5
1	E	257	LEU	2.5
1	Q	122	ALA	2.5
1	U	32	THR	2.5
1	M	436	GLY	2.5
1	I	261	LYS	2.5
1	M	401	LYS	2.5
1	S	354	ILE	2.5
1	O	355	GLY	2.5
1	G	392	PHE	2.5
1	G	462	GLU	2.5
1	C	355	GLY	2.5
1	Q	36	LYS	2.5
1	G	86	HIS	2.5
1	Y	352	GLU	2.5
1	K	293	GLY	2.5
1	K	356	GLY	2.5
1	U	296	PRO	2.5
1	I	465	ASN	2.5
1	E	63	ARG	2.5
1	S	353	THR	2.5
1	M	29	PRO	2.5
1	U	68	ASP	2.5
1	U	159	ILE	2.5
1	W	437	ILE	2.5
1	C	242	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	M	114	LEU	2.4
1	C	422	ASP	2.4
1	E	437	ILE	2.4
1	M	310	LYS	2.4
1	S	404	PHE	2.4
1	Q	114	LEU	2.4
1	O	52	TYR	2.4
1	W	389	PHE	2.4
1	Y	32	THR	2.4
1	C	297	LYS	2.4
1	Q	48	LYS	2.4
1	Y	296	PRO	2.4
1	O	414	PHE	2.4
1	Y	409	GLU	2.4
1	S	291	TYR	2.4
1	I	396	LEU	2.4
1	O	457	LEU	2.4
1	E	305	TYR	2.4
1	G	110	ASP	2.4
1	G	402	GLY	2.4
1	I	120	GLU	2.4
1	I	165	MET	2.4
1	S	308	VAL	2.4
1	W	75	VAL	2.4
1	A	81	ASN	2.4
1	C	300	THR	2.4
1	M	406	PRO	2.4
1	Y	309	ILE	2.4
1	E	307	SER	2.4
1	M	157	TYR	2.4
1	E	30	ASP	2.4
1	A	110	ASP	2.4
1	Y	355	GLY	2.4
1	C	53	TYR	2.4
1	K	291	TYR	2.4
1	A	32	THR	2.4
1	K	242	VAL	2.3
1	Q	315	GLY	2.3
1	C	122	ALA	2.3
1	E	288	LEU	2.3
1	Y	437	ILE	2.3
1	A	430	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	Y	399	THR	2.3
1	W	422	ASP	2.3
1	Y	165	MET	2.3
1	C	394	GLU	2.3
1	Y	398	ASN	2.3
1	A	358	ALA	2.3
1	W	467	TYR	2.3
1	Y	405	ASN	2.3
1	I	410	LEU	2.3
1	S	289	LYS	2.3
1	O	240	GLY	2.3
1	W	39	ASP	2.3
1	G	75	VAL	2.3
1	E	261	LYS	2.3
1	Q	121	LEU	2.3
1	A	157	TYR	2.3
1	E	169	TYR	2.3
1	C	148	PHE	2.3
1	G	156	ASP	2.3
1	W	396	LEU	2.3
1	E	256	ASP	2.3
1	G	119	ASN	2.3
1	K	371	ASP	2.3
1	O	64	ARG	2.3
1	W	438	MET	2.3
1	E	255	SER	2.3
1	O	377	ALA	2.3
1	U	389	PHE	2.3
1	U	391	PHE	2.3
1	E	29	PRO	2.3
1	Y	157	TYR	2.3
1	W	432	GLY	2.3
1	E	278	PHE	2.3
1	O	117	TYR	2.3
1	O	389	PHE	2.3
1	Y	278	PHE	2.3
1	K	149	VAL	2.2
1	K	391	PHE	2.2
1	G	85	SER	2.2
1	A	321	ARG	2.2
1	C	403	ASP	2.2
1	E	309	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	437	ILE	2.2
1	E	452	ASP	2.2
1	I	391	PHE	2.2
1	W	242	VAL	2.2
1	I	461	GLU	2.2
1	S	352	GLU	2.2
1	K	317	VAL	2.2
1	K	400	GLY	2.2
1	O	405	ASN	2.2
1	M	166	ILE	2.2
1	Y	389	PHE	2.2
1	K	66	TYR	2.2
1	K	302	ASN	2.2
1	M	66	TYR	2.2
1	O	39	ASP	2.2
1	S	405	ASN	2.2
1	Y	403	ASP	2.2
1	S	320	LEU	2.2
1	E	86	HIS	2.2
1	G	404	PHE	2.2
1	M	361	PRO	2.2
1	Q	449	PHE	2.2
1	A	118	VAL	2.2
1	K	122	ALA	2.2
1	Y	70	ALA	2.2
1	W	359	THR	2.2
1	Q	157	TYR	2.2
1	S	37	LEU	2.2
1	S	111	ASN	2.2
1	Q	294	GLU	2.2
1	O	458	ALA	2.2
1	C	349	ASN	2.2
1	K	438	MET	2.2
1	W	405	ASN	2.2
1	G	102	GLY	2.2
1	G	286	TYR	2.2
1	G	443	ALA	2.2
1	S	67	TYR	2.2
1	A	147	PRO	2.2
1	E	414	PHE	2.2
1	K	299	PHE	2.2
1	E	403	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	58	ASP	2.2
1	Y	41	HIS	2.2
