Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 06:13 AM EDT

PDB ID	:	4G0J
Title	:	Crystallographic Analysis of Rotavirus NSP2-RNA Complex Reveals Specific Recognition of 5'-GG Sequence for RTPase activity
Authors	:	Hu, L.; Prasad, B.V.V.
Deposited on	:	2012-07-09
Resolution	:	3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

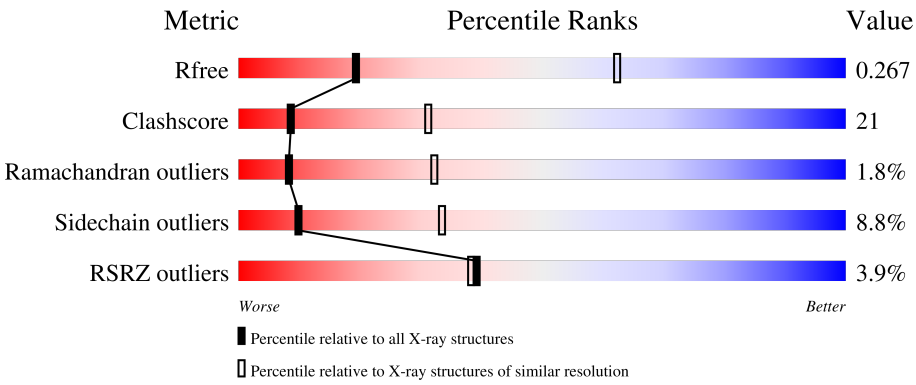
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=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	294	4% 50% 43% 5% •
1	B	294	4% 57% 36% 5% •
1	C	294	5% 54% 41% • •
1	D	294	3% 56% 41% • •
1	E	294	4% 57% 37% • •

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Mol	Chain	Length	Quality of chain
1	F	294	4% 58% 37%
1	G	294	3% 49% 45%
1	H	294	2% 63% 33%
1	I	294	3% 55% 40%
1	J	294	5% 56% 38%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 23600 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 Non-structural protein 2.

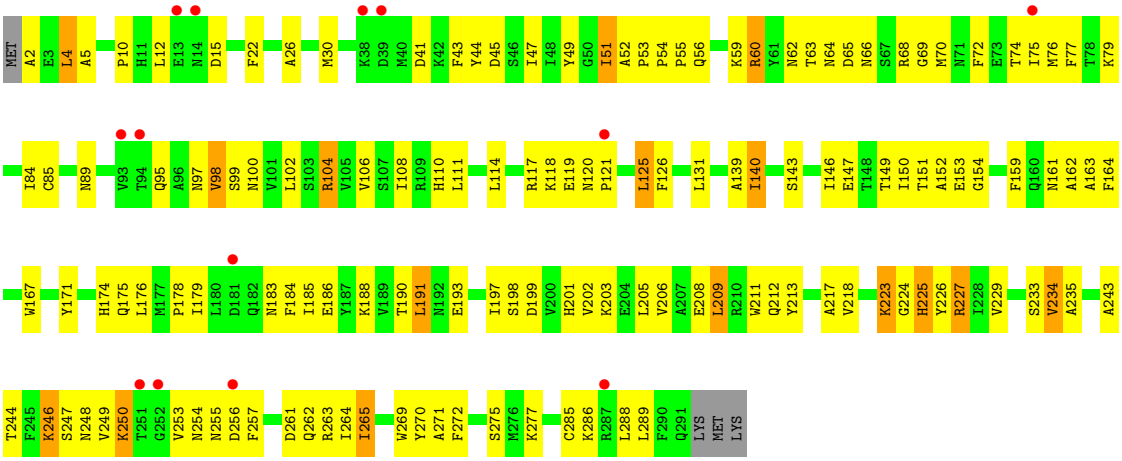
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	290	2360	1518	400	430	12	0	0	0
1	B	290	2360	1518	400	430	12	0	0	0
1	C	290	2360	1518	400	430	12	0	0	0
1	D	290	2360	1518	400	430	12	0	0	0
1	E	290	2360	1518	400	430	12	0	0	0
1	F	290	2360	1518	400	430	12	0	0	0
1	G	290	2360	1518	400	430	12	0	0	0
1	H	290	2360	1518	400	430	12	0	0	0
1	I	290	2360	1518	400	430	12	0	0	0
1	J	290	2360	1518	400	430	12	0	0	0

3 Residue-property plots (i)

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

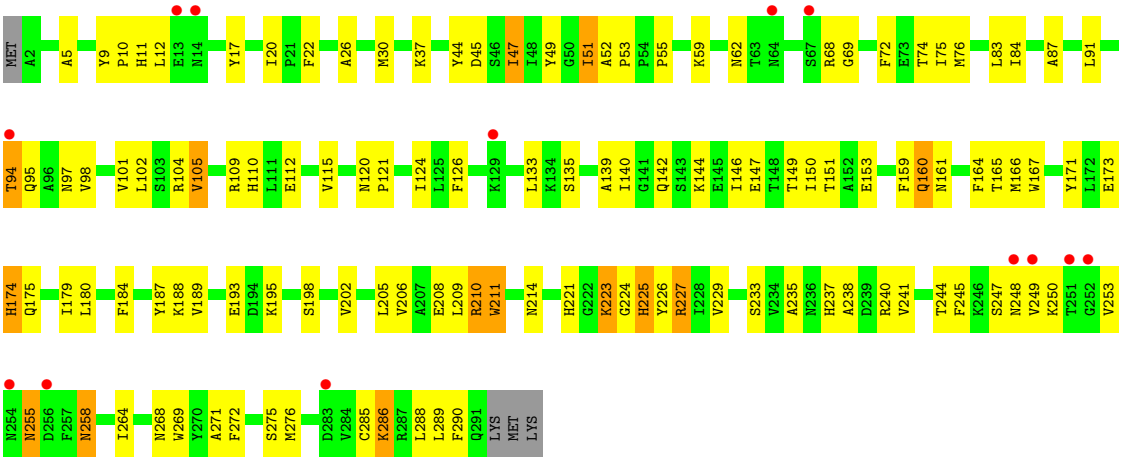
• Molecule 1: Non-structural protein 2

Chain A:



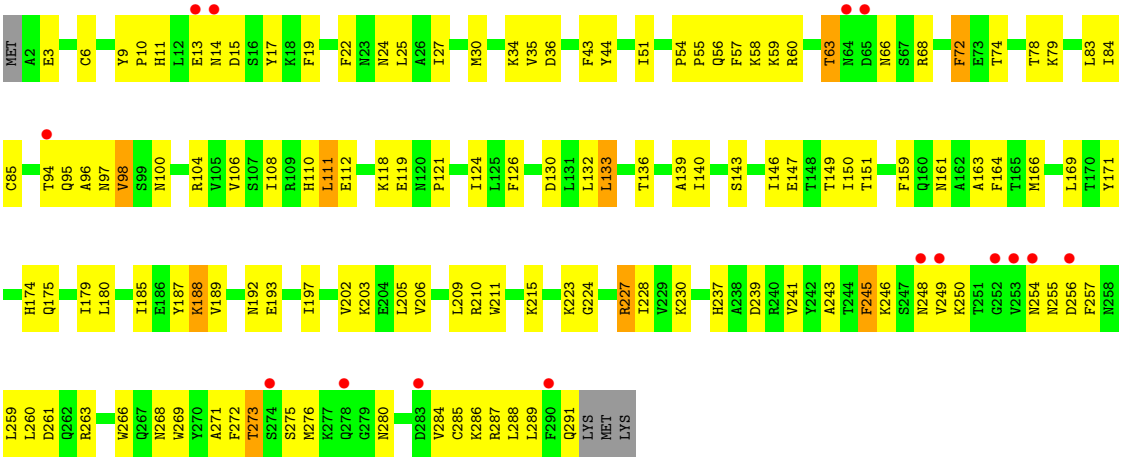
• Molecule 1: Non-structural protein 2

Chain B:



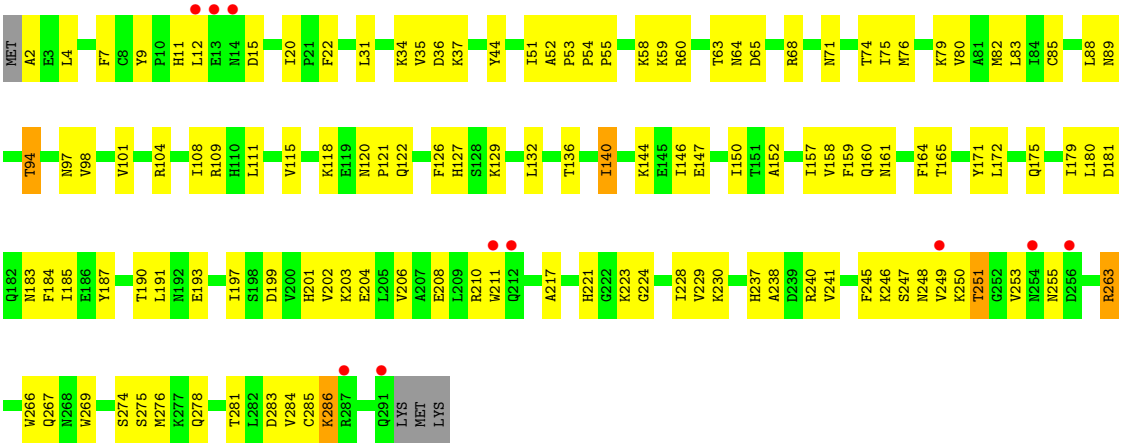
• Molecule 1: Non-structural protein 2

Chain C:



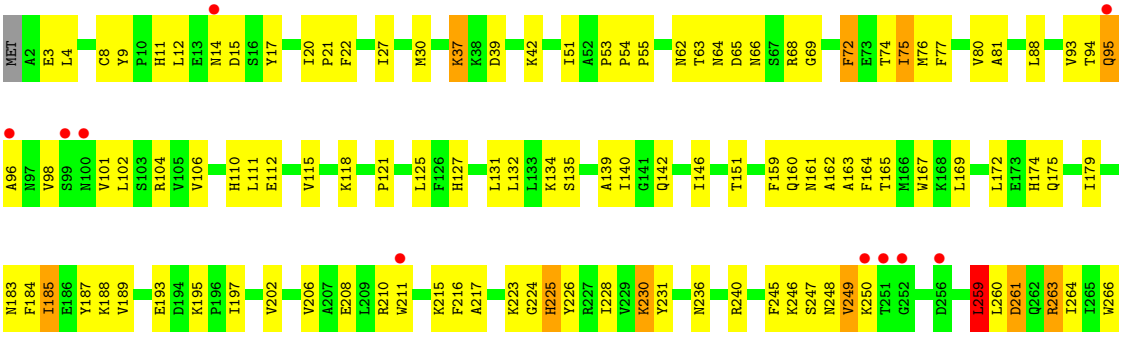
- Molecule 1: Non-structural protein 2

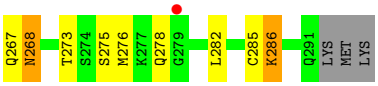
Chain D:



- Molecule 1: Non-structural protein 2

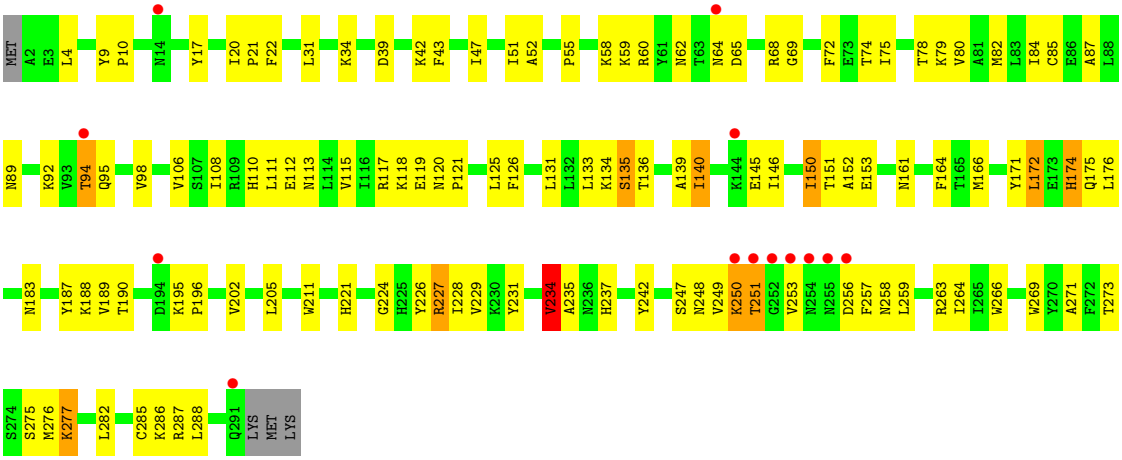
Chain E:





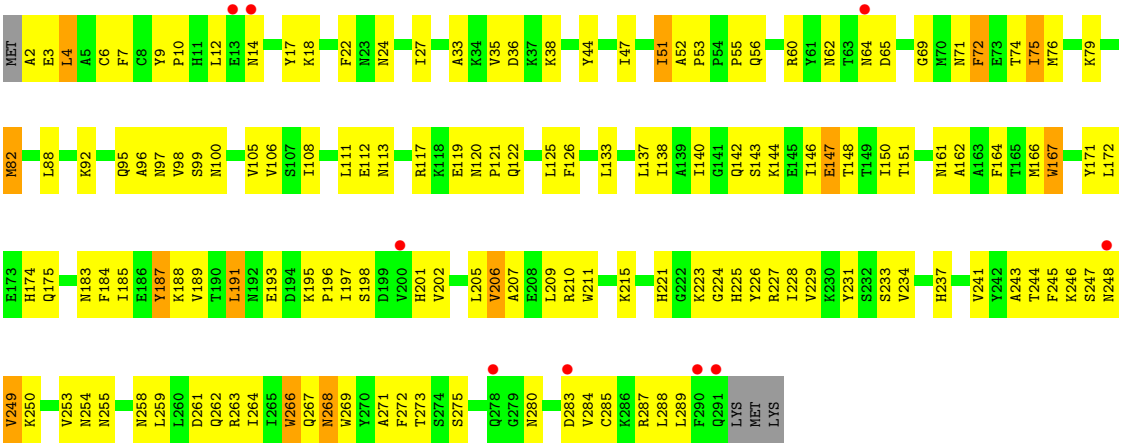
• Molecule 1: Non-structural protein 2

Chain F:



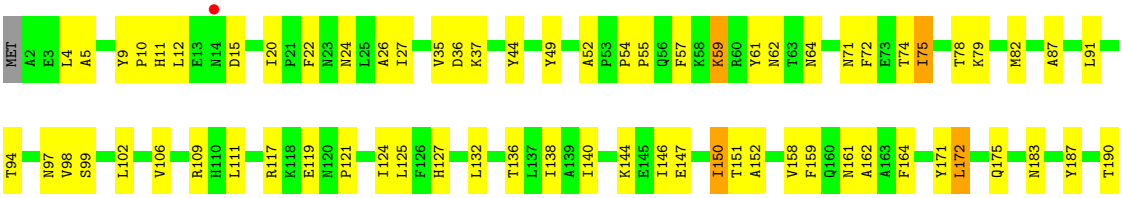
• Molecule 1: Non-structural protein 2

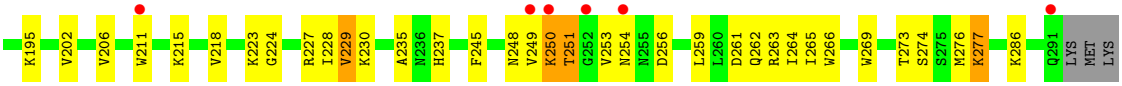
Chain G:



