



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 07:41 pm BST

PDB ID : 1D2R
Title : 2.9 Å CRYSTAL STRUCTURE OF LIGAND-FREE TRYPTOPHANYL-TRNA SYNTHETASE: DOMAIN MOVEMENTS FRAGMENT THE ADENINE NUCLEOTIDE BINDING SITE.
Authors : Ilyin, V.A.; Carter Jr., C.W.
Deposited on : 1999-09-27
Resolution : 2.90 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

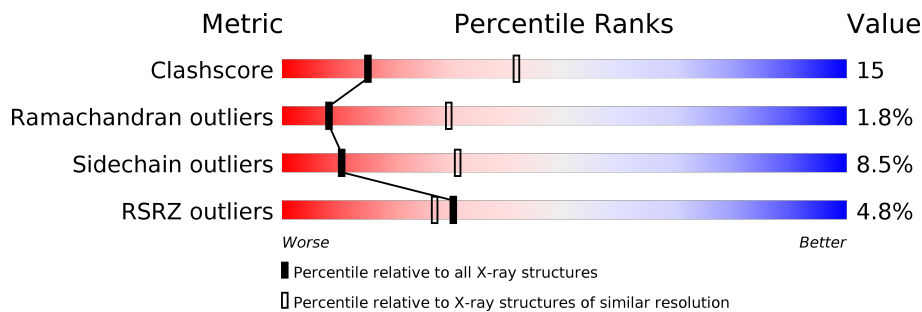
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 $\leq 5\%$. 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	326	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 63%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 32%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange;"></div> </div> <p style="text-align: center;">4% 63% 32% 5%</p>
1	B	326	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 67%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 28%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange;"></div> </div> <p style="text-align: center;">5% 67% 28% . .</p>
1	C	326	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 64%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 30%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange;"></div> </div> <p style="text-align: center;">5% 64% 30% 5%</p>
1	D	326	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 65%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 31%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange;"></div> </div> <p style="text-align: center;">5% 65% 31% .</p>
1	E	326	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 65%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 30%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange;"></div> </div> <p style="text-align: center;">5% 65% 30% 5%</p>
1	F	326	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 68%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 28%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange;"></div> </div> <p style="text-align: center;">5% 68% 28% .</p>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 15480 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.

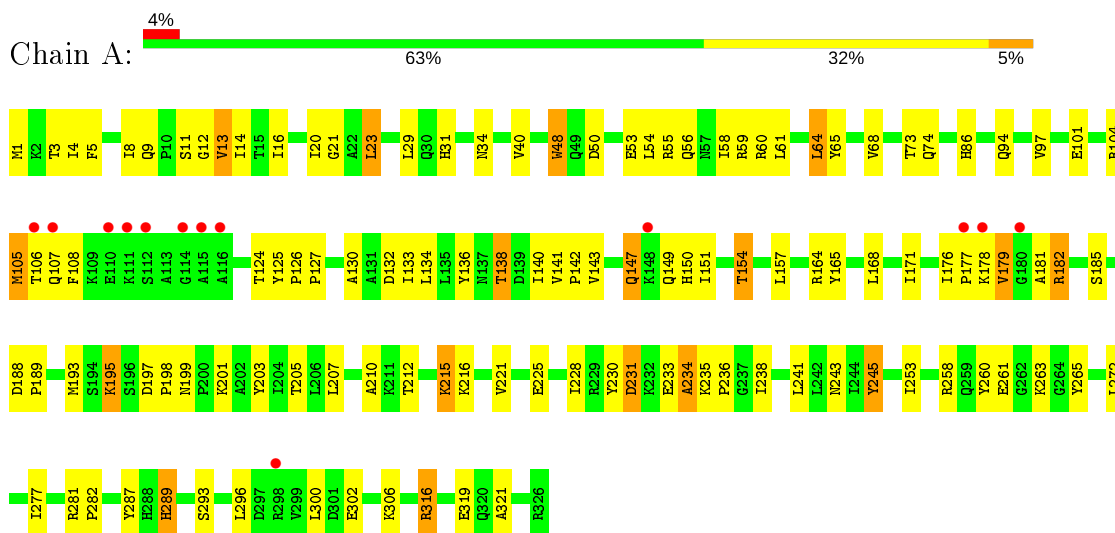
- Molecule 1 is a protein called PROTEIN (TRYPTOPHANYL TRNA SYNTHETASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	326	2580	1635	444	488	13	0	0	0
1	B	326	2580	1635	444	488	13	0	0	0
1	C	326	2580	1635	444	488	13	0	0	0
1	D	326	2580	1635	444	488	13	0	0	0
1	E	326	2580	1635	444	488	13	0	0	0
1	F	326	2580	1635	444	488	13	0	0	0

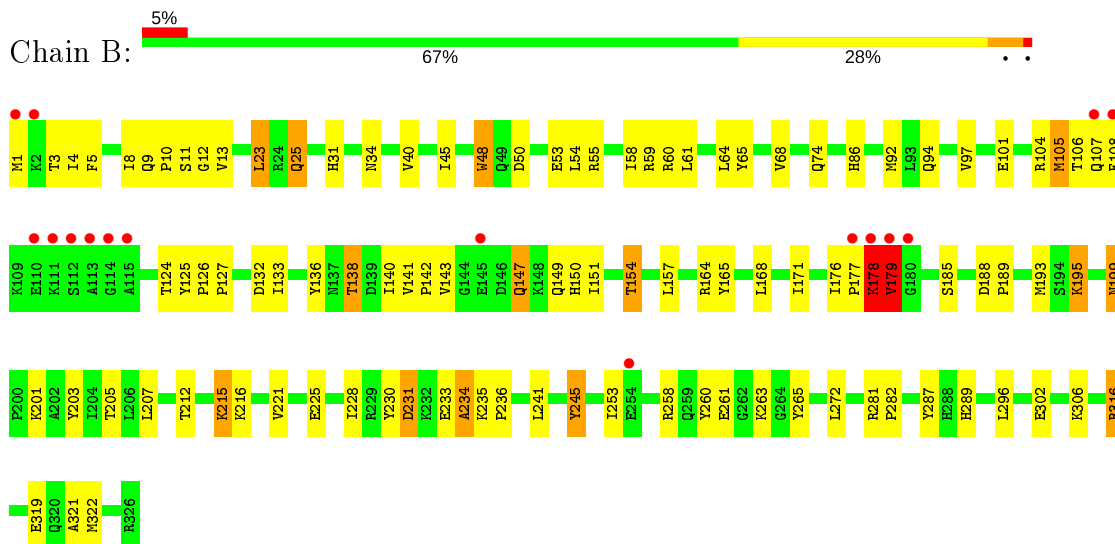
3 Residue-property plots [i](#)

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: PROTEIN (TRYPTOPHANYL TRNA SYNTHETASE)

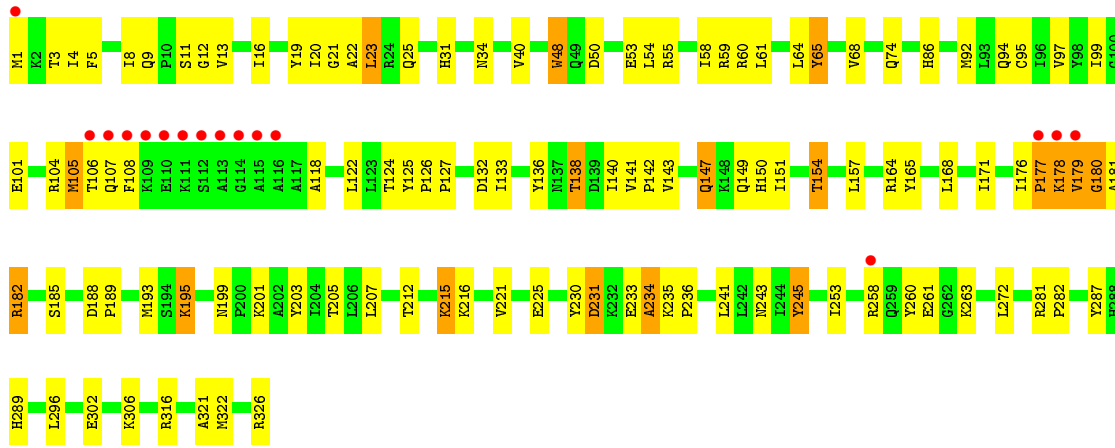


- Molecule 1: PROTEIN (TRYPTOPHANYL TRNA SYNTHETASE)

