



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 10:05 AM BST

PDB ID : 1MB2
Title : Crystal Structure of Tryptophanyl-tRNA Synthetase Complexed with Tryptophan in an Open Conformation
Authors : Retailleau, P.; Huang, X.; Yin, Y.; Hu, M.; Weinreb, V.; Vachette, P.; Vonrhein, C.; Bricogne, G.; Roversi, P.; Ilyin, V.; Carter Jr., C.W.
Deposited on : 2002-08-02
Resolution : 2.70 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.4.dev1
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) : 2.14.4.dev1

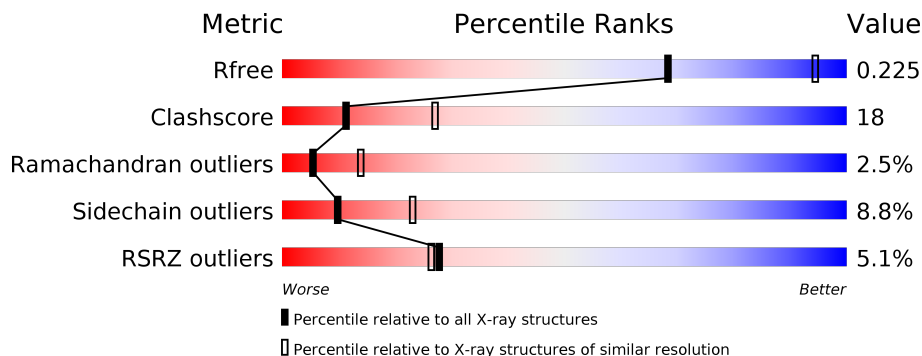
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	328	 5% 57% 40% ..
1	B	328	 5% 65% 30% ..
1	C	328	 4% 57% 39% ..
1	D	328	 6% 62% 33% ..
1	E	328	 5% 62% 32% 5% ..
1	F	328	 5% 64% 30% ..

2 Entry composition [i](#)

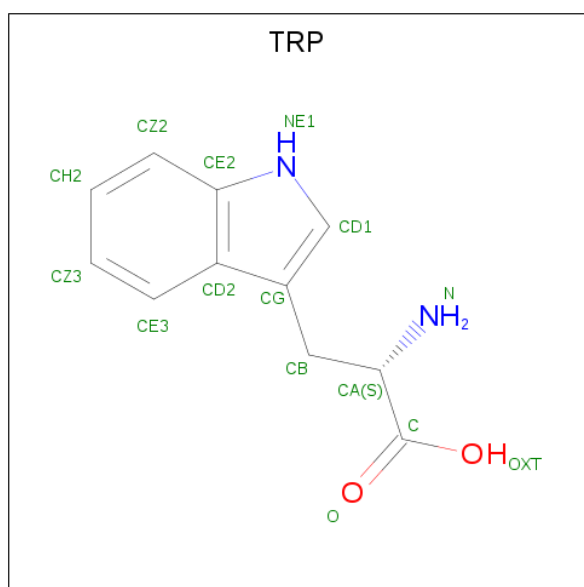
There are 2 unique types of molecules in this entry. The entry contains 15468 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TRYPTOPHAN-TRNA LIGASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	326	Total 2563	C 1624	N 442	O 484	S 13	0	0	0
1	B	326	Total 2563	C 1624	N 442	O 484	S 13	0	0	0
1	C	326	Total 2563	C 1624	N 442	O 484	S 13	0	0	0
1	D	326	Total 2563	C 1624	N 442	O 484	S 13	0	0	0
1	E	326	Total 2563	C 1624	N 442	O 484	S 13	0	0	0
1	F	326	Total 2563	C 1624	N 442	O 484	S 13	0	0	0

- Molecule 2 is TRYPTOPHAN (three-letter code: TRP) (formula: C₁₁H₁₂N₂O₂).

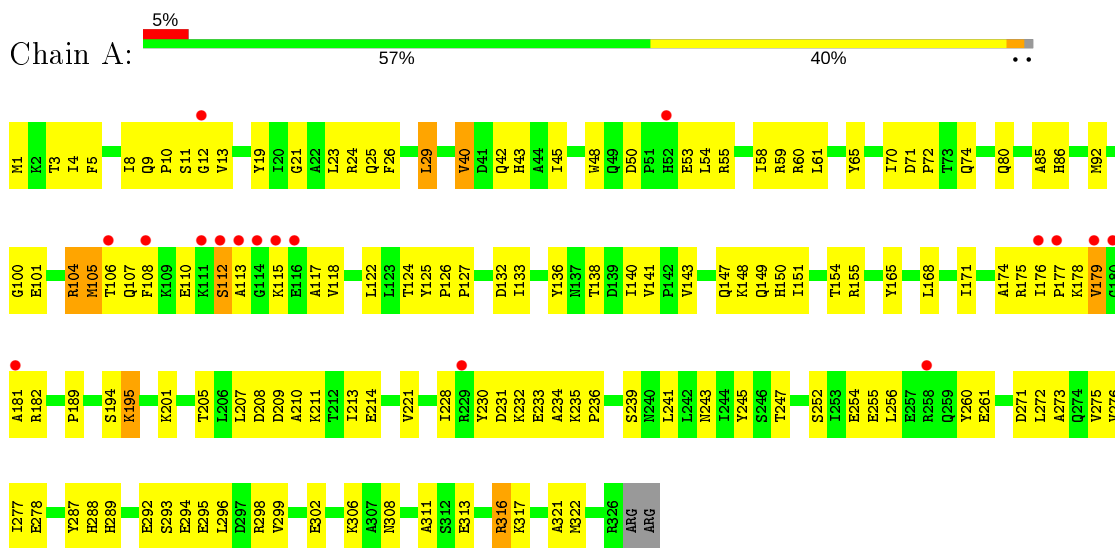


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	11	2	2		
2	B	1	Total	C	N	O	0	0
			15	11	2	2		
2	C	1	Total	C	N	O	0	0
			15	11	2	2		
2	D	1	Total	C	N	O	0	0
			15	11	2	2		
2	E	1	Total	C	N	O	0	0
			15	11	2	2		
2	F	1	Total	C	N	O	0	0
			15	11	2	2		

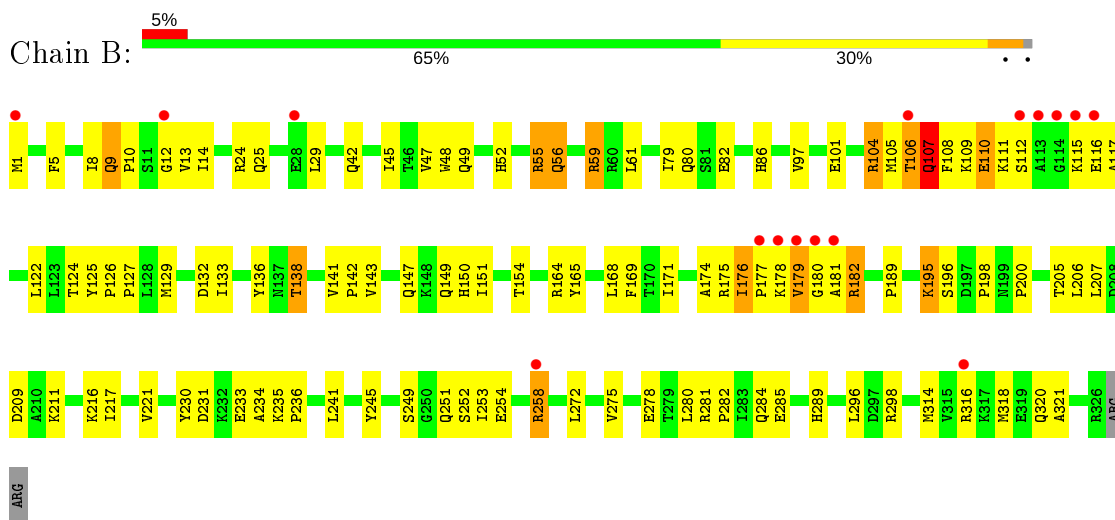
3 Residue-property plots [i](#)