• Molecule 1: Non-structural protein 2

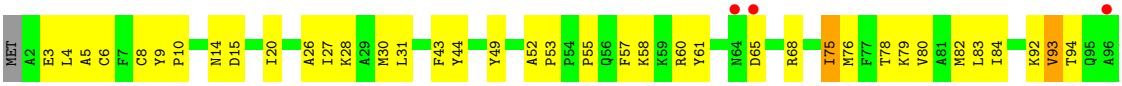
Chain H:

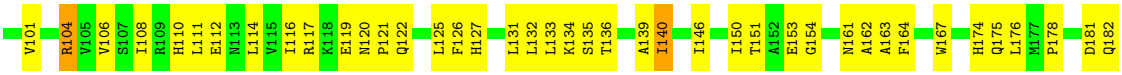


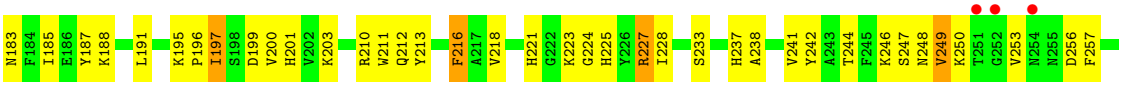


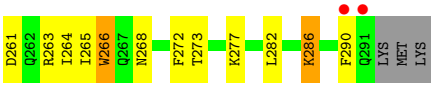
• Molecule 1: Non-structural protein 2

Chain I:



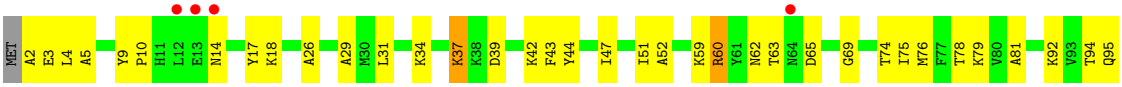


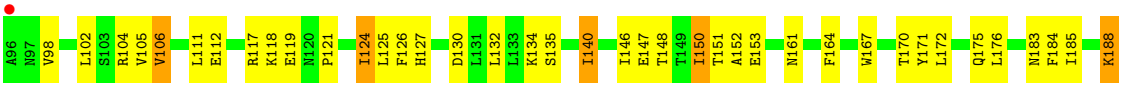


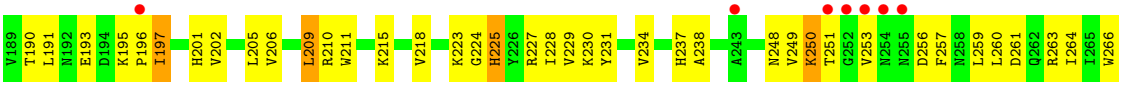


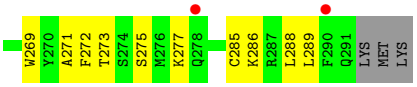
• Molecule 1: Non-structural protein 2

Chain J:









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4	Depositor
Cell constants a, b, c, α, β, γ	122.48Å 122.48Å 301.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	301.31 – 3.40 19.96 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (301.31-3.40) 99.9 (19.96-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.61 (at 3.44Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.237 , 0.294 0.214 , 0.267	Depositor DCC
R_{free} test set	3109 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å^2)	67.0	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 31.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.236 for h,-k,-l	Xtriage
Reported twinning fraction	0.299 for H, K, L 0.701 for -H, K, -L	Depositor
Outliers	0 of 60405 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	23600	wwPDB-VP
Average B, all atoms (Å^2)	78.0	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 33.80 % 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 7.5552e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (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	0.65	2/2411 (0.1%)	0.78	1/3261 (0.0%)
1	B	0.64	2/2411 (0.1%)	0.78	0/3261
1	C	0.64	1/2411 (0.0%)	0.80	0/3261
1	D	0.64	3/2411 (0.1%)	0.77	0/3261
1	E	0.67	4/2411 (0.2%)	0.78	1/3261 (0.0%)
1	F	0.64	3/2411 (0.1%)	0.74	0/3261
1	G	0.65	4/2411 (0.2%)	0.79	1/3261 (0.0%)
1	H	0.65	3/2411 (0.1%)	0.78	0/3261
1	I	0.64	2/2411 (0.1%)	0.77	0/3261
1	J	0.63	3/2411 (0.1%)	0.74	0/3261
All	All	0.64	27/24110 (0.1%)	0.77	3/32610 (0.0%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	266	TRP	CD2-CE2	6.11	1.48	1.41
1	A	269	TRP	CD2-CE2	6.10	1.48	1.41
1	H	269	TRP	CD2-CE2	6.10	1.48	1.41
1	I	211	TRP	CD2-CE2	6.07	1.48	1.41
1	D	211	TRP	CD2-CE2	6.01	1.48	1.41
1	A	211	TRP	CD2-CE2	5.92	1.48	1.41
1	J	211	TRP	CD2-CE2	5.90	1.48	1.41
1	H	266	TRP	CD2-CE2	5.89	1.48	1.41
1	H	211	TRP	CD2-CE2	5.77	1.48	1.41
1	G	211	TRP	CD2-CE2	5.76	1.48	1.41
1	F	211	TRP	CD2-CE2	5.72	1.48	1.41
1	G	269	TRP	CD2-CE2	5.69	1.48	1.41
1	G	167	TRP	CD2-CE2	5.61	1.48	1.41
1	E	95	GLN	CD-NE2	5.57	1.46	1.32
1	E	211	TRP	CD2-CE2	5.55	1.48	1.41
1	B	269	TRP	CD2-CE2	5.52	1.48	1.41
1	B	211	TRP	CD2-CE2	5.47	1.48	1.41
1	D	266	TRP	CD2-CE2	5.46	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	266	TRP	CD2-CE2	5.43	1.47	1.41
1	J	266	TRP	CD2-CE2	5.37	1.47	1.41
1	D	269	TRP	CD2-CE2	5.25	1.47	1.41
1	C	269	TRP	CD2-CE2	5.23	1.47	1.41
1	J	269	TRP	CD2-CE2	5.22	1.47	1.41
1	I	266	TRP	CD2-CE2	5.12	1.47	1.41
1	E	167	TRP	CD2-CE2	5.12	1.47	1.41
1	G	266	TRP	CD2-CE2	5.04	1.47	1.41
1	F	269	TRP	CD2-CE2	5.01	1.47	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	191	LEU	CA-CB-CG	6.96	131.30	115.30
1	E	259	LEU	CA-CB-CG	5.28	127.44	115.30
1	A	45	ASP	CB-CG-OD1	5.25	123.03	118.30

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	2360	0	2374	126	0
1	B	2360	0	2374	94	0
1	C	2360	0	2374	92	1
1	D	2360	0	2374	94	0
1	E	2360	0	2374	101	0
1	F	2360	0	2374	89	1
1	G	2360	0	2374	136	0
1	H	2360	0	2374	81	0
1	I	2360	0	2374	112	0
1	J	2360	0	2374	108	0
All	All	23600	0	23740	982	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 21.