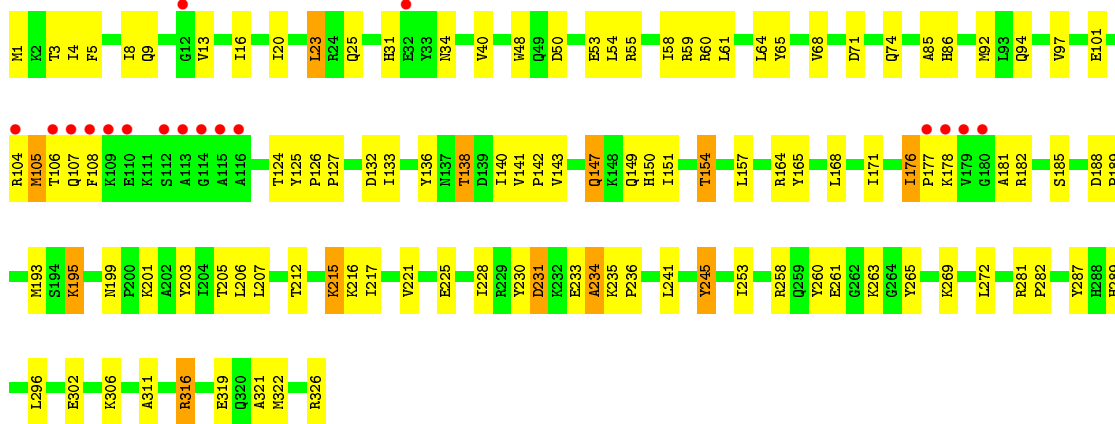


- Molecule 1: PROTEIN (TRYPTOPHANYL TRNA SYNTHETASE)

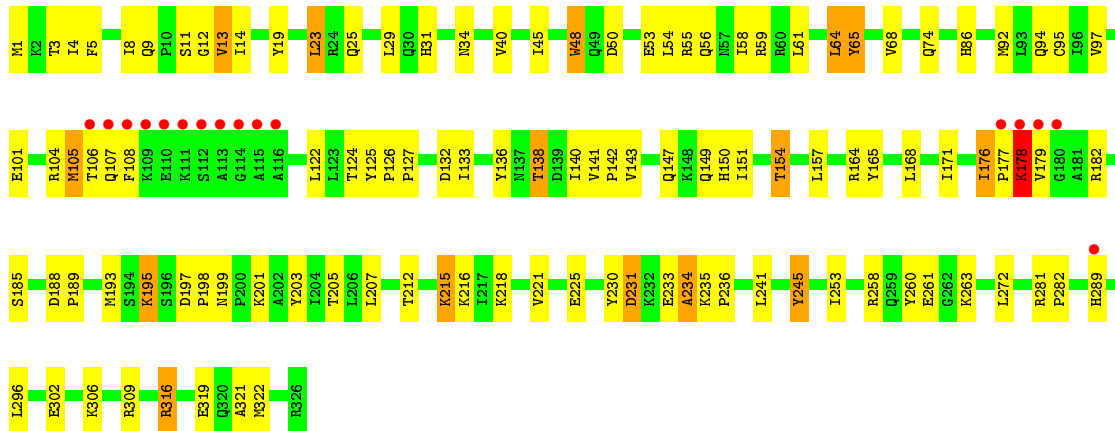




• Molecule 1: PROTEIN (TRYPTOPHANYL TRNA SYNTHETASE)

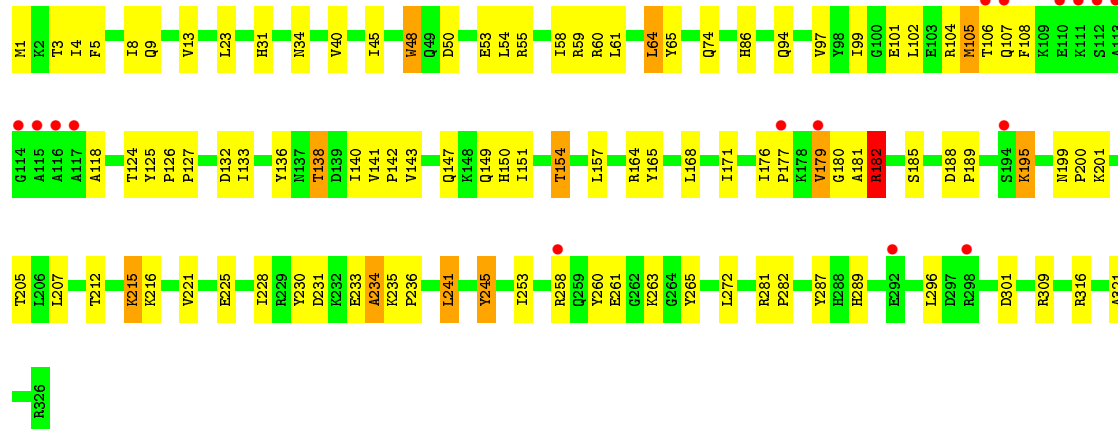


• Molecule 1: PROTEIN (TRYPTOPHANYL TRNA SYNTHETASE)



• Molecule 1: PROTEIN (TRYPTOPHANYL TRNA SYNTHETASE)

Chain F: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	226.76 Å 91.66 Å 156.97 Å 90.00° 132.66° 90.00°	Depositor
Resolution (Å)	10.00 – 2.90 33.85 – 2.90	Depositor EDS
% Data completeness (in resolution range)	74.3 (10.00-2.90) 74.5 (33.85-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.90 Å)	Xtrriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.237 , 0.262 0.220 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	45.6	Xtrriage
Anisotropy	0.100	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 58.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	0.036 for -h-2*1,-k,l	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	15480	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.11 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.3312e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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 i

5.1 Standard geometry i

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.46	0/2628	0.62	2/3552 (0.1%)
1	B	0.47	0/2628	0.67	3/3552 (0.1%)
1	C	0.45	0/2628	0.63	3/3552 (0.1%)
1	D	0.46	0/2628	0.62	2/3552 (0.1%)
1	E	0.45	0/2628	0.63	2/3552 (0.1%)
1	F	0.45	0/2628	0.61	3/3552 (0.1%)
All	All	0.46	0/15768	0.63	15/21312 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	179	VAL	O-C-N	-12.52	101.92	123.20
1	D	234	ALA	O-C-N	10.12	138.90	122.70
1	E	234	ALA	O-C-N	9.78	138.35	122.70
1	A	234	ALA	O-C-N	9.74	138.28	122.70
1	C	234	ALA	O-C-N	9.60	138.05	122.70
1	B	234	ALA	O-C-N	9.23	137.47	122.70
1	F	234	ALA	O-C-N	8.11	135.68	122.70
1	E	234	ALA	CA-C-N	-8.04	99.52	117.20
1	D	234	ALA	CA-C-N	-8.02	99.55	117.20
1	C	234	ALA	CA-C-N	-7.76	100.14	117.20
1	A	234	ALA	CA-C-N	-7.73	100.20	117.20
1	F	234	ALA	CA-C-N	-7.59	100.51	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	234	ALA	CA-C-N	-7.37	101.00	117.20
1	F	180	GLY	N-CA-C	-6.00	98.09	113.10
1	C	180	GLY	N-CA-C	-5.65	98.97	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	179	VAL	Mainchain

