Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 03:04 PM EDT

PDB ID	:	1DU3
Title	:	Crystal structure of TRAIL-SDR5
Authors	:	Cha, S.-S.; Sung, B.-J.; Oh, B.-H.
Deposited on	:	2000-01-14
Resolution	:	2.20 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 (i)) were used in the production of this report:

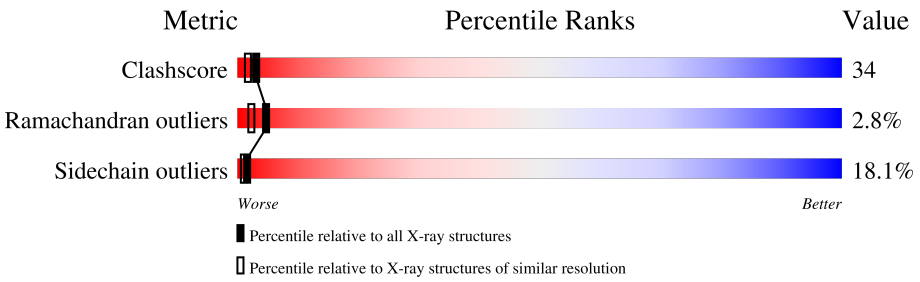
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	130	25% 36% 8% 31%
1	B	130	34% 39% 12% 15%
1	C	130	18% 38% 12% • 31%
1	G	130	33% 40% 10% 17%
1	H	130	28% 31% 10% • 31%
1	I	130	22% 34% 12% • 31%
2	D	168	46% 39% 5% • 10%
2	E	168	40% 39% 9% • 10%

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Mol	Chain	Length	Quality of chain
2	F	168	36% 48% 7% 10%
2	J	168	45% 40% • • 10%
2	K	168	43% 40% 5% • 10%
2	L	168	36% 45% 10% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ZN	E	1	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12108 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 DEATH RECEPTOR 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	90	701	419	122	148	12	0	0	0
1	B	110	833	497	148	172	16	0	0	0
1	C	90	697	417	121	147	12	0	0	0
1	G	108	833	498	150	169	16	0	0	0
1	H	90	691	414	118	147	12	0	0	0
1	I	90	701	419	122	148	12	0	0	0

- Molecule 2 is a protein called TNF-RELATED APOPTOSIS INDUCING LIGAND.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	152	1252	797	217	234	4	0	0	0
2	E	152	1252	797	217	234	4	0	0	0
2	F	152	1246	794	214	234	4	0	0	0
2	J	152	1248	795	217	232	4	0	0	0
2	K	152	1252	797	217	234	4	0	0	0
2	L	152	1238	789	212	233	4	0	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	E	1	1	1	0	0
			Total	Zn		
3	K	1	1	1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	26	26	26	0	0
			Total	O		
4	B	23	23	23	0	0
			Total	O		
4	C	6	6	6	0	0
			Total	O		
4	D	22	22	22	0	0
			Total	O		
4	E	14	14	14	0	0
			Total	O		
4	F	13	13	13	0	0
			Total	O		
4	G	16	16	16	0	0
			Total	O		
4	H	7	7	7	0	0
			Total	O		
4	I	11	11	11	0	0
			Total	O		
4	J	8	8	8	0	0
			Total	O		
4	K	9	9	9	0	0
			Total	O		
4	L	7	7	7	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. 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. 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.

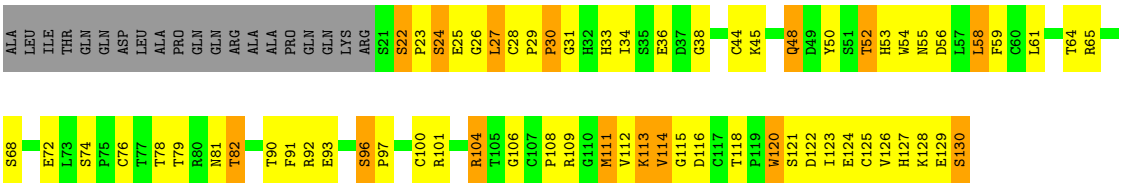
Note EDS was not executed.

• Molecule 1: DEATH RECEPTOR 5

Chain A: 25% 36% 8% 31%

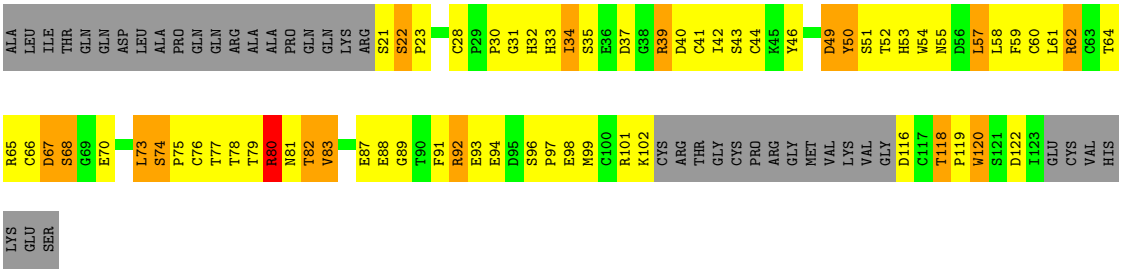
• Molecule 1: DEATH RECEPTOR 5

Chain B: 34% 39% 12% 15%



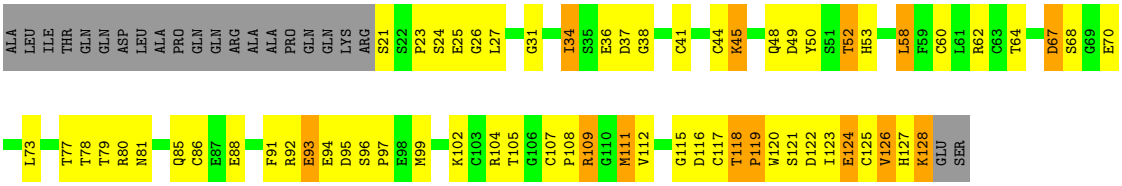
• Molecule 1: DEATH RECEPTOR 5

Chain C: 18% 38% 12% • 31%



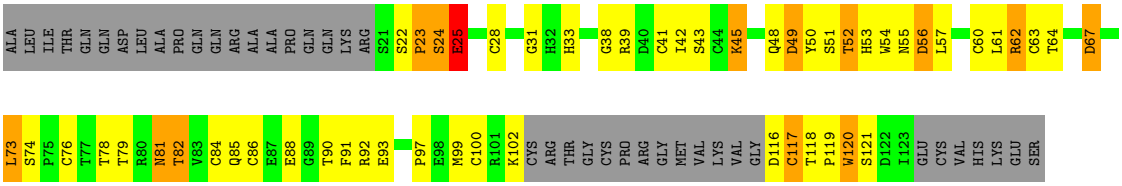
• Molecule 1: DEATH RECEPTOR 5

Chain G: 33% 40% 10% 17%



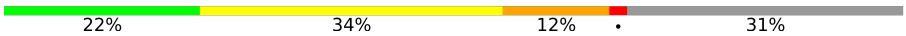
• Molecule 1: DEATH RECEPTOR 5

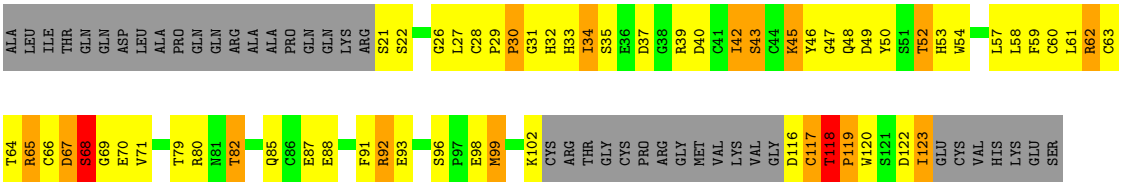
Chain H:



• Molecule 1: DEATH RECEPTOR 5

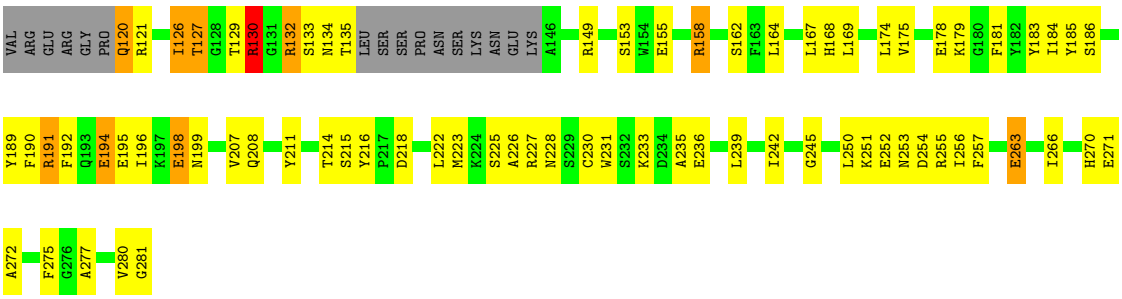
Chain I:





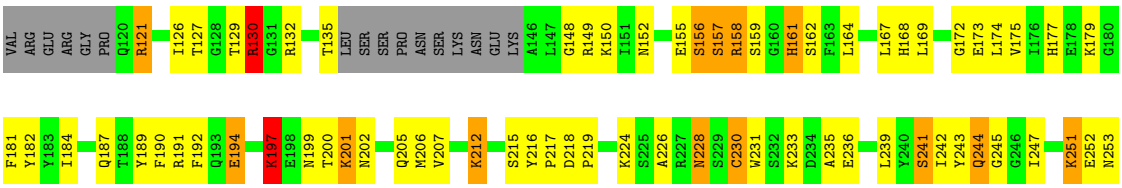
• Molecule 2: TNF-RELATED APOPTOSIS INDUCING LIGAND

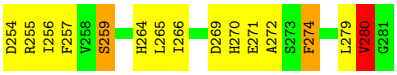
Chain D:



• Molecule 2: TNF-RELATED APOPTOSIS INDUCING LIGAND

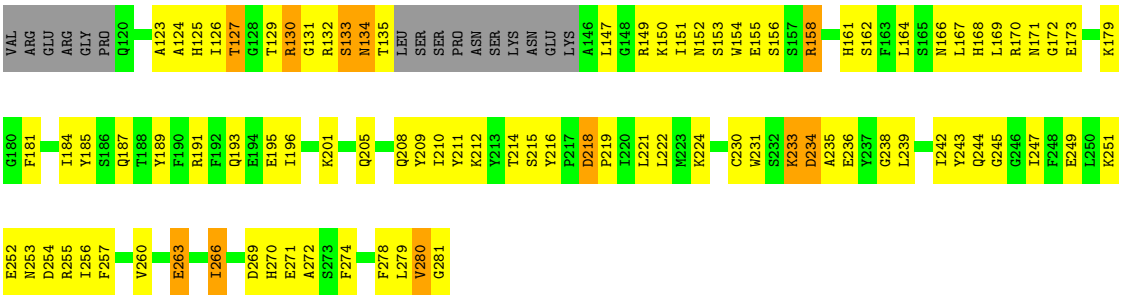
Chain E:





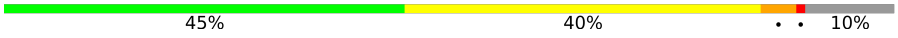
• Molecule 2: TNF-RELATED APOPTOSIS INDUCING LIGAND

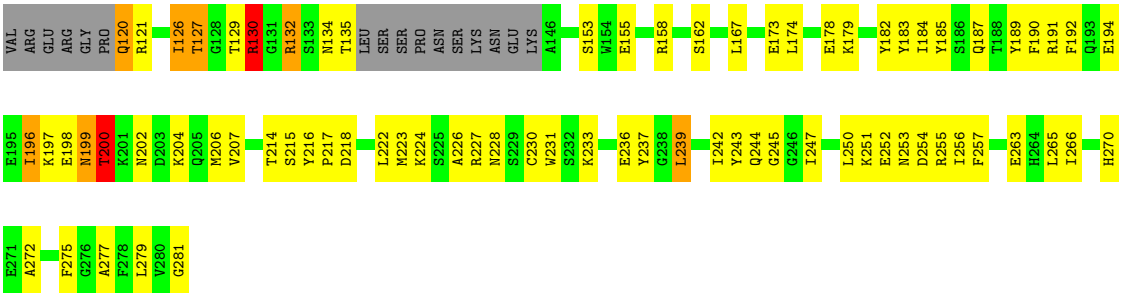
Chain F:



• Molecule 2: TNF-RELATED APOPTOSIS INDUCING LIGAND

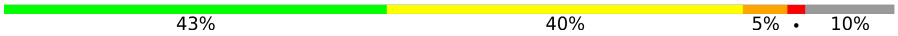
Chain J:

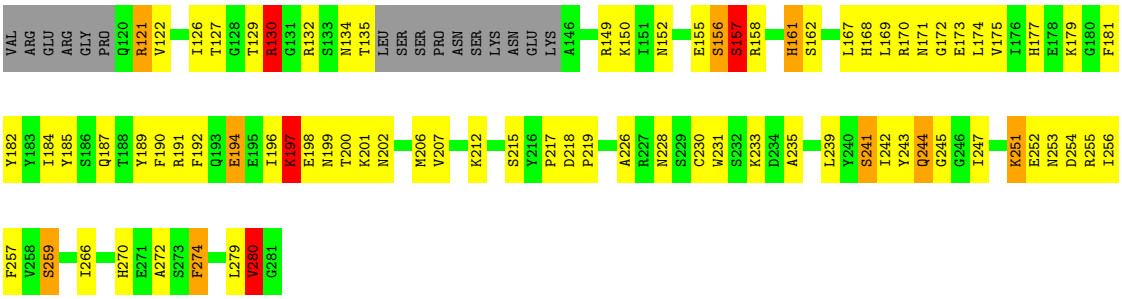




• Molecule 2: TNF-RELATED APOPTOSIS INDUCING LIGAND

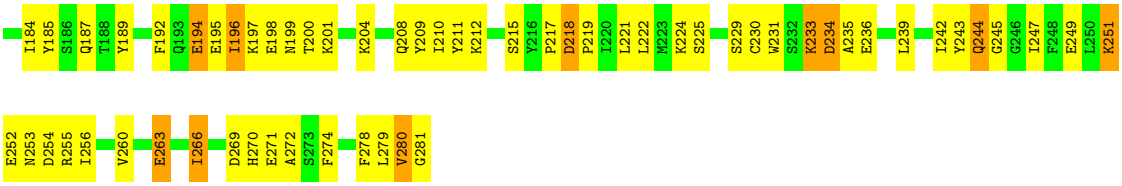
Chain K:





• Molecule 2: TNF-RELATED APOPTOSIS INDUCING LIGAND

Chain L:


I184
Y185
S186
Q187
T188
Y189
F192
Q193
E194
E195
I196
K197
E198
N199
T200
K201
K204
Q208
Y209
I210
Y211
K212
S215
Y216
P217
D218
P219
I220
L221
L222
M223
K224
S225
S229
C230
W231
S232
K233
D234
A235
E236
L239
I242
Y243
Q244
G245
G246
I247
F248
E249
L250
K251
E252
N253
D254
R255
I256
V260
E263
I266
D269
H270
E271
A272
S273
F274
F278
L279
V280
G281

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	68.63Å 124.81Å 128.37Å 90.00° 104.49° 90.00°	Depositor
Resolution (Å)	8.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.20)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.291 , 0.291	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12108	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.56	0/716	0.82	0/969
1	B	2.32	1/849 (0.1%)	1.89	2/1149 (0.2%)
1	C	0.51	0/712	0.72	0/964
1	G	0.62	0/851	0.80	0/1150
1	H	0.58	0/706	0.79	0/957
1	I	0.98	1/716 (0.1%)	1.35	3/969 (0.3%)
2	D	0.86	5/1282 (0.4%)	0.81	1/1724 (0.1%)
2	E	0.61	0/1282	0.79	0/1724
2	F	0.69	1/1276 (0.1%)	0.82	0/1717
2	J	0.62	0/1278	0.78	0/1719
2	K	0.61	0/1282	0.78	0/1724
2	L	0.64	0/1268	0.82	0/1708
All	All	0.89	8/12218 (0.1%)	0.95	6/16474 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	F	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	130	SER	C-O	-64.68	0.00	1.23
1	I	117	CYS	C-N	21.03	1.82	1.34
2	D	198	GLU	CG-CD	13.28	1.71	1.51
2	D	198	GLU	CD-OE1	9.92	1.36	1.25
2	F	191	ARG	C-N	-9.60	1.11	1.34
2	D	198	GLU	CD-OE2	6.92	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	191	ARG	C-N	-5.96	1.20	1.34
2	D	194	GLU	CB-CG	-5.29	1.42	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	130	SER	CA-C-O	-57.19	0.00	120.10
1	I	117	CYS	O-C-N	-25.30	82.22	122.70
1	I	117	CYS	C-N-CA	17.40	165.20	121.70
1	I	117	CYS	CA-C-N	17.17	154.98	117.20
1	B	127	HIS	O-C-N	-5.34	114.15	122.70
2	D	198	GLU	N-CA-C	5.22	125.10	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	205	GLN	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	701	0	619	46	0
1	B	833	0	735	75	1
1	C	697	0	613	94	0
1	G	833	0	755	63	0
1	H	691	0	602	55	0
1	I	701	0	618	65	0
2	D	1252	0	1197	80	0
2	E	1252	0	1200	81	0
2	F	1246	0	1188	99	0
2	J	1248	0	1196	73	0
2	K	1252	0	1200	75	0
2	L	1238	0	1172	105	0
3	E	1	0	0	2	0
3	K	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	26	0	0	0	0
4	B	23	0	0	3	2
4	C	6	0	0	2	0
4	D	22	0	0	7	0
4	E	14	0	0	2	0
4	F	13	0	0	2	0
4	G	16	0	0	0	1
4	H	7	0	0	0	3
4	I	11	0	0	1	1
4	J	8	0	0	0	0
4	K	9	0	0	1	0
4	L	7	0	0	2	0
All	All	12108	0	11095	772	4

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 34.