All (982) 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:H:74:THR:HB	1:H:175:GLN:HE21	1.12	1.14
1:I:65:ASP:HA	1:J:183:ASN:HD21	1.04	1.11
1:H:202:VAL:O	1:H:206:VAL:HG23	1.52	1.09
1:E:74:THR:HB	1:E:175:GLN:HE21	1.10	1.08
1:E:202:VAL:HG13	1:E:264:ILE:HD11	1.35	1.07
1:E:65:ASP:HA	1:F:183:ASN:HD21	0.93	1.07
1:D:161:ASN:HB3	1:D:164:PHE:H	1.19	1.06
1:B:146:ILE:HD11	1:B:224:GLY:H	1.07	1.05
1:G:146:ILE:HD11	1:G:224:GLY:H	1.16	1.05
1:E:183:ASN:HD21	1:F:65:ASP:HA	1.17	1.05
1:J:121:PRO:HA	1:J:126:PHE:CD1	1.92	1.04
1:E:74:THR:HB	1:E:175:GLN:NE2	1.73	1.02
1:E:65:ASP:HA	1:F:183:ASN:ND2	1.73	1.02
1:D:263:ARG:HG3	1:D:263:ARG:HH11	0.88	1.02
1:F:146:ILE:HD11	1:F:224:GLY:H	1.24	1.01
1:D:263:ARG:HG3	1:D:263:ARG:NH1	1.67	1.01
1:A:191:LEU:HD21	1:A:197:ILE:HD11	1.40	1.01
1:G:206:VAL:O	1:G:210:ARG:HG3	1.62	0.98
1:E:146:ILE:HD11	1:E:223:LYS:HB3	1.43	0.97
1:G:75:ILE:HD12	1:G:75:ILE:H	1.29	0.97
1:E:183:ASN:ND2	1:F:65:ASP:HA	1.81	0.94
1:D:144:LYS:HE3	1:E:162:ALA:O	1.66	0.94
1:F:195:LYS:HB2	1:F:196:PRO:HD2	1.49	0.93
1:G:146:ILE:CD1	1:G:224:GLY:H	1.81	0.93
1:D:263:ARG:HH11	1:D:263:ARG:CG	1.81	0.92
1:H:24:ASN:HA	1:H:27:ILE:HD12	1.51	0.92
1:J:205:LEU:O	1:J:209:LEU:HD12	1.70	0.91
1:B:101:VAL:HG22	1:B:142:GLN:HE22	1.35	0.91
1:E:146:ILE:CD1	1:E:223:LYS:HB3	2.01	0.90
1:A:250:LYS:O	1:A:253:VAL:HG12	1.72	0.90
1:G:24:ASN:HA	1:G:27:ILE:HD12	1.54	0.90
1:A:183:ASN:ND2	1:D:65:ASP:HA	1.87	0.89
1:G:146:ILE:CD1	1:G:223:LYS:HB3	2.02	0.89
1:I:65:ASP:HA	1:J:183:ASN:ND2	1.88	0.89
1:F:166:MET:HG3	1:F:189:VAL:HG22	1.55	0.89
1:F:202:VAL:HG21	1:F:263:ARG:NH2	1.88	0.89
1:E:261:ASP:OD1	1:E:263:ARG:HG3	1.72	0.88
1:J:125:LEU:HD22	1:J:132:LEU:HA	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:75:ILE:H	1:E:75:ILE:HD12	1.38	0.87
1:H:74:THR:HB	1:H:175:GLN:NE2	1.89	0.87
1:I:247:SER:O	1:I:253:VAL:HG11	1.74	0.86
1:I:65:ASP:CA	1:J:183:ASN:HD21	1.87	0.86
1:E:282:LEU:HD11	1:E:286:LYS:HE2	1.56	0.85
1:F:202:VAL:HG21	1:F:263:ARG:HH21	1.41	0.85
1:C:245:PHE:CE1	1:C:255:ASN:HB3	2.12	0.84
1:C:272:PHE:HB2	1:C:289:LEU:HD13	1.60	0.84
1:B:272:PHE:HB2	1:B:289:LEU:HD13	1.57	0.84
1:F:106:VAL:HG11	1:F:140:ILE:HD12	1.59	0.84
1:I:108:ILE:CG2	1:I:176:LEU:HD23	2.09	0.83
1:A:171:TYR:CB	1:A:179:ILE:HG13	2.08	0.83
1:J:146:ILE:HD12	1:J:147:GLU:H	1.42	0.83
1:C:202:VAL:O	1:C:206:VAL:HG23	1.77	0.83
1:G:259:LEU:HD22	1:G:273:THR:HB	1.59	0.83
1:A:198:SER:O	1:A:202:VAL:HG23	1.79	0.82
1:D:76:MET:O	1:D:80:VAL:HG23	1.78	0.82
1:G:166:MET:HG3	1:G:189:VAL:HG22	1.60	0.82
1:H:251:THR:HB	1:I:134:LYS:NZ	1.93	0.82
1:F:150:ILE:CG2	1:F:151:THR:HG23	2.10	0.81
1:B:146:ILE:HD11	1:B:224:GLY:N	1.91	0.81
1:G:146:ILE:HD11	1:G:224:GLY:N	1.94	0.81
1:C:146:ILE:HD11	1:C:224:GLY:H	1.43	0.81
1:D:75:ILE:HD12	1:D:75:ILE:H	1.44	0.81
1:G:72:PHE:H	1:G:72:PHE:HD2	1.28	0.81
1:I:183:ASN:HD21	1:J:65:ASP:HB3	1.46	0.81
1:F:150:ILE:HG23	1:F:151:THR:HG23	1.63	0.80
1:E:74:THR:CB	1:E:175:GLN:HE21	1.91	0.80
1:C:6:CYS:SG	1:C:60:ARG:HG3	2.23	0.79
1:A:247:SER:O	1:A:253:VAL:HG11	1.81	0.79
1:C:287:ARG:O	1:C:291:GLN:HG3	1.83	0.79
1:J:146:ILE:CD1	1:J:223:LYS:HB3	2.13	0.79
1:F:146:ILE:HD11	1:F:224:GLY:N	1.97	0.79
1:C:146:ILE:CD1	1:C:224:GLY:H	1.95	0.78
1:C:245:PHE:HE1	1:C:255:ASN:HB3	1.45	0.78
1:G:79:LYS:HE2	1:G:119:GLU:OE2	1.83	0.78
1:H:253:VAL:HG13	1:H:253:VAL:O	1.82	0.78
1:B:75:ILE:HD12	1:B:75:ILE:H	1.48	0.77
1:J:9:TYR:CE1	1:J:51:ILE:HB	2.19	0.77
1:G:64:ASN:O	1:H:183:ASN:ND2	2.18	0.77
1:D:44:TYR:HB3	1:D:52:ALA:HB3	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:146:ILE:HD13	1:J:223:LYS:HB3	1.67	0.77
1:I:183:ASN:HD21	1:J:65:ASP:CB	1.99	0.76
1:F:108:ILE:CG2	1:F:176:LEU:HD23	2.14	0.76
1:B:166:MET:HG3	1:B:189:VAL:HG22	1.66	0.76
1:B:47:ILE:HD12	1:B:47:ILE:H	1.51	0.76
1:E:275:SER:HB2	1:E:285:CYS:SG	2.26	0.76
1:G:248:ASN:C	1:G:250:LYS:H	1.89	0.76
1:A:65:ASP:HA	1:D:183:ASN:ND2	2.00	0.76
1:G:146:ILE:HD11	1:G:223:LYS:HB3	1.66	0.76
1:F:161:ASN:HD22	1:F:164:PHE:HD1	1.34	0.76
1:G:189:VAL:HG23	1:G:228:ILE:HD11	1.65	0.76
1:H:109:ARG:HB3	1:H:171:TYR:CE1	2.20	0.75
1:A:183:ASN:HD21	1:D:65:ASP:HA	1.49	0.75
1:G:253:VAL:O	1:G:253:VAL:HG13	1.84	0.75
1:B:159:PHE:CD2	1:B:208:GLU:HG2	2.21	0.75
1:D:197:ILE:HG22	1:D:202:VAL:HG23	1.69	0.75
1:A:171:TYR:HB3	1:A:179:ILE:HG13	1.69	0.74
1:I:146:ILE:HD11	1:I:223:LYS:HB3	1.66	0.74
1:E:17:TYR:CE1	1:E:98:VAL:HG11	2.23	0.74
1:F:195:LYS:HB2	1:F:196:PRO:CD	2.17	0.74
1:D:161:ASN:HB3	1:D:164:PHE:N	2.01	0.74
1:J:238:ALA:HB1	1:J:272:PHE:CZ	2.23	0.74
1:I:261:ASP:HB3	1:I:264:ILE:HD12	1.69	0.74
1:G:117:ARG:NH2	1:G:125:LEU:HG	2.02	0.73
1:G:171:TYR:HA	1:G:174:HIS:HD2	1.52	0.73
1:C:110:HIS:CE1	1:C:139:ALA:HB2	2.23	0.73
1:D:121:PRO:HA	1:D:126:PHE:CD1	2.23	0.73
1:H:251:THR:HA	1:H:253:VAL:HG12	1.68	0.73
1:I:4:LEU:HD11	1:I:140:ILE:HG13	1.69	0.72
1:B:44:TYR:HB3	1:B:52:ALA:HB3	1.70	0.72
1:E:110:HIS:CE1	1:E:139:ALA:HB2	2.25	0.72
1:D:31:LEU:HD13	1:D:63:THR:CG2	2.19	0.72
1:A:100:ASN:OD1	1:G:100:ASN:OD1	2.08	0.71
1:B:146:ILE:CD1	1:B:223:LYS:HB3	2.20	0.71
1:F:187:TYR:HB2	1:F:228:ILE:HB	1.72	0.71
1:F:117:ARG:NH2	1:F:125:LEU:HG	2.05	0.71
1:G:6:CYS:SG	1:G:60:ARG:HG3	2.31	0.71
1:G:150:ILE:HG23	1:G:151:THR:HG23	1.71	0.71
1:E:161:ASN:HB3	1:E:164:PHE:H	1.56	0.71
1:F:108:ILE:HG23	1:F:176:LEU:HD23	1.72	0.71
1:B:275:SER:HB2	1:B:285:CYS:SG	2.31	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:75:ILE:HD12	1:H:175:GLN:HE22	1.55	0.70
1:H:261:ASP:OD2	1:H:263:ARG:NH1	2.23	0.70
1:J:202:VAL:HG13	1:J:264:ILE:HD11	1.71	0.70
1:A:65:ASP:HA	1:D:183:ASN:HD21	1.56	0.70
1:D:245:PHE:O	1:D:248:ASN:HB2	1.90	0.70
1:J:225:HIS:CE1	1:J:227:ARG:HH21	2.09	0.70
1:C:261:ASP:OD1	1:C:263:ARG:HG3	1.90	0.70
1:H:146:ILE:HD11	1:H:223:LYS:HB3	1.71	0.70
1:A:275:SER:OG	1:A:288:LEU:HD11	1.91	0.70
1:B:101:VAL:HG22	1:B:142:GLN:NE2	2.05	0.69
1:B:150:ILE:HG23	1:B:151:THR:HG23	1.74	0.69
1:G:106:VAL:HG11	1:G:140:ILE:HA	1.73	0.69
1:C:146:ILE:HD11	1:C:223:LYS:HB3	1.74	0.69
1:G:245:PHE:HE1	1:G:255:ASN:HB3	1.55	0.69
1:H:251:THR:HB	1:I:134:LYS:HZ1	1.52	0.69
1:I:253:VAL:HG13	1:I:253:VAL:O	1.92	0.69
1:A:43:PHE:CD1	1:A:54:PRO:HD3	2.28	0.69
1:I:183:ASN:HD21	1:J:65:ASP:CA	2.04	0.69
1:J:106:VAL:HG11	1:J:140:ILE:HD12	1.72	0.69
1:B:248:ASN:C	1:B:250:LYS:H	1.96	0.69
1:B:146:ILE:HD11	1:B:223:LYS:HB3	1.75	0.69
1:C:266:TRP:CZ3	1:C:268:ASN:HB2	2.28	0.69
1:D:202:VAL:O	1:D:206:VAL:HG23	1.93	0.69
1:D:281:THR:OG1	1:D:284:VAL:HG23	1.93	0.69
1:F:259:LEU:HD13	1:F:273:THR:HG21	1.74	0.69
1:G:183:ASN:ND2	1:H:64:ASN:O	2.26	0.69
1:I:79:LYS:HE2	1:I:119:GLU:OE2	1.93	0.69
1:C:35:VAL:HG12	1:C:36:ASP:H	1.59	0.68
1:G:261:ASP:HB3	1:G:264:ILE:HD12	1.74	0.68
1:E:17:TYR:CD1	1:E:98:VAL:HG11	2.28	0.68
1:B:226:TYR:OH	1:B:264:ILE:HD12	1.94	0.68
1:B:5:ALA:HB2	1:B:102:LEU:HB3	1.76	0.68
1:C:159:PHE:HE1	1:C:161:ASN:HB2	1.59	0.68
1:G:72:PHE:N	1:G:72:PHE:CD2	2.62	0.68
1:G:275:SER:HB3	1:G:285:CYS:SG	2.33	0.68
1:F:259:LEU:HD22	1:F:273:THR:HG22	1.76	0.67
1:H:187:TYR:HB2	1:H:228:ILE:HB	1.75	0.67
1:A:171:TYR:HB3	1:A:179:ILE:CG1	2.24	0.67
1:B:210:ARG:HH22	1:J:42:LYS:HD3	1.57	0.67
1:G:205:LEU:HG	1:G:209:LEU:CD1	2.25	0.67
1:F:275:SER:HB2	1:F:285:CYS:SG	2.34	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:HIS:CE1	1:A:139:ALA:HB2	2.30	0.67
1:H:87:ALA:HB2	1:H:136:THR:HG21	1.75	0.67
1:A:99:SER:HB3	1:G:99:SER:HB3	1.77	0.66
1:H:261:ASP:OD1	1:H:263:ARG:HG2	1.96	0.66
1:E:146:ILE:HG12	1:E:224:GLY:H	1.59	0.66
1:C:161:ASN:HD22	1:C:164:PHE:HD1	1.44	0.66
1:E:185:ILE:HG13	1:E:230:LYS:HE3	1.78	0.66
1:G:17:TYR:CE1	1:G:98:VAL:HG11	2.31	0.66
1:A:171:TYR:HB2	1:A:179:ILE:HG13	1.75	0.66
1:A:205:LEU:O	1:A:209:LEU:HD12	1.96	0.66
1:B:210:ARG:NH2	1:J:42:LYS:HD3	2.10	0.66
1:B:84:ILE:O	1:B:87:ALA:HB3	1.96	0.66
1:G:111:LEU:HD11	1:G:140:ILE:CD1	2.26	0.66
1:I:183:ASN:ND2	1:J:65:ASP:HA	2.10	0.66
1:I:146:ILE:HG12	1:I:224:GLY:H	1.61	0.66
1:E:249:VAL:HG12	1:E:249:VAL:O	1.96	0.66
1:E:202:VAL:HG13	1:E:264:ILE:CD1	2.21	0.65
1:H:111:LEU:HD21	1:H:140:ILE:CD1	2.25	0.65
1:A:202:VAL:O	1:A:206:VAL:HG23	1.96	0.65
1:C:43:PHE:CE1	1:C:54:PRO:HD3	2.31	0.65
1:G:95:GLN:O	1:G:98:VAL:HG22	1.97	0.65
1:A:224:GLY:O	1:A:225:HIS:HB3	1.96	0.65
1:C:243:ALA:O	1:C:246:LYS:HB3	1.96	0.65
1:B:110:HIS:CE1	1:B:139:ALA:HB2	2.31	0.65
1:G:202:VAL:O	1:G:206:VAL:CG2	2.45	0.65
1:B:74:THR:HB	1:B:175:GLN:NE2	2.12	0.65
1:F:84:ILE:O	1:F:87:ALA:HB3	1.97	0.65
1:G:117:ARG:HH21	1:G:125:LEU:HG	1.60	0.65
1:F:271:ALA:HB1	1:F:288:LEU:HD22	1.79	0.65
1:G:189:VAL:CG2	1:G:228:ILE:HD11	2.27	0.65
1:F:226:TYR:OH	1:F:264:ILE:HD12	1.96	0.64
1:E:125:LEU:HB3	1:E:132:LEU:HD13	1.79	0.64
1:E:202:VAL:CG1	1:E:264:ILE:HD11	2.20	0.64
1:G:138:ILE:HG12	1:G:143:SER:HB3	1.77	0.64
1:C:17:TYR:CE1	1:C:98:VAL:HG11	2.31	0.64
1:G:44:TYR:HB3	1:G:52:ALA:HB3	1.79	0.64
1:A:146:ILE:HD12	1:A:147:GLU:H	1.61	0.64
1:I:14:ASN:O	1:I:15:ASP:HB2	1.97	0.64
1:J:37:LYS:CD	1:J:37:LYS:H	2.10	0.64
1:G:9:TYR:HB3	1:G:22:PHE:CZ	2.32	0.64
1:G:198:SER:O	1:G:202:VAL:HG23	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:283:ASP:O	1:G:287:ARG:HG3	1.97	0.64
1:I:108:ILE:HG21	1:I:176:LEU:HD23	1.79	0.64
1:E:206:VAL:HG12	1:E:210:ARG:HD2	1.79	0.64
1:B:160:GLN:HG3	1:B:165:THR:HG23	1.80	0.64
1:C:146:ILE:HD11	1:C:224:GLY:N	2.13	0.64
1:B:248:ASN:HB2	1:B:255:ASN:HD22	1.63	0.64
1:I:282:LEU:HD11	1:I:286:LYS:HE2	1.79	0.64
1:C:9:TYR:HB3	1:C:22:PHE:CZ	2.33	0.64
1:I:248:ASN:C	1:I:250:LYS:H	2.02	0.64
1:J:10:PRO:HD3	1:J:102:LEU:HD11	1.79	0.64
1:C:118:LYS:HG3	1:C:132:LEU:HD21	1.81	0.63
1:I:150:ILE:HG23	1:I:151:THR:HG23	1.79	0.63
1:J:125:LEU:HD22	1:J:132:LEU:CA	2.27	0.63
1:C:130:ASP:OD2	1:J:14:ASN:HA	1.98	0.63
1:D:246:LYS:C	1:D:248:ASN:H	2.01	0.63
1:G:261:ASP:OD1	1:G:263:ARG:HG3	1.98	0.63
1:J:117:ARG:NH2	1:J:125:LEU:HG	2.12	0.63
1:J:62:ASN:OD1	1:J:69:GLY:N	2.31	0.63
1:F:10:PRO:HB2	1:F:17:TYR:CD1	2.34	0.63
1:G:202:VAL:O	1:G:206:VAL:HG23	1.98	0.63
1:G:245:PHE:CE1	1:G:255:ASN:HB3	2.33	0.63
1:D:121:PRO:HA	1:D:126:PHE:CG	2.33	0.63
1:J:39:ASP:HA	1:J:42:LYS:HD2	1.81	0.62
1:G:75:ILE:H	1:G:75:ILE:CD1	2.05	0.62
1:E:224:GLY:O	1:E:225:HIS:HB3	2.00	0.62
1:J:111:LEU:HD21	1:J:140:ILE:HD13	1.81	0.62
1:A:51:ILE:HD13	1:A:51:ILE:N	2.15	0.62
1:C:17:TYR:CD1	1:C:98:VAL:HG11	2.35	0.62
1:E:185:ILE:HD12	1:E:216:PHE:HZ	1.63	0.62
1:I:183:ASN:HD21	1:J:65:ASP:HA	1.65	0.62
1:E:248:ASN:C	1:E:250:LYS:H	2.03	0.61
1:J:161:ASN:HD21	1:J:201:HIS:HB3	1.64	0.61
1:A:171:TYR:HA	1:A:174:HIS:CD2	2.34	0.61
1:I:225:HIS:NE2	1:I:227:ARG:NH2	2.47	0.61
1:E:183:ASN:HD21	1:F:65:ASP:CA	2.04	0.61
1:E:160:GLN:HG3	1:E:165:THR:HG23	1.81	0.61
1:G:183:ASN:OD1	1:H:64:ASN:O	2.19	0.61
1:I:121:PRO:HA	1:I:126:PHE:CG	2.35	0.61
1:A:10:PRO:HD3	1:A:102:LEU:HD11	1.83	0.61
1:C:257:PHE:CE1	1:C:273:THR:HG21	2.36	0.61