1	G	148	PHE	2.1
1	W	72	GLN	2.1
1	S	75	VAL	2.1
1	U	321	ARG	2.1
1	Y	244	ILE	2.1
1	I	400	GLY	2.1
1	A	291	TYR	2.1
1	Y	114	LEU	2.1
1	G	35	GLN	2.1
1	G	71	GLY	2.1
1	S	357	GLY	2.1
1	G	467	TYR	2.1
1	Y	145	TRP	2.1
1	M	466	GLN	2.1
1	A	37	LEU	2.1
1	C	128	ASP	2.1
1	O	403	ASP	2.1
1	K	113	THR	2.1
1	W	88	TRP	2.1
1	W	283	GLN	2.1
1	W	115	LEU	2.1
1	Y	117	TYR	2.1
1	Q	32	THR	2.1
1	W	354	ILE	2.1
1	E	115	LEU	2.1
1	O	74	LEU	2.1
1	I	109	SER	2.1
1	W	392	PHE	2.1
1	A	432	GLY	2.1
1	I	35	GLN	2.1
1	I	398	ASN	2.1
1	S	32	THR	2.1
1	Q	155	PHE	2.1
1	K	40	GLU	2.1
1	S	295	ASN	2.1
1	O	449	PHE	2.1
1	C	109	SER	2.1
1	I	427	GLN	2.1
1	A	399	THR	2.1
1	G	349	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	M	415	THR	2.1
1	C	419	ILE	2.1
1	C	281	PHE	2.1
1	S	359	THR	2.1
1	C	63	ARG	2.1
1	O	167	VAL	2.1
1	C	245	ILE	2.1
1	U	73	GLN	2.1
1	M	394	GLU	2.1
1	W	433	VAL	2.1
1	S	321	ARG	2.0
1	I	287	VAL	2.0
1	S	290	ASN	2.0
1	K	155	PHE	2.0
1	W	79	LYS	2.0
1	K	304	ARG	2.0
1	O	67	TYR	2.0
1	U	453	PRO	2.0
1	E	321	ARG	2.0
1	I	163	GLU	2.0
1	Y	294	GLU	2.0
1	Q	288	LEU	2.0
1	I	421	ASN	2.0
1	Y	29	PRO	2.0
1	W	56	GLU	2.0
1	E	312	SER	2.0
1	I	118	VAL	2.0
1	G	377	ALA	2.0
1	G	408	LYS	2.0
1	E	357	GLY	2.0
1	Q	313	GLY	2.0
1	C	54	MET	2.0
1	Y	412	MET	2.0
1	E	459	ARG	2.0
1	Q	244	ILE	2.0
1	E	349	ASN	2.0
1	U	163	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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, 95^{th} 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	O	701	1/1	0.71	0.14	140,140,140,140	1
4	CA	O	801	1/1	0.72	0.11	140,140,140,140	0
3	HG	S	701	1/1	0.73	0.13	140,140,140,140	1
4	CA	A	801	1/1	0.79	0.10	140,140,140,140	0
4	CA	M	801	1/1	0.82	0.15	140,140,140,140	0
3	HG	M	701	1/1	0.82	0.14	140,140,140,140	1
3	HG	I	701	1/1	0.86	0.12	140,140,140,140	1
4	CA	S	801	1/1	0.87	0.13	140,140,140,140	0
4	CA	C	801	1/1	0.88	0.08	140,140,140,140	0
3	HG	Q	701	1/1	0.88	0.12	140,140,140,140	1
3	HG	C	701	1/1	0.88	0.19	140,140,140,140	1
4	CA	K	801	1/1	0.90	0.12	140,140,140,140	0
4	CA	U	801	1/1	0.91	0.07	140,140,140,140	0
4	CA	Y	801	1/1	0.91	0.07	140,140,140,140	0
3	HG	A	701	1/1	0.92	0.17	140,140,140,140	1
4	CA	I	801	1/1	0.93	0.05	140,140,140,140	0
4	CA	W	801	1/1	0.93	0.17	140,140,140,140	0
3	HG	W	701	1/1	0.94	0.09	140,140,140,140	1
3	HG	E	701	1/1	0.95	0.28	140,140,140,140	1
4	CA	Q	801	1/1	0.95	0.08	140,140,140,140	0
3	HG	Y	701	1/1	0.95	0.12	140,140,140,140	1
4	CA	G	801	1/1	0.95	0.12	140,140,140,140	0
3	HG	G	701	1/1	0.96	0.11	140,140,140,140	1
3	HG	K	701	1/1	0.96	0.09	140,140,140,140	1
3	HG	U	701	1/1	0.96	0.10	140,140,140,140	1
4	CA	E	801	1/1	0.97	0.07	140,140,140,140	0

6.5 Other polymers (i)

There are no such residues in this entry.