All (772) 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:I:117:CYS:C	1:I:118:THR:N	1.82	1.33
1:C:75:PRO:HB3	2:L:170:ARG:HD3	1.30	1.13
1:B:58:LEU:HD23	4:B:3147:HOH:O	1.59	1.02
2:K:202:ASN:HB3	4:K:3043:HOH:O	1.60	1.01
2:K:230:CYS:SG	2:L:230:CYS:SG	2.59	1.01
1:C:76:CYS:CB	1:C:82:THR:HG22	1.91	1.00
2:D:192:PHE:CD1	2:D:194:GLU:HG2	1.97	1.00
1:C:76:CYS:HB2	1:C:82:THR:CG2	1.92	0.98
2:E:230:CYS:SG	2:F:230:CYS:SG	2.61	0.98
1:C:76:CYS:HB2	1:C:82:THR:HG22	1.00	0.97
2:J:129:THR:O	2:J:130:ARG:HB3	1.64	0.95
1:G:93:GLU:HG2	1:G:94:GLU:N	1.82	0.94
1:G:93:GLU:HG2	1:G:94:GLU:H	1.32	0.93
2:D:129:THR:O	2:D:130:ARG:HB3	1.68	0.93
1:H:118:THR:HG1	1:H:120:TRP:HE3	1.13	0.93
2:D:281:GLY:HA3	2:E:121:ARG:HG2	1.51	0.93
3:K:2:ZN:ZN	2:L:230:CYS:HG	0.62	0.91
1:C:92:ARG:HG3	1:C:92:ARG:HH11	1.34	0.91
2:J:230:CYS:SG	2:L:230:CYS:SG	2.69	0.90
2:J:281:GLY:HA3	2:K:121:ARG:HG2	1.54	0.90
2:J:121:ARG:HB3	2:L:281:GLY:HA2	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:24:SER:O	1:H:25:GLU:HB2	1.72	0.89
1:G:99:MET:HE1	2:J:191:ARG:HH11	1.37	0.88
1:C:118:THR:HG1	1:C:120:TRP:HE3	1.20	0.88
1:I:117:CYS:O	1:I:118:THR:N	2.06	0.88
2:D:230:CYS:SG	2:F:230:CYS:SG	2.72	0.88
1:B:31:GLY:HA2	1:B:78:THR:O	1.74	0.87
3:E:1:ZN:ZN	2:F:230:CYS:HG	0.85	0.86
1:A:36:GLU:HG3	1:A:58:LEU:HD21	1.56	0.86
1:G:52:THR:HB	1:G:79:THR:O	1.77	0.85
1:C:89:GLY:HA2	4:C:3028:HOH:O	1.74	0.85
1:B:113:LYS:HG2	1:B:115:GLY:O	1.77	0.85
1:H:90:THR:HG22	1:H:102:LYS:HA	1.59	0.85
1:G:85:GLN:NE2	1:G:119:PRO:HG3	1.92	0.84
1:B:64:THR:H	1:B:81:ASN:HD21	1.23	0.84
1:G:36:GLU:HG3	1:G:58:LEU:HD21	1.59	0.84
1:G:112:VAL:HG13	1:G:126:VAL:HG12	1.58	0.83
2:D:149:ARG:HB2	4:D:3025:HOH:O	1.77	0.83
2:D:228:ASN:ND2	2:E:239:LEU:H	1.77	0.83
1:H:61:LEU:HD13	2:K:132:ARG:HH12	1.44	0.82
1:H:76:CYS:HB2	1:H:82:THR:HG22	1.62	0.82
1:A:49:ASP:HB2	1:A:60:CYS:HB3	1.60	0.81
1:H:62:ARG:HG3	1:H:62:ARG:HH11	1.46	0.81
2:L:129:THR:O	2:L:130:ARG:HB3	1.80	0.81
1:C:92:ARG:HG3	1:C:92:ARG:NH1	1.92	0.81
2:E:230:CYS:HG	3:E:1:ZN:ZN	0.92	0.81
1:A:80:ARG:NH1	1:A:80:ARG:HG2	1.96	0.80
1:C:62:ARG:HD2	2:F:131:GLY:HA2	1.63	0.80
2:D:228:ASN:HD22	2:E:239:LEU:H	1.29	0.80
1:G:86:CYS:SG	1:G:92:ARG:HD3	2.21	0.80
1:B:31:GLY:N	1:B:79:THR:HG22	1.97	0.80
1:A:80:ARG:HG2	1:A:80:ARG:HH11	1.46	0.80
2:L:132:ARG:HG3	2:L:270:HIS:CE1	2.16	0.79
2:L:132:ARG:HG3	2:L:270:HIS:HE1	1.47	0.79
1:G:115:GLY:HA3	1:G:124:GLU:HB2	1.64	0.79
2:D:199:ASN:C	4:D:3157:HOH:O	2.21	0.79
2:D:121:ARG:HB3	2:F:281:GLY:HA2	1.62	0.79
2:K:129:THR:HG22	2:K:155:GLU:HG2	1.63	0.79
1:B:76:CYS:HB2	1:B:82:THR:HG22	1.65	0.79
2:L:132:ARG:HH21	2:L:135:THR:HG21	1.48	0.79
1:H:64:THR:O	1:H:82:THR:HG21	1.84	0.78
2:L:181:PHE:HB2	2:L:280:VAL:CG2	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:ARG:HG2	1:B:97:PRO:HA	1.66	0.77
1:C:46:TYR:CD1	2:L:168:HIS:HE1	2.02	0.77
2:F:181:PHE:HB2	2:F:280:VAL:CG2	2.15	0.77
2:D:132:ARG:HB2	2:D:270:HIS:CE1	2.20	0.77
1:A:44:CYS:SG	1:A:50:TYR:HA	2.26	0.76
2:L:132:ARG:HH21	2:L:135:THR:CG2	1.96	0.76
2:F:132:ARG:HH21	2:F:135:THR:HG21	1.48	0.76
2:J:132:ARG:HB2	2:J:270:HIS:CE1	2.21	0.76
1:C:28:CYS:SG	1:C:34:ILE:HD12	2.25	0.76
2:K:191:ARG:HG3	2:K:239:LEU:HD23	1.68	0.76
2:F:132:ARG:HH21	2:F:135:THR:CG2	1.98	0.76
1:I:48:GLN:O	1:I:63:CYS:SG	2.43	0.76
2:J:228:ASN:ND2	2:K:239:LEU:H	1.82	0.76
1:B:129:GLU:O	1:B:130:SER:OG	2.04	0.76
2:F:132:ARG:HG3	2:F:270:HIS:CE1	2.21	0.76
2:E:191:ARG:HG3	2:E:239:LEU:HD23	1.68	0.75
2:J:121:ARG:CB	2:L:281:GLY:HA2	2.16	0.75
1:G:93:GLU:OE1	1:G:95:ASP:HB2	1.87	0.75
2:E:129:THR:HG22	2:E:155:GLU:HG2	1.67	0.75
1:C:119:PRO:HD2	1:C:120:TRP:CZ3	2.21	0.75
1:A:49:ASP:HB2	1:A:60:CYS:CB	2.17	0.74
1:I:62:ARG:NH1	1:I:62:ARG:HB3	2.01	0.74
1:C:33:HIS:HD2	1:C:34:ILE:O	1.71	0.74
1:C:46:TYR:CE1	2:L:168:HIS:HE1	2.06	0.74
1:A:45:LYS:HE2	1:A:48:GLN:HE21	1.52	0.73
1:A:86:CYS:SG	1:A:92:ARG:HD3	2.27	0.73
2:D:132:ARG:HB2	2:D:270:HIS:HE1	1.54	0.73
1:G:91:PHE:CZ	1:G:122:ASP:HB2	2.24	0.72
1:B:112:VAL:HG22	1:B:126:VAL:HG23	1.72	0.72
2:J:231:TRP:CG	2:K:235:ALA:HA	2.25	0.72
2:K:132:ARG:HH21	2:K:135:THR:HG21	1.54	0.71
1:B:111:MET:HE2	1:B:125:CYS:HB2	1.71	0.71
1:G:99:MET:CE	2:J:191:ARG:HH11	2.02	0.71
2:J:228:ASN:HD22	2:K:239:LEU:H	1.37	0.71
1:C:62:ARG:O	2:F:132:ARG:HD3	1.91	0.70
1:G:99:MET:CE	2:J:191:ARG:HD2	2.21	0.70
1:I:49:ASP:HB2	1:I:60:CYS:HB2	1.72	0.70
1:B:113:LYS:HD3	1:B:116:ASP:OD1	1.90	0.70
2:D:126:ILE:HA	2:D:162:SER:HB2	1.73	0.70
1:H:62:ARG:HG3	1:H:62:ARG:NH1	2.03	0.70
1:H:42:ILE:HD12	1:H:42:ILE:H	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:175:VAL:HG22	2:K:255:ARG:HG2	1.74	0.70