5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2580	0	2598	86	0
1	B	2580	0	2598	79	0
1	C	2580	0	2598	90	0
1	D	2580	0	2598	75	0
1	E	2580	0	2598	82	0
1	F	2580	0	2598	71	0
All	All	15480	0	15588	466	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (466) 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:E:195:LYS:H	1:E:195:LYS:HD2	1.30	0.96
1:D:176:ILE:HG13	1:D:177:PRO:HD2	1.49	0.95
1:A:195:LYS:HD2	1:A:195:LYS:H	1.33	0.91
1:F:195:LYS:H	1:F:195:LYS:HD2	1.34	0.90
1:B:177:PRO:O	1:B:178:LYS:HB2	1.72	0.89
1:D:195:LYS:H	1:D:195:LYS:HD2	1.35	0.89
1:A:23:LEU:HD12	1:A:68:VAL:HG11	1.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ILE:HG22	1:A:61:LEU:HD21	1.55	0.87
1:E:11:SER:O	1:E:13:VAL:HG12	1.73	0.87
1:B:195:LYS:H	1:B:195:LYS:HD2	1.40	0.85
1:C:195:LYS:HD2	1:C:195:LYS:H	1.39	0.85
1:D:8:ILE:HG22	1:D:61:LEU:HD21	1.56	0.85
1:F:205:THR:HG22	1:F:207:LEU:H	1.42	0.83
1:F:260:TYR:HA	1:F:263:LYS:HG3	1.58	0.83
1:B:205:THR:HG22	1:B:207:LEU:H	1.44	0.83
1:B:8:ILE:HG22	1:B:61:LEU:HD21	1.60	0.82
1:C:205:THR:HG22	1:C:207:LEU:H	1.46	0.81
1:C:8:ILE:HG22	1:C:61:LEU:HD21	1.61	0.81
1:E:205:THR:HG22	1:E:207:LEU:H	1.45	0.81
1:C:86:HIS:HD2	1:C:132:ASP:OD1	1.64	0.80
1:E:86:HIS:HD2	1:E:132:ASP:OD1	1.64	0.80
1:E:8:ILE:HG22	1:E:61:LEU:HD21	1.63	0.80
1:B:177:PRO:O	1:B:178:LYS:CB	2.29	0.80
1:F:106:THR:H	1:F:149:GLN:HE22	1.30	0.79
1:A:106:THR:H	1:A:149:GLN:HE22	1.30	0.78
1:B:23:LEU:HD12	1:B:68:VAL:HG11	1.63	0.78
1:F:8:ILE:HG22	1:F:61:LEU:HD21	1.62	0.78
1:C:105:MET:HA	1:C:105:MET:HE2	1.64	0.78
1:C:180:GLY:C	1:C:182:ARG:H	1.86	0.78
1:E:105:MET:HA	1:E:105:MET:HE2	1.66	0.77
1:F:105:MET:HE2	1:F:105:MET:HA	1.67	0.77
1:D:106:THR:H	1:D:149:GLN:HE22	1.30	0.77
1:D:205:THR:HG22	1:D:207:LEU:H	1.49	0.77
1:D:8:ILE:CG2	1:D:61:LEU:HD21	2.14	0.77
1:E:106:THR:H	1:E:149:GLN:HE22	1.32	0.77
1:F:126:PRO:HB2	1:F:127:PRO:HD3	1.67	0.77
1:E:126:PRO:HB2	1:E:127:PRO:HD3	1.67	0.77
1:A:60:ARG:HG2	1:A:287:TYR:OH	1.85	0.77
1:D:105:MET:HA	1:D:105:MET:HE2	1.66	0.76
1:C:260:TYR:HA	1:C:263:LYS:HG3	1.67	0.76
1:A:260:TYR:HA	1:A:263:LYS:HG3	1.66	0.76
1:E:165:TYR:HB3	1:E:321:ALA:HB1	1.68	0.76
1:B:106:THR:H	1:B:149:GLN:HE22	1.33	0.76
1:A:165:TYR:HB3	1:A:321:ALA:HB1	1.67	0.76
1:D:165:TYR:HB3	1:D:321:ALA:HB1	1.68	0.75
1:A:86:HIS:HD2	1:A:132:ASP:OD1	1.69	0.75
1:F:165:TYR:HB3	1:F:321:ALA:HB1	1.69	0.75
1:C:165:TYR:HB3	1:C:321:ALA:HB1	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ARG:HD2	1:A:165:TYR:CE1	2.22	0.75
1:B:165:TYR:HB3	1:B:321:ALA:HB1	1.67	0.75
1:A:105:MET:HE2	1:A:105:MET:HA	1.68	0.74
1:A:8:ILE:CG2	1:A:61:LEU:HD21	2.17	0.74
1:B:164:ARG:HD2	1:B:165:TYR:CE1	2.23	0.74
1:B:126:PRO:HB2	1:B:127:PRO:HD3	1.70	0.74
1:E:176:ILE:HG13	1:E:177:PRO:HD2	1.67	0.74
1:B:105:MET:HA	1:B:105:MET:HE2	1.68	0.73
1:D:260:TYR:HA	1:D:263:LYS:HG3	1.69	0.73
1:E:260:TYR:HA	1:E:263:LYS:HG3	1.69	0.73
1:C:181:ALA:CB	1:C:243:ASN:HD21	2.02	0.73
1:F:164:ARG:HD2	1:F:165:TYR:CE1	2.22	0.73
1:C:106:THR:H	1:C:149:GLN:HE22	1.35	0.72
1:A:205:THR:HG22	1:A:207:LEU:H	1.52	0.72
1:C:31:HIS:CD2	1:C:74:GLN:HE21	2.07	0.72
1:B:86:HIS:HD2	1:B:132:ASP:OD1	1.73	0.72
1:D:126:PRO:HB2	1:D:127:PRO:HD3	1.72	0.71
1:A:29:LEU:HD11	1:A:178:LYS:HZ1	1.55	0.71
1:C:164:ARG:HD2	1:C:165:TYR:CE1	2.26	0.71
1:D:86:HIS:HD2	1:D:132:ASP:OD1	1.74	0.71
1:A:29:LEU:HD11	1:A:178:LYS:NZ	2.06	0.71
1:C:11:SER:O	1:C:13:VAL:HG12	1.90	0.71
1:F:86:HIS:HD2	1:F:132:ASP:OD1	1.74	0.71
1:B:260:TYR:HA	1:B:263:LYS:HG3	1.72	0.71
1:C:8:ILE:CG2	1:C:61:LEU:HD21	2.20	0.71
1:D:164:ARG:HD2	1:D:165:TYR:CE1	2.25	0.71
1:C:126:PRO:HB2	1:C:127:PRO:HD3	1.71	0.70
1:A:126:PRO:HB2	1:A:127:PRO:HD3	1.74	0.70
1:E:164:ARG:HD2	1:E:165:TYR:CE1	2.26	0.70
1:E:31:HIS:CD2	1:E:74:GLN:HE21	2.10	0.70
1:C:22:ALA:O	1:C:25:GLN:HG2	1.92	0.70
1:A:31:HIS:CD2	1:A:74:GLN:HE21	2.10	0.69
1:E:8:ILE:CG2	1:E:61:LEU:HD21	2.22	0.69
1:F:31:HIS:CD2	1:F:74:GLN:HE21	2.11	0.69
1:A:11:SER:O	1:A:13:VAL:HG12	1.93	0.69
1:B:8:ILE:CG2	1:B:61:LEU:HD21	2.22	0.69
1:E:195:LYS:CD	1:E:195:LYS:H	2.03	0.68
1:B:25:GLN:HA	1:B:25:GLN:HE21	1.59	0.68
1:F:8:ILE:CG2	1:F:61:LEU:HD21	2.24	0.67
1:C:176:ILE:HD12	1:C:177:PRO:HD2	1.76	0.67
1:D:31:HIS:CD2	1:D:74:GLN:HE21	2.13	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:LEU:O	1:A:58:ILE:HG13	1.95	0.67
1:A:73:THR:O	1:E:218:LYS:HD3	1.95	0.66
1:B:31:HIS:CD2	1:B:74:GLN:HE21	2.14	0.66
1:C:31:HIS:HD2	1:C:74:GLN:HE21	1.42	0.64
1:C:94:GLN:HE22	1:F:94:GLN:HE22	1.45	0.64
1:B:176:ILE:HD13	1:B:178:LYS:H	1.62	0.64
1:D:54:LEU:O	1:D:58:ILE:HG13	1.98	0.63
1:E:31:HIS:HD2	1:E:74:GLN:HE21	1.45	0.63
1:E:201:LYS:HE2	1:E:215:LYS:HE3	1.81	0.63
1:A:59:ARG:NH2	1:A:296:LEU:HD23	2.14	0.62
1:A:21:GLY:O	1:A:179:VAL:HG22	2.00	0.62
1:A:201:LYS:HE2	1:A:215:LYS:HE3	1.82	0.62
1:A:48:TRP:HE1	1:D:164:ARG:NH1	1.98	0.62
1:B:60:ARG:HG2	1:B:287:TYR:OH	1.99	0.62
1:A:31:HIS:HD2	1:A:74:GLN:HE21	1.46	0.61
1:D:201:LYS:HE2	1:D:215:LYS:HE3	1.82	0.61
1:C:195:LYS:CD	1:C:195:LYS:H	2.10	0.61
1:F:201:LYS:HE2	1:F:215:LYS:HE3	1.82	0.61
1:A:5:PHE:HB2	1:A:138:THR:HG21	1.82	0.61
1:E:195:LYS:N	1:E:195:LYS:HD2	2.11	0.61
1:E:23:LEU:HD21	1:E:65:TYR:CE1	2.35	0.61
1:A:179:VAL:HG12	1:A:181:ALA:H	1.65	0.61
1:D:13:VAL:O	1:D:13:VAL:HG13	2.01	0.60
1:E:86:HIS:CD2	1:E:132:ASP:OD1	2.53	0.60
1:A:300:LEU:HB2	1:D:326:ARG:NH1	2.17	0.60
1:A:181:ALA:O	1:A:182:ARG:HB2	2.02	0.60
1:F:31:HIS:HD2	1:F:74:GLN:HE21	1.47	0.60
1:C:54:LEU:O	1:C:58:ILE:HG13	2.02	0.59
1:D:25:GLN:OE1	1:D:178:LYS:HD3	2.02	0.59
1:B:13:VAL:HG13	1:B:13:VAL:O	2.02	0.59
1:A:1:MET:HE3	1:A:34:ASN:HD22	1.68	0.59
1:A:124:THR:O	1:A:127:PRO:HD2	2.02	0.59
1:F:13:VAL:O	1:F:13:VAL:HG13	2.02	0.59
1:A:94:GLN:HE22	1:D:94:GLN:HE22	1.51	0.59
1:A:13:VAL:O	1:A:13:VAL:HG13	2.03	0.59
1:D:31:HIS:HD2	1:D:74:GLN:HE21	1.50	0.59
1:B:94:GLN:HE22	1:E:94:GLN:HE22	1.51	0.59
1:F:59:ARG:NH2	1:F:296:LEU:HD23	2.18	0.59
1:B:31:HIS:HD2	1:B:74:GLN:HE21	1.51	0.58
1:C:13:VAL:O	1:C:13:VAL:HG13	2.03	0.58
1:B:59:ARG:NH2	1:B:296:LEU:HD23	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:PHE:HB2	1:B:138:THR:HG21	1.85	0.58
1:C:150:HIS:O	1:C:154:THR:HG22	2.03	0.58
1:F:54:LEU:O	1:F:58:ILE:HG13	2.04	0.58
1:C:86:HIS:CD2	1:C:132:ASP:OD1	2.52	0.58
1:D:4:ILE:HG12	1:D:140:ILE:HB	1.85	0.58
1:F:195:LYS:N	1:F:195:LYS:HD2	2.14	0.58
1:C:181:ALA:HB1	1:C:243:ASN:HD21	1.69	0.58
1:E:54:LEU:O	1:E:58:ILE:HG13	2.03	0.58
1:E:150:HIS:O	1:E:154:THR:HG22	2.04	0.58
1:F:4:ILE:HG12	1:F:140:ILE:HB	1.86	0.57
1:B:201:LYS:HE2	1:B:215:LYS:HE3	1.85	0.57
1:C:201:LYS:HE2	1:C:215:LYS:HE3	1.84	0.57
1:A:195:LYS:CD	1:A:195:LYS:H	2.04	0.57
1:C:4:ILE:HG12	1:C:140:ILE:HB	1.85	0.57
1:C:21:GLY:HA2	1:C:180:GLY:HA3	1.87	0.57
1:C:48:TRP:HE1	1:F:164:ARG:NH1	2.03	0.57
1:A:177:PRO:HB2	1:A:179:VAL:HG23	1.86	0.56
1:F:195:LYS:H	1:F:195:LYS:CD	2.06	0.56
1:C:101:GLU:HA	1:C:104:ARG:HH11	1.69	0.56
1:C:59:ARG:NH2	1:C:296:LEU:HD23	2.20	0.56
1:E:13:VAL:HG13	1:E:13:VAL:O	2.03	0.56
1:B:54:LEU:O	1:B:58:ILE:HG13	2.05	0.56
1:D:195:LYS:CD	1:D:195:LYS:H	2.06	0.56