1:E:95:GLN:HA	1:E:98:VAL:HG22	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:VAL:HG13	1:A:253:VAL:O	2.01	0.61
1:B:121:PRO:HA	1:B:126:PHE:CD2	2.35	0.61
1:G:171:TYR:HA	1:G:174:HIS:CD2	2.36	0.60
1:G:205:LEU:HG	1:G:209:LEU:HD11	1.82	0.60
1:E:14:ASN:O	1:E:15:ASP:HB2	2.01	0.60
1:F:135:SER:HB3	1:F:151:THR:O	2.01	0.60
1:H:11:HIS:HB2	1:H:20:ILE:HD11	1.84	0.60
1:A:285:CYS:HA	1:A:288:LEU:HD12	1.83	0.60
1:G:22:PHE:CD2	1:G:53:PRO:HG3	2.37	0.60
1:B:237:HIS:O	1:B:241:VAL:HG22	2.02	0.60
1:C:237:HIS:O	1:C:241:VAL:HG22	2.01	0.60
1:F:47:ILE:H	1:F:47:ILE:HD12	1.64	0.60
1:H:54:PRO:HG2	1:H:57:PHE:HE2	1.67	0.60
1:E:187:TYR:HB2	1:E:228:ILE:HB	1.83	0.60
1:J:14:ASN:HB2	1:J:18:LYS:NZ	2.17	0.60
1:J:188:LYS:HD3	1:J:225:HIS:HD2	1.67	0.60
1:J:231:TYR:O	1:J:234:VAL:HG22	2.01	0.60
1:A:62:ASN:OD1	1:A:69:GLY:N	2.30	0.59
1:B:275:SER:CB	1:B:285:CYS:SG	2.89	0.59
1:I:146:ILE:CG1	1:I:224:GLY:H	2.15	0.59
1:H:117:ARG:HB3	1:H:125:LEU:HD12	1.84	0.59
1:B:10:PRO:HD3	1:B:102:LEU:HD11	1.84	0.59
1:C:169:LEU:HD11	1:C:188:LYS:HG2	1.85	0.59
1:I:93:VAL:HG11	1:I:101:VAL:HG21	1.83	0.59
1:A:146:ILE:HD11	1:A:223:LYS:HB3	1.84	0.59
1:A:154:GLY:HA2	1:A:167:TRP:CE3	2.37	0.59
1:A:271:ALA:HB1	1:A:288:LEU:HD22	1.84	0.59
1:G:111:LEU:HD11	1:G:140:ILE:HD13	1.84	0.59
1:H:125:LEU:HD22	1:H:132:LEU:HA	1.84	0.59
1:J:248:ASN:O	1:J:250:LYS:N	2.34	0.59
1:A:117:ARG:NH2	1:A:125:LEU:HG	2.17	0.59
1:D:248:ASN:C	1:D:250:LYS:H	2.05	0.59
1:F:152:ALA:HB2	1:F:190:THR:HG21	1.84	0.59
1:A:183:ASN:OD1	1:D:64:ASN:O	2.21	0.59
1:H:75:ILE:HD12	1:H:175:GLN:NE2	2.17	0.59
1:D:146:ILE:HD12	1:D:147:GLU:H	1.67	0.59
1:G:285:CYS:HA	1:G:288:LEU:HD12	1.82	0.59
1:J:44:TYR:HB3	1:J:52:ALA:HB3	1.85	0.59
1:J:224:GLY:O	1:J:225:HIS:HB3	2.02	0.59
1:A:154:GLY:HA2	1:A:167:TRP:CZ3	2.38	0.59
1:J:146:ILE:HG12	1:J:224:GLY:H	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:249:VAL:O	1:I:249:VAL:HG12	2.02	0.59
1:I:261:ASP:OD1	1:I:263:ARG:HG3	2.02	0.59
1:J:121:PRO:HA	1:J:126:PHE:CE1	2.37	0.59
1:H:119:GLU:O	1:H:121:PRO:HD3	2.03	0.58
1:A:146:ILE:CD1	1:A:223:LYS:HB3	2.32	0.58
1:E:39:ASP:HA	1:E:42:LYS:HG3	1.84	0.58
1:A:111:LEU:HD21	1:A:140:ILE:HD13	1.85	0.58
1:E:188:LYS:HE2	1:E:225:HIS:NE2	2.17	0.58
1:F:21:PRO:HG3	1:F:85:CYS:SG	2.43	0.58
1:A:164:PHE:CZ	1:A:205:LEU:HD22	2.38	0.58
1:A:261:ASP:OD1	1:A:263:ARG:HG3	2.04	0.58
1:B:147:GLU:OE2	1:B:188:LYS:NZ	2.37	0.58
1:D:229:VAL:HG11	1:D:237:HIS:CD2	2.38	0.58
1:G:76:MET:HB2	1:G:175:GLN:OE1	2.04	0.58
1:J:146:ILE:HD11	1:J:223:LYS:HB3	1.85	0.58
1:C:146:ILE:HD12	1:C:147:GLU:H	1.69	0.58
1:G:76:MET:SD	1:G:112:GLU:HG3	2.44	0.58
1:I:154:GLY:HA2	1:I:167:TRP:CE3	2.39	0.58
1:F:121:PRO:HA	1:F:126:PHE:CG	2.38	0.58
1:G:207:ALA:HA	1:G:210:ARG:HD2	1.86	0.58
1:I:6:CYS:SG	1:I:60:ARG:HG3	2.44	0.58
1:C:79:LYS:HE2	1:C:119:GLU:OE2	2.04	0.58
1:F:195:LYS:CB	1:F:196:PRO:HD2	2.28	0.58
1:G:4:LEU:HD12	1:G:88:LEU:HD11	1.86	0.57
1:C:10:PRO:HB2	1:C:17:TYR:CD1	2.39	0.57
1:I:163:ALA:HB1	1:I:197:ILE:HD13	1.86	0.57
1:G:75:ILE:HD12	1:G:75:ILE:N	2.09	0.57
1:I:30:MET:HB2	1:I:44:TYR:CD2	2.40	0.57
1:J:171:TYR:HB2	1:J:184:PHE:CE2	2.40	0.57
1:E:9:TYR:HD1	1:E:22:PHE:CE1	2.22	0.57
1:B:202:VAL:O	1:B:206:VAL:HG23	2.05	0.57
1:C:271:ALA:HB1	1:C:288:LEU:HB3	1.85	0.57
1:D:118:LYS:HD2	1:D:132:LEU:HD21	1.85	0.57
1:I:146:ILE:CD1	1:I:224:GLY:H	2.18	0.57
1:I:161:ASN:HB3	1:I:164:PHE:H	1.69	0.57
1:B:225:HIS:NE2	1:B:227:ARG:NH2	2.52	0.57
1:C:72:PHE:N	1:C:72:PHE:CD2	2.73	0.57
1:E:3:GLU:N	1:E:3:GLU:OE1	2.38	0.57
1:C:118:LYS:O	1:C:118:LYS:HG2	2.03	0.57
1:A:41:ASP:HB3	1:A:56:GLN:HE22	1.69	0.57
1:E:76:MET:SD	1:E:112:GLU:HG3	2.45	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:10:PRO:HB2	1:F:17:TYR:HD1	1.68	0.57
1:H:146:ILE:HD12	1:H:147:GLU:H	1.70	0.57
1:B:74:THR:HB	1:B:175:GLN:HE21	1.70	0.56
1:B:121:PRO:HA	1:B:126:PHE:CG	2.39	0.56
1:F:111:LEU:HD21	1:F:140:ILE:HD13	1.86	0.56
1:I:125:LEU:HD13	1:I:132:LEU:HD12	1.87	0.56
1:B:150:ILE:CG2	1:B:151:THR:HG23	2.35	0.56
1:C:83:LEU:HD23	1:C:111:LEU:HD13	1.87	0.56
1:F:112:GLU:HB3	1:F:174:HIS:CE1	2.41	0.56
1:H:146:ILE:HD11	1:H:224:GLY:H	1.70	0.56
1:B:271:ALA:HB1	1:B:288:LEU:HD22	1.87	0.56
1:G:74:THR:HB	1:G:175:GLN:NE2	2.20	0.56
1:H:44:TYR:HB3	1:H:52:ALA:HB3	1.87	0.56
1:F:229:VAL:HG21	1:F:237:HIS:NE2	2.21	0.56
1:H:253:VAL:O	1:H:253:VAL:CG1	2.53	0.56
1:D:146:ILE:HG12	1:D:224:GLY:HA3	1.87	0.56
1:A:225:HIS:NE2	1:A:227:ARG:NH2	2.54	0.56
1:H:4:LEU:HD21	1:H:106:VAL:HG11	1.87	0.56
1:H:10:PRO:HD3	1:H:102:LEU:HD11	1.87	0.56
1:H:251:THR:HB	1:I:134:LYS:HZ3	1.68	0.56
1:I:191:LEU:HD23	1:I:197:ILE:HD11	1.87	0.56
1:A:186:GLU:OE2	1:A:227:ARG:HG2	2.05	0.56
1:A:202:VAL:HG21	1:A:263:ARG:HH21	1.70	0.56
1:H:172:LEU:HD12	1:H:172:LEU:H	1.70	0.56
1:D:275:SER:HB3	1:D:285:CYS:SG	2.45	0.56
1:A:272:PHE:HB2	1:A:289:LEU:HD13	1.87	0.55
1:C:205:LEU:O	1:C:209:LEU:HD12	2.06	0.55
1:D:109:ARG:HD3	1:D:171:TYR:CD1	2.42	0.55
1:I:237:HIS:O	1:I:241:VAL:HG13	2.07	0.55
1:F:31:LEU:CD2	1:F:58:LYS:HG3	2.36	0.55
1:C:94:THR:HG22	1:C:95:GLN:N	2.22	0.55
1:A:44:TYR:HB3	1:A:52:ALA:HB3	1.88	0.55
1:D:251:THR:HB	1:E:134:LYS:NZ	2.22	0.55
1:F:78:THR:O	1:F:82:MET:HG3	2.06	0.55
1:G:237:HIS:O	1:G:241:VAL:HG22	2.06	0.55
1:I:9:TYR:HB2	1:I:43:PHE:CZ	2.42	0.55
1:G:248:ASN:C	1:G:250:LYS:N	2.58	0.55
1:I:164:PHE:CZ	1:I:197:ILE:HD12	2.42	0.55
1:E:27:ILE:HG12	1:E:53:PRO:CD	2.37	0.55
1:I:75:ILE:HD12	1:I:175:GLN:HE22	1.71	0.55
1:B:198:SER:O	1:B:202:VAL:HG23	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:80:VAL:O	1:I:84:ILE:HD12	2.07	0.55
1:J:161:ASN:HB3	1:J:164:PHE:H	1.72	0.55
1:I:110:HIS:CE1	1:I:139:ALA:HB2	2.42	0.55
1:A:161:ASN:ND2	1:A:163:ALA:H	2.04	0.55
1:B:62:ASN:OD1	1:B:69:GLY:N	2.38	0.55
1:G:249:VAL:HG12	1:G:249:VAL:O	2.06	0.55
1:G:266:TRP:CZ3	1:G:268:ASN:HB2	2.42	0.55
1:H:79:LYS:HE2	1:H:119:GLU:OE2	2.07	0.55
1:B:44:TYR:O	1:B:51:ILE:HG22	2.07	0.55
1:A:75:ILE:HD12	1:A:75:ILE:H	1.72	0.54
1:G:250:LYS:O	1:G:253:VAL:HG12	2.07	0.54
1:A:10:PRO:HD3	1:A:102:LEU:CD1	2.38	0.54
1:A:257:PHE:HB3	1:A:277:LYS:HG3	1.88	0.54
1:A:79:LYS:HE2	1:A:119:GLU:OE2	2.07	0.54
1:C:72:PHE:N	1:C:72:PHE:HD2	2.04	0.54
1:E:275:SER:CB	1:E:285:CYS:SG	2.95	0.54
1:I:161:ASN:HD21	1:I:201:HIS:HB3	1.72	0.54
1:J:124:ILE:CD1	1:J:150:ILE:HG13	2.37	0.54
1:J:197:ILE:HD12	1:J:197:ILE:N	2.22	0.54
1:E:93:VAL:HG11	1:E:101:VAL:HG21	1.90	0.54
1:E:245:PHE:CE2	1:E:276:MET:O	2.61	0.54
1:D:253:VAL:O	1:D:253:VAL:HG13	2.07	0.54
1:B:210:ARG:NH2	1:J:42:LYS:CE	2.71	0.54
1:J:37:LYS:H	1:J:37:LYS:HD2	1.71	0.54
1:B:224:GLY:O	1:B:225:HIS:HB3	2.08	0.54
1:C:248:ASN:C	1:C:250:LYS:H	2.11	0.54
1:E:161:ASN:HD22	1:E:164:PHE:HD1	1.54	0.54
1:I:4:LEU:HD23	1:I:106:VAL:HG22	1.89	0.54
1:G:121:PRO:HA	1:G:126:PHE:CG	2.42	0.54
1:D:75:ILE:HD12	1:D:75:ILE:N	2.19	0.54
1:G:161:ASN:HB3	1:G:164:PHE:H	1.73	0.54
1:I:191:LEU:HD12	1:I:191:LEU:N	2.23	0.54
1:F:111:LEU:HD11	1:F:140:ILE:HD11	1.90	0.54
1:H:75:ILE:HD12	1:H:75:ILE:H	1.72	0.54
1:D:31:LEU:HD13	1:D:63:THR:HG22	1.88	0.53
1:E:94:THR:O	1:E:98:VAL:HG13	2.07	0.53
1:E:217:ALA:HB2	1:E:231:TYR:CE1	2.42	0.53
1:A:171:TYR:HA	1:A:174:HIS:HD2	1.73	0.53
1:E:268:ASN:OD1	1:E:268:ASN:N	2.42	0.53
1:C:112:GLU:HB3	1:C:174:HIS:CE1	2.43	0.53
1:E:62:ASN:OD1	1:E:69:GLY:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:51:ILE:N	1:G:51:ILE:HD13	2.23	0.53
1:G:272:PHE:HB2	1:G:289:LEU:HD13	1.91	0.53
1:H:111:LEU:HD21	1:H:140:ILE:HD11	1.91	0.53
1:E:63:THR:H	1:E:66:ASN:HB3	1.73	0.53
1:F:221:HIS:HB2	1:F:227:ARG:CZ	2.38	0.53
1:J:195:LYS:HB2	1:J:196:PRO:HD2	1.91	0.53
1:A:84:ILE:HD11	1:A:111:LEU:HD13	1.91	0.53
1:A:161:ASN:HB3	1:A:164:PHE:H	1.74	0.53
1:G:2:ALA:HB2	1:G:108:ILE:HD11	1.91	0.53
1:J:4:LEU:HD11	1:J:140:ILE:HG23	1.91	0.53
1:A:118:LYS:O	1:A:118:LYS:HG2	2.09	0.53
1:C:146:ILE:CD1	1:C:223:LYS:HB3	2.37	0.53
1:I:146:ILE:HG12	1:I:224:GLY:N	2.22	0.53
1:D:187:TYR:HB2	1:D:228:ILE:HB	1.89	0.53
1:E:225:HIS:H	1:E:260:LEU:HD11	1.73	0.53
1:G:146:ILE:HD13	1:G:223:LYS:HB3	1.88	0.53
1:G:205:LEU:HG	1:G:209:LEU:HD12	1.91	0.53
1:I:183:ASN:ND2	1:J:65:ASP:HB3	2.19	0.53
1:B:10:PRO:HB2	1:B:17:TYR:CD1	2.44	0.52
1:B:229:VAL:CG2	1:B:233:SER:HB2	2.39	0.52
1:D:245:PHE:O	1:D:248:ASN:CB	2.57	0.52
1:G:161:ASN:CG	1:G:162:ALA:H	2.12	0.52
1:A:74:THR:HB	1:A:175:GLN:NE2	2.24	0.52
1:C:272:PHE:CD1	1:C:272:PHE:C	2.82	0.52
1:E:249:VAL:O	1:E:249:VAL:CG1	2.57	0.52
1:H:229:VAL:HG11	1:H:237:HIS:CD2	2.43	0.52
1:C:280:ASN:OD1	1:C:284:VAL:HG11	2.08	0.52
1:G:120:ASN:HD21	1:G:122:GLN:HB2	1.74	0.52
1:I:55:PRO:O	1:I:58:LYS:HB2	2.10	0.52
1:D:31:LEU:HD13	1:D:63:THR:HG21	1.90	0.52
1:G:224:GLY:O	1:G:225:HIS:HB3	2.09	0.52
1:I:4:LEU:CD1	1:I:140:ILE:HG13	2.37	0.52
1:A:100:ASN:ND2	1:G:96:ALA:O	2.43	0.52
1:H:78:THR:O	1:H:82:MET:HG3	2.10	0.52
1:I:108:ILE:HG23	1:I:176:LEU:HD23	1.90	0.52
1:H:150:ILE:HG23	1:H:151:THR:HG23	1.90	0.52
1:I:27:ILE:HG12	1:I:53:PRO:HD2	1.92	0.52
1:C:171:TYR:HB3	1:C:179:ILE:HG13	1.92	0.52
1:G:14:ASN:HB2	1:G:18:LYS:NZ	2.25	0.52
1:J:146:ILE:HD12	1:J:147:GLU:N	2.18	0.52
1:J:153:GLU:HG2	1:J:188:LYS:NZ	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:ALA:O	1:A:246:LYS:HB3	2.10	0.52
1:B:188:LYS:HB3	1:B:227:ARG:HG3	1.92	0.52
1:B:205:LEU:CD1	1:B:209:LEU:HD11	2.40	0.52
1:A:5:ALA:HB2	1:A:102:LEU:HB3	1.91	0.51
1:G:185:ILE:HG22	1:G:187:TYR:CE1	2.44	0.51
1:J:9:TYR:C	1:J:9:TYR:CD2	2.84	0.51
1:J:14:ASN:HB2	1:J:18:LYS:HZ1	1.74	0.51
1:A:159:PHE:CD2	1:A:208:GLU:HG2	2.45	0.51
1:A:26:ALA:HB2	1:A:49:TYR:O	2.10	0.51
1:D:79:LYS:HA	1:D:82:MET:HE2	1.91	0.51
1:D:146:ILE:HD12	1:D:147:GLU:N	2.25	0.51
1:E:8:CYS:HB2	1:E:20:ILE:O	2.11	0.51
1:F:80:VAL:HG21	1:F:176:LEU:HD22	1.92	0.51
1:A:62:ASN:HB2	1:A:70:MET:O	2.10	0.51
1:B:76:MET:HG2	1:B:112:GLU:CD	2.30	0.51
1:I:187:TYR:HB2	1:I:228:ILE:HB	1.92	0.51
1:I:238:ALA:HB1	1:I:272:PHE:CZ	2.46	0.51
1:F:152:ALA:CB	1:F:190:THR:HG21	2.39	0.51
1:B:248:ASN:C	1:B:250:LYS:N	2.64	0.51
1:I:117:ARG:HB3	1:I:125:LEU:HD12	1.92	0.51
1:B:221:HIS:HE1	1:B:240:ARG:NH2	2.08	0.51
1:C:163:ALA:HA	1:C:192:ASN:HD22	1.74	0.51
1:G:184:PHE:C	1:G:185:ILE:HG13	2.30	0.51
1:J:2:ALA:HA	1:J:60:ARG:NH2	2.26	0.51
1:B:159:PHE:HE1	1:B:161:ASN:HB2	1.75	0.51
1:D:74:THR:HB	1:D:175:GLN:NE2	2.26	0.51
1:C:147:GLU:OE2	1:C:188:LYS:NZ	2.43	0.51
1:C:245:PHE:CD1	1:C:255:ASN:HB3	2.46	0.51
1:D:74:THR:HG21	1:D:175:GLN:HG2	1.92	0.51
1:G:248:ASN:HA	1:G:253:VAL:HG11	1.93	0.51
1:J:31:LEU:HD13	1:J:63:THR:CG2	2.41	0.51
1:C:164:PHE:CG	1:C:205:LEU:HD22	2.45	0.51
1:F:248:ASN:O	1:F:250:LYS:N	2.40	0.51
1:H:144:LYS:HE3	1:I:162:ALA:O	2.11	0.51
1:C:22:PHE:HZ	1:C:43:PHE:CE1	2.29	0.50
1:D:171:TYR:HD2	1:D:184:PHE:CZ	2.29	0.50
1:D:251:THR:HB	1:E:134:LYS:HZ1	1.77	0.50
1:G:138:ILE:HG12	1:G:143:SER:CB	2.41	0.50
1:H:117:ARG:CB	1:H:125:LEU:HD12	2.41	0.50
1:G:243:ALA:O	1:G:246:LYS:HB3	2.11	0.50