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

• Molecule 1: TRYPTOPHAN-TRNA LIGASE

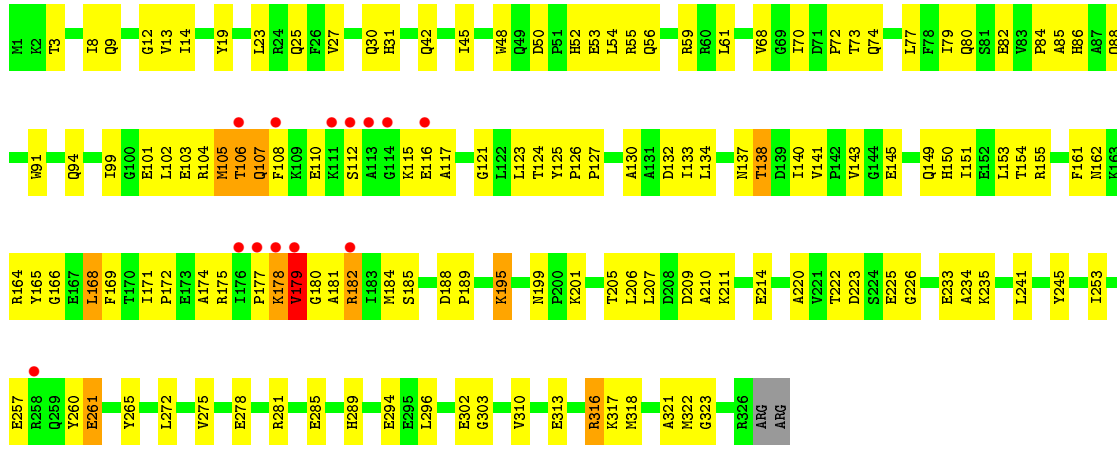


• Molecule 1: TRYPTOPHAN-TRNA LIGASE

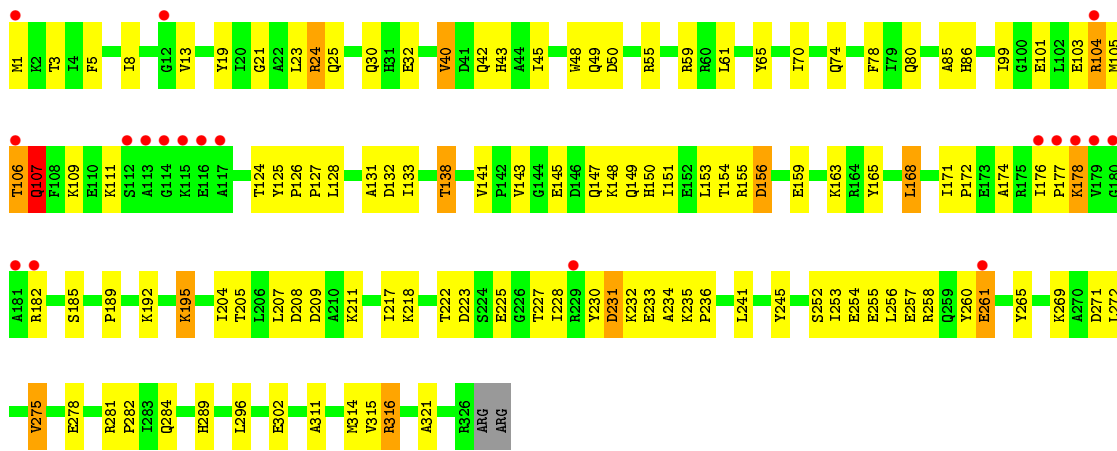


• Molecule 1: TRYPTOPHAN-TRNA LIGASE

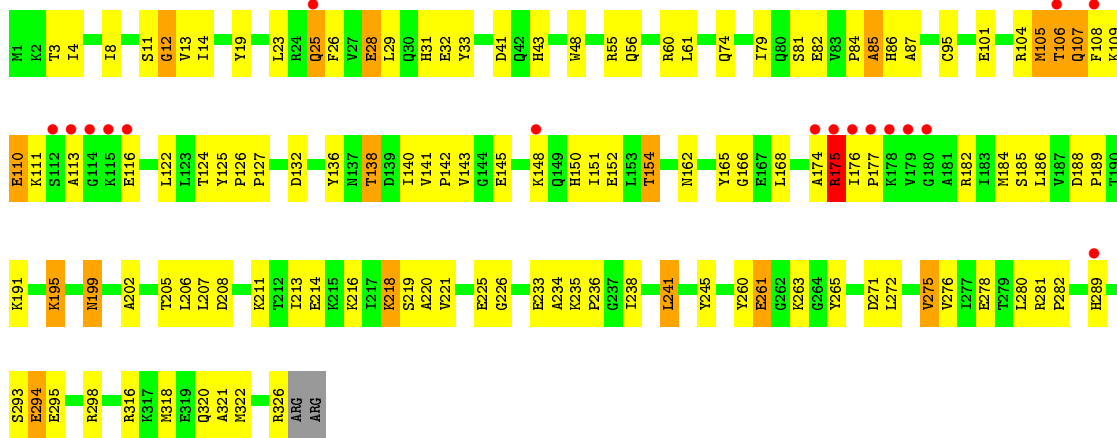




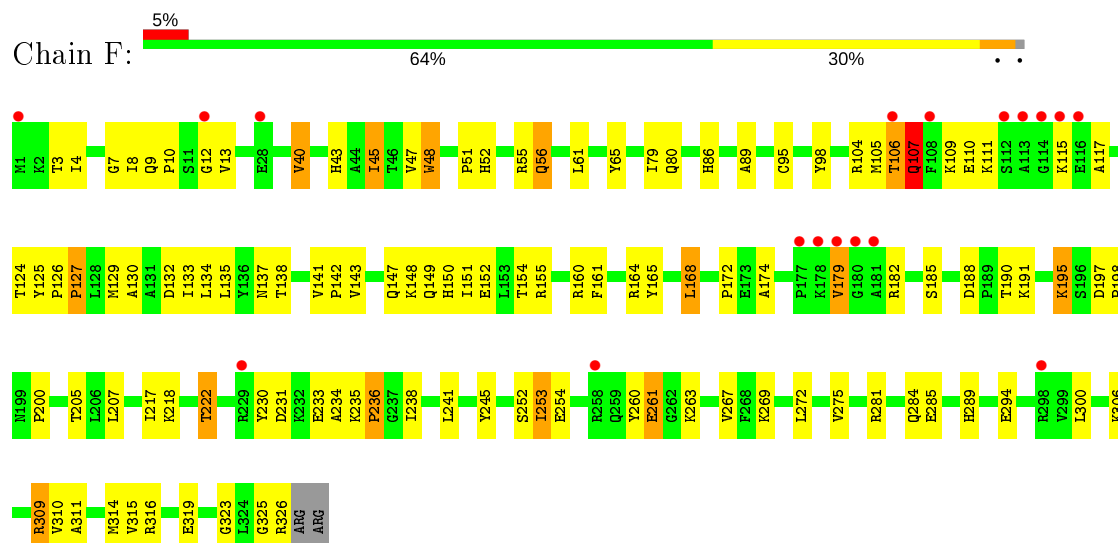
• Molecule 1: TRYPTOPHAN-TRNA LIGASE



• Molecule 1: TRYPTOPHAN-TRNA LIGASE



• Molecule 1: TRYPTOPHAN-TRNA LIGASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	228.73 Å 92.24 Å 157.59 Å 90.00° 132.71° 90.00°	Depositor
Resolution (Å)	14.98 – 2.70 15.02 – 2.58	Depositor EDS
% Data completeness (in resolution range)	83.9 (14.98-2.70) 78.0 (15.02-2.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.58 Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.220 , 0.254 0.194 , 0.225	Depositor DCC
R_{free} test set	4425 reflections (7.54%)	wwPDB-VP
Wilson B-factor (Å ²)	43.2	Xtrriage
Anisotropy	0.239	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 75.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.012 for -h-2*1,-k,l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15468	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 25.69 % 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 3.0244e-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 [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	0.44	0/2611	0.69	0/3532
1	B	0.42	0/2611	0.69	0/3532
1	C	0.45	0/2611	0.70	0/3532
1	D	0.43	0/2611	0.68	0/3532
1	E	0.47	0/2611	0.69	1/3532 (0.0%)
1	F	0.43	0/2611	0.67	0/3532
All	All	0.44	0/15666	0.69	1/21192 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	12	GLY	N-CA-C	5.59	127.08	113.10

There are no chirality outliers.

There are no planarity outliers.

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	2563	0	2554	100	0
1	B	2563	0	2554	92	0
1	C	2563	0	2554	93	0
1	D	2563	0	2554	107	0
1	E	2563	0	2554	85	0
1	F	2563	0	2554	86	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	15	0	9	0	0
2	B	15	0	9	3	0
2	C	15	0	9	0	0
2	D	15	0	9	1	0
2	E	15	0	9	0	0
2	F	15	0	9	2	0
All	All	15468	0	15378	548	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 18.