1:E:101:GLU:HA	1:E:104:ARG:HH11	1.71	0.56
1:A:4:ILE:HG12	1:A:140:ILE:HB	1.87	0.56
1:D:105:MET:O	1:D:108:PHE:HB3	2.06	0.56
1:D:59:ARG:NH2	1:D:296:LEU:HD23	2.19	0.56
1:A:181:ALA:HB1	1:A:243:ASN:ND2	2.21	0.56
1:B:4:ILE:HG12	1:B:140:ILE:HB	1.87	0.56
1:A:195:LYS:N	1:A:195:LYS:HD2	2.12	0.56
1:B:105:MET:O	1:B:108:PHE:HB3	2.06	0.55
1:E:105:MET:O	1:E:108:PHE:HB3	2.06	0.55
1:D:5:PHE:HB2	1:D:138:THR:HG21	1.86	0.55
1:B:25:GLN:NE2	1:B:25:GLN:HA	2.22	0.55
1:C:178:LYS:NZ	1:C:178:LYS:HB3	2.22	0.55
1:D:101:GLU:HA	1:D:104:ARG:HH11	1.70	0.55
1:D:176:ILE:CG1	1:D:177:PRO:HD2	2.31	0.55
1:A:105:MET:O	1:A:108:PHE:HB3	2.06	0.54
1:F:234:ALA:C	1:F:236:PRO:HD3	2.27	0.54
1:A:101:GLU:HA	1:A:104:ARG:HH11	1.72	0.54
1:E:234:ALA:C	1:E:236:PRO:HD3	2.27	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:TRP:HE1	1:E:164:ARG:NH1	2.06	0.54
1:F:105:MET:O	1:F:108:PHE:HB3	2.07	0.54
1:C:95:CYS:SG	1:F:45:ILE:HG23	2.48	0.54
1:F:5:PHE:HB2	1:F:138:THR:HG21	1.90	0.54
1:B:234:ALA:C	1:B:236:PRO:HD3	2.27	0.54
1:A:150:HIS:O	1:A:154:THR:HG22	2.08	0.54
1:A:302:GLU:O	1:A:306:LYS:HG3	2.07	0.54
1:E:4:ILE:HG12	1:E:140:ILE:HB	1.88	0.54
1:D:25:GLN:NE2	1:D:178:LYS:NZ	2.56	0.53
1:B:176:ILE:HB	1:B:177:PRO:HD2	1.90	0.53
1:C:105:MET:O	1:C:108:PHE:HB3	2.07	0.53
1:B:101:GLU:HA	1:B:104:ARG:HH11	1.72	0.53
1:C:164:ARG:NH1	1:F:48:TRP:HE1	2.06	0.53
1:F:101:GLU:HA	1:F:104:ARG:HH11	1.72	0.53
1:F:125:TYR:N	1:F:126:PRO:CD	2.71	0.53
1:C:11:SER:O	1:C:13:VAL:N	2.41	0.53
1:E:86:HIS:HE1	1:E:136:TYR:OH	1.91	0.53
1:B:171:ILE:HD12	1:B:171:ILE:N	2.24	0.53
1:C:195:LYS:HD2	1:C:195:LYS:N	2.18	0.52
1:C:5:PHE:HB2	1:C:138:THR:HG21	1.91	0.52
1:E:59:ARG:NH2	1:E:296:LEU:HD23	2.24	0.52
1:E:5:PHE:HB2	1:E:138:THR:HG21	1.91	0.52
1:B:177:PRO:O	1:B:178:LYS:CG	2.58	0.52
1:B:177:PRO:O	1:B:178:LYS:HG2	2.09	0.52
1:C:234:ALA:C	1:C:236:PRO:HD3	2.30	0.52
1:D:125:TYR:N	1:D:126:PRO:CD	2.73	0.52
1:D:195:LYS:HD2	1:D:195:LYS:N	2.15	0.52
1:C:181:ALA:O	1:C:182:ARG:HB2	2.08	0.52
1:F:230:TYR:CD2	1:F:253:ILE:HD13	2.45	0.52
1:E:230:TYR:CD2	1:E:253:ILE:HD13	2.45	0.52
1:B:125:TYR:N	1:B:126:PRO:CD	2.73	0.51
1:B:195:LYS:CD	1:B:195:LYS:H	2.10	0.51
1:D:234:ALA:C	1:D:236:PRO:HD3	2.31	0.51
1:E:97:VAL:HB	1:E:157:LEU:HD21	1.92	0.51
1:A:234:ALA:C	1:A:236:PRO:HD3	2.30	0.51
1:A:125:TYR:N	1:A:126:PRO:CD	2.74	0.51
1:E:125:TYR:N	1:E:126:PRO:CD	2.73	0.51
1:C:136:TYR:HB2	1:C:138:THR:HG22	1.93	0.51
1:B:176:ILE:CD1	1:B:178:LYS:H	2.23	0.51
1:A:212:THR:CG2	1:A:216:LYS:HE3	2.41	0.51
1:C:178:LYS:O	1:C:179:VAL:HG13	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:150:HIS:O	1:F:154:THR:HG22	2.10	0.51
1:B:151:ILE:HA	1:B:154:THR:HG23	1.93	0.50
1:E:171:ILE:N	1:E:171:ILE:HD12	2.26	0.50
1:E:23:LEU:HD21	1:E:65:TYR:CZ	2.47	0.50
1:F:151:ILE:HA	1:F:154:THR:HG23	1.93	0.50
1:E:25:GLN:OE1	1:E:178:LYS:HG2	2.10	0.50
1:B:245:TYR:HB2	1:B:272:LEU:HD13	1.94	0.50
1:C:151:ILE:HA	1:C:154:THR:HG23	1.93	0.50
1:B:195:LYS:N	1:B:195:LYS:HD2	2.19	0.50
1:D:25:GLN:NE2	1:D:178:LYS:HZ3	2.10	0.50
1:D:3:THR:HB	1:D:138:THR:HA	1.94	0.50
1:D:60:ARG:HG2	1:D:287:TYR:OH	2.12	0.50
1:D:86:HIS:CD2	1:D:132:ASP:OD1	2.61	0.50
1:D:245:TYR:HB2	1:D:272:LEU:HD13	1.94	0.50
1:F:185:SER:HB3	1:F:188:ASP:O	2.11	0.50
1:F:86:HIS:HE1	1:F:136:TYR:OH	1.95	0.50
1:A:14:ILE:HD11	1:A:64:LEU:HD22	1.94	0.49
1:D:150:HIS:O	1:D:154:THR:HG22	2.11	0.49
1:E:4:ILE:HG23	1:E:142:PRO:HD3	1.94	0.49
1:F:171:ILE:N	1:F:171:ILE:HD12	2.26	0.49
1:B:164:ARG:NH1	1:E:48:TRP:HE1	2.10	0.49
1:C:125:TYR:N	1:C:126:PRO:CD	2.75	0.49
1:C:4:ILE:HG23	1:C:142:PRO:HD3	1.94	0.49
1:D:124:THR:O	1:D:127:PRO:HD2	2.13	0.49
1:A:97:VAL:HB	1:A:157:LEU:HD21	1.95	0.49
1:D:151:ILE:HA	1:D:154:THR:HG23	1.93	0.49
1:D:212:THR:CG2	1:D:216:LYS:HE3	2.43	0.49
1:B:4:ILE:HG23	1:B:142:PRO:HD3	1.95	0.49
1:C:225:GLU:OE1	1:C:235:LYS:HD2	2.12	0.49
1:C:60:ARG:HG2	1:C:287:TYR:OH	2.13	0.49
1:E:136:TYR:HB2	1:E:138:THR:HG22	1.94	0.49
1:F:179:VAL:O	1:F:179:VAL:HG12	2.12	0.49
1:C:97:VAL:HB	1:C:157:LEU:HD21	1.95	0.49
1:D:302:GLU:O	1:D:306:LYS:HG3	2.11	0.49
1:F:179:VAL:HG13	1:F:182:ARG:HB2	1.94	0.49
1:A:245:TYR:HB2	1:A:272:LEU:HD13	1.94	0.48
1:B:230:TYR:CD2	1:B:253:ILE:HD13	2.47	0.48
1:C:212:THR:CG2	1:C:216:LYS:HE3	2.43	0.48
1:C:231:ASP:OD2	1:C:234:ALA:HB3	2.13	0.48
1:A:3:THR:HB	1:A:138:THR:HA	1.95	0.48
1:A:151:ILE:HA	1:A:154:THR:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:ILE:O	1:B:138:THR:HG23	2.13	0.48
1:E:151:ILE:HA	1:E:154:THR:HG23	1.95	0.48
1:F:133:ILE:O	1:F:138:THR:HG23	2.12	0.48
1:F:231:ASP:OD2	1:F:234:ALA:HB3	2.14	0.48
1:A:106:THR:N	1:A:149:GLN:HE22	2.06	0.48
1:A:193:MET:CE	1:A:203:TYR:HA	2.43	0.48
1:C:141:VAL:HG12	1:C:143:VAL:HG13	1.96	0.48
1:E:19:TYR:HE2	1:E:68:VAL:HG13	1.77	0.48
1:F:235:LYS:N	1:F:236:PRO:HD3	2.29	0.48
1:B:1:MET:CE	1:B:34:ASN:HD22	2.27	0.48
1:C:1:MET:CE	1:C:34:ASN:HD22	2.26	0.48
1:E:185:SER:HB3	1:E:188:ASP:O	2.14	0.48
1:F:106:THR:N	1:F:149:GLN:HE22	2.07	0.48
1:D:171:ILE:N	1:D:171:ILE:HD12	2.29	0.48
1:B:225:GLU:OE1	1:B:235:LYS:HD2	2.14	0.48
1:E:141:VAL:HG12	1:E:143:VAL:HG13	1.96	0.48
1:B:11:SER:O	1:B:13:VAL:HG12	2.13	0.48
1:B:25:GLN:CA	1:B:25:GLN:HE21	2.26	0.48
1:E:212:THR:CG2	1:E:216:LYS:HE3	2.43	0.48
1:C:230:TYR:CD2	1:C:253:ILE:HD13	2.49	0.48
1:D:4:ILE:HG23	1:D:142:PRO:HD3	1.96	0.48
1:D:231:ASP:OD2	1:D:234:ALA:HB3	2.13	0.47
1:F:136:TYR:HB2	1:F:138:THR:HG22	1.96	0.47
1:F:60:ARG:HG2	1:F:287:TYR:OH	2.14	0.47
1:F:1:MET:CE	1:F:34:ASN:HD22	2.26	0.47
1:C:171:ILE:N	1:C:171:ILE:HD12	2.29	0.47
1:C:181:ALA:HB3	1:C:243:ASN:HD21	1.79	0.47
1:B:235:LYS:N	1:B:236:PRO:HD3	2.30	0.47
1:C:3:THR:HB	1:C:138:THR:HA	1.96	0.47
1:A:185:SER:HB3	1:A:188:ASP:O	2.14	0.47
1:B:136:TYR:HB2	1:B:138:THR:HG22	1.96	0.47
1:C:185:SER:HB3	1:C:188:ASP:O	2.13	0.47
1:D:136:TYR:HB2	1:D:138:THR:HG22	1.96	0.47
1:C:181:ALA:HB3	1:C:243:ASN:ND2	2.29	0.47
1:E:225:GLU:OE1	1:E:235:LYS:HD2	2.15	0.47
1:F:179:VAL:HG13	1:F:182:ARG:CG	2.45	0.47
1:E:235:LYS:N	1:E:236:PRO:HD3	2.29	0.47
1:F:225:GLU:OE1	1:F:235:LYS:HD2	2.14	0.47
1:B:176:ILE:C	1:B:176:ILE:HD12	2.34	0.47
1:C:95:CYS:SG	1:F:45:ILE:CG2	3.02	0.47
1:A:176:ILE:HG23	1:A:177:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:HIS:O	1:B:154:THR:HG22	2.14	0.47
1:B:177:PRO:C	1:B:178:LYS:HG2	2.35	0.47
1:B:97:VAL:HB	1:B:157:LEU:HD21	1.97	0.47
1:E:133:ILE:O	1:E:138:THR:HG23	2.15	0.47
1:E:105:MET:CE	1:E:149:GLN:HE21	2.28	0.47
1:E:3:THR:HB	1:E:138:THR:HA	1.96	0.47
1:F:4:ILE:HG23	1:F:142:PRO:HD3	1.96	0.47
1:D:133:ILE:O	1:D:138:THR:HG23	2.15	0.46
1:D:230:TYR:CD2	1:D:253:ILE:HD13	2.49	0.46
1:A:230:TYR:CD2	1:A:253:ILE:HD13	2.51	0.46
1:F:64:LEU:HG	1:F:287:TYR:CD2	2.50	0.46
1:B:281:ARG:N	1:B:282:PRO:HD2	2.31	0.46
1:D:189:PRO:HD3	1:D:221:VAL:HG21	1.98	0.46
1:E:231:ASP:OD2	1:E:234:ALA:HB3	2.15	0.46
1:F:245:TYR:HB2	1:F:272:LEU:HD13	1.98	0.46
1:A:86:HIS:CD2	1:A:132:ASP:OD1	2.58	0.46
1:D:141:VAL:HG12	1:D:143:VAL:HG13	1.97	0.46
1:C:118:ALA:O	1:F:99:ILE:HG13	2.15	0.46
1:D:86:HIS:HE1	1:D:136:TYR:OH	1.98	0.46
1:F:97:VAL:HB	1:F:157:LEU:HD21	1.97	0.46
