



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:07 PM UTC

PDB ID : 1D2R / pdb_00001d2r
Title : 2.9 Å CRYSTAL STRUCTURE OF LIGAND-FREE TRYPTOPHANYL-
TRNA SYNTHETASE: DOMAIN MOVEMENTS FRAGMENT THE ADE-
NINE 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 types of validation reports are described at

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

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

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

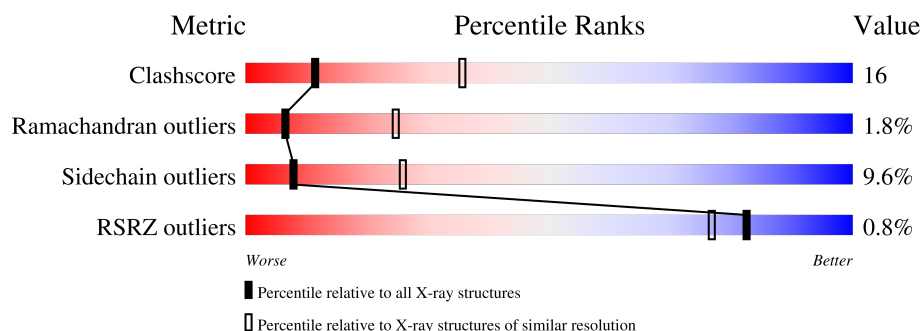
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	326	61% 32% 7%
1	B	326	2% 65% 29% 5%
1	C	326	2% 62% 32% 6%
1	D	326	2% 63% 32% 3%
1	E	326	2% 63% 30% 6%
1	F	326	2% 66% 30% 2%

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.

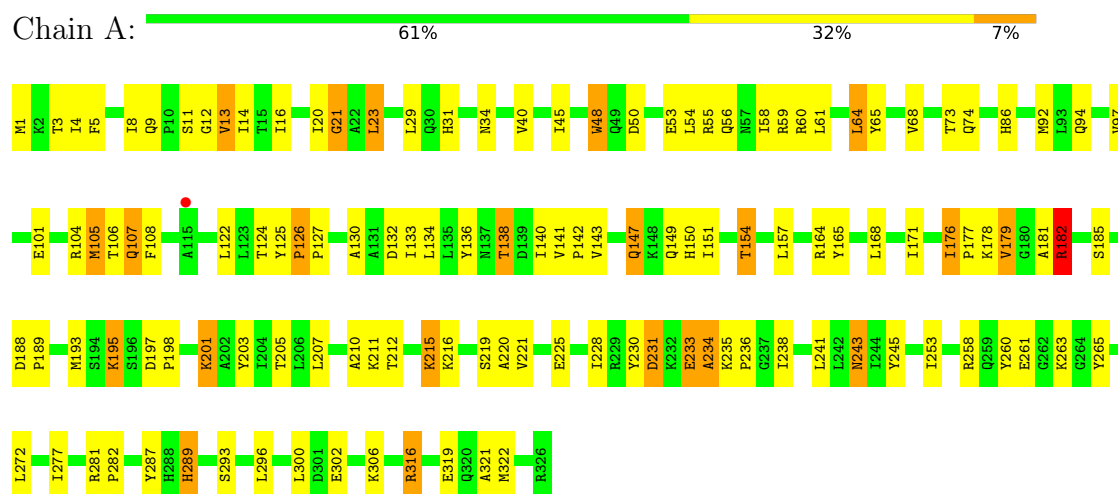
- Molecule 1 is a protein called PROTEIN (TRYPTOPHANYL TRNA SYNTHETASE).