1:D:111:LEU:HD21	1:D:140:ILE:CD1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:17:TYR:CZ	1:G:98:VAL:HG11	2.45	0.50
1:J:117:ARG:HH21	1:J:125:LEU:HG	1.75	0.50
1:F:75:ILE:HD12	1:F:175:GLN:HE22	1.76	0.50
1:G:271:ALA:HB1	1:G:288:LEU:HD22	1.93	0.50
1:J:3:GLU:HG3	1:J:105:VAL:HG22	1.92	0.50
1:B:205:LEU:HG	1:B:209:LEU:HD11	1.93	0.50
1:C:106:VAL:HG11	1:C:140:ILE:HA	1.91	0.50
1:G:62:ASN:OD1	1:G:69:GLY:N	2.45	0.50
1:J:253:VAL:HG13	1:J:253:VAL:O	2.11	0.50
1:C:74:THR:HG21	1:C:175:GLN:HG2	1.93	0.50
1:E:159:PHE:CD2	1:E:208:GLU:HG2	2.47	0.50
1:F:62:ASN:OD1	1:F:69:GLY:N	2.40	0.50
1:I:191:LEU:HD12	1:I:191:LEU:H	1.76	0.50
1:I:146:ILE:HG12	1:I:224:GLY:HA3	1.92	0.50
1:J:202:VAL:O	1:J:206:VAL:HG23	2.11	0.50
1:A:217:ALA:N	1:A:229:VAL:O	2.43	0.50
1:A:254:ASN:N	1:A:254:ASN:HD22	2.09	0.50
1:D:109:ARG:CZ	1:D:179:ILE:HG12	2.42	0.50
1:G:14:ASN:HB2	1:G:18:LYS:HZ1	1.77	0.50
1:B:44:TYR:CD2	1:B:45:ASP:N	2.80	0.50
1:D:4:LEU:HD12	1:D:101:VAL:O	2.12	0.50
1:E:76:MET:O	1:E:80:VAL:HG23	2.12	0.50
1:E:146:ILE:HD13	1:E:223:LYS:HB3	1.90	0.50
1:F:43:PHE:HD1	1:F:52:ALA:O	1.94	0.49
1:H:87:ALA:HB2	1:H:136:THR:CG2	2.41	0.49
1:G:22:PHE:CE2	1:G:53:PRO:HG3	2.47	0.49
1:G:72:PHE:HD2	1:G:72:PHE:N	1.98	0.49
1:A:22:PHE:CE2	1:A:53:PRO:HG3	2.47	0.49
1:C:118:LYS:O	1:C:126:PHE:HD2	1.95	0.49
1:D:88:LEU:HD21	1:D:140:ILE:HG21	1.94	0.49
1:D:199:ASP:O	1:D:203:LYS:HG3	2.12	0.49
1:F:87:ALA:HB2	1:F:136:THR:HG21	1.95	0.49
1:G:113:ASN:ND2	1:G:171:TYR:HE1	2.10	0.49
1:G:188:LYS:HB3	1:G:227:ARG:HG3	1.95	0.49
1:H:121:PRO:O	1:H:127:HIS:HE1	1.95	0.49
1:I:4:LEU:CD2	1:I:106:VAL:HG22	2.42	0.49
1:B:83:LEU:HD22	1:B:115:VAL:HG23	1.94	0.49
1:J:261:ASP:OD2	1:J:263:ARG:NH2	2.45	0.49
1:F:150:ILE:HG22	1:F:151:THR:HG23	1.91	0.49
1:H:218:VAL:HG12	1:H:265:ILE:HA	1.95	0.49
1:H:250:LYS:O	1:H:253:VAL:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:250:LYS:O	1:I:253:VAL:HG12	2.11	0.49
1:B:245:PHE:CD2	1:B:276:MET:HG2	2.48	0.49
1:B:272:PHE:CD2	1:B:289:LEU:HD22	2.47	0.49
1:D:274:SER:O	1:D:278:GLN:HB2	2.13	0.49
1:E:197:ILE:HG22	1:E:202:VAL:HG23	1.94	0.49
1:A:205:LEU:HG	1:A:209:LEU:CD1	2.41	0.49
1:A:275:SER:HB2	1:A:285:CYS:SG	2.53	0.49
1:E:183:ASN:ND2	1:F:64:ASN:O	2.46	0.49
1:G:195:LYS:HB2	1:G:196:PRO:HD2	1.94	0.49
1:I:121:PRO:O	1:I:127:HIS:HE1	1.96	0.49
1:J:26:ALA:O	1:J:29:ALA:HB3	2.12	0.49
1:A:106:VAL:HG11	1:A:140:ILE:HD12	1.93	0.49
1:C:11:HIS:CE1	1:C:13:GLU:HB3	2.47	0.49
1:C:246:LYS:C	1:C:248:ASN:H	2.16	0.49
1:D:221:HIS:HE2	1:D:237:HIS:HD1	1.61	0.49
1:E:94:THR:HG22	1:E:96:ALA:H	1.78	0.49
1:E:246:LYS:C	1:E:248:ASN:H	2.17	0.49
1:F:74:THR:HB	1:F:175:GLN:NE2	2.26	0.49
1:I:112:GLU:O	1:I:116:ILE:HG13	2.13	0.49
1:J:9:TYR:CD1	1:J:51:ILE:HB	2.48	0.49
1:J:111:LEU:HD21	1:J:140:ILE:CD1	2.42	0.49
1:A:184:PHE:O	1:A:185:ILE:HG13	2.13	0.49
1:B:30:MET:SD	1:B:55:PRO:HA	2.53	0.49
1:C:97:ASN:O	1:C:98:VAL:C	2.50	0.49
1:F:202:VAL:CG2	1:F:263:ARG:HH21	2.19	0.49
1:I:8:CYS:HB2	1:I:20:ILE:O	2.13	0.49
1:A:161:ASN:ND2	1:A:164:PHE:HD1	2.11	0.48
1:A:248:ASN:C	1:A:250:LYS:H	2.15	0.48
1:F:231:TYR:O	1:F:234:VAL:HG22	2.12	0.48
1:G:184:PHE:O	1:G:185:ILE:HG13	2.13	0.48
1:I:224:GLY:O	1:I:225:HIS:HB3	2.13	0.48
1:D:283:ASP:HA	1:D:286:LYS:HB2	1.95	0.48
1:E:9:TYR:HB3	1:E:22:PHE:CZ	2.48	0.48
1:E:245:PHE:CD2	1:E:276:MET:HG2	2.48	0.48
1:I:153:GLU:HG2	1:I:188:LYS:NZ	2.28	0.48
1:J:111:LEU:HD11	1:J:140:ILE:HD11	1.94	0.48
1:H:9:TYR:CE1	1:H:20:ILE:HB	2.48	0.48
1:B:159:PHE:CD1	1:B:159:PHE:C	2.86	0.48
1:C:275:SER:CB	1:C:285:CYS:SG	3.02	0.48
1:E:4:LEU:HD21	1:E:106:VAL:HG11	1.95	0.48
1:G:187:TYR:CD1	1:G:187:TYR:N	2.82	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:27:ILE:HG12	1:I:53:PRO:CD	2.43	0.48
1:J:75:ILE:H	1:J:75:ILE:HD12	1.78	0.48
1:B:229:VAL:HG22	1:B:233:SER:HB2	1.94	0.48
1:C:206:VAL:O	1:C:210:ARG:HG3	2.13	0.48
1:E:4:LEU:HB2	1:E:102:LEU:HA	1.95	0.48
1:G:167:TRP:O	1:G:187:TYR:HB3	2.13	0.48
1:H:74:THR:CB	1:H:175:GLN:HE21	2.04	0.48
1:I:216:PHE:N	1:I:216:PHE:CD1	2.81	0.48
1:A:95:GLN:HE22	1:G:56:GLN:HE22	1.60	0.48
1:A:205:LEU:HG	1:A:209:LEU:HD12	1.95	0.48
1:A:229:VAL:HG21	1:A:233:SER:HB2	1.95	0.48
1:B:104:ARG:HE	1:B:104:ARG:HA	1.79	0.48
1:G:275:SER:OG	1:G:288:LEU:HD11	2.13	0.48
1:I:161:ASN:CG	1:I:162:ALA:H	2.17	0.48
1:I:246:LYS:C	1:I:248:ASN:H	2.17	0.48
1:J:79:LYS:NZ	1:J:119:GLU:OE1	2.47	0.48
1:J:188:LYS:HD3	1:J:225:HIS:CD2	2.46	0.48
1:J:218:VAL:HG22	1:J:228:ILE:HD12	1.96	0.48
1:B:109:ARG:NH2	1:B:179:ILE:HG12	2.29	0.48
1:C:94:THR:HG22	1:C:96:ALA:H	1.79	0.48
1:H:261:ASP:OD1	1:H:261:ASP:C	2.52	0.48
1:D:159:PHE:CD2	1:D:208:GLU:HG2	2.48	0.48
1:E:146:ILE:CG1	1:E:224:GLY:H	2.25	0.48
1:I:218:VAL:HG11	1:I:264:ILE:HG22	1.95	0.48
1:F:259:LEU:HD13	1:F:273:THR:CG2	2.43	0.48
1:H:75:ILE:CD1	1:H:175:GLN:HE22	2.24	0.48
1:A:72:PHE:HA	1:A:77:PHE:CD1	2.49	0.47
1:A:262:GLN:HG3	1:A:270:TYR:CD2	2.49	0.47
1:D:37:LYS:H	1:D:37:LYS:HG3	1.47	0.47
1:D:9:TYR:CE1	1:D:20:ILE:HB	2.49	0.47
1:E:189:VAL:HB	1:E:226:TYR:HB2	1.95	0.47
1:G:183:ASN:CG	1:H:64:ASN:O	2.52	0.47
1:I:10:PRO:HD2	1:I:43:PHE:CE2	2.50	0.47
1:F:31:LEU:HD23	1:F:58:LYS:HG3	1.96	0.47
1:J:17:TYR:HE2	1:J:95:GLN:HG2	1.78	0.47
1:C:146:ILE:HG12	1:C:224:GLY:HA3	1.97	0.47
1:D:31:LEU:CD1	1:D:63:THR:HG22	2.44	0.47
1:F:221:HIS:HB2	1:F:227:ARG:NH2	2.30	0.47
1:G:137:LEU:O	1:G:142:GLN:N	2.41	0.47
1:H:59:LYS:H	1:H:59:LYS:HD3	1.79	0.47
1:D:75:ILE:H	1:D:75:ILE:CD1	2.20	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:259:LEU:HD13	1:E:273:THR:CG2	2.45	0.47
1:H:26:ALA:HB2	1:H:49:TYR:O	2.14	0.47
1:H:152:ALA:HB2	1:H:190:THR:HG21	1.96	0.47
1:I:111:LEU:HD23	1:I:114:LEU:HD12	1.96	0.47
1:I:174:HIS:O	1:I:178:PRO:HG3	2.14	0.47
1:J:197:ILE:HD12	1:J:197:ILE:H	1.78	0.47
1:B:44:TYR:O	1:B:51:ILE:CG2	2.62	0.47
1:B:104:ARG:HH21	1:B:105:VAL:HG23	1.79	0.47
1:D:109:ARG:HB3	1:D:171:TYR:CE1	2.49	0.47
1:F:273:THR:O	1:F:277:LYS:HB2	2.14	0.47
1:H:54:PRO:HG2	1:H:57:PHE:CE2	2.48	0.47
1:I:120:ASN:HD21	1:I:122:GLN:HB2	1.79	0.47
1:I:146:ILE:HD11	1:I:224:GLY:H	1.78	0.47
1:I:212:GLN:HB3	1:I:213:TYR:CD2	2.48	0.47
1:G:161:ASN:CG	1:G:162:ALA:N	2.68	0.47
1:I:242:TYR:CE1	1:I:282:LEU:HA	2.50	0.47
1:A:184:PHE:C	1:A:185:ILE:HG13	2.34	0.47
1:A:226:TYR:CE1	1:A:264:ILE:HB	2.50	0.47
1:B:164:PHE:CG	1:B:205:LEU:HD22	2.49	0.47
1:B:210:ARG:O	1:B:214:ASN:HB3	2.14	0.47
1:D:85:CYS:O	1:D:89:ASN:ND2	2.48	0.47
1:I:26:ALA:HB2	1:I:49:TYR:O	2.15	0.47
1:J:257:PHE:O	1:J:277:LYS:HE3	2.15	0.47
1:A:104:ARG:HE	1:A:104:ARG:HA	1.80	0.47
1:B:161:ASN:HB3	1:B:164:PHE:H	1.80	0.47
1:C:15:ASP:OD2	1:J:134:LYS:HE2	2.15	0.47
1:D:35:VAL:HG12	1:D:36:ASP:H	1.78	0.47
1:A:191:LEU:CD2	1:A:197:ILE:HD11	2.28	0.47
1:A:261:ASP:OD1	1:A:263:ARG:N	2.33	0.47
1:G:172:LEU:HD11	1:G:184:PHE:HB3	1.96	0.47
1:H:259:LEU:HD13	1:H:273:THR:CG2	2.45	0.47
1:J:121:PRO:HA	1:J:126:PHE:CG	2.46	0.47
1:G:146:ILE:HD12	1:G:147:GLU:H	1.80	0.46
1:H:97:ASN:O	1:H:98:VAL:C	2.53	0.46
1:E:193:GLU:HB2	1:E:195:LYS:HG2	1.96	0.46
1:J:202:VAL:HG21	1:J:263:ARG:HH21	1.80	0.46
1:C:3:GLU:OE1	1:C:3:GLU:N	2.45	0.46
1:G:205:LEU:O	1:G:209:LEU:HD12	2.15	0.46
1:I:200:VAL:HA	1:I:203:LYS:HE3	1.98	0.46
1:I:253:VAL:O	1:I:253:VAL:CG1	2.63	0.46
1:A:229:VAL:CG2	1:A:233:SER:HB2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:PRO:HB2	1:C:17:TYR:CE1	2.51	0.46
1:C:35:VAL:HG12	1:C:36:ASP:N	2.28	0.46
1:E:236:ASN:O	1:E:240:ARG:HG3	2.16	0.46
1:F:121:PRO:HA	1:F:126:PHE:CD2	2.50	0.46
1:G:202:VAL:O	1:G:206:VAL:HG22	2.15	0.46
1:A:65:ASP:HA	1:D:183:ASN:CG	2.36	0.46
1:C:54:PRO:HA	1:C:55:PRO:HD3	1.80	0.46
1:C:97:ASN:O	1:C:100:ASN:N	2.48	0.46
1:D:94:THR:OG1	1:D:97:ASN:ND2	2.48	0.46
1:A:121:PRO:HA	1:A:126:PHE:CG	2.50	0.46
1:A:140:ILE:HD12	1:A:140:ILE:HA	1.64	0.46
1:C:24:ASN:HA	1:C:27:ILE:HD12	1.97	0.46
1:E:21:PRO:HB3	1:E:81:ALA:HB1	1.97	0.46
1:G:253:VAL:O	1:G:253:VAL:CG1	2.55	0.46
1:C:259:LEU:HD13	1:C:273:THR:HB	1.98	0.46
1:D:2:ALA:HA	1:D:60:ARG:NH2	2.30	0.46
1:J:135:SER:OG	1:J:151:THR:HG22	2.16	0.46
1:D:54:PRO:HA	1:D:55:PRO:HD3	1.84	0.46
1:E:164:PHE:CZ	1:E:197:ILE:HD12	2.51	0.46
1:G:3:GLU:HG3	1:G:105:VAL:HG22	1.98	0.46
1:G:3:GLU:N	1:G:3:GLU:OE1	2.49	0.46
1:H:35:VAL:HG12	1:H:36:ASP:H	1.81	0.46
1:H:87:ALA:CB	1:H:136:THR:CG2	2.94	0.46
1:G:10:PRO:HB2	1:G:17:TYR:CD1	2.51	0.45
1:G:97:ASN:O	1:G:98:VAL:C	2.53	0.45
1:J:183:ASN:O	1:J:185:ILE:HG13	2.15	0.45
1:D:79:LYS:HA	1:D:82:MET:CE	2.45	0.45
1:D:181:ASP:C	1:D:181:ASP:OD1	2.54	0.45
1:G:4:LEU:HD21	1:G:140:ILE:HG13	1.97	0.45
1:I:117:ARG:CZ	1:I:125:LEU:HG	2.46	0.45
1:A:63:THR:H	1:A:66:ASN:HB3	1.80	0.45
1:C:83:LEU:HG	1:C:136:THR:HG21	1.98	0.45
1:G:280:ASN:OD1	1:G:284:VAL:HG11	2.16	0.45
1:J:229:VAL:HG21	1:J:237:HIS:NE2	2.32	0.45
1:A:117:ARG:NH1	1:A:152:ALA:O	2.38	0.45
1:B:268:ASN:O	1:B:271:ALA:HB3	2.17	0.45
1:C:72:PHE:HD2	1:C:72:PHE:H	1.63	0.45
1:C:150:ILE:HG23	1:C:151:THR:HG23	1.99	0.45
1:D:275:SER:CB	1:D:285:CYS:SG	3.05	0.45
1:E:111:LEU:HD21	1:E:140:ILE:CD1	2.46	0.45
1:F:39:ASP:HA	1:F:42:LYS:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:7:PHE:HZ	1:G:108:ILE:HG12	1.82	0.45
1:J:10:PRO:HD2	1:J:43:PHE:CE2	2.51	0.45
1:A:183:ASN:CG	1:D:65:ASP:HA	2.37	0.45
1:A:212:GLN:HB3	1:A:213:TYR:CD2	2.51	0.45
1:E:125:LEU:HB3	1:E:132:LEU:CD1	2.45	0.45
1:E:140:ILE:HG22	1:E:142:GLN:HG2	1.98	0.45
1:J:76:MET:SD	1:J:112:GLU:HG3	2.56	0.45
1:J:248:ASN:C	1:J:250:LYS:N	2.70	0.45
1:B:75:ILE:H	1:B:75:ILE:CD1	2.22	0.45
1:B:146:ILE:CD1	1:B:224:GLY:H	1.99	0.45
1:D:22:PHE:HD1	1:D:51:ILE:O	2.00	0.45
1:H:111:LEU:HD21	1:H:140:ILE:HD12	1.99	0.45
1:I:146:ILE:HG12	1:I:224:GLY:CA	2.47	0.45
1:I:265:ILE:HD13	1:I:265:ILE:HA	1.80	0.45
1:A:248:ASN:C	1:A:250:LYS:N	2.70	0.45
1:J:9:TYR:CD2	1:J:9:TYR:O	2.70	0.45
1:J:152:ALA:HB2	1:J:190:THR:HG21	1.98	0.45
1:B:159:PHE:CD2	1:B:208:GLU:CG	2.94	0.45
1:C:171:TYR:HB3	1:C:179:ILE:CG1	2.47	0.45
1:E:135:SER:OG	1:E:151:THR:HG22	2.17	0.45
1:E:185:ILE:HG13	1:E:230:LYS:CE	2.45	0.45
1:H:218:VAL:HG11	1:H:264:ILE:O	2.17	0.45
1:I:3:GLU:C	1:I:5:ALA:N	2.70	0.45
1:I:154:GLY:HA2	1:I:167:TRP:CZ3	2.52	0.45
1:F:85:CYS:O	1:F:89:ASN:ND2	2.50	0.45
1:G:33:ALA:HB2	1:G:44:TYR:OH	2.17	0.45
1:G:247:SER:O	1:G:253:VAL:HG11	2.16	0.45
1:A:97:ASN:HD21	1:G:250:LYS:NZ	2.15	0.45
1:A:146:ILE:HG13	1:A:147:GLU:N	2.32	0.45
1:B:210:ARG:NH2	1:J:42:LYS:CD	2.78	0.45
1:C:187:TYR:HB2	1:C:228:ILE:HB	1.98	0.45
1:C:245:PHE:O	1:C:248:ASN:HB2	2.17	0.45
1:F:221:HIS:HB2	1:F:227:ARG:NH1	2.31	0.45
1:F:257:PHE:O	1:F:259:LEU:N	2.48	0.45
1:G:261:ASP:OD1	1:G:261:ASP:C	2.55	0.45
1:J:94:THR:O	1:J:98:VAL:HG13	2.16	0.45
1:A:275:SER:CB	1:A:285:CYS:SG	3.05	0.44
1:B:9:TYR:CE2	1:B:20:ILE:HD12	2.52	0.44
1:C:275:SER:HB2	1:C:285:CYS:SG	2.57	0.44
1:E:88:LEU:HA	1:E:88:LEU:HD23	1.77	0.44
1:A:164:PHE:CE1	1:A:205:LEU:HD22	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:TRP:O	1:B:187:TYR:HB3	2.17	0.44