1:A:228:ILE:HD13	1:A:265:TYR:CE1	2.51	0.46
1:B:3:THR:HB	1:B:138:THR:HA	1.97	0.46
1:A:136:TYR:HB2	1:A:138:THR:HG22	1.96	0.46
1:A:171:ILE:HD12	1:A:171:ILE:N	2.30	0.46
1:B:50:ASP:HB3	1:B:53:GLU:HB2	1.97	0.46
1:C:133:ILE:O	1:C:138:THR:HG23	2.16	0.46
1:C:281:ARG:N	1:C:282:PRO:HD2	2.31	0.46
1:D:97:VAL:HB	1:D:157:LEU:HD21	1.98	0.46
1:F:281:ARG:N	1:F:282:PRO:HD2	2.30	0.46
1:C:23:LEU:HD21	1:C:65:TYR:CE1	2.51	0.45
1:E:1:MET:CE	1:E:34:ASN:HD22	2.29	0.45
1:E:245:TYR:HB2	1:E:272:LEU:HD13	1.99	0.45
1:E:14:ILE:HD11	1:E:64:LEU:HD22	1.97	0.45
1:A:231:ASP:OD2	1:A:234:ALA:HB3	2.15	0.45
1:C:105:MET:CE	1:C:149:GLN:HE21	2.30	0.45
1:A:281:ARG:N	1:A:282:PRO:HD2	2.31	0.45
1:B:212:THR:CG2	1:B:216:LYS:HE3	2.46	0.45
1:E:50:ASP:HB3	1:E:53:GLU:HG3	1.98	0.45
1:C:235:LYS:N	1:C:236:PRO:HD3	2.31	0.45
1:D:193:MET:CE	1:D:203:TYR:HA	2.46	0.45
1:B:302:GLU:O	1:B:306:LYS:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:HIS:HE1	1:B:136:TYR:OH	2.00	0.45
1:E:302:GLU:O	1:E:306:LYS:HG3	2.16	0.45
1:A:225:GLU:OE1	1:A:235:LYS:HD2	2.17	0.45
1:E:177:PRO:O	1:E:179:VAL:HG23	2.16	0.45
1:A:50:ASP:HB3	1:A:53:GLU:HG3	1.98	0.45
1:B:231:ASP:OD2	1:B:234:ALA:HB3	2.16	0.45
1:D:16:ILE:O	1:D:20:ILE:HG13	2.17	0.45
1:D:1:MET:CE	1:D:34:ASN:HD22	2.30	0.45
1:A:133:ILE:O	1:A:138:THR:HG23	2.17	0.45
1:A:141:VAL:HG12	1:A:143:VAL:HG13	1.98	0.44
1:A:4:ILE:HG23	1:A:142:PRO:HD3	1.98	0.44
1:B:105:MET:CE	1:B:149:GLN:HE21	2.30	0.44
1:B:147:GLN:HB3	1:B:147:GLN:HE21	1.59	0.44
1:D:228:ILE:HD13	1:D:265:TYR:CE1	2.52	0.44
1:D:225:GLU:OE1	1:D:235:LYS:HD2	2.17	0.44
1:D:281:ARG:N	1:D:282:PRO:HD2	2.32	0.44
1:E:126:PRO:CB	1:E:127:PRO:HD3	2.44	0.44
1:E:176:ILE:CG1	1:E:177:PRO:HD2	2.41	0.44
1:D:92:MET:HB3	1:D:322:MET:HE1	1.98	0.44
1:A:125:TYR:CG	1:A:126:PRO:HD3	2.53	0.44
1:D:316:ARG:NH1	1:D:319:GLU:OE1	2.50	0.44
1:E:92:MET:HB3	1:E:322:MET:HE1	1.99	0.44
1:F:3:THR:HB	1:F:138:THR:HA	1.99	0.44
1:A:16:ILE:O	1:A:20:ILE:HG13	2.17	0.44
1:A:235:LYS:N	1:A:236:PRO:HD3	2.33	0.44
1:A:86:HIS:HE1	1:A:136:TYR:OH	2.00	0.44
1:A:130:ALA:O	1:A:134:LEU:HG	2.18	0.44
1:A:1:MET:CE	1:A:34:ASN:HD22	2.28	0.43
1:D:185:SER:HB3	1:D:188:ASP:O	2.18	0.43
1:E:281:ARG:N	1:E:282:PRO:HD2	2.33	0.43
1:C:124:THR:O	1:C:127:PRO:HD2	2.18	0.43
1:C:176:ILE:O	1:C:176:ILE:HG23	2.18	0.43
1:D:126:PRO:CB	1:D:127:PRO:HD3	2.47	0.43
1:C:50:ASP:HB3	1:C:53:GLU:HG3	2.00	0.43
1:E:151:ILE:HA	1:E:154:THR:CG2	2.48	0.43
1:A:181:ALA:O	1:A:182:ARG:CB	2.65	0.43
1:E:25:GLN:O	1:E:29:LEU:HG	2.19	0.43
1:E:50:ASP:HB3	1:E:53:GLU:HB2	2.01	0.43
1:F:105:MET:CE	1:F:149:GLN:HE21	2.31	0.43
1:F:141:VAL:HG12	1:F:143:VAL:HG13	1.99	0.43
1:C:151:ILE:HA	1:C:154:THR:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:86:HIS:CD2	1:F:132:ASP:OD1	2.62	0.43
1:A:147:GLN:HE21	1:A:147:GLN:HB3	1.60	0.43
1:A:210:ALA:HB1	1:A:277:ILE:HD13	2.01	0.43
1:B:141:VAL:HG12	1:B:143:VAL:HG13	2.00	0.43
1:E:124:THR:O	1:E:127:PRO:HD2	2.18	0.43
1:C:302:GLU:O	1:C:306:LYS:HG3	2.18	0.43
1:E:125:TYR:CG	1:E:126:PRO:HD3	2.53	0.43
1:F:171:ILE:H	1:F:171:ILE:HD12	1.84	0.43
1:F:212:THR:CG2	1:F:216:LYS:HE3	2.49	0.43
1:A:50:ASP:HB3	1:A:53:GLU:HB2	2.00	0.43
1:B:316:ARG:NH1	1:B:319:GLU:OE1	2.51	0.43
1:E:126:PRO:HB2	1:E:127:PRO:CD	2.45	0.43
1:A:105:MET:HE2	1:A:105:MET:CA	2.43	0.43
1:A:289:HIS:O	1:A:293:SER:HB2	2.18	0.43
1:C:125:TYR:CG	1:C:126:PRO:HD3	2.53	0.43
1:C:8:ILE:HD12	1:C:65:TYR:OH	2.19	0.43
1:C:147:GLN:HB3	1:C:147:GLN:HE21	1.59	0.43
1:D:50:ASP:HB3	1:D:53:GLU:HG3	2.00	0.43
1:B:124:THR:O	1:B:127:PRO:HD2	2.19	0.42
1:B:50:ASP:HB3	1:B:53:GLU:HG3	2.00	0.42
1:A:56:GLN:NE2	1:A:56:GLN:HA	2.33	0.42
1:B:171:ILE:H	1:B:171:ILE:HD12	1.84	0.42
1:D:105:MET:HE2	1:D:105:MET:CA	2.43	0.42
1:B:45:ILE:HG23	1:E:95:CYS:SG	2.59	0.42
1:C:106:THR:N	1:C:149:GLN:HE22	2.10	0.42
1:C:245:TYR:HB2	1:C:272:LEU:HD13	2.00	0.42
1:E:45:ILE:HG23	1:E:45:ILE:O	2.19	0.42
1:C:181:ALA:CB	1:C:243:ASN:ND2	2.75	0.42
1:C:19:TYR:HE2	1:C:68:VAL:HG13	1.85	0.42
1:D:105:MET:CE	1:D:149:GLN:HE21	2.32	0.42
1:E:56:GLN:HA	1:E:56:GLN:NE2	2.34	0.42
1:F:228:ILE:HD13	1:F:265:TYR:CE1	2.55	0.42
1:A:105:MET:CE	1:A:149:GLN:HE21	2.32	0.42
1:E:125:TYR:CD2	1:E:126:PRO:HD3	2.55	0.42
1:E:105:MET:CA	1:E:105:MET:HE2	2.44	0.42
1:A:189:PRO:HD3	1:A:221:VAL:HG21	2.01	0.42
1:B:185:SER:HB3	1:B:188:ASP:O	2.19	0.42
1:E:106:THR:N	1:E:149:GLN:HE22	2.09	0.42
1:A:316:ARG:NH1	1:A:319:GLU:OE1	2.52	0.42
1:F:50:ASP:HB3	1:F:53:GLU:HG3	2.01	0.42
1:C:86:HIS:HE1	1:C:136:TYR:OH	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:ILE:HB	1:B:177:PRO:CD	2.50	0.41
1:E:171:ILE:HD12	1:E:171:ILE:H	1.85	0.41
1:E:193:MET:CE	1:E:203:TYR:HA	2.50	0.41
1:A:197:ASP:HA	1:A:198:PRO:HD3	1.90	0.41
1:B:45:ILE:HG23	1:B:45:ILE:O	2.20	0.41
1:C:125:TYR:CD2	1:C:126:PRO:HD3	2.56	0.41
1:B:193:MET:CE	1:B:203:TYR:HA	2.50	0.41
1:E:316:ARG:NH1	1:E:319:GLU:OE1	2.53	0.41
1:A:125:TYR:CD2	1:A:126:PRO:HD3	2.55	0.41
1:A:189:PRO:HB2	1:A:236:PRO:HB2	2.02	0.41
1:C:189:PRO:HB2	1:C:236:PRO:HB2	2.01	0.41
1:F:102:LEU:HD21	1:F:127:PRO:HD3	2.02	0.41
1:C:50:ASP:HB3	1:C:53:GLU:HB2	2.01	0.41
1:C:92:MET:HB3	1:C:322:MET:HE1	2.02	0.41
1:D:193:MET:HE1	1:D:203:TYR:HA	2.02	0.41
1:D:205:THR:HG22	1:D:206:LEU:N	2.35	0.41
1:E:189:PRO:HD3	1:E:221:VAL:HG21	2.03	0.41
1:F:164:ARG:HD2	1:F:165:TYR:CZ	2.55	0.41
1:F:241:LEU:HG	1:F:272:LEU:CD2	2.51	0.41
1:A:48:TRP:HE1	1:D:164:ARG:HH11	1.68	0.41
1:C:21:GLY:HA2	1:C:180:GLY:CA	2.48	0.41
1:B:199:ASN:ND2	1:B:201:LYS:H	2.19	0.41
1:D:125:TYR:CG	1:D:126:PRO:HD3	2.56	0.41
1:D:147:GLN:HB3	1:D:147:GLN:HE21	1.61	0.41
1:F:176:ILE:HA	1:F:177:PRO:HD3	1.92	0.41
1:F:200:PRO:O	1:F:216:LYS:HE2	2.21	0.41
1:C:326:ARG:NH2	1:F:301:ASP:OD1	2.54	0.41
1:B:228:ILE:HD13	1:B:265:TYR:CE1	2.56	0.41
1:B:92:MET:HB3	1:B:322:MET:HE1	2.03	0.41
1:C:180:GLY:O	1:C:181:ALA:HB3	2.21	0.41
1:C:193:MET:HE1	1:C:203:TYR:HA	2.02	0.41
1:D:85:ALA:HB3	1:D:311:ALA:HB1	2.03	0.41
1:F:189:PRO:HD3	1:F:221:VAL:HG21	2.03	0.41
1:A:238:ILE:HD13	1:A:238:ILE:HA	1.99	0.40
1:C:19:TYR:HA	1:C:23:LEU:HB3	2.02	0.40
1:C:99:ILE:HG13	1:F:118:ALA:O	2.20	0.40
1:F:151:ILE:HA	1:F:154:THR:CG2	2.51	0.40
1:B:189:PRO:HD3	1:B:221:VAL:HG21	2.03	0.40
1:D:50:ASP:HB3	1:D:53:GLU:HB2	2.02	0.40
1:E:197:ASP:HA	1:E:198:PRO:HD3	1.93	0.40
1:E:189:PRO:HB2	1:E:236:PRO:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:19:TYR:CE2	1:E:68:VAL:HG13	2.54	0.40
1:C:189:PRO:HD3	1:C:221:VAL:HG21	2.04	0.40
1:B:10:PRO:HA	1:B:61:LEU:HD22	2.04	0.40
1:D:71:ASP:HB3	1:D:74:GLN:HB3	2.03	0.40
1:F:124:THR:O	1:F:127:PRO:HD2	2.21	0.40
1:C:16:ILE:O	1:C:20:ILE:HG13	2.22	0.40
1:D:217:ILE:O	1:D:269:LYS:HD2	2.22	0.40
1:D:23:LEU:HD12	1:D:68:VAL:HG11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	324/326 (99%)	299 (92%)	18 (6%)	7 (2%)	6	24
1	B	324/326 (99%)	299 (92%)	19 (6%)	6 (2%)	8	28
1	C	324/326 (99%)	298 (92%)	19 (6%)	7 (2%)	6	24
1	D	324/326 (99%)	300 (93%)	20 (6%)	4 (1%)	13	40
1	E	324/326 (99%)	298 (92%)	20 (6%)	6 (2%)	8	28
1	F	324/326 (99%)	300 (93%)	19 (6%)	5 (2%)	10	34
All	All	1944/1956 (99%)	1794 (92%)	115 (6%)	35 (2%)	8	29