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

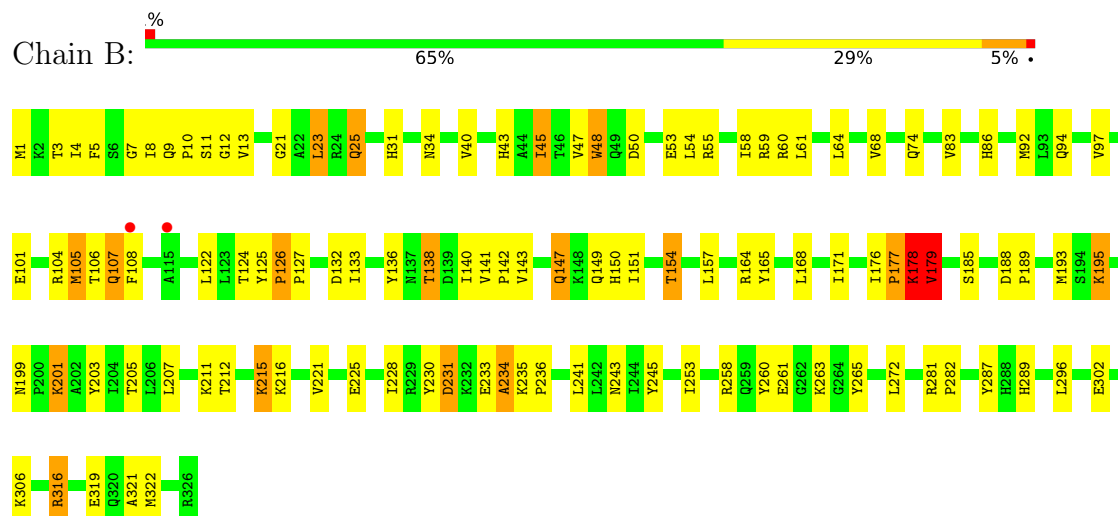
3 Residue-property plots

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

• Molecule 1: PROTEIN (TRYPTOPHANYL TRNA SYNTHETASE)

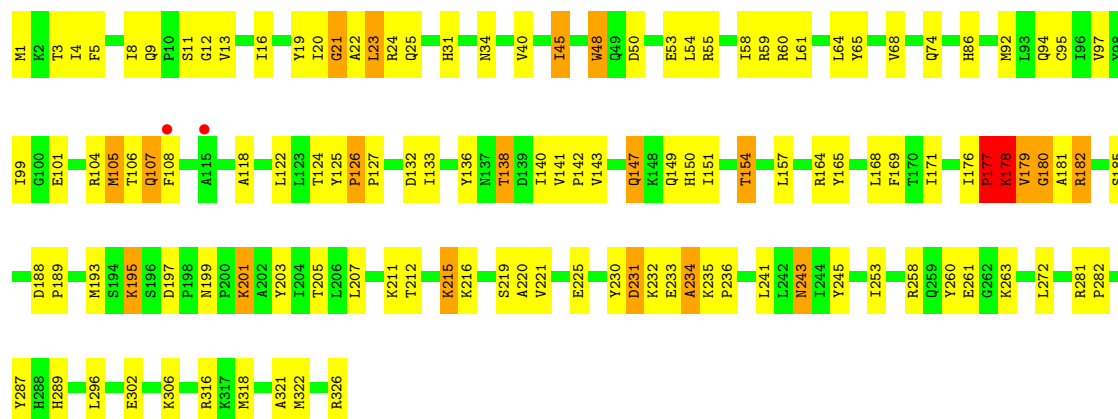


• Molecule 1: PROTEIN (TRYPTOPHANYL TRNA SYNTHETASE)

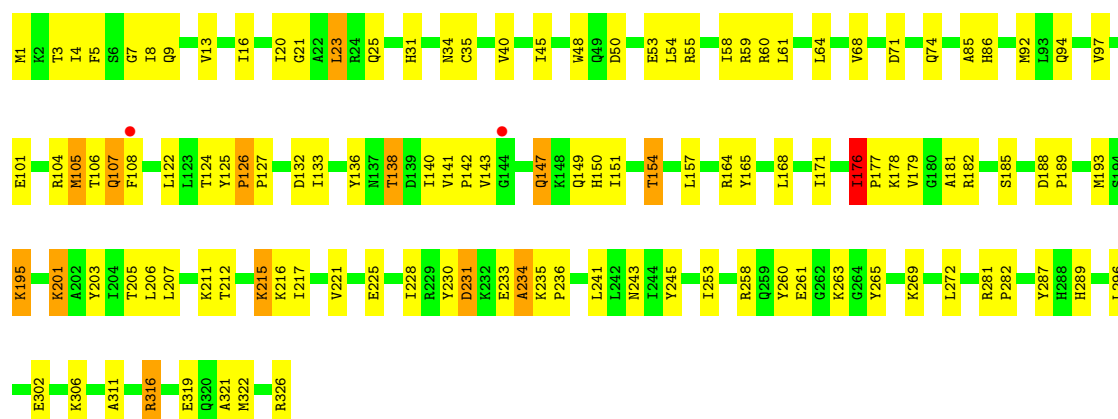


• Molecule 1: PROTEIN (TRYPTOPHANYL TRNA SYNTHETASE)