2:F:132:ARG:HG3	2:F:270:HIS:HE1	1.57	0.70
1:I:119:PRO:HD2	1:I:120:TRP:CZ3	2.27	0.70
1:B:27:LEU:HD22	1:B:55:ASN:O	1.91	0.69
2:J:126:ILE:HA	2:J:162:SER:HB2	1.74	0.69
1:I:118:THR:HG1	1:I:120:TRP:HE3	1.40	0.69
1:C:99:MET:HG3	2:F:239:LEU:HD21	1.74	0.69
1:G:31:GLY:HA2	1:G:78:THR:O	1.91	0.69
2:J:132:ARG:HB2	2:J:270:HIS:HE1	1.57	0.69
2:J:194:GLU:HG3	2:J:204:LYS:HE2	1.75	0.69
1:C:65:ARG:HD2	2:F:130:ARG:O	1.93	0.69
1:C:92:ARG:HH11	1:C:92:ARG:CG	2.06	0.69
2:J:120:GLN:HA	2:J:120:GLN:OE1	1.92	0.69
2:D:121:ARG:CB	2:F:281:GLY:HA2	2.23	0.69
2:J:192:PHE:CD1	2:J:194:GLU:HB2	2.28	0.69
1:B:61:LEU:HD13	2:E:132:ARG:HH12	1.57	0.68
1:B:111:MET:HG3	2:D:199:ASN:ND2	2.09	0.68
1:C:49:ASP:O	1:C:50:TYR:HB3	1.92	0.68
1:B:59:PHE:HZ	2:E:158:ARG:HD2	1.59	0.68
1:C:78:THR:HG21	4:L:3018:HOH:O	1.94	0.68
1:A:80:ARG:HH11	1:A:80:ARG:CG	2.06	0.68
2:D:120:GLN:OE1	2:D:120:GLN:HA	1.93	0.68
1:G:73:LEU:HD21	1:G:85:GLN:OE1	1.94	0.67
1:C:46:TYR:CD1	2:L:168:HIS:CE1	2.83	0.67
2:F:129:THR:O	2:F:130:ARG:HB3	1.93	0.67
1:B:33:HIS:HD2	1:B:34:ILE:O	1.77	0.67
1:C:53:HIS:HB3	2:E:217:PRO:HG2	1.77	0.67
1:I:64:THR:O	1:I:82:THR:HG21	1.94	0.67
1:I:26:GLY:O	1:I:27:LEU:HD12	1.93	0.67
2:L:170:ARG:O	2:L:171:ASN:HB2	1.94	0.67
2:E:279:LEU:O	2:E:280:VAL:HG13	1.93	0.67
1:G:125:CYS:HB2	2:L:199:ASN:HD21	1.60	0.67
1:I:33:HIS:HD2	1:I:34:ILE:O	1.77	0.67
2:K:129:THR:CG2	2:K:155:GLU:HG2	2.24	0.67
2:D:185:TYR:OH	2:F:247:ILE:HG13	1.95	0.67
1:G:26:GLY:O	1:G:27:LEU:HD23	1.95	0.66
1:B:111:MET:CE	2:D:199:ASN:ND2	2.58	0.66
2:F:133:SER:OG	2:F:271:GLU:OE1	2.13	0.66
1:H:64:THR:H	1:H:81:ASN:HD21	1.42	0.66
2:J:192:PHE:HD1	2:J:194:GLU:HB2	1.61	0.66
2:F:170:ARG:O	2:F:171:ASN:HB2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:231:TRP:CH2	2:L:236:GLU:HB2	2.31	0.66
1:C:64:THR:HG21	2:F:134:ASN:HA	1.78	0.65
2:K:279:LEU:O	2:K:280:VAL:HG13	1.97	0.65
2:D:129:THR:HG23	2:D:155:GLU:HG2	1.78	0.65
2:D:192:PHE:HD1	2:D:194:GLU:HG2	1.57	0.65
2:F:166:ASN:O	2:F:167:LEU:HD12	1.97	0.65
1:B:108:PRO:HG3	2:D:199:ASN:O	1.96	0.65
2:E:175:VAL:HG22	2:E:255:ARG:HG2	1.79	0.65
1:B:44:CYS:HA	4:B:3144:HOH:O	1.96	0.65
2:D:129:THR:CG2	2:D:155:GLU:HG2	2.27	0.64
1:G:36:GLU:HA	1:G:58:LEU:HD11	1.77	0.64
1:B:111:MET:HB2	1:B:125:CYS:HB3	1.79	0.64
1:H:33:HIS:HB2	1:H:57:LEU:O	1.98	0.64
1:B:114:VAL:N	1:B:124:GLU:O	2.31	0.64
1:G:50:TYR:O	1:G:60:CYS:HB3	1.97	0.64
2:E:132:ARG:HH21	2:E:135:THR:HG21	1.63	0.64
2:K:247:ILE:HD11	2:L:278:PHE:HD2	1.63	0.64
2:E:231:TRP:CG	2:F:235:ALA:HA	2.33	0.63
1:A:45:LYS:HB3	1:A:48:GLN:HB2	1.80	0.63
1:I:42:ILE:HG22	1:I:43:SER:N	2.13	0.63
1:A:99:MET:HE2	2:D:191:ARG:HD2	1.79	0.63
1:B:64:THR:N	1:B:81:ASN:HD21	1.96	0.63
1:B:111:MET:HA	1:B:126:VAL:O	1.99	0.63
2:D:132:ARG:HH21	2:D:135:THR:HG21	1.64	0.63
2:E:231:TRP:CH2	2:F:236:GLU:HB2	2.34	0.62
2:J:121:ARG:HG2	2:L:281:GLY:CA	2.29	0.62
2:D:231:TRP:CG	2:E:235:ALA:HA	2.34	0.62
1:G:104:ARG:HD2	1:G:122:ASP:OD2	1.99	0.62
2:K:192:PHE:HD1	2:K:194:GLU:HB3	1.65	0.62
2:L:152:ASN:HA	2:L:172:GLY:HA3	1.82	0.62
1:A:45:LYS:HE2	1:A:48:GLN:NE2	2.14	0.62
2:E:181:PHE:O	2:E:279:LEU:HD12	2.00	0.62
2:K:168:HIS:HD1	2:K:177:HIS:HE2	1.46	0.62
2:D:174:LEU:HD12	2:D:275:PHE:CE2	2.35	0.62
2:E:190:PHE:CD1	2:E:206:MET:HG2	2.34	0.62
1:I:45:LYS:HD3	1:I:48:GLN:NE2	2.14	0.62
1:C:77:THR:HG21	1:C:80:ARG:NH1	2.14	0.62
1:I:26:GLY:C	1:I:27:LEU:HD12	2.20	0.62
1:I:31:GLY:N	1:I:79:THR:HG22	2.15	0.62
2:J:129:THR:HG23	2:J:155:GLU:HG2	1.82	0.61
2:L:166:ASN:O	2:L:167:LEU:HD12	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:121:ARG:CG	2:L:281:GLY:HA2	2.30	0.61
1:A:99:MET:HE1	2:D:191:ARG:HG3	1.82	0.61
1:B:28:CYS:O	1:B:54:TRP:HA	2.00	0.61
2:J:129:THR:O	2:J:130:ARG:CB	2.42	0.61
1:I:53:HIS:CG	2:K:217:PRO:HG2	2.35	0.61
1:B:59:PHE:CZ	2:E:158:ARG:HD2	2.35	0.61
2:J:174:LEU:HD12	2:J:275:PHE:CE2	2.36	0.61
1:H:33:HIS:HD2	1:H:60:CYS:SG	2.24	0.61
2:E:247:ILE:HG13	2:F:185:TYR:OH	2.00	0.61
2:D:129:THR:O	2:D:130:ARG:CB	2.45	0.61
2:D:252:GLU:O	2:D:253:ASN:HB2	2.00	0.60
2:D:281:GLY:HA3	2:E:121:ARG:CG	2.27	0.60
1:I:62:ARG:HB3	1:I:62:ARG:HH11	1.64	0.60
1:C:50:TYR:HE2	1:C:61:LEU:HD12	1.66	0.60
1:I:61:LEU:HD13	2:L:132:ARG:NH1	2.15	0.60
2:J:192:PHE:HB3	2:J:265:LEU:HD22	1.82	0.60
1:A:90:THR:HB	1:A:100:CYS:HB3	1.83	0.60
2:J:121:ARG:HG2	2:L:281:GLY:HA2	1.82	0.60
2:L:233:LYS:HG3	2:L:234:ASP:OD1	2.01	0.60
1:A:44:CYS:SG	1:A:50:TYR:CA	2.89	0.60
2:E:129:THR:CG2	2:E:155:GLU:HG2	2.31	0.60
1:H:62:ARG:HH11	1:H:62:ARG:CG	2.15	0.60
1:B:59:PHE:CE2	2:E:159:SER:HA	2.36	0.60