All (548) 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:C:205:THR:HG22	1:C:207:LEU:H	1.25	0.97
1:A:195:LYS:HD2	1:A:195:LYS:H	1.31	0.94
1:F:205:THR:HG22	1:F:207:LEU:H	1.32	0.93
1:A:5:PHE:HB2	1:A:138:THR:HG21	1.49	0.92
1:C:86:HIS:HD2	1:C:132:ASP:OD1	1.54	0.91
1:F:195:LYS:HD2	1:F:195:LYS:H	1.35	0.90
1:E:86:HIS:HD2	1:E:132:ASP:OD1	1.54	0.89
1:F:126:PRO:HB2	1:F:127:PRO:HD3	1.53	0.88
1:D:205:THR:HG22	1:D:207:LEU:H	1.37	0.88
1:C:145:GLU:CD	1:C:145:GLU:H	1.77	0.88
1:D:195:LYS:H	1:D:195:LYS:HD2	1.38	0.87
1:A:151:ILE:HG21	1:A:174:ALA:HB2	1.56	0.87
1:D:106:THR:H	1:D:149:GLN:HE22	1.24	0.84
1:B:176:ILE:HB	1:B:177:PRO:CD	2.07	0.84
1:B:205:THR:HG22	1:B:207:LEU:H	1.40	0.84
1:D:176:ILE:HG23	1:D:177:PRO:HD2	1.58	0.84
1:A:92:MET:HG2	1:A:322:MET:CE	2.09	0.82
1:D:5:PHE:HB2	1:D:138:THR:HG21	1.61	0.82
1:C:184:MET:HG3	1:C:189:PRO:O	1.82	0.80
1:B:281:ARG:O	1:B:285:GLU:HG3	1.81	0.80
1:B:25:GLN:OE1	1:B:178:LYS:HE2	1.82	0.79
1:C:195:LYS:HD2	1:C:195:LYS:H	1.46	0.79
1:A:205:THR:HG22	1:A:207:LEU:H	1.48	0.78
1:F:309:ARG:HH11	1:F:310:VAL:HG23	1.49	0.78
1:D:106:THR:N	1:D:149:GLN:HE22	1.81	0.77
1:A:125:TYR:CD2	1:A:126:PRO:HD3	2.19	0.77
1:C:133:ILE:HD13	1:C:141:VAL:HG21	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:THR:O	1:D:127:PRO:HD2	1.83	0.77
1:A:124:THR:O	1:A:127:PRO:HD2	1.84	0.76
1:E:188:ASP:OD2	1:E:191:LYS:HB2	1.85	0.76
1:E:205:THR:HG22	1:E:207:LEU:H	1.50	0.76
1:C:150:HIS:O	1:C:154:THR:HG23	1.86	0.75
1:D:59:ARG:NH2	1:D:296:LEU:HD23	2.00	0.75
1:B:29:LEU:HD21	1:B:175:ARG:HH22	1.51	0.75
1:E:205:THR:HB	1:E:208:ASP:OD1	1.87	0.75
1:F:195:LYS:H	1:F:195:LYS:CD	1.99	0.74
1:A:195:LYS:CD	1:A:195:LYS:H	1.95	0.74
1:B:177:PRO:O	1:B:178:LYS:HB2	1.88	0.73
1:A:86:HIS:HD2	1:A:132:ASP:OD1	1.72	0.72
1:B:82:GLU:OE2	1:E:326:ARG:HD3	1.90	0.72
1:D:106:THR:H	1:D:149:GLN:NE2	1.88	0.72
1:E:195:LYS:H	1:E:195:LYS:HD2	1.55	0.71
1:B:198:PRO:O	1:B:200:PRO:HD3	1.90	0.71
1:D:271:ASP:O	1:D:275:VAL:HG12	1.90	0.71
1:E:25:GLN:NE2	1:E:29:LEU:HD13	2.06	0.71
1:C:54:LEU:HD23	1:F:323:GLY:O	1.91	0.71
1:B:86:HIS:HD2	1:B:132:ASP:OD1	1.73	0.71
1:A:195:LYS:N	1:A:195:LYS:HD2	2.05	0.70
1:C:151:ILE:HG21	1:C:174:ALA:HB2	1.73	0.70
1:A:231:ASP:HB3	1:A:235:LYS:HB2	1.72	0.70
1:D:176:ILE:HG23	1:D:177:PRO:CD	2.22	0.70
1:E:25:GLN:O	1:E:29:LEU:HB2	1.92	0.70
1:A:181:ALA:O	1:A:182:ARG:HB2	1.90	0.70
1:B:126:PRO:HB2	1:B:127:PRO:HD3	1.74	0.70
1:E:195:LYS:N	1:E:195:LYS:HD2	2.07	0.70
1:C:165:TYR:HB3	1:C:321:ALA:HB1	1.74	0.70
1:F:106:THR:H	1:F:149:GLN:HE22	1.38	0.69
1:B:124:THR:HG21	1:E:124:THR:HG21	1.74	0.69
1:F:179:VAL:O	1:F:179:VAL:HG12	1.92	0.69
1:B:234:ALA:C	1:B:236:PRO:HD3	2.12	0.69
1:A:92:MET:HG2	1:A:322:MET:HE1	1.75	0.68
1:C:14:ILE:HD11	1:C:206:LEU:HD12	1.74	0.68
1:D:195:LYS:HD2	1:D:195:LYS:N	2.09	0.68
1:D:55:ARG:HG2	1:D:55:ARG:HH11	1.58	0.68
1:E:3:THR:HB	1:E:138:THR:HA	1.75	0.68
1:B:143:VAL:HB	1:B:147:GLN:HB2	1.75	0.68
1:C:195:LYS:H	1:C:195:LYS:CD	2.06	0.68
1:E:126:PRO:HB2	1:E:127:PRO:HD3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:GLY:O	1:A:179:VAL:HG22	1.93	0.68
1:E:195:LYS:CD	1:E:195:LYS:H	2.07	0.67
1:F:272:LEU:O	1:F:275:VAL:HG12	1.94	0.67
1:C:105:MET:HA	1:C:149:GLN:HE22	1.59	0.66
1:A:92:MET:HG2	1:A:322:MET:HE2	1.78	0.66
1:A:55:ARG:HG2	1:A:55:ARG:HH11	1.60	0.66
1:C:323:GLY:HA2	1:F:55:ARG:HE	1.59	0.66
1:D:254:GLU:H	1:D:254:GLU:CD	1.99	0.66
1:A:4:ILE:HG12	1:A:140:ILE:HB	1.78	0.66
1:F:150:HIS:O	1:F:154:THR:HG23	1.95	0.65
1:D:13:VAL:O	1:D:13:VAL:HG22	1.96	0.65
1:F:86:HIS:HD2	1:F:132:ASP:OD1	1.80	0.65
1:D:86:HIS:HD2	1:D:132:ASP:OD1	1.80	0.65
1:F:55:ARG:HG2	1:F:55:ARG:HH11	1.62	0.64
1:D:143:VAL:HB	1:D:147:GLN:HB2	1.80	0.64
1:F:185:SER:HB3	1:F:188:ASP:O	1.97	0.64
1:C:126:PRO:HB2	1:C:127:PRO:HD3	1.79	0.64
1:C:27:VAL:O	1:C:30:GLN:HG2	1.97	0.64
1:F:10:PRO:HA	1:F:61:LEU:HD22	1.78	0.63
1:E:101:GLU:O	1:E:104:ARG:HG2	1.98	0.63
1:B:29:LEU:HD21	1:B:175:ARG:NH2	2.13	0.63
1:C:86:HIS:CD2	1:C:132:ASP:OD1	2.44	0.63
1:E:184:MET:HG3	1:E:189:PRO:O	1.98	0.63
1:A:176:ILE:HG23	1:A:177:PRO:HD2	1.80	0.63
1:B:179:VAL:HG12	1:B:180:GLY:H	1.62	0.63
1:D:165:TYR:HB3	1:D:321:ALA:HB1	1.81	0.63
1:A:150:HIS:O	1:A:154:THR:HG23	1.98	0.62
1:A:25:GLN:OE1	1:A:178:LYS:HD2	1.98	0.62
1:B:141:VAL:HG12	1:B:143:VAL:HG13	1.81	0.62
1:C:55:ARG:HE	1:F:323:GLY:HA2	1.63	0.62
1:A:165:TYR:HB3	1:A:321:ALA:HB1	1.81	0.62
1:A:272:LEU:HA	1:A:275:VAL:HG12	1.81	0.62
1:C:31:HIS:ND1	1:C:74:GLN:HG2	2.15	0.62
1:D:85:ALA:HB3	1:D:311:ALA:HB1	1.82	0.62
1:F:309:ARG:HH11	1:F:310:VAL:CG2	2.13	0.62
1:A:233:GLU:O	1:A:234:ALA:HB3	1.99	0.62
1:F:309:ARG:NH1	1:F:310:VAL:HG23	2.14	0.62
1:B:176:ILE:HB	1:B:177:PRO:HD2	1.82	0.62
1:E:162:ASN:HA	1:E:166:GLY:O	2.00	0.62
1:C:225:GLU:OE1	1:C:235:LYS:NZ	2.23	0.62
1:B:25:GLN:HG3	1:B:29:LEU:HD13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:165:TYR:HB3	1:E:321:ALA:HB1	1.80	0.61
1:B:195:LYS:N	1:B:195:LYS:HD2	2.15	0.61
1:E:141:VAL:HG12	1:E:143:VAL:HG13	1.82	0.61
1:C:178:LYS:HE3	1:C:179:VAL:HG22	1.83	0.61
1:E:140:ILE:HG21	1:E:175:ARG:HG3	1.83	0.61
1:C:3:THR:HB	1:C:138:THR:HA	1.82	0.60
1:B:195:LYS:CD	1:B:195:LYS:H	2.13	0.60
1:D:133:ILE:O	1:D:138:THR:HG23	2.02	0.60
1:A:254:GLU:H	1:A:254:GLU:CD	2.05	0.60
1:B:5:PHE:HB2	1:B:138:THR:HG21	1.83	0.60
1:B:195:LYS:H	1:B:195:LYS:HD2	1.67	0.60
1:C:91:TRP:O	1:C:94:GLN:HB2	2.02	0.59
1:E:214:GLU:O	1:E:218:LYS:HG3	2.02	0.59
1:A:29:LEU:HD21	1:A:175:ARG:HH12	1.66	0.59
1:E:140:ILE:CG2	1:E:175:ARG:HG3	2.33	0.59
1:E:11:SER:O	1:E:13:VAL:HG12	2.02	0.59
1:B:47:VAL:O	1:B:49:GLN:HG2	2.03	0.59
1:D:205:THR:N	1:D:208:ASP:OD2	2.30	0.59
1:A:228:ILE:HG13	1:A:260:TYR:HB3	1.85	0.59
1:B:258:ARG:HA	1:B:258:ARG:HE	1.68	0.58
1:C:8:ILE:CG2	1:C:61:LEU:HD21	2.33	0.58
1:B:106:THR:H	1:B:149:GLN:HE22	1.52	0.58
1:A:140:ILE:HG23	1:A:175:ARG:HB2	1.86	0.58
1:F:217:ILE:O	1:F:269:LYS:HD3	2.04	0.58
1:B:230:TYR:CD2	1:B:253:ILE:HD13	2.39	0.57
1:C:133:ILE:O	1:C:138:THR:HG23	2.04	0.57
1:C:85:ALA:HA	1:C:88:GLN:OE1	2.04	0.57
1:E:86:HIS:CD2	1:E:132:ASP:OD1	2.47	0.57
1:F:306:LYS:HA	1:F:309:ARG:NE	2.19	0.57
1:B:179:VAL:HG12	1:B:180:GLY:N	2.20	0.57
1:D:105:MET:HA	1:D:149:GLN:HE22	1.69	0.57
1:E:272:LEU:O	1:E:276:VAL:HG23	2.05	0.57
1:A:8:ILE:CG2	1:A:61:LEU:HD21	2.34	0.57
1:B:55:ARG:HH11	1:B:55:ARG:HG2	1.70	0.57
1:D:150:HIS:O	1:D:154:THR:HG23	2.04	0.57
1:D:3:THR:HB	1:D:138:THR:HA	1.87	0.57
1:A:24:ARG:HH12	1:A:247:THR:HB	1.70	0.57
1:D:195:LYS:CD	1:D:195:LYS:H	2.00	0.57
1:F:8:ILE:HG22	1:F:61:LEU:HD21	1.86	0.57
1:A:288:HIS:O	1:A:292:GLU:HG2	2.04	0.56
1:D:65:TYR:O	1:D:70:ILE:HG12	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:109:LYS:C	1:F:111:LYS:H	2.09	0.56
1:F:306:LYS:O	1:F:309:ARG:NH1	2.38	0.56
1:A:176:ILE:HG23	1:A:177:PRO:CD	2.34	0.56
1:C:155:ARG:NH1	1:C:172:PRO:O	2.38	0.56
1:F:233:GLU:O	1:F:234:ALA:HB3	2.06	0.56
1:D:42:GLN:HB2	1:D:80:GLN:OE1	2.05	0.56
1:D:231:ASP:CB	1:D:235:LYS:HB2	2.35	0.56
1:F:98:TYR:CE2	1:F:160:ARG:NH1	2.73	0.56
1:C:205:THR:HG22	1:C:207:LEU:N	2.09	0.56
1:E:23:LEU:HA	1:E:26:PHE:HD2	1.70	0.56
1:A:230:TYR:CE2	1:A:239:SER:HB3	2.40	0.56
1:B:8:ILE:HG22	1:B:61:LEU:HD21	1.88	0.56
1:E:32:GLU:HG3	1:E:33:TYR:CD1	2.40	0.56
1:B:235:LYS:N	1:B:236:PRO:HD3	2.21	0.56
1:F:129:MET:HG3	2:F:405:TRP:CD1	2.41	0.56
1:D:151:ILE:O	1:D:155:ARG:HG3	2.06	0.56
1:C:211:LYS:HB3	1:C:211:LYS:NZ	2.21	0.56
1:D:231:ASP:HB3	1:D:235:LYS:HB2	1.87	0.56
1:B:231:ASP:HB3	1:B:235:LYS:HB2	1.88	0.55
1:C:195:LYS:HD2	1:C:195:LYS:N	2.19	0.55
1:B:133:ILE:O	1:B:138:THR:HG23	2.07	0.55
1:B:14:ILE:HG13	1:B:14:ILE:O	2.05	0.55
1:C:102:LEU:O	1:C:105:MET:HB2	2.07	0.55
1:C:124:THR:HG21	1:F:124:THR:HG21	1.87	0.55
1:F:272:LEU:HD12	1:F:275:VAL:CG1	2.36	0.55
1:A:50:ASP:HB3	1:A:53:GLU:HB2	1.88	0.55
1:C:226:GLY:HA2	1:C:265:TYR:CZ	2.42	0.55
1:D:233:GLU:O	1:D:234:ALA:HB3	2.07	0.55
1:B:233:GLU:O	1:B:234:ALA:HB3	2.07	0.55
1:D:86:HIS:CD2	1:D:132:ASP:OD1	2.59	0.55
1:E:225:GLU:OE1	1:E:235:LYS:NZ	2.35	0.55
1:E:41:ASP:OD2	1:E:81:SER:OG	2.18	0.55
1:D:182:ARG:CZ	1:D:192:LYS:HD3	2.37	0.55
1:D:228:ILE:HD13	1:D:265:TYR:CE1	2.41	0.55