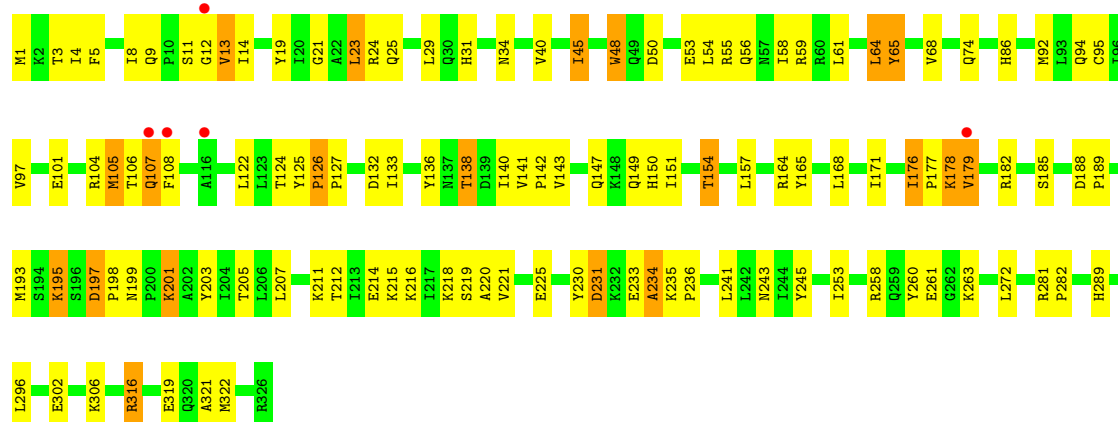




• Molecule 1: PROTEIN (TRYPTOPHANYL TRNA SYNTHETASE)

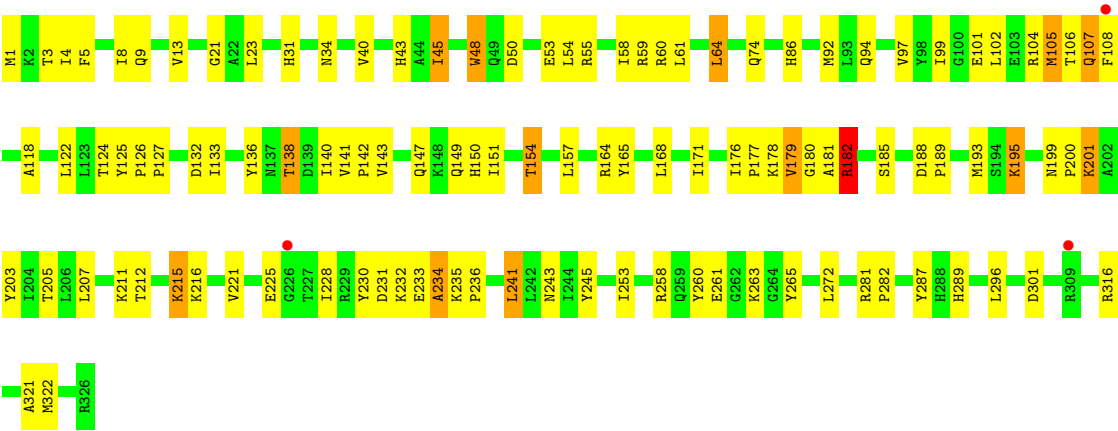


• Molecule 1: PROTEIN (TRYPTOPHANYL TRNA SYNTHETASE)



• Molecule 1: PROTEIN (TRYPTOPHANYL TRNA SYNTHETASE)





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	226.76Å 91.66Å 156.97Å 90.00° 132.66° 90.00°	Depositor
Resolution (Å)	10.00 – 2.90 10.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	74.3 (10.00-2.90) 72.5 (10.00-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.90Å)	Xtriage
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	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 62.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.036 for -h-2*k,l	Xtriage
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

Xtriage'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 2.3313e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.59	1/2628 (0.0%)	0.90	3/3552 (0.1%)
1	B	0.59	1/2628 (0.0%)	0.97	9/3552 (0.3%)
1	C	0.58	0/2628	0.91	7/3552 (0.2%)
1	D	0.60	0/2628	0.91	7/3552 (0.2%)
1	E	0.60	0/2628	0.91	7/3552 (0.2%)
1	F	0.56	0/2628	0.89	4/3552 (0.1%)
All	All	0.59	2/15768 (0.0%)	0.92	37/21312 (0.2%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	179	VAL	CA-CB	5.88	1.62	1.54
1	A	233	GLU	CA-C	5.18	1.59	1.52