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	179	VAL
1	D	40	VAL
1	D	181	ALA
1	A	40	VAL

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Mol	Chain	Res	Type
1	A	179	VAL
1	A	261	GLU
1	B	40	VAL
1	B	178	LYS
1	B	261	GLU
1	C	12	GLY
1	C	177	PRO
1	C	178	LYS
1	C	261	GLU
1	D	261	GLU
1	E	261	GLU
1	F	40	VAL
1	F	261	GLU
1	C	182	ARG
1	E	13	VAL
1	E	40	VAL
1	E	178	LYS
1	C	40	VAL
1	C	231	ASP
1	E	12	GLY
1	A	182	ARG
1	B	12	GLY
1	D	231	ASP
1	E	231	ASP
1	F	182	ARG
1	A	231	ASP
1	B	231	ASP
1	F	181	ALA
1	A	12	GLY
1	A	13	VAL
1	F	179	VAL

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	274/274 (100%)	253 (92%)	21 (8%)	13	35
1	B	274/274 (100%)	250 (91%)	24 (9%)	10	30
1	C	274/274 (100%)	251 (92%)	23 (8%)	11	31
1	D	274/274 (100%)	251 (92%)	23 (8%)	11	31
1	E	274/274 (100%)	248 (90%)	26 (10%)	8	26
1	F	274/274 (100%)	251 (92%)	23 (8%)	11	31
All	All	1644/1644 (100%)	1504 (92%)	140 (8%)	10	31