2:F:164:LEU:HD22	2:F:168:HIS:HA	1.82	0.60
1:H:117:CYS:SG	1:H:118:THR:N	2.74	0.60
1:I:42:ILE:N	1:I:42:ILE:HD12	2.16	0.60
2:F:152:ASN:HA	2:F:172:GLY:HA3	1.84	0.60
1:B:111:MET:HE2	2:D:199:ASN:ND2	2.17	0.60
1:I:91:PHE:HD2	1:I:92:ARG:O	1.85	0.60
2:F:233:LYS:HG3	2:F:234:ASP:OD1	2.02	0.60
1:H:55:ASN:HB2	1:H:57:LEU:HG	1.84	0.60
2:L:149:ARG:HD3	2:L:263:GLU:CD	2.22	0.59
2:L:280:VAL:HG23	2:L:281:GLY:N	2.15	0.59
1:C:61:LEU:HD13	2:F:132:ARG:HH12	1.68	0.59
2:K:197:LYS:N	2:K:202:ASN:HD21	2.00	0.59
2:E:197:LYS:N	2:E:202:ASN:HD21	2.00	0.59
1:I:59:PHE:CZ	2:L:158:ARG:HD2	2.37	0.59
1:A:58:LEU:HD22	2:D:158:ARG:NH1	2.18	0.59
1:B:58:LEU:O	4:B:3141:HOH:O	2.17	0.59
1:I:61:LEU:HD13	2:L:132:ARG:HH12	1.67	0.59
2:L:200:THR:HG22	2:L:201:LYS:N	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:TYR:CZ	1:B:81:ASN:HB2	2.38	0.59
1:G:50:TYR:CZ	1:G:81:ASN:HB2	2.38	0.59
1:A:48:GLN:O	1:A:63:CYS:SG	2.61	0.59
1:A:118:THR:HB	1:A:119:PRO:HD2	1.83	0.58
2:D:263:GLU:HB3	4:D:3025:HOH:O	2.03	0.58
2:E:189:TYR:OH	2:E:239:LEU:HD22	2.03	0.58
2:K:181:PHE:O	2:K:279:LEU:HD12	2.03	0.58
2:J:129:THR:CG2	2:J:155:GLU:HG2	2.32	0.58
2:J:130:ARG:O	2:J:130:ARG:HG3	2.03	0.58
2:L:149:ARG:NH1	4:L:3074:HOH:O	2.35	0.58
2:L:252:GLU:O	2:L:253:ASN:HB2	2.03	0.58
2:L:164:LEU:HD22	2:L:168:HIS:HA	1.85	0.58
2:K:173:GLU:HG2	2:K:257:PHE:HB3	1.86	0.58
1:A:42:ILE:N	1:A:42:ILE:HD12	2.18	0.58
2:D:130:ARG:HG3	2:D:130:ARG:O	2.03	0.58
1:G:99:MET:HG2	2:J:237:TYR:CD1	2.38	0.58
1:B:56:ASP:N	1:B:56:ASP:OD1	2.37	0.58
2:D:121:ARG:CG	2:F:281:GLY:HA2	2.33	0.58
1:I:33:HIS:HB2	1:I:57:LEU:O	2.04	0.58
1:B:81:ASN:ND2	1:B:82:THR:H	2.02	0.57
2:F:149:ARG:HD3	2:F:263:GLU:CD	2.25	0.57
2:J:281:GLY:HA3	2:K:121:ARG:CG	2.30	0.57
1:G:93:GLU:CD	1:G:95:ASP:HB2	2.24	0.57
1:H:52:THR:HB	1:H:79:THR:O	2.03	0.57
2:D:121:ARG:HG2	2:F:281:GLY:HA2	1.85	0.57
1:C:50:TYR:CE2	1:C:61:LEU:HD12	2.40	0.57
2:E:173:GLU:HG2	2:E:257:PHE:HB3	1.86	0.57
1:B:90:THR:HB	1:B:100:CYS:HB3	1.85	0.57
1:C:92:ARG:HD3	1:C:97:PRO:HA	1.86	0.57
1:I:52:THR:HB	1:I:79:THR:O	2.04	0.57
2:K:231:TRP:CG	2:L:235:ALA:HA	2.39	0.57
1:A:64:THR:HA	2:D:132:ARG:O	2.04	0.57
1:C:87:GLU:CD	1:C:88:GLU:H	2.07	0.57
2:D:194:GLU:HG3	4:D:3088:HOH:O	2.05	0.57
1:H:23:PRO:HD3	1:H:41:CYS:SG	2.45	0.57
1:C:73:LEU:HB3	1:C:83:VAL:HG12	1.85	0.57
1:C:33:HIS:CD2	1:C:34:ILE:O	2.57	0.57
2:L:200:THR:HG22	2:L:201:LYS:H	1.70	0.57
1:G:52:THR:OG1	1:G:52:THR:O	2.23	0.56
2:K:161:HIS:N	2:K:161:HIS:CD2	2.73	0.56
1:C:44:CYS:SG	1:C:50:TYR:HA	2.45	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:161:HIS:N	2:E:161:HIS:CD2	2.73	0.56
2:E:187:GLN:NE2	2:E:274:PHE:CZ	2.73	0.56
2:F:126:ILE:HD12	2:F:154:TRP:CB	2.34	0.56
2:F:209:TYR:HD1	2:F:221:LEU:HD11	1.70	0.56
2:D:121:ARG:HG2	2:F:281:GLY:CA	2.35	0.56
2:L:125:HIS:HE1	2:L:274:PHE:CD1	2.23	0.56
2:K:192:PHE:CD1	2:K:194:GLU:HB3	2.39	0.56
2:E:127:THR:HG22	2:E:274:PHE:HB3	1.85	0.56
2:E:264:HIS:O	2:E:265:LEU:HD23	2.05	0.56
1:B:24:SER:O	1:B:25:GLU:HB2	2.05	0.56
2:F:147:LEU:HB2	2:F:211:TYR:OH	2.05	0.56
1:H:31:GLY:HA2	1:H:78:THR:O	2.04	0.56
1:C:55:ASN:HB2	1:C:57:LEU:HG	1.88	0.56
1:C:78:THR:HG23	1:C:79:THR:HG23	1.88	0.56
1:C:57:LEU:HD21	2:E:216:TYR:CD1	2.41	0.56
2:L:280:VAL:HG23	2:L:281:GLY:H	1.70	0.56
1:C:67:ASP:O	1:C:70:GLU:HB2	2.05	0.56
1:B:91:PHE:CE1	1:B:122:ASP:HB2	2.41	0.55
1:C:53:HIS:CB	2:E:217:PRO:HG2	2.36	0.55
1:C:34:ILE:HG23	1:C:35:SER:N	2.22	0.55
1:H:67:ASP:CG	2:K:191:ARG:HH22	2.09	0.55
2:F:252:GLU:O	2:F:253:ASN:HB2	2.07	0.55
2:F:280:VAL:HG23	2:F:281:GLY:N	2.20	0.55
1:C:118:THR:OG1	1:C:120:TRP:HE3	1.86	0.55
1:C:122:ASP:OD2	2:E:201:LYS:HD2	2.07	0.55
2:J:226:ALA:H	2:K:241:SER:HB2	1.72	0.55
1:H:22:SER:HB3	1:H:23:PRO:HD2	1.88	0.55
2:L:127:THR:OG1	2:L:270:HIS:HB2	2.07	0.55
1:B:112:VAL:O	1:B:125:CYS:HA	2.07	0.55
1:I:93:GLU:HB3	1:I:96:SER:OG	2.07	0.55
2:L:133:SER:OG	2:L:271:GLU:OE1	2.25	0.55
2:F:126:ILE:HA	2:F:162:SER:HB2	1.89	0.54
1:G:23:PRO:HB3	1:G:34:ILE:HD12	1.88	0.54
1:A:26:GLY:O	1:A:27:LEU:HD23	2.07	0.54
4:E:3118:HOH:O	2:F:270:HIS:HD2	1.90	0.54
1:I:28:CYS:O	1:I:54:TRP:HA	2.08	0.54
2:D:174:LEU:HD12	2:D:275:PHE:CZ	2.43	0.54
2:J:132:ARG:HH21	2:J:135:THR:HG21	1.73	0.54
2:K:247:ILE:HG13	2:L:185:TYR:OH	2.07	0.54
1:H:52:THR:O	1:H:52:THR:OG1	2.24	0.54
1:C:99:MET:HG3	2:F:239:LEU:CD2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:TYR:CD2	1:C:50:TYR:C	2.82	0.54
1:C:87:GLU:HG3	1:C:88:GLU:N	2.23	0.54
2:K:156:SER:HB3	2:K:169:LEU:HD23	1.89	0.53
2:E:189:TYR:HD2	2:E:272:ALA:HB1	1.73	0.53
1:C:87:GLU:CG	1:C:88:GLU:N	2.72	0.53
1:H:23:PRO:HG2	1:H:38:GLY:O	2.09	0.53