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	179	VAL	O-C-N	-16.52	101.92	122.57
1	D	234	ALA	O-C-N	12.34	138.90	122.36
1	A	234	ALA	O-C-N	11.88	138.28	122.36
1	B	234	ALA	O-C-N	11.28	137.47	122.36
1	E	234	ALA	O-C-N	11.26	138.35	122.36
1	C	234	ALA	O-C-N	11.05	138.05	122.36
1	F	234	ALA	O-C-N	9.94	135.68	122.36
1	D	179	VAL	N-CA-C	7.26	118.47	108.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	179	VAL	N-CA-C	7.08	124.06	109.34
1	E	179	VAL	N-CA-C	7.06	118.20	108.89
1	F	180	GLY	N-CA-C	-6.37	98.09	113.18
1	B	177	PRO	N-CA-CB	6.07	108.54	102.17
1	C	107	GLN	N-CA-C	-6.01	105.44	112.89
1	C	180	GLY	N-CA-C	-6.00	98.97	113.18
1	E	107	GLN	N-CA-C	-5.91	105.56	112.89
1	E	21	GLY	N-CA-C	5.86	119.58	112.49
1	B	21	GLY	N-CA-C	5.85	119.56	112.49
1	B	107	GLN	N-CA-C	-5.84	105.64	112.89
1	B	179	VAL	CA-C-O	5.81	128.04	120.78
1	A	107	GLN	N-CA-C	-5.80	105.69	112.89
1	D	107	GLN	N-CA-C	-5.72	105.80	112.89
1	A	21	GLY	N-CA-C	5.67	119.35	112.49
1	F	107	GLN	N-CA-C	-5.64	105.89	112.89
1	F	21	GLY	N-CA-C	5.42	119.04	112.49
1	D	21	GLY	N-CA-C	5.24	118.83	112.49
1	C	21	GLY	N-CA-C	5.22	118.81	112.49
1	E	24	ARG	N-CA-C	5.21	116.64	111.07
1	C	197	ASP	CA-C-N	5.16	124.88	119.82
1	C	197	ASP	C-N-CA	5.16	124.88	119.82
1	C	24	ARG	N-CA-C	5.09	116.83	111.28
1	E	197	ASP	CA-C-N	5.08	124.80	119.82
1	E	197	ASP	C-N-CA	5.08	124.80	119.82
1	D	176	ILE	CA-C-N	5.08	125.35	119.92
1	D	176	ILE	C-N-CA	5.08	125.35	119.92
1	B	83	VAL	CA-C-N	5.07	125.35	119.47
1	B	83	VAL	C-N-CA	5.07	125.35	119.47
1	D	35	CYS	N-CA-C	5.06	118.19	110.20

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

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	91	0
1	B	2580	0	2598	88	0
1	C	2580	0	2598	99	0
1	D	2580	0	2598	79	0
1	E	2580	0	2598	88	0
1	F	2580	0	2598	78	0
All	All	15480	0	15588	499	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 16.