1:B:14:ILE:HD11	1:B:206:LEU:HD12	1.89	0.55
1:F:195:LYS:N	1:F:195:LYS:HD2	2.14	0.55
1:A:141:VAL:HG12	1:A:143:VAL:HG13	1.89	0.54
1:F:198:PRO:O	1:F:200:PRO:HD3	2.08	0.54
1:B:211:LYS:HB3	1:B:211:LYS:NZ	2.21	0.54
1:A:85:ALA:HB3	1:A:311:ALA:HB1	1.90	0.54
1:A:86:HIS:HE1	1:A:136:TYR:OH	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:LEU:O	1:B:284:GLN:HG3	2.07	0.54
1:C:99:ILE:O	1:C:103:GLU:HG3	2.08	0.54
1:C:211:LYS:HZ3	1:C:211:LYS:HB3	1.72	0.54
1:E:101:GLU:HA	1:E:104:ARG:HH11	1.73	0.54
1:D:189:PRO:HB2	1:D:236:PRO:HB2	1.88	0.54
1:B:177:PRO:C	1:B:179:VAL:H	2.11	0.54
1:F:52:HIS:O	1:F:56:GLN:HB2	2.08	0.54
1:B:181:ALA:O	1:B:182:ARG:C	2.46	0.53
1:E:136:TYR:HB2	1:E:138:THR:HG22	1.90	0.53
1:C:253:ILE:O	1:C:257:GLU:HG3	2.08	0.53
1:F:125:TYR:N	1:F:126:PRO:CD	2.71	0.53
1:A:211:LYS:HB3	1:A:211:LYS:NZ	2.22	0.53
1:E:176:ILE:HG13	1:E:177:PRO:HD2	1.90	0.53
1:A:316:ARG:HA	1:A:316:ARG:NH1	2.23	0.53
1:D:21:GLY:O	1:D:177:PRO:HB3	2.08	0.53
1:A:295:GLU:O	1:A:299:VAL:HG23	2.09	0.53
1:D:40:VAL:O	1:D:40:VAL:HG23	2.08	0.53
1:D:126:PRO:HB2	1:D:127:PRO:HD3	1.90	0.53
1:F:149:GLN:O	1:F:149:GLN:HG2	2.07	0.53
1:D:105:MET:HA	1:D:149:GLN:NE2	2.24	0.53
1:D:43:HIS:HD2	1:D:125:TYR:HB2	1.75	0.53
1:E:176:ILE:HG13	1:E:177:PRO:CD	2.39	0.53
1:E:79:ILE:HB	1:E:82:GLU:HG3	1.91	0.53
1:C:184:MET:CG	1:C:189:PRO:O	2.54	0.52
1:F:309:ARG:NH1	1:F:310:VAL:CG2	2.72	0.52
1:C:59:ARG:NH2	1:C:296:LEU:HD23	2.25	0.52
1:E:43:HIS:HE1	1:E:132:ASP:OD2	1.93	0.52
1:D:43:HIS:CD2	1:D:125:TYR:HB2	2.44	0.52
1:E:150:HIS:O	1:E:154:THR:CG2	2.57	0.52
1:C:108:PHE:CZ	1:C:123:LEU:HD13	2.44	0.52
1:C:55:ARG:HG2	1:C:55:ARG:HH11	1.73	0.52
1:D:8:ILE:CG2	1:D:61:LEU:HD21	2.40	0.52
1:B:272:LEU:HA	1:B:275:VAL:HG12	1.91	0.52
1:C:145:GLU:CD	1:C:145:GLU:N	2.54	0.52
1:C:42:GLN:OE1	1:C:80:GLN:HG2	2.10	0.52
1:C:108:PHE:C	1:C:110:GLU:N	2.61	0.52
1:F:161:PHE:HE2	1:F:168:LEU:HD12	1.74	0.51
1:F:89:ALA:HB2	1:F:135:LEU:HD21	1.92	0.51
1:F:13:VAL:O	1:F:13:VAL:HG13	2.11	0.51
1:F:155:ARG:NH1	1:F:172:PRO:O	2.42	0.51
1:F:234:ALA:O	1:F:236:PRO:HD3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:ARG:O	1:C:285:GLU:HG3	2.09	0.51
1:D:228:ILE:HD13	1:D:265:TYR:HE1	1.73	0.51
1:F:45:ILE:HG23	1:F:45:ILE:O	2.11	0.51
1:C:105:MET:O	1:C:107:GLN:N	2.44	0.51
1:A:40:VAL:O	1:A:40:VAL:HG23	2.11	0.51
1:A:143:VAL:HB	1:A:147:GLN:HB2	1.92	0.50
1:D:316:ARG:HA	1:D:316:ARG:NH1	2.25	0.50
1:F:252:SER:HB2	1:F:254:GLU:OE1	2.11	0.50
1:A:59:ARG:NH2	1:A:296:LEU:HD23	2.27	0.50
1:C:13:VAL:O	1:C:13:VAL:HG13	2.11	0.50
1:F:8:ILE:HD12	1:F:65:TYR:OH	2.12	0.50
1:C:108:PHE:C	1:C:110:GLU:H	2.14	0.50
1:F:141:VAL:HG12	1:F:143:VAL:HG13	1.93	0.50
1:F:143:VAL:HB	1:F:147:GLN:HB2	1.93	0.50
1:D:258:ARG:NH2	1:D:261:GLU:OE1	2.45	0.50
1:B:165:TYR:HB3	1:B:321:ALA:HB1	1.94	0.50
1:C:140:ILE:HG23	1:C:175:ARG:HB2	1.93	0.50
1:D:125:TYR:CD2	1:D:126:PRO:HD3	2.47	0.50
1:A:260:TYR:OH	1:A:271:ASP:OD2	2.24	0.49
1:B:125:TYR:N	1:B:126:PRO:CD	2.74	0.49
1:F:105:MET:O	1:F:107:GLN:N	2.45	0.49
1:A:245:TYR:CD2	1:A:272:LEU:HD13	2.46	0.49
1:D:155:ARG:NH1	1:D:172:PRO:O	2.45	0.49
1:D:252:SER:OG	1:D:255:GLU:HB2	2.12	0.49
1:B:107:GLN:C	1:B:109:LYS:H	2.16	0.49
1:A:100:GLY:O	1:A:104:ARG:HG2	2.12	0.49
1:A:302:GLU:O	1:A:306:LYS:HG3	2.11	0.49
1:C:141:VAL:HG12	1:C:143:VAL:HG13	1.93	0.49
1:E:233:GLU:O	1:E:234:ALA:HB3	2.13	0.49
1:E:4:ILE:HG23	1:E:142:PRO:HD3	1.95	0.49
1:D:55:ARG:HG2	1:D:55:ARG:NH1	2.25	0.49
1:A:3:THR:HB	1:A:138:THR:HA	1.95	0.49
1:C:272:LEU:O	1:C:275:VAL:HG12	2.13	0.49
1:D:103:GLU:C	1:D:105:MET:H	2.16	0.49
1:D:228:ILE:HD11	1:D:265:TYR:HD1	1.77	0.49
1:F:309:ARG:HD3	1:F:310:VAL:HG23	1.94	0.49
1:A:189:PRO:HD3	1:A:221:VAL:CG2	2.42	0.49
1:A:108:PHE:HZ	1:D:99:ILE:HD13	1.78	0.49
1:A:126:PRO:HB2	1:A:127:PRO:HD3	1.95	0.49
1:C:323:GLY:HA2	1:F:55:ARG:NE	2.27	0.49
1:A:25:GLN:O	1:A:29:LEU:HD12	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:HIS:HE1	1:A:132:ASP:OD2	1.95	0.49
1:A:151:ILE:O	1:A:155:ARG:HG3	2.13	0.48
1:D:223:ASP:OD2	1:D:235:LYS:HG2	2.12	0.48
1:A:181:ALA:O	1:A:182:ARG:CB	2.61	0.48
1:A:189:PRO:HD3	1:A:221:VAL:HG21	1.94	0.48
1:C:55:ARG:HG2	1:C:55:ARG:NH1	2.29	0.48
1:A:272:LEU:HA	1:A:275:VAL:CG1	2.42	0.48
1:A:40:VAL:HA	1:A:80:GLN:HB2	1.95	0.48
1:B:115:LYS:O	1:B:117:ALA:N	2.47	0.48
1:F:230:TYR:CD2	1:F:253:ILE:HD13	2.48	0.48
1:F:315:VAL:HG12	1:F:319:GLU:OE2	2.13	0.48
1:B:281:ARG:N	1:B:282:PRO:HD2	2.29	0.48
1:B:59:ARG:CZ	1:B:296:LEU:HD23	2.44	0.48
1:D:40:VAL:HA	1:D:80:GLN:HB2	1.95	0.48
1:F:115:LYS:C	1:F:117:ALA:H	2.16	0.48
1:F:51:PRO:O	1:F:55:ARG:HB2	2.12	0.48
1:B:45:ILE:CG2	1:E:95:CYS:SG	3.01	0.48
1:D:223:ASP:CG	1:D:235:LYS:HZ2	2.16	0.48
1:A:23:LEU:HA	1:A:26:PHE:HD1	1.77	0.48
1:B:9:GLN:NE2	1:B:10:PRO:HD2	2.29	0.48
1:E:151:ILE:HG21	1:E:174:ALA:HB2	1.96	0.48
1:F:207:LEU:HA	1:F:284:GLN:HE21	1.78	0.48
1:B:105:MET:HA	1:B:149:GLN:HE22	1.78	0.48
1:C:14:ILE:HD11	1:C:206:LEU:CD1	2.44	0.48
1:D:211:LYS:HB3	1:D:211:LYS:NZ	2.29	0.48
1:F:126:PRO:HB2	1:F:127:PRO:CD	2.34	0.48
1:C:225:GLU:HB3	1:C:235:LYS:NZ	2.29	0.48
1:D:225:GLU:O	1:D:227:THR:HG23	2.14	0.48
1:D:230:TYR:HE1	1:D:232:LYS:HG2	1.78	0.48
1:A:245:TYR:CE1	1:A:256:LEU:HD21	2.49	0.48
1:C:171:ILE:N	1:C:171:ILE:CD1	2.77	0.48
1:C:82:GLU:O	1:C:84:PRO:HD3	2.14	0.48
1:E:109:LYS:C	1:E:111:LYS:H	2.16	0.48
1:C:101:GLU:HA	1:C:104:ARG:HH11	1.78	0.47
1:A:133:ILE:HD13	1:A:141:VAL:HG21	1.95	0.47
1:D:19:TYR:HA	1:D:23:LEU:HB2	1.95	0.47
1:A:292:GLU:HG3	1:A:293:SER:N	2.30	0.47
1:B:209:ASP:OD1	1:B:211:LYS:HB3	2.14	0.47
1:E:19:TYR:HA	1:E:23:LEU:HB3	1.96	0.47
1:F:79:ILE:HD11	1:F:300:LEU:HD13	1.96	0.47
1:A:42:GLN:O	1:A:45:ILE:HG22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:ILE:N	1:C:171:ILE:HD12	2.29	0.47
1:D:159:GLU:O	1:D:163:LYS:HG3	2.15	0.47
1:F:179:VAL:HG13	1:F:182:ARG:HG3	1.95	0.47
1:A:205:THR:N	1:A:208:ASP:OD2	2.34	0.47
1:B:45:ILE:HG23	1:E:95:CYS:SG	2.55	0.47
1:D:45:ILE:HD12	1:D:49:GLN:HG3	1.96	0.47
1:F:222:THR:HG22	1:F:238:ILE:HG12	1.97	0.47
1:A:122:LEU:O	1:A:125:TYR:HD2	1.98	0.47
1:D:217:ILE:HD12	1:D:272:LEU:HD23	1.96	0.46
1:C:169:PHE:HZ	1:C:318:MET:SD	2.38	0.46
1:C:19:TYR:HE2	1:C:68:VAL:HG13	1.80	0.46
1:D:176:ILE:CG2	1:D:177:PRO:N	2.77	0.46
1:F:263:LYS:HB3	1:F:267:VAL:HG21	1.97	0.46
1:D:141:VAL:HG12	1:D:143:VAL:HG13	1.97	0.46
1:D:5:PHE:HB2	1:D:138:THR:CG2	2.41	0.46
1:E:125:TYR:N	1:E:126:PRO:CD	2.79	0.46
1:E:185:SER:HB2	1:E:202:ALA:HB1	1.97	0.46
1:A:5:PHE:HB2	1:A:138:THR:CG2	2.34	0.46
1:B:171:ILE:HD12	1:B:171:ILE:N	2.31	0.46
1:E:25:GLN:HE21	1:E:29:LEU:HD13	1.77	0.46
1:E:150:HIS:O	1:E:154:THR:HG22	2.15	0.46
1:F:191:LYS:NZ	1:F:197:ASP:OD2	2.48	0.46
1:A:19:TYR:HA	1:A:23:LEU:HB3	1.98	0.46
1:A:313:GLU:HG3	1:A:317:LYS:NZ	2.30	0.46
1:C:161:PHE:HE2	1:C:168:LEU:HD12	1.81	0.46
1:C:25:GLN:HE22	1:C:177:PRO:HB3	1.81	0.46
1:E:241:LEU:HD12	1:E:241:LEU:HA	1.85	0.46
1:B:115:LYS:C	1:B:117:ALA:H	2.18	0.46
1:B:126:PRO:O	1:B:129:MET:N	2.45	0.46
1:C:222:THR:OG1	1:C:223:ASP:N	2.49	0.46
1:D:218:LYS:HA	1:D:269:LYS:HD3	1.98	0.46
1:E:234:ALA:C	1:E:236:PRO:HD3	2.35	0.46
1:F:7:GLY:N	2:F:405:TRP:CH2	2.84	0.46
1:B:189:PRO:HD3	1:B:221:VAL:HG21	1.98	0.46
1:E:151:ILE:HA	1:E:154:THR:HG23	1.97	0.46
1:C:45:ILE:HG23	1:F:95:CYS:SG	2.56	0.45
1:A:8:ILE:HG22	1:A:61:LEU:HD21	1.98	0.45
1:C:153:LEU:O	1:C:153:LEU:HG	2.14	0.45
1:C:8:ILE:HG22	1:C:61:LEU:HD21	1.98	0.45
1:E:271:ASP:O	1:E:275:VAL:HG12	2.16	0.45
1:F:8:ILE:CG2	1:F:61:LEU:HD21	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:199:ASN:C	1:E:199:ASN:HD22	2.19	0.45
1:B:101:GLU:HA	1:B:104:ARG:HH11	1.82	0.45
1:C:130:ALA:O	1:C:134:LEU:HG	2.16	0.45
1:C:140:ILE:CG2	1:C:175:ARG:HB2	2.47	0.45
1:C:260:TYR:O	1:C:261:GLU:C	2.54	0.45
1:E:148:LYS:O	1:E:152:GLU:HG2	2.17	0.45
1:F:260:TYR:O	1:F:261:GLU:C	2.54	0.45
1:A:55:ARG:NH1	1:A:55:ARG:HG2	2.30	0.45
1:B:42:GLN:HB2	1:B:80:GLN:OE1	2.16	0.45
1:F:306:LYS:O	1:F:309:ARG:CD	2.65	0.45
1:F:40:VAL:HB	1:F:43:HIS:HB2	1.97	0.45
1:A:54:LEU:O	1:A:58:ILE:HG13	2.17	0.45
1:B:86:HIS:CD2	1:B:132:ASP:OD1	2.62	0.45
1:C:125:TYR:N	1:C:126:PRO:CD	2.80	0.45