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	23	LEU
1	A	48	TRP
1	A	55	ARG
1	A	64	LEU
1	A	65	TYR
1	A	105	MET
1	A	107	GLN
1	A	138	THR
1	A	147	GLN
1	A	154	THR
1	A	168	LEU
1	A	195	LYS
1	A	199	ASN
1	A	215	LYS
1	A	233	GLU
1	A	241	LEU
1	A	245	TYR
1	A	258	ARG
1	A	289	HIS
1	A	316	ARG
1	B	9	GLN
1	B	23	LEU
1	B	25	GLN
1	B	48	TRP
1	B	55	ARG
1	B	64	LEU

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Mol	Chain	Res	Type
1	B	65	TYR
1	B	105	MET
1	B	107	GLN
1	B	138	THR
1	B	147	GLN
1	B	154	THR
1	B	168	LEU
1	B	178	LYS
1	B	179	VAL
1	B	195	LYS
1	B	199	ASN
1	B	215	LYS
1	B	233	GLU
1	B	241	LEU
1	B	245	TYR
1	B	258	ARG
1	B	289	HIS
1	B	316	ARG
1	C	9	GLN
1	C	23	LEU
1	C	48	TRP
1	C	55	ARG
1	C	64	LEU
1	C	65	TYR
1	C	105	MET
1	C	107	GLN
1	C	122	LEU
1	C	138	THR
1	C	147	GLN
1	C	154	THR
1	C	168	LEU
1	C	179	VAL
1	C	195	LYS
1	C	199	ASN
1	C	215	LYS
1	C	233	GLU
1	C	241	LEU
1	C	245	TYR
1	C	258	ARG
1	C	289	HIS
1	C	316	ARG
1	D	9	GLN