All (499) 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:A:193:MET:HE2	1:A:203:TYR:HA	1.48	0.95
1:D:176:ILE:HG13	1:D:177:PRO:HD2	1.49	0.95
1:A:195:LYS:H	1:A:195:LYS:HD2	1.33	0.91
1:D:193:MET:HE2	1:D:203:TYR:HA	1.50	0.91
1:F:195:LYS:H	1:F:195:LYS:HD2	1.34	0.90
1:B:105:MET:HE2	1:B:149:GLN:HE21	1.35	0.90
1:E:105:MET:HE2	1:E:149:GLN:HE21	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:D:105:MET:HE2	1:D:149:GLN:HE21	1.37	0.88
1:B:193:MET:HE2	1:B:203:TYR:HA	1.55	0.88
1:A:23:LEU:HD12	1:A:68:VAL:HG11	1.56	0.88
1:C:105:MET:HE2	1:C:149:GLN:HE21	1.35	0.88
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:F:105:MET:HE2	1:F:149:GLN:HE21	1.36	0.86
1:A:105:MET:HE2	1:A:149:GLN:HE21	1.39	0.86
1:B:195:LYS:H	1:B:195:LYS:HD2	1.40	0.85
1:C:193:MET:HE2	1:C:203:TYR:HA	1.58	0.85
1:C:195:LYS:H	1:C:195:LYS:HD2	1.39	0.85
1:F:193:MET:HE2	1:F:203:TYR:HA	1.57	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:E:193:MET:HE2	1:E:203:TYR:HA	1.58	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:180:GLY:C	1:C:182:ARG:H	1.86	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:8:ILE:HG22	1:E:61:LEU:HD21	1.63	0.80
1:E:86:HIS:HD2	1:E:132:ASP:OD1	1.64	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:D:106:THR:H	1:D:149:GLN:HE22	1.30	0.77
1:D:8:ILE:CG2	1:D:61:LEU:HD21	2.14	0.77
1:D:205:THR:HG22	1:D:207:LEU:H	1.49	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: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:29:LEU:HD11	1:A:178:LYS:HZ1	1.51	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:31:HIS:CD2	1:E:74:GLN:HE21	2.10	0.70
1:E:164:ARG:HD2	1:E:165:TYR:CE1	2.26	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:H	1:E:195:LYS:CD	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
1:A:54:LEU:O	1:A:58:ILE:HG13	1.95	0.67
1:A:45:ILE:HG12	1:D:322:MET:HE3	1.77	0.66
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:E:92:MET:HB3	1:E:322:MET:HE2	1.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:TRP:HE1	1:D:164:ARG:NH1	1.98	0.62
1:A:201:LYS:HE2	1:A:215:LYS:HE3	1.82	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:D:92:MET:HB3	1:D:322:MET:HE2	1.82	0.61
1:C:195:LYS:H	1:C:195:LYS:CD	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:23:LEU:HD21	1:E:65:TYR:CE1	2.35	0.61
1:E:195:LYS:HD2	1:E:195:LYS:N	2.11	0.61
1:A:179:VAL:HG12	1:A:181:ALA:H	1.65	0.61
1:D:13:VAL:HG13	1:D:13:VAL:O	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:E:105:MET:HE2	1:E:149:GLN:NE2	2.12	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:O	1:B:13:VAL:HG13	2.02	0.59
1:A:1:MET:HE2	1:E:214:GLU:OE1	2.02	0.59
1:A:124:THR:O	1:A:127:PRO:HD2	2.02	0.59
1:F:13:VAL:HG13	1:F:13:VAL:O	2.02	0.59
1:F:234:ALA:C	1:F:236:PRO:HD3	2.27	0.59
1:A:94:GLN:HE22	1:D:94:GLN:HE22	1.51	0.59
1:B:105:MET:HE2	1:B:149:GLN:NE2	2.14	0.59
1:E:234:ALA:C	1:E:236:PRO:HD3	2.27	0.59
1:A:13:VAL:O	1:A:13:VAL:HG13	2.03	0.59
1:B:234:ALA:C	1:B:236:PRO:HD3	2.27	0.59
1:B:94:GLN:HE22	1:E:94:GLN:HE22	1.51	0.59
1:D:31:HIS:HD2	1:D:74:GLN:HE21	1.50	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:195:LYS:HD2	1:F:195:LYS:N	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:H	1:A:195:LYS:CD	2.04	0.57
1:C:4:ILE:HG12	1:C:140:ILE:HB	1.85	0.57
1:A:234:ALA:C	1:A:236:PRO:HD3	2.30	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:B:92:MET:HB3	1:B:322:MET:HE2	1.87	0.56
1:C:234:ALA:C	1:C:236:PRO:HD3	2.30	0.56
1:F:195:LYS:H	1:F:195:LYS:CD	2.06	0.56
1:C:59:ARG:NH2	1:C:296:LEU:HD23	2.20	0.56
1:C:101:GLU:HA	1:C:104:ARG:HH11	1.69	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:H	1:D:195:LYS:CD	2.06	0.56
1:C:105:MET:HE2	1:C:149:GLN:NE2	2.14	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:234:ALA:C	1:D:236:PRO:HD3	2.31	0.56