1:D:125:TYR:N	1:D:126:PRO:CD	2.80	0.45
1:A:233:GLU:O	1:A:234:ALA:CB	2.65	0.45
1:B:52:HIS:O	1:B:56:GLN:HB2	2.17	0.45
1:D:107:GLN:C	1:D:109:LYS:H	2.19	0.45
1:D:225:GLU:OE1	1:D:235:LYS:HD2	2.17	0.45
1:E:281:ARG:HH11	1:E:281:ARG:HG3	1.82	0.45
1:B:108:PHE:C	1:B:110:GLU:N	2.70	0.45
1:B:13:VAL:HG13	1:B:13:VAL:O	2.16	0.45
1:C:133:ILE:O	1:C:138:THR:CG2	2.65	0.45
1:E:108:PHE:C	1:E:110:GLU:N	2.69	0.45
1:E:176:ILE:HG23	1:E:177:PRO:O	2.16	0.45
1:E:235:LYS:N	1:E:236:PRO:HD3	2.32	0.45
1:F:151:ILE:HG21	1:F:174:ALA:HB2	1.98	0.45
1:A:234:ALA:C	1:A:236:PRO:HD3	2.37	0.44
1:B:8:ILE:CG2	1:B:61:LEU:HD21	2.47	0.44
1:B:169:PHE:HZ	1:B:318:MET:SD	2.41	0.44
1:B:150:HIS:O	1:B:154:THR:HG23	2.17	0.44
1:C:209:ASP:OD1	1:C:211:LYS:HB3	2.17	0.44
1:C:77:LEU:O	1:C:303:GLY:HA3	2.17	0.44
1:F:137:ASN:OD1	1:F:314:MET:CE	2.65	0.44
1:B:151:ILE:HG21	1:B:174:ALA:HB2	2.00	0.44
1:D:8:ILE:HG22	1:D:61:LEU:HD21	1.98	0.44
1:E:213:ILE:CD1	1:E:280:LEU:HD12	2.47	0.44
1:A:60:ARG:HG2	1:A:287:TYR:OH	2.18	0.44
1:B:126:PRO:CB	1:B:127:PRO:HD3	2.46	0.44
1:D:25:GLN:OE1	1:D:178:LYS:NZ	2.50	0.44
1:A:118:VAL:O	1:D:99:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:164:ARG:HD2	1:F:165:TYR:CZ	2.52	0.44
1:A:209:ASP:OD1	1:A:211:LYS:HB3	2.18	0.44
1:D:256:LEU:O	1:D:260:TYR:HD1	2.00	0.44
1:B:195:LYS:CD	1:B:195:LYS:N	2.78	0.44
1:B:200:PRO:O	1:B:216:LYS:HE2	2.17	0.44
1:C:162:ASN:O	1:C:166:GLY:N	2.43	0.44
1:A:273:ALA:O	1:A:277:ILE:HG13	2.18	0.44
1:C:179:VAL:HB	1:C:180:GLY:H	1.61	0.44
1:D:189:PRO:CB	1:D:236:PRO:HB2	2.47	0.44
1:A:210:ALA:HB1	1:A:277:ILE:HD13	2.00	0.43
1:B:14:ILE:HD11	1:B:206:LEU:CD1	2.48	0.43
1:B:249:SER:OG	1:B:251:GLN:HG3	2.18	0.43
1:C:210:ALA:O	1:C:214:GLU:HB2	2.17	0.43
1:B:272:LEU:HD12	1:B:275:VAL:CG1	2.48	0.43
1:C:14:ILE:HG13	1:C:206:LEU:HG	2.00	0.43
1:C:52:HIS:O	1:C:56:GLN:HB2	2.18	0.43
1:D:128:LEU:O	1:D:131:ALA:HB3	2.18	0.43
1:D:105:MET:HE1	1:D:153:LEU:HD22	1.99	0.43
1:D:253:ILE:O	1:D:257:GLU:HG3	2.17	0.43
1:B:314:MET:O	1:B:318:MET:HG3	2.18	0.43
1:C:233:GLU:O	1:C:234:ALA:HB3	2.19	0.43
1:C:79:ILE:HG21	1:F:325:GLY:HA2	2.00	0.43
1:D:153:LEU:O	1:D:156:ASP:HB2	2.18	0.43
1:E:226:GLY:HA2	1:E:265:TYR:CE2	2.53	0.43
1:F:133:ILE:O	1:F:138:THR:HG23	2.18	0.43
1:C:50:ASP:HB3	1:C:53:GLU:HB2	1.99	0.43
1:D:24:ARG:HH11	1:D:24:ARG:HB3	1.83	0.43
1:E:43:HIS:CE1	1:E:132:ASP:OD2	2.72	0.43
1:E:293:SER:OG	1:E:295:GLU:HB2	2.18	0.43
1:B:177:PRO:O	1:B:178:LYS:CB	2.62	0.43
1:B:217:ILE:HA	1:B:217:ILE:HD13	1.92	0.43
1:E:211:LYS:HB3	1:E:211:LYS:NZ	2.34	0.43
1:E:8:ILE:CG2	1:E:61:LEU:HD21	2.49	0.43
1:A:65:TYR:O	1:A:70:ILE:HG12	2.18	0.43
1:D:171:ILE:N	1:D:171:ILE:HD12	2.34	0.43
1:D:25:GLN:HB2	1:D:25:GLN:HE21	1.58	0.43
1:E:25:GLN:O	1:E:28:GLU:OE1	2.37	0.43
1:F:109:LYS:C	1:F:111:LYS:N	2.72	0.43
1:A:140:ILE:HG23	1:A:175:ARG:CB	2.49	0.43
1:A:230:TYR:OH	1:A:232:LYS:HE3	2.19	0.43
1:D:5:PHE:CB	1:D:138:THR:HG21	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:ILE:HA	1:D:208:ASP:OD2	2.18	0.43
1:E:238:ILE:HD13	1:E:238:ILE:HA	1.87	0.43
1:F:3:THR:HB	1:F:138:THR:HA	2.00	0.43
1:C:316:ARG:HA	1:C:316:ARG:NH1	2.34	0.43
1:E:189:PRO:HD3	1:E:221:VAL:HG21	1.99	0.43
1:B:79:ILE:CD1	1:E:326:ARG:HD2	2.49	0.43
1:F:80:GLN:NE2	1:F:132:ASP:OD1	2.52	0.43
1:A:45:ILE:HA	1:A:45:ILE:HD12	1.84	0.42
1:E:208:ASP:OD2	1:E:216:LYS:NZ	2.40	0.42
1:A:213:ILE:HD13	1:A:276:VAL:HG12	2.01	0.42
1:B:252:SER:HB2	1:B:254:GLU:OE1	2.18	0.42
1:C:115:LYS:C	1:C:117:ALA:H	2.22	0.42
1:A:43:HIS:CE1	1:A:132:ASP:OD2	2.73	0.42
1:A:231:ASP:CB	1:A:235:LYS:HB2	2.45	0.42
1:E:31:HIS:HA	1:E:74:GLN:HE21	1.84	0.42
1:C:226:GLY:HA2	1:C:265:TYR:CE2	2.54	0.42
1:E:219:SER:O	1:E:220:ALA:C	2.57	0.42
1:D:30:GLN:O	1:D:74:GLN:HG3	2.20	0.42
1:D:78:PHE:CD1	1:D:78:PHE:N	2.87	0.42
1:E:281:ARG:HB3	1:E:282:PRO:CD	2.50	0.42
1:D:176:ILE:HG22	1:D:177:PRO:O	2.20	0.42
1:A:43:HIS:HD2	1:A:125:TYR:HB2	1.84	0.42
1:C:42:GLN:HB2	1:C:80:GLN:OE1	2.20	0.42
1:D:86:HIS:CD2	1:D:132:ASP:HA	2.55	0.42
1:E:162:ASN:O	1:E:166:GLY:N	2.45	0.42
1:E:186:LEU:O	1:E:221:VAL:HG22	2.19	0.42
1:A:122:LEU:HA	1:A:122:LEU:HD13	1.87	0.42
1:B:109:LYS:C	1:B:111:LYS:H	2.23	0.42
1:B:176:ILE:CB	1:B:177:PRO:CD	2.83	0.42
1:B:97:VAL:HG13	1:B:97:VAL:O	2.20	0.42
1:D:281:ARG:HB3	1:D:282:PRO:CD	2.50	0.42
1:E:84:PRO:O	1:E:86:HIS:N	2.53	0.42
1:F:109:LYS:O	1:F:111:LYS:N	2.52	0.42
1:F:4:ILE:HG23	1:F:142:PRO:HD3	2.01	0.42
1:F:45:ILE:O	1:F:45:ILE:CG2	2.68	0.42
1:A:74:GLN:HA	1:E:218:LYS:NZ	2.35	0.41
1:D:109:LYS:C	1:D:111:LYS:H	2.23	0.41
1:E:174:ALA:O	1:E:175:ARG:O	2.38	0.41
1:F:311:ALA:O	1:F:315:VAL:HG23	2.20	0.41
1:A:11:SER:O	1:A:13:VAL:HG12	2.20	0.41
1:B:176:ILE:CB	1:B:177:PRO:HD3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:MET:HE3	2:B:401:TRP:CE3	2.55	0.41
1:B:61:LEU:HD12	1:B:61:LEU:HA	1.88	0.41
1:C:70:ILE:O	1:C:72:PRO:HD3	2.20	0.41
1:D:147:GLN:O	1:D:148:LYS:C	2.58	0.41
1:D:228:ILE:HD11	1:D:265:TYR:CD1	2.53	0.41
1:D:40:VAL:HG11	2:D:403:TRP:NE1	2.35	0.41
1:E:23:LEU:HA	1:E:26:PHE:CD2	2.52	0.41
1:A:101:GLU:HA	1:A:104:ARG:NH1	2.35	0.41
1:A:105:MET:HE3	1:A:105:MET:HA	2.02	0.41
1:B:124:THR:O	1:B:127:PRO:HD2	2.20	0.41
1:A:10:PRO:HA	1:A:61:LEU:HD22	2.02	0.41
1:B:129:MET:HG3	2:B:401:TRP:CD1	2.55	0.41
1:D:101:GLU:HA	1:D:104:ARG:HH11	1.85	0.41
1:E:56:GLN:HG3	1:E:60:ARG:NH1	2.36	0.41
1:B:254:GLU:CD	1:B:254:GLU:H	2.21	0.41
1:C:25:GLN:OE1	1:C:178:LYS:HB2	2.21	0.41
1:C:179:VAL:C	1:C:181:ALA:H	2.24	0.41
1:D:272:LEU:O	1:D:275:VAL:HG13	2.21	0.41
1:D:302:GLU:HG2	1:D:302:GLU:O	2.20	0.41
1:E:260:TYR:O	1:E:261:GLU:C	2.59	0.41
1:E:318:MET:O	1:E:322:MET:HG2	2.20	0.41
1:A:71:ASP:HA	1:A:72:PRO:HD2	1.98	0.41
1:C:165:TYR:CE2	1:C:322:MET:HA	2.56	0.41
1:E:84:PRO:O	1:E:87:ALA:N	2.53	0.41
1:F:107:GLN:C	1:F:109:LYS:H	2.24	0.41
1:F:230:TYR:CD1	1:F:231:ASP:N	2.87	0.41
1:B:86:HIS:HE1	1:B:136:TYR:OH	2.04	0.41
1:C:185:SER:HB3	1:C:188:ASP:O	2.21	0.41
1:B:105:MET:O	1:B:107:GLN:N	2.53	0.41
1:B:110:GLU:C	1:B:112:SER:H	2.24	0.41
1:E:84:PRO:O	1:E:85:ALA:C	2.56	0.41
1:F:130:ALA:O	1:F:134:LEU:HG	2.21	0.41
1:F:55:ARG:HG2	1:F:55:ARG:NH1	2.34	0.41
1:B:176:ILE:HB	1:B:177:PRO:HD3	1.95	0.41
1:D:151:ILE:HG21	1:D:174:ALA:HB2	2.03	0.41
1:F:148:LYS:O	1:F:152:GLU:HG2	2.21	0.41
1:F:263:LYS:HB3	1:F:267:VAL:CG2	2.51	0.41
1:B:142:PRO:HA	1:B:175:ARG:O	2.21	0.41
1:F:306:LYS:O	1:F:309:ARG:CZ	2.69	0.41
1:A:110:GLU:C	1:A:112:SER:H	2.24	0.41
1:D:176:ILE:HG23	1:D:177:PRO:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:211:LYS:HZ3	1:D:211:LYS:HB3	1.86	0.41
1:D:85:ALA:HB1	1:D:315:VAL:CG2	2.51	0.41
1:E:189:PRO:HB2	1:E:236:PRO:HB2	2.02	0.41
1:F:231:ASP:HB3	1:F:235:LYS:HB2	2.03	0.41
1:A:42:GLN:HB2	1:A:80:GLN:OE1	2.20	0.40
1:B:86:HIS:CD2	1:B:132:ASP:HA	2.56	0.40
1:D:24:ARG:HH11	1:D:24:ARG:CB	2.34	0.40
1:E:206:LEU:O	1:E:207:LEU:HD23	2.20	0.40
1:F:47:VAL:O	1:F:48:TRP:C	2.59	0.40
1:A:313:GLU:HG3	1:A:317:LYS:HZ1	1.86	0.40
1:C:313:GLU:HG3	1:C:317:LYS:HZ2	1.86	0.40
1:D:105:MET:CA	1:D:149:GLN:HE22	2.33	0.40
1:D:168:LEU:CD2	1:D:314:MET:SD	3.10	0.40
1:D:99:ILE:HG13	1:D:99:ILE:H	1.77	0.40
1:E:14:ILE:O	1:E:14:ILE:HG13	2.21	0.40
1:E:294:GLU:HG3	1:E:294:GLU:H	1.67	0.40
1:A:108:PHE:C	1:A:110:GLU:H	2.24	0.40
1:D:168:LEU:HD22	1:D:168:LEU:O	2.21	0.40
1:A:171:ILE:N	1:A:171:ILE:HD12	2.37	0.40
1:A:272:LEU:O	1:A:275:VAL:HG12	2.21	0.40
1:B:129:MET:CE	2:B:401:TRP:CE3	3.05	0.40
1:C:121:GLY:HA2	1:C:124:THR:OG1	2.21	0.40
1:C:310:VAL:O	1:C:313:GLU:HB3	2.22	0.40
1:A:115:LYS:C	1:A:117:ALA:H	2.24	0.40
1:A:252:SER:OG	1:A:255:GLU:HB2	2.22	0.40
1:D:225:GLU:HG2	1:D:225:GLU:O	2.21	0.40
1:D:272:LEU:HA	1:D:275:VAL:CG1	2.52	0.40
1:D:59:ARG:CZ	1:D:296:LEU:HD23	2.52	0.40
1:F:281:ARG:O	1:F:285:GLU:HG3	2.21	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	324/328 (99%)	287 (89%)	30 (9%)	7 (2%)	6	17
1	B	324/328 (99%)	285 (88%)	31 (10%)	8 (2%)	5	14
1	C	324/328 (99%)	290 (90%)	23 (7%)	11 (3%)	3	8
1	D	324/328 (99%)	280 (86%)	40 (12%)	4 (1%)	13	32
1	E	324/328 (99%)	281 (87%)	33 (10%)	10 (3%)	4	9
1	F	324/328 (99%)	289 (89%)	27 (8%)	8 (2%)	5	14
All	All	1944/1968 (99%)	1712 (88%)	184 (10%)	48 (2%)	5	14