1:C:30:MET:SD	1:C:30:MET:C	2.96	0.44
1:D:120:ASN:OD1	1:D:121:PRO:HD2	2.17	0.44
1:D:126:PHE:HD1	1:D:127:HIS:CE1	2.35	0.44
1:G:2:ALA:CB	1:G:108:ILE:HD11	2.47	0.44
1:I:221:HIS:HB2	1:I:227:ARG:NH2	2.33	0.44
1:A:85:CYS:O	1:A:89:ASN:ND2	2.50	0.44
1:B:247:SER:O	1:B:253:VAL:CG1	2.65	0.44
1:D:111:LEU:HD21	1:D:140:ILE:HD13	1.99	0.44
1:B:233:SER:O	1:B:235:ALA:N	2.50	0.44
1:E:75:ILE:HD12	1:E:75:ILE:N	2.20	0.44
1:F:20:ILE:HA	1:F:21:PRO:HD3	1.81	0.44
1:J:225:HIS:N	1:J:260:LEU:HD11	2.33	0.44
1:J:275:SER:HB2	1:J:285:CYS:SG	2.57	0.44
1:D:31:LEU:CD1	1:D:63:THR:CG2	2.93	0.44
1:G:221:HIS:HB2	1:G:227:ARG:NH2	2.33	0.44
1:J:215:LYS:HE2	1:J:215:LYS:HB3	1.82	0.44
1:C:43:PHE:CD1	1:C:54:PRO:HD3	2.52	0.44
1:D:152:ALA:HB2	1:D:190:THR:HG21	2.00	0.44
1:D:221:HIS:HE1	1:D:240:ARG:NH2	2.16	0.44
1:E:75:ILE:H	1:E:75:ILE:CD1	2.10	0.44
1:F:164:PHE:CE2	1:F:205:LEU:HD22	2.52	0.44
1:F:172:LEU:HD12	1:F:172:LEU:H	1.82	0.44
1:I:57:PHE:O	1:I:60:ARG:HB2	2.18	0.44
1:I:183:ASN:ND2	1:J:65:ASP:CB	2.75	0.44
1:F:94:THR:O	1:F:98:VAL:HG13	2.17	0.44
1:F:115:VAL:O	1:F:119:GLU:HG3	2.18	0.44
1:F:134:LYS:NZ	1:F:145:GLU:OE2	2.49	0.44
1:G:183:ASN:OD1	1:H:64:ASN:C	2.56	0.44
1:J:153:GLU:HG2	1:J:188:LYS:HZ2	1.83	0.44
1:B:164:PHE:CD1	1:B:205:LEU:HD22	2.53	0.44
1:C:268:ASN:HB3	1:C:289:LEU:HA	2.00	0.44
1:E:172:LEU:HD11	1:E:184:PHE:O	2.17	0.44
1:F:110:HIS:CE1	1:F:139:ALA:HB2	2.53	0.44
1:I:83:LEU:HD11	1:I:136:THR:OG1	2.18	0.44
1:A:84:ILE:HD11	1:A:111:LEU:CD1	2.48	0.43
1:I:106:VAL:HG11	1:I:140:ILE:HA	2.00	0.43
1:A:233:SER:O	1:A:235:ALA:N	2.51	0.43
1:C:149:THR:HB	1:C:192:ASN:HA	1.99	0.43
1:F:110:HIS:CE1	1:F:153:GLU:HB3	2.53	0.43
1:H:9:TYR:CZ	1:H:20:ILE:HD12	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:215:LYS:HE2	1:H:215:LYS:HB3	1.61	0.43
1:H:229:VAL:HG21	1:H:237:HIS:NE2	2.33	0.43
1:I:146:ILE:HD11	1:I:223:LYS:CB	2.43	0.43
1:A:272:PHE:CB	1:A:289:LEU:HD13	2.48	0.43
1:C:227:ARG:HE	1:C:227:ARG:HB2	1.57	0.43
1:H:230:LYS:HE3	1:H:230:LYS:HB3	1.82	0.43
1:J:225:HIS:HE1	1:J:227:ARG:HH21	1.61	0.43
1:C:56:GLN:C	1:C:58:LYS:H	2.22	0.43
1:F:161:ASN:ND2	1:F:164:PHE:HD1	2.10	0.43
1:I:181:ASP:OD1	1:I:182:GLN:N	2.51	0.43
1:J:259:LEU:HD22	1:J:273:THR:HG22	1.99	0.43
1:F:106:VAL:HG11	1:F:140:ILE:HA	2.00	0.43
1:E:76:MET:SD	1:E:115:VAL:HG11	2.59	0.43
1:E:161:ASN:HB3	1:E:163:ALA:H	1.82	0.43
1:I:216:PHE:N	1:I:216:PHE:HD1	2.16	0.43
1:I:266:TRP:CZ2	1:I:268:ASN:HB2	2.54	0.43
1:J:31:LEU:HD13	1:J:63:THR:HG21	1.99	0.43
1:A:114:LEU:HD21	1:A:153:GLU:HA	2.00	0.43
1:B:235:ALA:O	1:B:238:ALA:HB3	2.19	0.43
1:D:217:ALA:N	1:D:229:VAL:O	2.52	0.43
1:G:207:ALA:O	1:G:210:ARG:HB2	2.19	0.43
1:G:253:VAL:O	1:G:255:ASN:N	2.51	0.43
1:I:248:ASN:C	1:I:250:LYS:N	2.71	0.43
1:J:78:THR:O	1:J:81:ALA:HB3	2.18	0.43
1:A:106:VAL:HG11	1:A:140:ILE:CD1	2.49	0.43
1:B:26:ALA:HB2	1:B:49:TYR:O	2.18	0.43
1:D:53:PRO:HA	1:D:54:PRO:HD3	1.91	0.43
1:E:22:PHE:HE1	1:E:51:ILE:HG22	1.83	0.43
1:E:121:PRO:O	1:E:127:HIS:HE1	2.01	0.43
1:F:134:LYS:NZ	1:F:145:GLU:OE1	2.49	0.43
1:A:76:MET:HG3	1:A:176:LEU:HB2	2.00	0.43
1:C:10:PRO:HB2	1:C:17:TYR:HD1	1.84	0.43
1:H:259:LEU:HD13	1:H:273:THR:HG21	2.01	0.43
1:B:205:LEU:O	1:B:209:LEU:HD12	2.18	0.43
1:D:144:LYS:CE	1:E:162:ALA:O	2.53	0.43
1:G:82:MET:HE2	1:G:82:MET:HB2	1.79	0.43
1:J:106:VAL:HG11	1:J:140:ILE:HA	2.00	0.43
1:J:171:TYR:HB2	1:J:184:PHE:HE2	1.82	0.43
1:A:150:ILE:HG23	1:A:151:THR:HG23	2.01	0.42
1:A:261:ASP:OD1	1:A:263:ARG:CB	2.67	0.42
1:B:247:SER:O	1:B:253:VAL:HG11	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:PHE:HZ	1:D:108:ILE:HG12	1.84	0.42
1:E:72:PHE:HA	1:E:77:PHE:CD1	2.54	0.42
1:E:261:ASP:OD1	1:E:261:ASP:C	2.58	0.42
1:F:117:ARG:HH21	1:F:125:LEU:HG	1.78	0.42
1:I:195:LYS:HB2	1:I:196:PRO:HD2	2.01	0.42
1:J:271:ALA:HB1	1:J:288:LEU:HD13	2.00	0.42
1:A:4:LEU:CD2	1:A:106:VAL:HG21	2.49	0.42
1:B:153:GLU:HG2	1:B:188:LYS:HZ2	1.83	0.42
1:C:121:PRO:HA	1:C:126:PHE:CG	2.54	0.42
1:C:275:SER:HB3	1:C:285:CYS:SG	2.58	0.42
1:E:30:MET:SD	1:E:30:MET:C	2.98	0.42
1:E:37:LYS:H	1:E:37:LYS:HZ3	1.66	0.42
1:E:215:LYS:HE2	1:E:215:LYS:HB3	1.83	0.42
1:F:9:TYR:CE1	1:F:51:ILE:HB	2.55	0.42
1:G:193:GLU:HB3	1:G:195:LYS:HE3	2.01	0.42
1:I:4:LEU:CD2	1:I:106:VAL:CG2	2.97	0.42
1:C:25:LEU:HD23	1:C:25:LEU:HA	1.78	0.42
1:B:229:VAL:HG11	1:B:237:HIS:HD2	1.83	0.42
1:E:202:VAL:O	1:E:206:VAL:HG23	2.19	0.42
1:G:10:PRO:HB2	1:G:17:TYR:CE1	2.54	0.42
1:G:248:ASN:HB2	1:G:255:ASN:HD22	1.83	0.42
1:J:5:ALA:HB2	1:J:102:LEU:HB3	2.01	0.42
1:A:265:ILE:H	1:A:265:ILE:HG12	1.72	0.42
1:C:84:ILE:O	1:C:85:CYS:C	2.58	0.42
1:C:136:THR:O	1:C:140:ILE:HB	2.19	0.42
1:A:149:THR:HA	1:A:190:THR:OG1	2.20	0.42
1:A:218:VAL:HG11	1:A:264:ILE:HG22	2.02	0.42
1:B:144:LYS:H	1:B:144:LYS:HG2	1.60	0.42
1:C:245:PHE:HD2	1:C:276:MET:HG2	1.84	0.42
1:D:83:LEU:HD22	1:D:115:VAL:HG23	2.01	0.42
1:D:184:PHE:O	1:D:185:ILE:HG13	2.19	0.42
1:J:47:ILE:HD12	1:J:47:ILE:H	1.85	0.42
1:J:272:PHE:CD2	1:J:289:LEU:HB2	2.54	0.42
1:D:238:ALA:O	1:D:241:VAL:HG22	2.20	0.42
1:E:27:ILE:HG12	1:E:53:PRO:HD3	2.02	0.42
1:G:9:TYR:HB3	1:G:22:PHE:CE1	2.54	0.42
1:G:198:SER:OG	1:G:201:HIS:CD2	2.73	0.42
1:H:4:LEU:HD11	1:H:140:ILE:HG23	2.02	0.42
1:J:185:ILE:HB	1:J:230:LYS:HE3	2.02	0.42
1:C:9:TYR:HB3	1:C:22:PHE:CE1	2.55	0.42
1:D:201:HIS:O	1:D:204:GLU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:9:TYR:HD1	1:F:22:PHE:CE1	2.37	0.42
1:G:64:ASN:O	1:H:183:ASN:CG	2.57	0.42
1:G:261:ASP:OD1	1:G:262:GLN:N	2.53	0.42
1:H:274:SER:O	1:H:277:LYS:HB2	2.19	0.42
1:A:64:ASN:O	1:D:183:ASN:OD1	2.38	0.42
1:E:54:PRO:HA	1:E:55:PRO:HD3	1.77	0.42
1:I:10:PRO:HD2	1:I:43:PHE:CZ	2.54	0.42
1:B:171:TYR:HA	1:B:174:HIS:CD2	2.55	0.42
1:B:271:ALA:HB1	1:B:288:LEU:HB3	2.01	0.42
1:C:63:THR:H	1:C:66:ASN:HB3	1.84	0.42
1:E:261:ASP:OD1	1:E:263:ARG:CG	2.57	0.42
1:H:9:TYR:HB3	1:H:22:PHE:CE1	2.54	0.42
1:H:250:LYS:O	1:H:253:VAL:CG1	2.67	0.42
1:B:9:TYR:HD1	1:B:22:PHE:CE1	2.38	0.41
1:B:9:TYR:HB3	1:B:22:PHE:CE1	2.55	0.41
1:D:245:PHE:HE2	1:D:276:MET:O	2.03	0.41
1:F:253:VAL:O	1:F:253:VAL:HG13	2.20	0.41
1:F:257:PHE:CE1	1:F:273:THR:HG23	2.55	0.41
1:G:97:ASN:O	1:G:100:ASN:N	2.52	0.41
1:G:272:PHE:CD1	1:G:272:PHE:C	2.93	0.41
1:B:94:THR:HG22	1:B:95:GLN:H	1.85	0.41
1:C:19:PHE:CD1	1:C:19:PHE:N	2.88	0.41
1:D:83:LEU:HD11	1:D:136:THR:OG1	2.21	0.41
1:D:140:ILE:HA	1:D:140:ILE:HD12	1.69	0.41
1:G:229:VAL:CG2	1:G:233:SER:HB2	2.50	0.41
1:H:61:TYR:HB3	1:H:72:PHE:CD2	2.55	0.41
1:H:161:ASN:CG	1:H:162:ALA:H	2.23	0.41
1:I:4:LEU:HG	1:I:104:ARG:O	2.20	0.41
1:I:78:THR:O	1:I:82:MET:HG3	2.20	0.41
1:B:179:ILE:HG21	1:B:184:PHE:CG	2.56	0.41
1:F:140:ILE:HD12	1:F:140:ILE:HA	1.64	0.41
1:J:74:THR:HG21	1:J:175:GLN:HG2	2.02	0.41
1:A:54:PRO:HA	1:A:55:PRO:HD3	1.55	0.41
1:A:121:PRO:HA	1:A:126:PHE:CD2	2.55	0.41
1:A:224:GLY:O	1:A:225:HIS:CB	2.67	0.41
1:A:225:HIS:CD2	1:A:227:ARG:HH21	2.37	0.41
1:B:120:ASN:HA	1:B:121:PRO:HD2	1.96	0.41
1:D:120:ASN:HD21	1:D:122:GLN:HB2	1.85	0.41
1:F:188:LYS:HE2	1:F:188:LYS:HB2	1.88	0.41
1:F:248:ASN:C	1:F:250:LYS:N	2.73	0.41
1:I:233:SER:HB3	1:I:237:HIS:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:257:PHE:CE1	1:I:273:THR:CG2	3.04	0.41
1:J:10:PRO:HB2	1:J:17:TYR:CE1	2.55	0.41
1:A:146:ILE:CG1	1:A:147:GLU:N	2.83	0.41
1:A:183:ASN:ND2	1:D:64:ASN:O	2.54	0.41
1:C:161:ASN:HB3	1:C:164:PHE:H	1.86	0.41
1:D:160:GLN:HG3	1:D:165:THR:HG23	2.03	0.41
1:F:79:LYS:HB3	1:F:115:VAL:HG11	2.02	0.41
1:F:275:SER:CB	1:F:285:CYS:SG	3.08	0.41
1:G:215:LYS:O	1:G:231:TYR:HD2	2.03	0.41
1:I:248:ASN:O	1:I:250:LYS:N	2.52	0.41
1:J:140:ILE:HD12	1:J:140:ILE:HA	1.82	0.41
1:C:30:MET:HB2	1:C:44:TYR:CD2	2.55	0.41
1:F:242:TYR:CE1	1:F:282:LEU:HA	2.55	0.41
1:G:36:ASP:C	1:G:38:LYS:N	2.73	0.41
1:G:106:VAL:HG11	1:G:140:ILE:HD12	2.02	0.41
1:I:14:ASN:O	1:I:15:ASP:CB	2.63	0.41
1:A:30:MET:HB2	1:A:44:TYR:CD2	2.55	0.41
1:C:166:MET:CA	1:C:189:VAL:HG13	2.51	0.41
1:E:12:LEU:HD12	1:E:17:TYR:CE2	2.56	0.41
1:E:282:LEU:HD11	1:E:286:LYS:CE	2.38	0.41
1:H:5:ALA:O	1:H:22:PHE:HE2	2.03	0.41
1:H:245:PHE:HE2	1:H:276:MET:O	2.02	0.41
1:J:126:PHE:HD1	1:J:127:HIS:CE1	2.39	0.41
1:A:2:ALA:HA	1:A:60:ARG:CZ	2.51	0.41
1:A:4:LEU:HD22	1:A:84:ILE:HD13	2.03	0.41
1:A:174:HIS:O	1:A:178:PRO:HB3	2.20	0.41
1:A:226:TYR:CD2	1:A:226:TYR:N	2.88	0.41
1:B:149:THR:HG21	1:B:165:THR:OG1	2.20	0.41
1:D:109:ARG:NH2	1:D:179:ILE:HA	2.36	0.41
1:D:146:ILE:CD1	1:D:224:GLY:H	2.34	0.41
1:A:117:ARG:HH21	1:A:125:LEU:HG	1.84	0.41
1:A:120:ASN:HA	1:A:121:PRO:HD3	1.99	0.41
1:A:199:ASP:O	1:A:203:LYS:HB2	2.21	0.41
1:B:94:THR:HG22	1:B:95:GLN:N	2.35	0.41
1:B:272:PHE:CB	1:B:289:LEU:HD13	2.39	0.41
1:E:12:LEU:O	1:E:12:LEU:HD23	2.21	0.41
1:E:169:LEU:HD21	1:E:188:LYS:HG2	2.02	0.41
1:F:4:LEU:HD23	1:F:4:LEU:HA	1.85	0.41
1:F:31:LEU:HA	1:F:58:LYS:HE2	2.03	0.41
1:G:226:TYR:N	1:G:226:TYR:CD2	2.88	0.41
1:G:246:LYS:O	1:G:249:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:272:PHE:CB	1:G:289:LEU:HD13	2.51	0.41
1:H:223:LYS:HD2	1:H:223:LYS:N	2.35	0.41
1:H:261:ASP:OD1	1:H:262:GLN:N	2.53	0.41
1:J:257:PHE:CE1	1:J:273:THR:HG21	2.56	0.41
1:A:146:ILE:HD13	1:A:223:LYS:HB3	2.02	0.41
1:G:75:ILE:CD1	1:G:75:ILE:N	2.78	0.41
1:H:161:ASN:HB3	1:H:164:PHE:H	1.86	0.41
1:H:218:VAL:HG22	1:H:228:ILE:HD12	2.03	0.41
1:B:10:PRO:HB2	1:B:17:TYR:CE1	2.56	0.40
1:B:229:VAL:HG11	1:B:237:HIS:CD2	2.57	0.40
1:F:276:MET:N	1:F:285:CYS:SG	2.94	0.40
1:H:62:ASN:ND2	1:H:71:ASN:OD1	2.52	0.40
1:I:6:CYS:HA	1:I:61:TYR:OH	2.21	0.40
1:I:120:ASN:ND2	1:I:122:GLN:HB2	2.36	0.40
1:I:153:GLU:OE2	1:I:188:LYS:NZ	2.44	0.40
1:J:230:LYS:HE2	1:J:230:LYS:HB3	1.82	0.40
1:A:250:LYS:O	1:A:250:LYS:HG3	2.22	0.40
1:B:22:PHE:CE2	1:B:53:PRO:HG3	2.56	0.40
1:B:272:PHE:HD2	1:B:289:LEU:HD22	1.86	0.40
1:D:229:VAL:HG22	1:D:230:LYS:H	1.85	0.40
1:G:65:ASP:OD1	1:G:65:ASP:N	2.46	0.40
1:I:199:ASP:O	1:I:203:LYS:HG3	2.21	0.40
1:J:275:SER:CB	1:J:285:CYS:SG	3.09	0.40
1:A:162:ALA:HB3	1:A:201:HIS:CE1	2.57	0.40
1:D:97:ASN:O	1:D:101:VAL:HG23	2.20	0.40
1:F:113:ASN:HD21	1:F:171:TYR:HE1	1.69	0.40
1:I:161:ASN:CG	1:I:162:ALA:N	2.74	0.40
1:A:56:GLN:HE21	1:A:56:GLN:HB3	1.53	0.40
1:A:161:ASN:CG	1:A:162:ALA:N	2.75	0.40
1:D:157:ILE:HD13	1:D:165:THR:HG21	2.02	0.40
1:E:118:LYS:HB2	1:E:132:LEU:HD11	2.02	0.40
1:E:259:LEU:HD13	1:E:273:THR:HG21	2.04	0.40
1:G:144:LYS:H	1:G:144:LYS:HG2	1.73	0.40
1:H:54:PRO:HA	1:H:55:PRO:HD3	1.86	0.40
1:A:97:ASN:O	1:A:98:VAL:C	2.60	0.40
1:A:146:ILE:HG12	1:A:224:GLY:H	1.86	0.40
1:C:14:ASN:HA	1:J:130:ASP:OD2	2.22	0.40
1:D:161:ASN:HD21	1:D:201:HIS:HB3	1.85	0.40
1:F:120:ASN:HA	1:F:121:PRO:HD3	1.99	0.40
1:I:44:TYR:HB3	1:I:52:ALA:HB3	2.04	0.40
1:I:76:MET:O	1:I:80:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:76:MET:HG3	1:J:176:LEU:HB2	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:ASP:OD2	1:F:251:THR:OG1[2_654]	2.14	0.06