1:C:92:MET:HB3	1:C:322:MET:HE2	1.87	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:HD2	1:A:195:LYS:N	2.12	0.56
1:B:322:MET:HE3	1:E:45:ILE:HG12	1.88	0.56
1:A:92:MET:HB3	1:A:322:MET:HE2	1.88	0.55
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:HA	1:B:25:GLN:NE2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:GLU:HA	1:A:104:ARG:HH11	1.72	0.54
1:C:45:ILE:HG12	1:F:322:MET:HE3	1.89	0.54
1:F:105:MET:HE2	1:F:149:GLN:NE2	2.15	0.54
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:45:ILE:HG12	1:E:322:MET:HE3	1.90	0.54
1:D:105:MET:HE2	1:D:149:GLN:NE2	2.15	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:N	1:B:171:ILE:HD12	2.24	0.53
1:C:5:PHE:HB2	1:C:138:THR:HG21	1.91	0.52
1:C:195:LYS:HD2	1:C:195:LYS:N	2.18	0.52
1:E:5:PHE:HB2	1:E:138:THR:HG21	1.91	0.52
1:E:59:ARG:NH2	1:E:296:LEU:HD23	2.24	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: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:B:176:ILE:C	1:B:176:ILE:HD12	2.34	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:177:PRO:C	1:B:178:LYS:HG2	2.35	0.51
1:B:195:LYS:H	1:B:195:LYS:CD	2.10	0.51
1:E:97:VAL:HB	1:E:157:LEU:HD21	1.92	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:A:105:MET:HE2	1:A:149:GLN:NE2	2.17	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:23:LEU:HD21	1:E:65:TYR:CZ	2.47	0.50
1:E:171:ILE:N	1:E:171:ILE:HD12	2.26	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:HD2	1:B:195:LYS:N	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:HD12	1:F:171:ILE:N	2.26	0.49
1:B:164:ARG:NH1	1:E:48:TRP:HE1	2.10	0.49
1:C:4:ILE:HG23	1:C:142:PRO:HD3	1.94	0.49
1:C:125:TYR:N	1:C:126:PRO:CD	2.75	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:179:VAL:HG12	1:F:179:VAL:O	2.12	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:HE21	1:B:25:GLN:CA	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:E:92:MET:CB	1:E:322:MET:HE2	2.43	0.48
1:D:231:ASP:OD2	1:D:234:ALA:HB3	2.13	0.47
1:F:92:MET:HB3	1:F:322:MET:HE2	1.96	0.47
1:F:1:MET:CE	1:F:34:ASN:HD22	2.26	0.47
1:F:60:ARG:HG2	1:F:287:TYR:OH	2.14	0.47
1:F:136:TYR:HB2	1:F:138:THR:HG22	1.96	0.47
1:C:171:ILE:HD12	1:C:171:ILE:N	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:A:1:MET:CE	1:A:34:ASN:HD22	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:179:VAL:HG13	1:F:182:ARG:CG	2.45	0.47
1:C:95:CYS:SG	1:F:45:ILE:CG2	3.02	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:A:176:ILE:HG23	1:A:177:PRO:HD2	1.96	0.47
1:B:150:HIS:O	1:B:154:THR:HG22	2.14	0.47
1:B:97:VAL:HB	1:B:157:LEU:HD21	1.97	0.47
1:D:92:MET:CB	1:D:322:MET:HE2	2.45	0.47
1:E:3:THR:HB	1:E:138:THR:HA	1.96	0.47
1:E:133:ILE:O	1:E:138:THR:HG23	2.15	0.47
1:C:322:MET:HE3	1:F:45:ILE:HG12	1.97	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:A:322:MET:HE3	1:D:45:ILE:HG12	1.98	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:14:ILE:HD11	1:E:64:LEU:HD22	1.97	0.45
1:E:245:TYR:HB2	1:E:272:LEU:HD13	1.99	0.45
1:A:231:ASP:OD2	1:A:234:ALA:HB3	2.15	0.45
1:A:281:ARG:N	1:A:282:PRO:HD2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:92:MET:CB	1:A:322:MET:HE2	2.47	0.45
1:C:235:LYS:N	1:C:236:PRO:HD3	2.31	0.45
1:B:302:GLU:O	1:B:306:LYS:HG3	2.17	0.45
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:1:MET:CE	1:D:34:ASN:HD22	2.30	0.45
1:D:16:ILE:O	1:D:20:ILE:HG13	2.17	0.45
1:A:133:ILE:O	1:A:138:THR:HG23	2.17	0.45
1:C:11:SER:C	1:C:13:VAL:H	2.25	0.45
1:A:4:ILE:HG23	1:A:142:PRO:HD3	1.98	0.44
1:A:141:VAL:HG12	1:A:143:VAL:HG13	1.98	0.44
1:B:147:GLN:HE21	1:B:147:GLN:HB3	1.59	0.44
1:C:199:ASN:C	1:C:199:ASN:HD22	2.25	0.44
1:D:228:ILE:HD13	1:D:265:TYR:CE1	2.52	0.44
1:C:1:MET:HE3	1:C:34:ASN:HD22	1.81	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:A:125:TYR:CG	1:A:126:PRO:HD3	2.53	0.44
1:B:199:ASN:C	1:B:199:ASN:HD22	2.24	0.44