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	SER
1	A	113	ALA
1	A	179	VAL
1	A	261	GLU
1	B	179	VAL
1	C	261	GLU
1	D	40	VAL
1	E	12	GLY
1	E	107	GLN
1	E	175	ARG
1	E	261	GLU
1	F	106	THR
1	F	261	GLU
1	A	40	VAL
1	B	106	THR
1	B	107	GLN
1	B	116	GLU
1	B	182	ARG
1	C	112	SER
1	C	137	ASN
1	C	179	VAL
1	C	220	ALA
1	D	106	THR
1	D	107	GLN
1	E	106	THR
1	F	12	GLY
1	F	107	GLN
1	F	110	GLU
1	C	107	GLN
1	C	116	GLU

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Mol	Chain	Res	Type
1	D	261	GLU
1	E	113	ALA
1	E	116	GLU
1	B	12	GLY
1	C	12	GLY
1	C	106	THR
1	C	182	ARG
1	E	85	ALA
1	E	110	GLU
1	C	105	MET
1	E	105	MET
1	F	179	VAL
1	F	236	PRO
1	A	12	GLY
1	A	148	LYS
1	B	110	GLU
1	F	40	VAL
1	B	176	ILE

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	270/280 (96%)	248 (92%)	22 (8%)	11	27
1	B	270/280 (96%)	247 (92%)	23 (8%)	10	24
1	C	270/280 (96%)	249 (92%)	21 (8%)	12	29
1	D	270/280 (96%)	246 (91%)	24 (9%)	9	22
1	E	270/280 (96%)	243 (90%)	27 (10%)	7	18
1	F	270/280 (96%)	250 (93%)	20 (7%)	13	32
All	All	1620/1680 (96%)	1483 (92%)	137 (8%)	10	24