1:A:101:ARG:HH21	2:F:201:LYS:HE2	1.73	0.53
2:D:236:GLU:HB2	2:F:231:TRP:CH2	2.44	0.53
2:E:192:PHE:HD1	2:E:194:GLU:HB3	1.73	0.53
1:B:96:SER:N	1:B:97:PRO:HD3	2.24	0.53
1:H:64:THR:N	1:H:81:ASN:HD21	2.06	0.53
1:I:59:PHE:HZ	2:L:158:ARG:HD2	1.73	0.53
2:K:189:TYR:HD2	2:K:272:ALA:HB1	1.74	0.53
1:B:111:MET:CA	1:B:126:VAL:O	2.57	0.53
1:G:108:PRO:O	1:G:111:MET:HB2	2.09	0.53
2:J:184:ILE:HD11	2:J:250:LEU:HD11	1.91	0.53
1:C:32:HIS:ND1	1:C:43:SER:HB3	2.24	0.53
1:C:33:HIS:HB2	1:C:57:LEU:O	2.09	0.53
1:C:44:CYS:HB3	1:C:49:ASP:OD1	2.09	0.53
2:F:156:SER:HB3	2:F:169:LEU:HD23	1.90	0.53
1:H:63:CYS:HA	1:H:81:ASN:ND2	2.24	0.53
1:I:42:ILE:N	1:I:42:ILE:CD1	2.72	0.53
2:D:127:THR:OG1	2:D:270:HIS:HB2	2.09	0.52
2:J:184:ILE:O	2:J:245:GLY:HA2	2.09	0.52
2:L:126:ILE:HA	2:L:162:SER:HB2	1.90	0.52
1:C:62:ARG:CD	2:F:131:GLY:HA2	2.34	0.52
1:G:122:ASP:OD1	1:G:123:ILE:N	2.42	0.52
2:J:127:THR:OG1	2:J:270:HIS:HB2	2.08	0.52
2:L:126:ILE:CD1	2:L:169:LEU:HD13	2.40	0.52
1:A:85:GLN:NE2	1:A:119:PRO:HG3	2.24	0.52
1:B:52:THR:O	1:B:52:THR:OG1	2.26	0.52
1:B:129:GLU:C	1:B:130:SER:OG	2.48	0.52
1:H:61:LEU:HD13	2:K:132:ARG:NH1	2.20	0.52
1:B:108:PRO:HD2	1:B:111:MET:HG3	1.91	0.52
1:H:99:MET:CE	2:K:191:ARG:HE	2.22	0.52
1:I:34:ILE:HG13	1:I:35:SER:H	1.75	0.52
2:L:209:TYR:HD1	2:L:221:LEU:HD11	1.75	0.52
1:B:128:LYS:O	1:B:128:LYS:HG3	2.10	0.52
2:F:126:ILE:HD12	2:F:154:TRP:HB3	1.91	0.52
1:A:50:TYR:CZ	1:A:81:ASN:HB2	2.44	0.52
1:H:28:CYS:O	1:H:54:TRP:HA	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:73:LEU:HD21	1:H:85:GLN:OE1	2.09	0.52
1:I:30:PRO:O	1:I:32:HIS:HD2	1.93	0.52
2:L:147:LEU:HB2	2:L:211:TYR:OH	2.10	0.52
2:L:208:GLN:NE2	2:L:210:ILE:HD11	2.25	0.52
1:B:91:PHE:CZ	1:B:122:ASP:HB2	2.45	0.52
2:D:121:ARG:CZ	2:F:181:PHE:CE2	2.93	0.52
2:E:168:HIS:HD1	2:E:177:HIS:HE2	1.58	0.52
2:F:132:ARG:NH2	2:F:135:THR:HG21	2.22	0.52
1:I:59:PHE:HZ	2:L:158:ARG:HH11	1.55	0.52
2:L:270:HIS:CD2	2:L:271:GLU:HG3	2.45	0.52
1:C:77:THR:OG1	1:C:80:ARG:HB3	2.10	0.51
1:G:92:ARG:HG2	1:G:97:PRO:HA	1.92	0.51
1:I:70:GLU:HA	1:I:85:GLN:O	2.10	0.51
1:I:99:MET:HG3	2:L:239:LEU:HD21	1.91	0.51
2:J:247:ILE:HD12	2:K:185:TYR:OH	2.10	0.51
1:B:112:VAL:CG2	1:B:126:VAL:HG23	2.40	0.51
1:B:61:LEU:HD13	2:E:132:ARG:NH1	2.24	0.51
1:C:96:SER:N	1:C:97:PRO:HD3	2.26	0.51
2:E:247:ILE:HD11	2:F:278:PHE:HD2	1.76	0.51
2:E:187:GLN:NE2	2:E:274:PHE:HZ	2.09	0.51
1:H:49:ASP:OD1	1:H:60:CYS:HB2	2.11	0.51
2:J:190:PHE:CZ	2:J:266:ILE:HD11	2.46	0.51
1:B:114:VAL:HB	1:B:126:VAL:HG22	1.92	0.51
2:D:190:PHE:CZ	2:D:266:ILE:HD11	2.45	0.51
2:F:270:HIS:CD2	2:F:271:GLU:HG3	2.46	0.51
2:J:236:GLU:HB2	2:L:231:TRP:CH2	2.45	0.51
1:H:99:MET:HE1	2:K:191:ARG:HG2	1.91	0.51
2:K:187:GLN:NE2	2:K:274:PHE:CZ	2.79	0.51
2:L:192:PHE:HE1	2:L:194:GLU:OE2	1.94	0.51
2:F:125:HIS:HE1	2:F:274:PHE:CD1	2.30	0.50
2:E:252:GLU:HG2	2:E:253:ASN:OD1	2.11	0.50
1:G:70:GLU:OE2	2:J:134:ASN:ND2	2.44	0.50
2:F:127:THR:OG1	2:F:270:HIS:HB2	2.10	0.50
2:F:181:PHE:HB2	2:F:280:VAL:HG21	1.91	0.50
2:F:187:GLN:HA	2:F:242:ILE:O	2.12	0.50
1:I:64:THR:HG22	1:I:65:ARG:N	2.26	0.50
1:A:122:ASP:OD1	1:A:123:ILE:HG13	2.11	0.50
2:E:199:ASN:O	2:E:200:THR:HG23	2.11	0.50
1:G:37:ASP:C	1:G:37:ASP:OD1	2.50	0.50
1:G:45:LYS:HD3	1:G:48:GLN:CD	2.31	0.50
1:H:53:HIS:CG	2:J:217:PRO:HG2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:189:TYR:OH	2:D:239:LEU:HD22	2.11	0.50
2:E:251:LYS:O	2:E:254:ASP:HB2	2.12	0.50
1:G:97:PRO:HG2	2:L:209:TYR:OH	2.12	0.50
2:E:218:ASP:HB3	2:E:219:PRO:HD2	1.93	0.50
2:F:278:PHE:HD1	2:F:279:LEU:O	1.95	0.50
2:E:192:PHE:CD1	2:E:194:GLU:HB3	2.47	0.50
1:H:119:PRO:HD2	1:H:120:TRP:CZ3	2.47	0.50
2:F:155:GLU:OE1	2:F:161:HIS:HE1	1.94	0.50
2:D:194:GLU:CB	4:D:3088:HOH:O	2.59	0.50
2:E:189:TYR:HH	2:E:239:LEU:HD22	1.77	0.50
2:J:185:TYR:OH	2:L:247:ILE:HG13	2.11	0.50
2:L:132:ARG:NH2	2:L:135:THR:HG21	2.21	0.50
1:C:59:PHE:HZ	2:F:158:ARG:HH11	1.59	0.49
1:I:31:GLY:C	1:I:32:HIS:CD2	2.85	0.49
2:K:127:THR:HG22	2:K:274:PHE:HB3	1.93	0.49
1:B:122:ASP:OD1	1:B:123:ILE:N	2.45	0.49
2:E:194:GLU:O	2:E:194:GLU:HG3	2.09	0.49
2:L:184:ILE:O	2:L:245:GLY:HA2	2.11	0.49
1:A:56:ASP:OD1	1:A:56:ASP:N	2.45	0.49
1:B:113:LYS:CD	1:B:116:ASP:OD1	2.60	0.49
2:F:209:TYR:HB3	2:F:221:LEU:CD1	2.42	0.49
1:A:44:CYS:SG	1:A:50:TYR:C	2.91	0.49
2:E:190:PHE:CE1	2:E:266:ILE:HD11	2.48	0.49
1:H:92:ARG:HG2	1:H:97:PRO:HA	1.95	0.49
1:I:92:ARG:HG2	1:I:93:GLU:H	1.77	0.49
1:C:23:PRO:HD3	1:C:39:ARG:O	2.13	0.49
2:E:182:TYR:O	2:E:247:ILE:HA	2.13	0.49
1:G:49:ASP:O	1:G:50:TYR:HB3	2.13	0.49
1:I:67:ASP:O	1:I:70:GLU:HB2	2.12	0.49