1:D:316:ARG:NH1	1:D:319:GLU:OE1	2.50	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:86:HIS:HE1	1:A:136:TYR:OH	2.00	0.44
1:A:235:LYS:N	1:A:236:PRO:HD3	2.33	0.44
1:B:177:PRO:C	1:B:178:LYS:CG	2.91	0.44
1:A:1:MET:HE3	1:A:34:ASN:HD22	1.82	0.44
1:A:130:ALA:O	1:A:134:LEU:HG	2.18	0.44
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:HG23	1:C:176:ILE:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:141:VAL:HG12	1:F:143:VAL:HG13	1.99	0.43
1:C:92:MET:CB	1:C:322:MET:HE2	2.48	0.43
1:C:151:ILE:HA	1:C:154:THR:CG2	2.48	0.43
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:E:199:ASN:C	1:E:199:ASN:HD22	2.27	0.43
1:F:171:ILE:HD12	1:F:171:ILE:H	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:289:HIS:O	1:A:293:SER:HB2	2.18	0.43
1:B:178:LYS:O	1:B:179:VAL:C	2.60	0.43
1:C:8:ILE:HD12	1:C:65:TYR:OH	2.19	0.43
1:C:125:TYR:CG	1:C:126:PRO:HD3	2.53	0.43
1:C:147:GLN:HE21	1:C:147:GLN:HB3	1.59	0.43
1:D:50:ASP:HB3	1:D:53:GLU:HG3	2.00	0.43
1:E:1:MET:HE3	1:E:34:ASN:HD22	1.84	0.43
1:B:50:ASP:HB3	1:B:53:GLU:HG3	2.00	0.42
1:B:124:THR:O	1:B:127:PRO:HD2	2.19	0.42
1:A:56:GLN:HA	1:A:56:GLN:NE2	2.33	0.42
1:B:1:MET:HE3	1:B:34:ASN:HD22	1.83	0.42
1:B:92:MET:CB	1:B:322:MET:HE2	2.48	0.42
1:B:171:ILE:HD12	1:B:171:ILE:H	1.84	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:19:TYR:HE2	1:C:68:VAL:HG13	1.85	0.42
1:C:169:PHE:HZ	1:C:318:MET:HE3	1.85	0.42
1:C:181:ALA:CB	1:C:243:ASN:ND2	2.75	0.42
1:E:56:GLN:HA	1:E:56:GLN:NE2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:228:ILE:HD13	1:F:265:TYR:CE1	2.55	0.42
1:E:125:TYR:CD2	1:E:126:PRO:HD3	2.55	0.42
1:D:1:MET:HE3	1:D:34:ASN:HD22	1.83	0.42
1:D:7:GLY:C	1:D:8:ILE:HD13	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:B:7:GLY:C	1:B:8:ILE:HD13	2.44	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
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:A:197:ASP:HA	1:A:198:PRO:HD3	1.90	0.41
1:C:125:TYR:CD2	1:C:126:PRO:HD3	2.56	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:A:219:SER:O	1:A:220:ALA:C	2.63	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:B:47:VAL:O	1:B:48:TRP:C	2.61	0.41
1:C:50:ASP:HB3	1:C:53:GLU:HB2	2.01	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:1:MET:HE3	1:F:34:ASN:HD22	1.85	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:F:199:ASN:C	1:F:199:ASN:HD22	2.27	0.41
1:B:199:ASN:ND2	1:B:201:LYS:H	2.19	0.41
1:C:326:ARG:NH2	1:F:301:ASP:OD1	2.54	0.41
1:D:125:TYR:CG	1:D:126:PRO:HD3	2.56	0.41
1:D:147:GLN:HE21	1:D:147:GLN:HB3	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:B:228:ILE:HD13	1:B:265:TYR:CE1	2.56	0.41
1:C:180:GLY:O	1:C:181:ALA:HB3	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:219:SER:O	1:E:220:ALA:C	2.63	0.40
1:F:151:ILE:HA	1:F:154:THR:CG2	2.51	0.40
1:B:45:ILE:HG23	1:B:45:ILE:O	2.20	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:19:TYR:CE2	1:E:68:VAL:HG13	2.54	0.40
1:E:189:PRO:HB2	1:E:236:PRO:HB2	2.04	0.40
1:E:197:ASP:HA	1:E:198:PRO:HD3	1.93	0.40
1:C:189:PRO:HD3	1:C:221:VAL:HG21	2.04	0.40
1:C:219:SER:O	1:C:220:ALA:C	2.64	0.40
1:B:10:PRO:HA	1:B:61:LEU:HD22	2.04	0.40
1:D:25:GLN:CD	1:D:178:LYS:HD3	2.47	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:F:231:ASP:O	1:F:232:LYS:C	2.63	0.40
1:C:16:ILE:O	1:C:20:ILE:HG13	2.22	0.40
1:C:231:ASP:O	1:C:232:LYS:C	2.65	0.40
1:D:23:LEU:HD12	1:D:68:VAL:HG11	2.04	0.40
1:D:217:ILE:O	1:D:269:LYS:HD2	2.22	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%)	5	20
1	B	324/326 (99%)	299 (92%)	19 (6%)	6 (2%)	6	23
1	C	324/326 (99%)	298 (92%)	19 (6%)	7 (2%)	5	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	324/326 (99%)	300 (93%)	20 (6%)	4 (1%)	10	34
1	E	324/326 (99%)	298 (92%)	20 (6%)	6 (2%)	6	23
1	F	324/326 (99%)	300 (93%)	19 (6%)	5 (2%)	8	28
All	All	1944/1956 (99%)	1794 (92%)	115 (6%)	35 (2%)	6	25