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	9	GLN
1	A	29	LEU
1	A	48	TRP
1	A	104	ARG
1	A	105	MET
1	A	106	THR
1	A	107	GLN
1	A	149	GLN
1	A	168	LEU
1	A	194	SER
1	A	195	LYS
1	A	201	LYS
1	A	214	GLU
1	A	241	LEU
1	A	243	ASN
1	A	278	GLU
1	A	289	HIS
1	A	294	GLU
1	A	298	ARG
1	A	308	ASN
1	A	316	ARG
1	B	1	MET
1	B	9	GLN
1	B	24	ARG
1	B	48	TRP
1	B	55	ARG
1	B	56	GLN
1	B	59	ARG
1	B	104	ARG
1	B	107	GLN
1	B	122	LEU
1	B	138	THR
1	B	164	ARG
1	B	168	LEU
1	B	195	LYS
1	B	196	SER
1	B	241	LEU
1	B	245	TYR
1	B	258	ARG
1	B	278	GLU
1	B	289	HIS
1	B	298	ARG

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Mol	Chain	Res	Type
1	B	316	ARG
1	B	320	GLN
1	C	9	GLN
1	C	23	LEU
1	C	48	TRP
1	C	73	THR
1	C	106	THR
1	C	138	THR
1	C	164	ARG
1	C	168	LEU
1	C	178	LYS
1	C	179	VAL
1	C	182	ARG
1	C	195	LYS
1	C	199	ASN
1	C	201	LYS
1	C	241	LEU
1	C	245	TYR
1	C	278	GLU
1	C	289	HIS
1	C	294	GLU
1	C	302	GLU
1	C	316	ARG
1	D	1	MET
1	D	24	ARG
1	D	32	GLU
1	D	48	TRP
1	D	50	ASP
1	D	104	ARG
1	D	107	GLN
1	D	138	THR
1	D	145	GLU
1	D	156	ASP
1	D	168	LEU
1	D	178	LYS
1	D	185	SER
1	D	195	LYS
1	D	209	ASP
1	D	222	THR
1	D	231	ASP
1	D	241	LEU
1	D	245	TYR

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Mol	Chain	Res	Type
1	D	275	VAL
1	D	278	GLU
1	D	284	GLN
1	D	289	HIS
1	D	316	ARG
1	E	25	GLN
1	E	28	GLU
1	E	48	TRP
1	E	55	ARG
1	E	105	MET
1	E	106	THR
1	E	107	GLN
1	E	122	LEU
1	E	138	THR
1	E	145	GLU
1	E	154	THR
1	E	168	LEU
1	E	175	ARG
1	E	182	ARG
1	E	195	LYS
1	E	199	ASN
1	E	218	LYS
1	E	241	LEU
1	E	245	TYR
1	E	263	LYS
1	E	275	VAL
1	E	278	GLU
1	E	289	HIS
1	E	294	GLU
1	E	298	ARG
1	E	316	ARG
1	E	320	GLN
1	F	9	GLN
1	F	45	ILE
1	F	48	TRP
1	F	56	GLN
1	F	104	ARG
1	F	107	GLN
1	F	127	PRO
1	F	168	LEU
1	F	190	THR
1	F	195	LYS

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Mol	Chain	Res	Type
1	F	218	LYS
1	F	222	THR
1	F	241	LEU
1	F	245	TYR
1	F	253	ILE
1	F	289	HIS
1	F	294	GLU
1	F	309	ARG
1	F	316	ARG
1	F	326	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	43	HIS
1	A	56	GLN
1	A	86	HIS
1	A	320	GLN
1	B	9	GLN
1	B	43	HIS
1	B	56	GLN
1	B	86	HIS
1	B	149	GLN
1	C	9	GLN
1	C	34	ASN
1	C	56	GLN
1	C	86	HIS
1	C	199	ASN
1	C	251	GLN
1	C	259	GLN
1	D	9	GLN
1	D	34	ASN
1	D	86	HIS
1	D	149	GLN
1	D	199	ASN
1	D	251	GLN
1	D	259	GLN
1	E	25	GLN
1	E	31	HIS
1	E	34	ASN
1	E	43	HIS