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	288/294 (98%)	246 (85%)	35 (12%)	7 (2%)	6	28
1	B	288/294 (98%)	246 (85%)	36 (12%)	6 (2%)	7	30
1	C	288/294 (98%)	243 (84%)	41 (14%)	4 (1%)	11	37
1	D	288/294 (98%)	256 (89%)	29 (10%)	3 (1%)	15	46
1	E	288/294 (98%)	260 (90%)	22 (8%)	6 (2%)	7	30
1	F	288/294 (98%)	252 (88%)	27 (9%)	9 (3%)	4	23
1	G	288/294 (98%)	252 (88%)	32 (11%)	4 (1%)	11	37
1	H	288/294 (98%)	254 (88%)	28 (10%)	6 (2%)	7	30
1	I	288/294 (98%)	257 (89%)	28 (10%)	3 (1%)	15	46
1	J	288/294 (98%)	256 (89%)	28 (10%)	4 (1%)	11	37
All	All	2880/2940 (98%)	2522 (88%)	306 (11%)	52 (2%)	8	32

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	249	VAL

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Mol	Chain	Res	Type
1	E	249	VAL
1	F	235	ALA
1	F	250	LYS
1	G	249	VAL
1	H	250	LYS
1	I	249	VAL
1	J	249	VAL
1	J	250	LYS
1	A	250	LYS
1	B	72	PHE
1	B	249	VAL
1	B	255	ASN
1	B	258	ASN
1	D	249	VAL
1	E	72	PHE
1	E	259	LEU
1	F	72	PHE
1	F	249	VAL
1	F	258	ASN
1	G	254	ASN
1	H	235	ALA
1	H	249	VAL
1	I	256	ASP
1	A	225	HIS
1	A	256	ASP
1	C	256	ASP
1	D	247	SER
1	E	225	HIS
1	H	256	ASP
1	J	256	ASP
1	A	234	VAL
1	B	286	LYS
1	C	57	PHE
1	C	133	LEU
1	D	255	ASN
1	F	256	ASP
1	I	31	LEU
1	A	12	LEU
1	B	225	HIS
1	C	249	VAL
1	E	247	SER
1	E	261	ASP