1:A:30:PRO:O	1:A:32:HIS:HD2	1.95	0.49
1:B:50:TYR:OH	1:B:81:ASN:HB2	2.12	0.49
1:C:32:HIS:CE1	1:C:43:SER:HB3	2.46	0.49
2:F:260:VAL:HG21	2:F:266:ILE:HD11	1.95	0.49
1:G:64:THR:HA	2:J:132:ARG:O	2.13	0.49
2:K:251:LYS:O	2:K:254:ASP:HB2	2.13	0.49
2:L:155:GLU:OE1	2:L:161:HIS:HE1	1.95	0.49
2:D:184:ILE:O	2:D:245:GLY:HA2	2.12	0.49
1:I:70:GLU:OE2	2:L:134:ASN:ND2	2.45	0.49
1:G:99:MET:HG2	2:J:237:TYR:CG	2.48	0.49
1:I:92:ARG:O	1:I:93:GLU:HB2	2.13	0.49
2:J:121:ARG:CG	2:L:281:GLY:CA	2.90	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:133:SER:OG	2:D:271:GLU:OE1	2.21	0.49
2:L:204:LYS:HB2	2:L:229:SER:HB3	1.93	0.49
2:L:218:ASP:HB3	2:L:219:PRO:HD2	1.94	0.49
1:B:33:HIS:CD2	1:B:34:ILE:O	2.63	0.48
2:K:199:ASN:O	2:K:200:THR:HG23	2.13	0.48
2:L:209:TYR:HB3	2:L:221:LEU:CD1	2.42	0.48
1:H:119:PRO:HG2	1:H:120:TRP:CE2	2.48	0.48
1:A:118:THR:HB	1:A:119:PRO:CD	2.43	0.48
2:D:231:TRP:CH2	2:E:236:GLU:HB2	2.48	0.48
1:H:22:SER:HA	1:H:41:CYS:SG	2.54	0.48
1:A:65:ARG:HD3	1:A:66:CYS:O	2.13	0.48
1:C:32:HIS:HA	1:C:42:ILE:O	2.13	0.48
2:E:187:GLN:HA	2:E:242:ILE:O	2.14	0.48
1:I:29:PRO:O	1:I:30:PRO:C	2.50	0.48
2:K:190:PHE:CE1	2:K:266:ILE:HD11	2.48	0.48
1:C:52:THR:HG22	1:C:79:THR:C	2.34	0.48
2:K:182:TYR:CZ	2:K:279:LEU:HD13	2.49	0.48
1:C:32:HIS:HA	1:C:43:SER:HA	1.95	0.48
1:C:89:GLY:CA	4:C:3028:HOH:O	2.48	0.48
2:D:226:ALA:H	2:E:241:SER:HB2	1.79	0.48
2:F:126:ILE:CD1	2:F:169:LEU:HD13	2.44	0.48
2:F:280:VAL:HG23	2:F:281:GLY:H	1.77	0.48
1:I:42:ILE:CG2	1:I:43:SER:N	2.77	0.48
1:I:62:ARG:O	2:L:132:ARG:HD3	2.14	0.48
2:L:126:ILE:HD13	2:L:169:LEU:HD13	1.95	0.48
1:C:91:PHE:HE1	1:C:102:LYS:O	1.97	0.48
1:I:53:HIS:CB	2:K:217:PRO:HG2	2.44	0.48
2:J:199:ASN:C	2:J:200:THR:HG22	2.33	0.48
2:L:179:LYS:O	2:L:179:LYS:HG3	2.12	0.48
1:B:92:ARG:CG	1:B:97:PRO:HA	2.41	0.48
2:L:181:PHE:HB2	2:L:280:VAL:HG21	1.94	0.48
2:D:184:ILE:HD11	2:D:250:LEU:HD11	1.96	0.48
2:F:243:TYR:CD1	2:F:243:TYR:C	2.87	0.48
2:J:182:TYR:CZ	2:J:279:LEU:HD13	2.49	0.48
2:E:130:ARG:HG2	2:E:130:ARG:HH11	1.79	0.47
2:F:179:LYS:O	2:F:179:LYS:HG3	2.14	0.47
1:H:90:THR:HB	1:H:100:CYS:HB3	1.96	0.47
1:I:118:THR:C	1:I:120:TRP:H	2.18	0.47
2:J:174:LEU:HD12	2:J:275:PHE:CZ	2.48	0.47
1:G:73:LEU:HD22	1:G:85:GLN:HB2	1.96	0.47
2:K:228:ASN:ND2	2:L:239:LEU:H	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:150:LYS:HA	2:E:259:SER:HA	1.97	0.47
2:J:207:VAL:HG13	2:J:226:ALA:HB2	1.95	0.47
2:J:231:TRP:CD2	2:K:235:ALA:HA	2.49	0.47
2:E:228:ASN:ND2	2:F:239:LEU:H	2.12	0.47
2:F:184:ILE:O	2:F:245:GLY:HA2	2.14	0.47
2:E:184:ILE:O	2:E:245:GLY:HA2	2.14	0.47
1:H:84:CYS:HB2	2:K:134:ASN:HD21	1.80	0.47
1:H:86:CYS:HB3	1:H:90:THR:O	2.15	0.47
1:I:46:TYR:CD1	1:I:47:GLY:N	2.82	0.47
1:I:98:GLU:HG2	2:K:207:VAL:HG21	1.97	0.47
2:J:121:ARG:HG2	2:L:281:GLY:HA3	1.96	0.47
2:L:278:PHE:HD1	2:L:279:LEU:O	1.98	0.47
1:B:108:PRO:HG3	2:D:199:ASN:C	2.29	0.47
1:C:50:TYR:HE1	1:C:81:ASN:OD1	1.98	0.47
2:J:197:LYS:HB3	2:J:200:THR:CG2	2.45	0.47
1:C:57:LEU:HB2	1:C:59:PHE:O	2.15	0.47
2:D:225:SER:OG	2:D:227:ARG:NH1	2.48	0.47
2:E:156:SER:HB3	2:E:169:LEU:HD23	1.97	0.47
1:G:45:LYS:HB2	1:G:48:GLN:HB2	1.96	0.47
1:H:67:ASP:OD2	2:K:191:ARG:NH2	2.39	0.47
2:J:190:PHE:CD2	2:J:206:MET:HG2	2.50	0.47
1:C:31:GLY:HA2	1:C:78:THR:O	2.15	0.47
1:C:76:CYS:H	2:L:170:ARG:NH1	2.13	0.47
2:J:222:LEU:C	2:J:223:MET:HG3	2.36	0.46
1:C:30:PRO:HD3	1:C:54:TRP:NE1	2.30	0.46
2:F:169:LEU:HG	2:F:170:ARG:N	2.30	0.46
2:K:194:GLU:O	2:K:194:GLU:HG3	2.11	0.46
2:F:208:GLN:NE2	2:F:210:ILE:HD11	2.30	0.46
2:F:238:GLY:C	2:F:239:LEU:HD23	2.35	0.46
1:G:112:VAL:HB	1:G:128:LYS:HD2	1.96	0.46
1:B:29:PRO:HA	1:B:54:TRP:CD2	2.51	0.46
2:F:126:ILE:HD13	2:F:169:LEU:HD13	1.98	0.46
1:G:36:GLU:C	1:G:38:GLY:N	2.69	0.46
1:H:50:TYR:C	1:H:50:TYR:CD2	2.88	0.46
1:C:61:LEU:HD13	2:F:132:ARG:NH1	2.31	0.46
1:C:87:GLU:CG	1:C:88:GLU:H	2.28	0.46
1:C:99:MET:HE1	2:F:193:GLN:HG3	1.96	0.46
1:G:67:ASP:OD1	1:G:67:ASP:C	2.54	0.46
2:E:182:TYR:CZ	2:E:279:LEU:HD13	2.50	0.46
2:F:280:VAL:CG2	2:F:281:GLY:H	2.29	0.46
1:I:31:GLY:CA	1:I:79:THR:HG22	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:133:SER:O	2:L:134:ASN:C	2.54	0.46
1:A:46:TYR:CE2	1:A:77:THR:HA	2.51	0.46
1:A:49:ASP:HB2	1:A:60:CYS:HB2	1.95	0.46
1:B:52:THR:O	1:B:53:HIS:CG	2.69	0.46
1:C:96:SER:HB2	2:E:205:GLN:CD	2.36	0.46
1:G:50:TYR:OH	1:G:81:ASN:HB2	2.16	0.46
1:H:24:SER:HB2	1:H:54:TRP:HZ3	1.81	0.46
1:H:45:LYS:HG2	1:H:48:GLN:CB	2.46	0.46
2:L:156:SER:HB3	2:L:169:LEU:HD23	1.97	0.46
1:A:97:PRO:HG2	2:F:209:TYR:OH	2.16	0.46
2:D:222:LEU:C	2:D:223:MET:HG3	2.35	0.46