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Mol	Chain	Res	Type
1	E	56	GLN
1	E	86	HIS
1	E	199	ASN
1	E	251	GLN
1	E	259	GLN
1	F	9	GLN
1	F	25	GLN
1	F	43	HIS
1	F	56	GLN
1	F	86	HIS
1	F	149	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	TRP	D	403	-	12,16,16	1.61	3 (25%)	12,22,22	4.02	8 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	TRP	C	402	-	12,16,16	1.37	2 (16%)	12,22,22	3.49	6 (50%)
2	TRP	F	405	-	12,16,16	1.44	2 (16%)	12,22,22	3.61	5 (41%)
2	TRP	A	400	-	12,16,16	1.56	3 (25%)	12,22,22	3.33	5 (41%)
2	TRP	B	401	-	12,16,16	1.36	3 (25%)	12,22,22	3.60	4 (33%)
2	TRP	E	404	-	12,16,16	1.57	3 (25%)	12,22,22	3.71	7 (58%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TRP	D	403	-	-	1/3/8/8	0/2/2/2
2	TRP	C	402	-	-	1/3/8/8	0/2/2/2
2	TRP	F	405	-	-	1/3/8/8	0/2/2/2
2	TRP	A	400	-	-	1/3/8/8	0/2/2/2
2	TRP	B	401	-	-	2/3/8/8	0/2/2/2
2	TRP	E	404	-	-	1/3/8/8	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	404	TRP	CH2-CZ2	3.52	1.44	1.36
2	D	403	TRP	CH2-CZ2	3.38	1.44	1.36
2	F	405	TRP	CH2-CZ2	3.19	1.44	1.36
2	E	404	TRP	CH2-CZ3	3.02	1.46	1.38
2	F	405	TRP	CH2-CZ3	3.00	1.46	1.38
2	C	402	TRP	CH2-CZ2	3.00	1.43	1.36
2	A	400	TRP	CH2-CZ3	2.94	1.45	1.38
2	A	400	TRP	CH2-CZ2	2.77	1.43	1.36
2	B	401	TRP	CH2-CZ3	2.73	1.45	1.38
2	B	401	TRP	CH2-CZ2	2.70	1.42	1.36
2	C	402	TRP	CH2-CZ3	2.61	1.44	1.38
2	A	400	TRP	CZ2-CE2	-2.61	1.37	1.41
2	E	404	TRP	CA-N	2.43	1.52	1.47
2	D	403	TRP	CD2-CE2	-2.16	1.36	1.42
2	B	401	TRP	CZ2-CE2	-2.09	1.38	1.41
2	D	403	TRP	CB-CG	-2.07	1.45	1.51

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	TRP	CB-CA-C	10.50	127.69	110.69
2	F	405	TRP	CB-CA-C	9.36	125.85	110.69
2	D	403	TRP	CB-CA-C	8.22	124.00	110.69
2	E	404	TRP	CB-CA-C	8.02	123.67	110.69
2	A	400	TRP	CB-CA-C	7.98	123.61	110.69
2	C	402	TRP	CB-CA-C	6.74	121.61	110.69
2	C	402	TRP	CB-CG-CD1	-6.62	119.78	127.97
2	A	400	TRP	CB-CG-CD1	-6.44	120.00	127.97
2	D	403	TRP	CB-CG-CD1	-6.29	120.19	127.97
2	E	404	TRP	CB-CG-CD1	-6.00	120.55	127.97
2	F	405	TRP	CB-CG-CD1	-5.41	121.28	127.97
2	D	403	TRP	CZ3-CE3-CD2	-5.14	113.76	120.89
2	B	401	TRP	CB-CG-CD1	-5.12	121.64	127.97
2	E	404	TRP	CB-CG-CD2	5.06	134.12	126.25
2	D	403	TRP	CB-CG-CD2	4.90	133.87	126.25
2	C	402	TRP	CB-CG-CD2	4.86	133.81	126.25
2	D	403	TRP	CE3-CD2-CE2	4.19	123.72	118.17
2	F	405	TRP	CB-CG-CD2	4.05	132.55	126.25
2	C	402	TRP	CZ3-CE3-CD2	-3.69	115.78	120.89
2	E	404	TRP	CZ3-CE3-CD2	-3.59	115.91	120.89
2	E	404	TRP	CE3-CD2-CE2	3.57	122.91	118.17
2	A	400	TRP	CB-CG-CD2	3.40	131.54	126.25
2	F	405	TRP	CE3-CD2-CE2	2.87	121.97	118.17
2	C	402	TRP	CH2-CZ3-CE3	2.86	124.45	120.44
2	D	403	TRP	CH2-CZ2-CE2	-2.60	116.34	120.08
2	F	405	TRP	CZ3-CE3-CD2	-2.54	117.37	120.89
2	A	400	TRP	CZ3-CE3-CD2	-2.53	117.38	120.89
2	D	403	TRP	CE3-CD2-CG	-2.50	129.83	134.42
2	C	402	TRP	CE3-CD2-CE2	2.45	121.42	118.17
2	B	401	TRP	CB-CG-CD2	2.36	129.92	126.25
2	A	400	TRP	CE3-CD2-CE2	2.25	121.15	118.17
2	B	401	TRP	CZ3-CE3-CD2	-2.25	117.78	120.89
2	D	403	TRP	CH2-CZ3-CE3	2.20	123.53	120.44
2	E	404	TRP	CH2-CZ3-CE3	2.09	123.38	120.44
2	E	404	TRP	CH2-CZ2-CE2	-2.04	117.15	120.08

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	403	TRP	CA-CB-CG-CD1
2	C	402	TRP	CA-CB-CG-CD1
2	F	405	TRP	CA-CB-CG-CD1

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Mol	Chain	Res	Type	Atoms
2	A	400	TRP	CA-CB-CG-CD1
2	E	404	TRP	CA-CB-CG-CD1
2	B	401	TRP	CA-CB-CG-CD1
2	B	401	TRP	C-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	403	TRP	1	0
2	F	405	TRP	2	0
2	B	401	TRP	3	0

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	326/328 (99%)	-0.16	17 (5%) 27 25	21, 45, 85, 110	0
1	B	326/328 (99%)	-0.17	16 (4%) 29 28	10, 44, 82, 116	0
1	C	326/328 (99%)	-0.29	13 (3%) 38 37	19, 42, 84, 112	0
1	D	326/328 (99%)	-0.16	19 (5%) 23 22	21, 45, 89, 120	0
1	E	326/328 (99%)	-0.25	17 (5%) 27 25	19, 40, 82, 123	0
1	F	326/328 (99%)	-0.15	18 (5%) 25 24	6, 48, 86, 120	0
All	All	1956/1968 (99%)	-0.20	100 (5%) 28 26	6, 44, 87, 123	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	179	VAL	12.3
1	D	179	VAL	10.8
1	F	114	GLY	9.6
1	F	113	ALA	9.2
1	B	114	GLY	8.8
1	F	180	GLY	8.5
1	A	177	PRO	8.4
1	D	114	GLY	8.1
1	B	179	VAL	7.4
1	E	177	PRO	6.8
1	D	113	ALA	6.8
1	D	180	GLY	6.4
1	C	179	VAL	6.4
1	E	114	GLY	6.4
1	C	178	LYS	6.2
1	F	179	VAL	6.2
1	B	177	PRO	5.8
1	B	180	GLY	5.6
1	E	113	ALA	5.5

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Mol	Chain	Res	Type	RSRZ
1	E	178	LYS	5.5
1	A	180	GLY	5.3
1	B	113	ALA	5.1
1	A	114	GLY	5.1
1	D	178	LYS	5.0
1	A	113	ALA	5.0
1	C	112	SER	5.0
1	B	258	ARG	4.6
1	A	112	SER	4.5
1	D	112	SER	4.3
1	C	113	ALA	4.2
1	C	177	PRO	4.2
1	A	179	VAL	4.1
1	F	106	THR	4.1
1	A	176	ILE	4.1
1	B	112	SER	4.1
1	F	177	PRO	4.0
1	C	176	ILE	3.9
1	E	180	GLY	3.9
1	B	178	LYS	3.7
1	E	116	GLU	3.7
1	A	106	THR	3.7
1	A	12	GLY	3.7
1	E	112	SER	3.6
1	C	114	GLY	3.6
1	E	176	ILE	3.5
1	D	181	ALA	3.4
1	D	177	PRO	3.3
1	A	181	ALA	3.1
1	F	298	ARG	3.1
1	B	116	GLU	3.1
1	C	116	GLU	3.0
1	E	106	THR	3.0
1	F	181	ALA	3.0
1	C	182	ARG	2.9
1	B	181	ALA	2.9
1	D	104	ARG	2.9
1	A	258	ARG	2.8
1	F	12	GLY	2.8
1	F	178	LYS	2.8
1	A	116	GLU	2.8
1	F	108	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	316	ARG	2.7
1	B	115	LYS	2.7
1	E	175	ARG	2.7
1	A	52	HIS	2.6
1	C	106	THR	2.6
1	F	115	LYS	2.6
1	F	1	MET	2.6
1	D	12	GLY	2.5
1	F	116	GLU	2.5
1	D	176	ILE	2.5
1	D	116	GLU	2.4
1	B	1	MET	2.4
1	D	261	GLU	2.4
1	B	106	THR	2.4
1	A	229	ARG	2.4
1	A	115	LYS	2.4
1	D	115	LYS	2.3
1	E	25	GLN	2.3
1	E	108	PHE	2.3
1	F	229	ARG	2.3
1	A	111	LYS	2.2
1	F	28	GLU	2.2
1	C	111	LYS	2.2
1	F	258	ARG	2.2
1	C	258	ARG	2.2
1	E	148	LYS	2.1
1	D	1	MET	2.1
1	C	108	PHE	2.1
1	D	106	THR	2.1
1	F	112	SER	2.1
1	E	289	HIS	2.1
1	D	182	ARG	2.1
1	B	28	GLU	2.1
1	D	229	ARG	2.1
1	A	108	PHE	2.1
1	E	115	LYS	2.0
1	D	117	ALA	2.0
1	B	12	GLY	2.0
1	E	174	ALA	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 monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	TRP	B	401	15/15	0.82	0.22	47,48,50,50	0
2	TRP	A	400	15/15	0.85	0.24	49,51,54,56	0
2	TRP	F	405	15/15	0.86	0.26	57,59,60,60	0
2	TRP	C	402	15/15	0.87	0.19	41,42,44,47	0
2	TRP	D	403	15/15	0.87	0.22	42,44,45,46	0
2	TRP	E	404	15/15	0.89	0.18	38,41,53,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.