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
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

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Mol	Chain	Res	Type
1	A	13	VAL
1	F	179	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	274/274 (100%)	248 (90%)	26 (10%)	8	26
1	B	274/274 (100%)	246 (90%)	28 (10%)	7	23
1	C	274/274 (100%)	247 (90%)	27 (10%)	7	24
1	D	274/274 (100%)	249 (91%)	25 (9%)	9	28
1	E	274/274 (100%)	248 (90%)	26 (10%)	8	26
1	F	274/274 (100%)	248 (90%)	26 (10%)	8	26
All	All	1644/1644 (100%)	1486 (90%)	158 (10%)	8	26

All (158) 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	122	LEU
1	A	126	PRO
1	A	138	THR
1	A	147	GLN
1	A	154	THR
1	A	168	LEU
1	A	176	ILE
1	A	182	ARG

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Mol	Chain	Res	Type
1	A	195	LYS
1	A	201	LYS
1	A	211	LYS
1	A	215	LYS
1	A	233	GLU
1	A	241	LEU
1	A	243	ASN
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	43	HIS
1	B	45	ILE
1	B	48	TRP
1	B	55	ARG
1	B	64	LEU
1	B	105	MET
1	B	107	GLN
1	B	122	LEU
1	B	126	PRO
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	201	LYS
1	B	211	LYS
1	B	215	LYS
1	B	233	GLU
1	B	241	LEU
1	B	243	ASN
1	B	258	ARG
1	B	289	HIS
1	B	316	ARG
1	C	9	GLN
1	C	23	LEU
1	C	45	ILE
1	C	48	TRP

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Mol	Chain	Res	Type
1	C	55	ARG
1	C	64	LEU
1	C	105	MET
1	C	107	GLN
1	C	122	LEU
1	C	126	PRO
1	C	138	THR
1	C	147	GLN
1	C	154	THR
1	C	168	LEU
1	C	177	PRO
1	C	178	LYS
1	C	179	VAL
1	C	195	LYS
1	C	201	LYS
1	C	211	LYS
1	C	215	LYS
1	C	233	GLU
1	C	241	LEU
1	C	243	ASN
1	C	258	ARG
1	C	289	HIS
1	C	316	ARG
1	D	9	GLN
1	D	23	LEU
1	D	48	TRP
1	D	55	ARG
1	D	64	LEU
1	D	105	MET
1	D	107	GLN
1	D	122	LEU
1	D	126	PRO
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	201	LYS
1	D	211	LYS
1	D	215	LYS

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Mol	Chain	Res	Type
1	D	233	GLU
1	D	241	LEU
1	D	243	ASN
1	D	258	ARG
1	D	289	HIS
1	D	316	ARG
1	E	9	GLN
1	E	23	LEU
1	E	45	ILE
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	126	PRO
1	E	138	THR
1	E	147	GLN
1	E	154	THR
1	E	168	LEU
1	E	176	ILE
1	E	182	ARG
1	E	195	LYS
1	E	201	LYS
1	E	211	LYS
1	E	233	GLU
1	E	241	LEU
1	E	243	ASN
1	E	258	ARG
1	E	289	HIS
1	E	316	ARG
1	F	9	GLN
1	F	23	LEU
1	F	43	HIS
1	F	45	ILE
1	F	48	TRP
1	F	55	ARG
1	F	64	LEU
1	F	105	MET
1	F	107	GLN
1	F	122	LEU

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Mol	Chain	Res	Type
1	F	138	THR
1	F	147	GLN
1	F	154	THR
1	F	168	LEU
1	F	178	LYS
1	F	182	ARG
1	F	195	LYS
1	F	201	LYS
1	F	211	LYS
1	F	215	LYS
1	F	233	GLU
1	F	241	LEU
1	F	243	ASN
1	F	258	ARG
1	F	289	HIS
1	F	316	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	18	ASN
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
1	A	149	GLN
1	A	199	ASN
1	A	243	ASN
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

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Mol	Chain	Res	Type
1	B	86	HIS
1	B	107	GLN
1	B	147	GLN
1	B	149	GLN
1	B	199	ASN
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	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
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	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

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Mol	Chain	Res	Type
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	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	243	ASN
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 oligosaccharides 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%)	-0.49	1 (0%) 90 87	14, 41, 89, 141	0
1	B	326/326 (100%)	-0.47	2 (0%) 85 81	14, 41, 89, 141	0
1	C	326/326 (100%)	-0.39	2 (0%) 85 81	18, 41, 89, 141	0
1	D	326/326 (100%)	-0.40	2 (0%) 85 81	17, 42, 90, 140	0
1	E	326/326 (100%)	-0.40	5 (1%) 72 64	15, 40, 90, 141	0
1	F	326/326 (100%)	-0.40	3 (0%) 81 75	15, 43, 89, 141	0
All	All	1956/1956 (100%)	-0.43	15 (0%) 82 77	14, 41, 90, 141	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	179	VAL	3.8
1	B	115	ALA	3.6
1	F	108	PHE	3.4
1	E	108	PHE	3.1
1	C	108	PHE	3.0
1	E	116	ALA	2.9
1	E	107	GLN	2.8
1	C	115	ALA	2.6
1	D	108	PHE	2.6
1	F	226	GLY	2.3
1	E	12	GLY	2.3
1	F	309	ARG	2.2
1	B	108	PHE	2.2
1	A	115	ALA	2.2
1	D	144	GLY	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.