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Mol	Chain	Res	Type
1	D	23	LEU
1	D	48	TRP
1	D	55	ARG
1	D	64	LEU
1	D	65	TYR
1	D	105	MET
1	D	107	GLN
1	D	138	THR
1	D	147	GLN
1	D	154	THR
1	D	168	LEU
1	D	176	ILE
1	D	182	ARG
1	D	195	LYS
1	D	199	ASN
1	D	215	LYS
1	D	233	GLU
1	D	241	LEU
1	D	245	TYR
1	D	258	ARG
1	D	289	HIS
1	D	316	ARG
1	E	9	GLN
1	E	23	LEU
1	E	48	TRP
1	E	55	ARG
1	E	64	LEU
1	E	65	TYR
1	E	105	MET
1	E	107	GLN
1	E	122	LEU
1	E	138	THR
1	E	147	GLN
1	E	154	THR
1	E	168	LEU
1	E	176	ILE
1	E	178	LYS
1	E	182	ARG
1	E	195	LYS
1	E	199	ASN
1	E	215	LYS
1	E	233	GLU

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Mol	Chain	Res	Type
1	E	241	LEU
1	E	245	TYR
1	E	258	ARG
1	E	289	HIS
1	E	309	ARG
1	E	316	ARG
1	F	9	GLN
1	F	23	LEU
1	F	48	TRP
1	F	55	ARG
1	F	64	LEU
1	F	65	TYR
1	F	105	MET
1	F	107	GLN
1	F	138	THR
1	F	147	GLN
1	F	154	THR
1	F	168	LEU
1	F	182	ARG
1	F	195	LYS
1	F	199	ASN
1	F	215	LYS
1	F	233	GLU
1	F	241	LEU
1	F	245	TYR
1	F	258	ARG
1	F	289	HIS
1	F	309	ARG
1	F	316	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	31	HIS
1	A	34	ASN
1	A	43	HIS
1	A	56	GLN
1	A	86	HIS
1	A	94	GLN
1	A	107	GLN
1	A	147	GLN

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Mol	Chain	Res	Type
1	A	149	GLN
1	A	199	ASN
1	A	243	ASN
1	A	251	GLN
1	A	259	GLN
1	A	284	GLN
1	B	9	GLN
1	B	18	ASN
1	B	25	GLN
1	B	31	HIS
1	B	34	ASN
1	B	43	HIS
1	B	56	GLN
1	B	86	HIS
1	B	107	GLN
1	B	147	GLN
1	B	149	GLN
1	B	199	ASN
1	B	251	GLN
1	B	259	GLN
1	B	284	GLN
1	C	9	GLN
1	C	18	ASN
1	C	31	HIS
1	C	34	ASN
1	C	43	HIS
1	C	56	GLN
1	C	86	HIS
1	C	94	GLN
1	C	107	GLN
1	C	147	GLN
1	C	149	GLN
1	C	199	ASN
1	C	243	ASN
1	C	251	GLN
1	C	259	GLN
1	C	284	GLN
1	D	9	GLN
1	D	18	ASN
1	D	25	GLN
1	D	31	HIS
1	D	34	ASN

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Mol	Chain	Res	Type
1	D	43	HIS
1	D	56	GLN
1	D	86	HIS
1	D	107	GLN
1	D	147	GLN
1	D	149	GLN
1	D	199	ASN
1	D	251	GLN
1	D	259	GLN
1	D	284	GLN
1	E	9	GLN
1	E	18	ASN
1	E	31	HIS
1	E	34	ASN
1	E	43	HIS
1	E	56	GLN
1	E	86	HIS
1	E	94	GLN
1	E	107	GLN
1	E	147	GLN
1	E	149	GLN
1	E	199	ASN
1	E	251	GLN
1	E	259	GLN
1	E	284	GLN
1	F	9	GLN
1	F	18	ASN
1	F	31	HIS
1	F	34	ASN
1	F	43	HIS
1	F	56	GLN
1	F	86	HIS
1	F	107	GLN
1	F	147	GLN
1	F	149	GLN
1	F	199	ASN
1	F	251	GLN
1	F	259	GLN
1	F	284	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	326/326 (100%)	-0.10	13 (3%) 38 33	14, 41, 89, 141	0
1	B	326/326 (100%)	-0.13	16 (4%) 29 26	14, 41, 89, 141	0
1	C	326/326 (100%)	-0.12	16 (4%) 29 26	18, 41, 89, 141	0
1	D	326/326 (100%)	-0.04	17 (5%) 27 23	17, 42, 90, 140	0
1	E	326/326 (100%)	-0.08	16 (4%) 29 26	15, 40, 90, 141	0
1	F	326/326 (100%)	-0.06	16 (4%) 29 26	15, 43, 89, 141	0
All	All	1956/1956 (100%)	-0.09	94 (4%) 30 27	14, 41, 90, 141	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	179	VAL	8.7
1	E	110	GLU	8.7
1	A	115	ALA	7.9
1	C	110	GLU	7.6
1	B	115	ALA	7.3
1	F	110	GLU	6.6
1	C	115	ALA	6.4
1	A	110	GLU	6.1
1	D	179	VAL	6.0
1	C	178	LYS	5.8
1	B	113	ALA	5.7
1	C	116	ALA	5.6
1	D	114	GLY	5.5
1	D	106	THR	5.3
1	C	112	SER	5.3
1	E	113	ALA	5.3
1	A	177	PRO	5.2
1	A	107	GLN	5.0
1	D	115	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	114	GLY	4.7
1	E	106	THR	4.7
1	D	109	LYS	4.6
1	F	114	GLY	4.6
1	F	117	ALA	4.6
1	C	114	GLY	4.5
1	E	178	LYS	4.5
1	D	116	ALA	4.5
1	E	112	SER	4.5
1	E	107	GLN	4.3
1	C	108	PHE	4.3
1	A	116	ALA	4.3
1	D	112	SER	4.2
1	F	115	ALA	4.2
1	B	107	GLN	4.2
1	C	113	ALA	4.1
1	A	106	THR	4.1
1	D	110	GLU	4.0
1	F	107	GLN	4.0
1	D	177	PRO	3.8
1	C	106	THR	3.8
1	E	180	GLY	3.7
1	F	116	ALA	3.7
1	B	110	GLU	3.7
1	A	111	LYS	3.7
1	D	107	GLN	3.7
1	F	113	ALA	3.6
1	C	109	LYS	3.4
1	E	116	ALA	3.4
1	C	111	LYS	3.4
1	E	114	GLY	3.3
1	F	179	VAL	3.3
1	B	178	LYS	3.2
1	D	180	GLY	3.2
1	B	179	VAL	3.2
1	C	107	GLN	3.1
1	B	112	SER	3.1
1	E	115	ALA	3.1
1	F	292	GLU	3.1
1	E	111	LYS	3.0
1	B	111	LYS	3.0
1	E	177	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	108	PHE	3.0
1	B	254	GLU	3.0
1	D	104	ARG	2.9
1	A	112	SER	2.8
1	C	177	PRO	2.8
1	C	258	ARG	2.7
1	B	1	MET	2.6
1	C	179	VAL	2.6
1	F	194	SER	2.6
1	B	177	PRO	2.6
1	D	113	ALA	2.5
1	F	112	SER	2.4
1	B	180	GLY	2.4
1	A	178	LYS	2.4
1	F	177	PRO	2.4
1	D	178	LYS	2.3
1	A	148	LYS	2.3
1	B	145	GLU	2.2
1	D	32	GLU	2.2
1	A	298	ARG	2.2
1	D	12	GLY	2.2
1	E	289	HIS	2.2
1	B	114	GLY	2.2
1	D	108	PHE	2.2
1	E	109	LYS	2.2
1	F	298	ARG	2.1
1	F	258	ARG	2.1
1	C	1	MET	2.1
1	B	2	LYS	2.1
1	F	111	LYS	2.0
1	B	108	PHE	2.0
1	A	180	GLY	2.0
1	F	106	THR	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.