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Mol	Chain	Res	Type
1	F	247	SER
1	H	254	ASN
1	A	255	ASN
1	G	55	PRO
1	G	147	GLU
1	H	159	PHE
1	J	225	HIS
1	F	234	VAL
1	F	55	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	262/266 (98%)	237 (90%)	25 (10%)	8	29
1	B	262/266 (98%)	232 (88%)	30 (12%)	5	20
1	C	262/266 (98%)	233 (89%)	29 (11%)	6	22
1	D	262/266 (98%)	237 (90%)	25 (10%)	8	29
1	E	262/266 (98%)	246 (94%)	16 (6%)	18	48
1	F	262/266 (98%)	241 (92%)	21 (8%)	12	38
1	G	262/266 (98%)	241 (92%)	21 (8%)	12	38
1	H	262/266 (98%)	242 (92%)	20 (8%)	13	41
1	I	262/266 (98%)	242 (92%)	20 (8%)	13	41
1	J	262/266 (98%)	239 (91%)	23 (9%)	10	33
All	All	2620/2660 (98%)	2390 (91%)	230 (9%)	10	33

All (230) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	15	ASP
1	A	47	ILE
1	A	51	ILE

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Mol	Chain	Res	Type
1	A	59	LYS
1	A	60	ARG
1	A	68	ARG
1	A	98	VAL
1	A	104	ARG
1	A	108	ILE
1	A	125	LEU
1	A	131	LEU
1	A	140	ILE
1	A	143	SER
1	A	188	LYS
1	A	191	LEU
1	A	193	GLU
1	A	209	LEU
1	A	223	LYS
1	A	227	ARG
1	A	234	VAL
1	A	244	THR
1	A	246	LYS
1	A	265	ILE
1	A	286	LYS
1	B	11	HIS
1	B	12	LEU
1	B	37	LYS
1	B	47	ILE
1	B	51	ILE
1	B	59	LYS
1	B	68	ARG
1	B	91	LEU
1	B	94	THR
1	B	97	ASN
1	B	98	VAL
1	B	105	VAL
1	B	124	ILE
1	B	133	LEU
1	B	135	SER
1	B	140	ILE
1	B	160	GLN
1	B	173	GLU
1	B	174	HIS
1	B	180	LEU
1	B	193	GLU

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Mol	Chain	Res	Type
1	B	195	LYS
1	B	210	ARG
1	B	211	TRP
1	B	223	LYS
1	B	227	ARG
1	B	244	THR
1	B	258	ASN
1	B	286	LYS
1	B	290	PHE
1	C	34	LYS
1	C	51	ILE
1	C	59	LYS
1	C	63	THR
1	C	68	ARG
1	C	72	PHE
1	C	78	THR
1	C	98	VAL
1	C	104	ARG
1	C	108	ILE
1	C	111	LEU
1	C	124	ILE
1	C	133	LEU
1	C	143	SER
1	C	180	LEU
1	C	185	ILE
1	C	188	LYS
1	C	193	GLU
1	C	197	ILE
1	C	203	LYS
1	C	211	TRP
1	C	215	LYS
1	C	227	ARG
1	C	230	LYS
1	C	245	PHE
1	C	254	ASN
1	C	260	LEU
1	C	273	THR
1	C	286	LYS
1	D	11	HIS
1	D	12	LEU
1	D	15	ASP
1	D	34	LYS

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Mol	Chain	Res	Type
1	D	58	LYS
1	D	59	LYS
1	D	68	ARG
1	D	71	ASN
1	D	94	THR
1	D	98	VAL
1	D	104	ARG
1	D	129	LYS
1	D	140	ILE
1	D	150	ILE
1	D	158	VAL
1	D	172	LEU
1	D	180	LEU
1	D	191	LEU
1	D	193	GLU
1	D	210	ARG
1	D	223	LYS
1	D	251	THR
1	D	263	ARG
1	D	267	GLN
1	D	286	LYS
1	E	11	HIS
1	E	37	LYS
1	E	64	ASN
1	E	68	ARG
1	E	75	ILE
1	E	104	ARG
1	E	131	LEU
1	E	174	HIS
1	E	179	ILE
1	E	185	ILE
1	E	230	LYS
1	E	263	ARG
1	E	267	GLN
1	E	268	ASN
1	E	278	GLN
1	E	286	LYS
1	F	34	LYS
1	F	59	LYS
1	F	60	ARG
1	F	68	ARG
1	F	92	LYS

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Mol	Chain	Res	Type
1	F	94	THR
1	F	95	GLN
1	F	118	LYS
1	F	131	LEU
1	F	133	LEU
1	F	135	SER
1	F	140	ILE
1	F	150	ILE
1	F	172	LEU
1	F	174	HIS
1	F	227	ARG
1	F	234	VAL
1	F	251	THR
1	F	277	LYS
1	F	286	LYS
1	F	287	ARG
1	G	4	LEU
1	G	12	LEU
1	G	35	VAL
1	G	47	ILE
1	G	51	ILE
1	G	71	ASN
1	G	72	PHE
1	G	75	ILE
1	G	82	MET
1	G	92	LYS
1	G	133	LEU
1	G	148	THR
1	G	187	TYR
1	G	191	LEU
1	G	197	ILE
1	G	206	VAL
1	G	234	VAL
1	G	244	THR
1	G	258	ASN
1	G	267	GLN
1	G	268	ASN
1	H	12	LEU
1	H	15	ASP
1	H	37	LYS
1	H	59	LYS
1	H	75	ILE

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Mol	Chain	Res	Type
1	H	91	LEU
1	H	94	THR
1	H	99	SER
1	H	124	ILE
1	H	138	ILE
1	H	150	ILE
1	H	158	VAL
1	H	172	LEU
1	H	195	LYS
1	H	227	ARG
1	H	229	VAL
1	H	248	ASN
1	H	251	THR
1	H	277	LYS
1	H	286	LYS
1	I	28	LYS
1	I	68	ARG
1	I	75	ILE
1	I	92	LYS
1	I	93	VAL
1	I	94	THR
1	I	104	ARG
1	I	131	LEU
1	I	133	LEU
1	I	135	SER
1	I	140	ILE
1	I	185	ILE
1	I	197	ILE
1	I	210	ARG
1	I	216	PHE
1	I	227	ARG
1	I	244	THR
1	I	277	LYS
1	I	286	LYS
1	I	290	PHE
1	J	34	LYS
1	J	37	LYS
1	J	59	LYS
1	J	60	ARG
1	J	92	LYS
1	J	104	ARG
1	J	106	VAL

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Mol	Chain	Res	Type
1	J	118	LYS
1	J	124	ILE
1	J	140	ILE
1	J	148	THR
1	J	150	ILE
1	J	167	TRP
1	J	170	THR
1	J	172	LEU
1	J	188	LYS
1	J	191	LEU
1	J	193	GLU
1	J	197	ILE
1	J	209	LEU
1	J	210	ARG
1	J	251	THR
1	J	286	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	95	GLN
1	A	100	ASN
1	A	161	ASN
1	A	175	GLN
1	A	201	HIS
1	A	254	ASN
1	B	56	GLN
1	B	142	GLN
1	B	160	GLN
1	B	175	GLN
1	B	201	HIS
1	B	254	ASN
1	B	255	ASN
1	C	56	GLN
1	C	142	GLN
1	C	160	GLN
1	C	192	ASN
1	D	11	HIS
1	D	97	ASN
1	D	127	HIS
1	D	161	ASN

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Mol	Chain	Res	Type
1	D	225	HIS
1	D	267	GLN
1	E	14	ASN
1	E	56	GLN
1	E	127	HIS
1	E	160	GLN
1	E	175	GLN
1	E	192	ASN
1	E	267	GLN
1	F	11	HIS
1	F	56	GLN
1	F	127	HIS
1	F	161	ASN
1	F	175	GLN
1	F	183	ASN
1	F	201	HIS
1	F	254	ASN
1	F	267	GLN
1	G	120	ASN
1	G	161	ASN
1	G	201	HIS
1	G	225	HIS
1	G	254	ASN
1	H	56	GLN
1	H	97	ASN
1	H	127	HIS
1	H	161	ASN
1	H	174	HIS
1	H	175	GLN
1	I	56	GLN
1	I	127	HIS
1	I	161	ASN
1	I	175	GLN
1	I	183	ASN
1	I	267	GLN
1	J	161	ASN
1	J	175	GLN
1	J	183	ASN
1	J	225	HIS

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)

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	290/294 (98%)	-0.11	13 (4%)	33	33	37, 73, 144, 188	0
1	B	290/294 (98%)	-0.13	13 (4%)	33	33	43, 72, 141, 183	0
1	C	290/294 (98%)	-0.13	15 (5%)	27	27	40, 70, 143, 180	0
1	D	290/294 (98%)	-0.18	10 (3%)	45	44	41, 71, 123, 182	0
1	E	290/294 (98%)	-0.21	11 (3%)	40	39	37, 66, 136, 212	0
1	F	290/294 (98%)	-0.08	13 (4%)	33	33	43, 73, 124, 206	0
1	G	290/294 (98%)	-0.22	9 (3%)	49	48	41, 71, 137, 196	0
1	H	290/294 (98%)	-0.25	7 (2%)	59	57	38, 70, 122, 205	0
1	I	290/294 (98%)	-0.30	8 (2%)	53	51	39, 67, 131, 224	0
1	J	290/294 (98%)	-0.08	14 (4%)	30	31	41, 71, 140, 240	0
All	All	2900/2940 (98%)	-0.17	113 (3%)	39	38	37, 71, 138, 240	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	252	GLY	8.7
1	F	254	ASN	8.3
1	C	64	ASN	6.2
1	E	251	THR	6.2
1	I	252	GLY	5.8
1	E	252	GLY	5.7
1	J	253	VAL	5.6
1	I	251	THR	5.5
1	F	253	VAL	5.5
1	C	254	ASN	5.4
1	B	249	VAL	5.2
1	H	252	GLY	5.1
1	H	254	ASN	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	13	GLU	4.7
1	J	14	ASN	4.6
1	D	256	ASP	4.6
1	G	13	GLU	4.5
1	C	13	GLU	4.4
1	C	248	ASN	4.3
1	F	250	LYS	4.2
1	A	252	GLY	4.2
1	I	254	ASN	4.2
1	F	14	ASN	4.1
1	I	96	ALA	4.1
1	J	254	ASN	4.0
1	A	181	ASP	3.9
1	A	94	THR	3.9
1	A	251	THR	3.8
1	H	291	GLN	3.7
1	F	256	ASP	3.7
1	B	248	ASN	3.6
1	F	251	THR	3.6
1	A	256	ASP	3.5
1	F	252	GLY	3.5
1	D	13	GLU	3.5
1	A	14	ASN	3.5
1	J	64	ASN	3.5
1	F	94	THR	3.5
1	F	291	GLN	3.5
1	D	249	VAL	3.4
1	B	94	THR	3.4
1	B	252	GLY	3.4
1	D	14	ASN	3.3
1	E	279	GLY	3.3
1	J	290	PHE	3.3
1	D	211	TRP	3.2
1	C	256	ASP	3.2
1	F	144	LYS	3.2
1	J	196	PRO	3.2
1	A	39	ASP	3.2
1	C	253	VAL	3.2
1	C	249	VAL	3.1
1	E	96	ALA	3.1
1	B	14	ASN	3.1
1	C	278	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	94	THR	3.0
1	B	283	ASP	3.0
1	I	64	ASN	3.0
1	G	291	GLN	2.9
1	G	283	ASP	2.9
1	E	256	ASP	2.9
1	E	95	GLN	2.8
1	C	252	GLY	2.8
1	D	291	GLN	2.8
1	D	12	LEU	2.8
1	A	93	VAL	2.7
1	B	129	LYS	2.7
1	E	100	ASN	2.7
1	H	14	ASN	2.7
1	A	38	LYS	2.6
1	D	212	GLN	2.6
1	D	254	ASN	2.6
1	G	278	GLN	2.6
1	B	251	THR	2.6
1	F	255	ASN	2.6
1	C	14	ASN	2.5
1	J	278	GLN	2.5
1	J	243	ALA	2.5
1	G	14	ASN	2.5
1	A	13	GLU	2.5
1	A	121	PRO	2.5
1	J	255	ASN	2.4
1	E	250	LYS	2.4
1	I	65	ASP	2.4
1	B	67	SER	2.4
1	J	13	GLU	2.4
1	F	64	ASN	2.4
1	C	290	PHE	2.3
1	D	287	ARG	2.3
1	G	248	ASN	2.3
1	J	96	ALA	2.3
1	C	283	ASP	2.3
1	F	194	ASP	2.3
1	E	14	ASN	2.3
1	H	250	LYS	2.3
1	E	99	SER	2.3
1	G	64	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	291	GLN	2.2
1	A	287	ARG	2.2
1	G	290	PHE	2.2
1	B	254	ASN	2.2
1	H	249	VAL	2.1
1	C	65	ASP	2.1
1	E	211	TRP	2.1
1	H	211	TRP	2.1
1	J	12	LEU	2.1
1	C	274	SER	2.1
1	I	290	PHE	2.1
1	A	75	ILE	2.0
1	J	251	THR	2.0
1	B	64	ASN	2.0
1	B	256	ASP	2.0
1	G	200	VAL	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.