1:I:33:HIS:CD2	1:I:34:ILE:O	2.65	0.46
1:C:49:ASP:O	1:C:50:TYR:CB	2.63	0.46
2:D:127:THR:HG23	2:D:162:SER:HB3	1.98	0.46
2:E:189:TYR:CD2	2:E:272:ALA:HB1	2.51	0.46
2:E:207:VAL:HG13	2:E:226:ALA:HB2	1.96	0.46
2:F:209:TYR:CD1	2:F:221:LEU:HD11	2.50	0.46
1:G:96:SER:N	1:G:97:PRO:HD3	2.31	0.46
2:J:127:THR:HG23	2:J:162:SER:HB3	1.98	0.46
2:D:207:VAL:HG13	2:D:226:ALA:HB2	1.98	0.45
2:F:189:TYR:HD2	2:F:272:ALA:HB1	1.81	0.45
2:F:214:THR:O	2:F:216:TYR:N	2.48	0.45
1:H:99:MET:HE1	2:K:191:ARG:HE	1.80	0.45
1:I:85:GLN:NE2	1:I:119:PRO:HG2	2.31	0.45
2:J:187:GLN:HA	2:J:242:ILE:O	2.16	0.45
1:G:118:THR:C	1:G:120:TRP:H	2.19	0.45
2:L:243:TYR:CD1	2:L:243:TYR:C	2.89	0.45
1:B:27:LEU:HD22	1:B:55:ASN:C	2.37	0.45
2:D:175:VAL:HG22	2:D:255:ARG:HG2	1.97	0.45
2:D:214:THR:O	2:D:216:TYR:N	2.48	0.45
2:K:130:ARG:HH11	2:K:130:ARG:HG2	1.80	0.45
1:A:58:LEU:HD22	2:D:158:ARG:HH12	1.80	0.45
1:C:67:ASP:O	1:C:68:SER:C	2.54	0.45
2:F:149:ARG:NH1	4:F:3017:HOH:O	2.48	0.45
1:G:44:CYS:HB3	1:G:49:ASP:OD1	2.16	0.45
1:B:29:PRO:O	1:B:30:PRO:O	2.34	0.45
1:C:21:SER:HA	1:C:41:CYS:H	1.81	0.45
1:C:37:ASP:OD2	1:C:39:ARG:HB2	2.17	0.45
2:D:235:ALA:HA	2:F:231:TRP:CG	2.52	0.45
1:A:28:CYS:O	1:A:54:TRP:HA	2.17	0.45
1:B:104:ARG:HE	1:B:104:ARG:HB2	1.71	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:VAL:O	1:B:114:VAL:N	2.50	0.45
1:I:52:THR:HG21	4:I:3040:HOH:O	2.16	0.45
2:J:189:TYR:OH	2:J:239:LEU:HD22	2.16	0.45
1:B:111:MET:CB	1:B:125:CYS:HB3	2.45	0.45
1:C:74:SER:HA	1:C:75:PRO:HD2	1.74	0.45
2:D:121:ARG:CG	2:F:281:GLY:CA	2.95	0.45
2:F:218:ASP:HB3	2:F:219:PRO:HD2	1.97	0.45
1:I:50:TYR:CE2	1:I:61:LEU:HD12	2.52	0.45
2:K:152:ASN:HA	2:K:172:GLY:HA3	1.99	0.45
2:L:208:GLN:O	2:L:224:LYS:HA	2.16	0.45
1:B:112:VAL:N	1:B:126:VAL:O	2.49	0.45
2:D:164:LEU:HD22	2:D:168:HIS:HA	1.97	0.45
2:J:254:ASP:O	2:J:255:ARG:HG3	2.17	0.45
2:K:189:TYR:OH	2:K:239:LEU:HD22	2.17	0.45
1:C:98:GLU:OE2	2:E:224:LYS:NZ	2.47	0.45
2:F:169:LEU:HD11	2:F:172:GLY:HA2	1.99	0.45
2:K:168:HIS:ND1	2:K:177:HIS:NE2	2.58	0.45
1:C:61:LEU:HB3	2:F:132:ARG:NH1	2.32	0.44
2:E:161:HIS:ND1	2:E:270:HIS:CD2	2.85	0.44
2:F:127:THR:HG23	2:F:162:SER:HB3	1.98	0.44
2:J:252:GLU:O	2:J:253:ASN:HB2	2.16	0.44
1:C:91:PHE:HD2	1:C:92:ARG:O	1.99	0.44
1:C:92:ARG:O	1:C:93:GLU:HB2	2.17	0.44
2:D:263:GLU:HA	2:D:266:ILE:HG12	1.99	0.44
2:K:218:ASP:HB3	2:K:219:PRO:HD2	2.00	0.44
2:L:189:TYR:CD2	2:L:272:ALA:HB1	2.51	0.44
2:E:152:ASN:HA	2:E:172:GLY:HA3	1.99	0.44
2:K:187:GLN:HA	2:K:242:ILE:O	2.17	0.44
1:C:77:THR:C	1:C:79:THR:H	2.21	0.44
2:E:231:TRP:CD2	2:F:235:ALA:HA	2.53	0.44
1:H:91:PHE:HE1	1:H:102:LYS:O	2.00	0.44
1:G:24:SER:O	1:G:25:GLU:HB2	2.17	0.44
1:G:104:ARG:CD	1:G:122:ASP:OD2	2.66	0.44
1:H:53:HIS:CB	2:J:217:PRO:HG2	2.48	0.44
2:E:161:HIS:ND1	2:E:270:HIS:CG	2.85	0.44
2:K:190:PHE:CD1	2:K:206:MET:HG2	2.53	0.44
1:C:50:TYR:CE1	1:C:81:ASN:HA	2.53	0.44
1:G:107:CYS:HB3	1:G:108:PRO:HD2	1.99	0.44
1:I:98:GLU:O	1:I:99:MET:HG2	2.17	0.44
1:B:45:LYS:HB2	1:B:48:GLN:HB3	1.99	0.44
2:D:211:TYR:HB2	2:D:257:PHE:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:254:ASP:O	2:D:255:ARG:HG3	2.18	0.44
2:J:121:ARG:CZ	2:L:181:PHE:CE2	3.01	0.44
2:K:247:ILE:HD11	2:L:278:PHE:CD2	2.49	0.44
2:L:131:GLY:O	2:L:269:ASP:HA	2.18	0.44
2:L:208:GLN:NE2	2:L:244:GLN:HE21	2.16	0.44
1:A:62:ARG:HH22	2:D:129:THR:HG22	1.83	0.44
2:E:197:LYS:H	2:E:202:ASN:HD21	1.66	0.44
2:L:212:LYS:HG2	2:L:222:LEU:HD21	1.99	0.44
1:B:22:SER:HA	1:B:23:PRO:HD3	1.88	0.43
1:C:66:CYS:HB3	1:C:70:GLU:HB3	2.00	0.43
2:E:265:LEU:HA	4:E:3016:HOH:O	2.18	0.43
1:G:49:ASP:HB2	1:G:60:CYS:HB2	2.00	0.43
1:G:125:CYS:HB2	2:L:199:ASN:ND2	2.31	0.43
1:H:99:MET:HG3	1:H:100:CYS:N	2.33	0.43
1:A:24:SER:OG	1:A:54:TRP:CZ3	2.71	0.43
1:A:62:ARG:NH2	2:D:155:GLU:OE1	2.50	0.43
2:F:254:ASP:C	2:F:255:ARG:HG3	2.39	0.43
1:I:118:THR:O	1:I:120:TRP:N	2.51	0.43
1:C:77:THR:HG21	1:C:80:ARG:HH12	1.81	0.43
1:C:93:GLU:HG2	1:C:94:GLU:H	1.83	0.43
1:G:73:LEU:CD2	1:G:85:GLN:HB2	2.48	0.43
2:L:187:GLN:HA	2:L:242:ILE:O	2.17	0.43
1:A:119:PRO:HD2	1:A:120:TRP:CZ3	2.53	0.43
1:B:29:PRO:HB3	1:B:54:TRP:CH2	2.53	0.43
2:F:133:SER:O	2:F:134:ASN:C	2.57	0.43
1:H:56:ASP:OD1	1:H:56:ASP:N	2.52	0.43
2:J:183:TYR:O	2:J:277:ALA:HA	2.17	0.43
1:A:70:GLU:OE2	2:D:134:ASN:ND2	2.51	0.43
1:C:30:PRO:HD3	1:C:54:TRP:CD1	2.53	0.43
2:F:181:PHE:CD1	2:F:249:GLU:HG3	2.54	0.43
2:F:189:TYR:CD2	2:F:272:ALA:HB1	2.53	0.43
1:I:122:ASP:OD1	1:I:123:ILE:HG13	2.19	0.43
1:C:64:THR:HG22	1:C:65:ARG:N	2.34	0.43
2:E:279:LEU:HD12	2:E:279:LEU:HA	1.78	0.43
1:G:36:GLU:C	1:G:38:GLY:H	2.22	0.43
1:I:69:GLY:O	1:I:87:GLU:N	2.50	0.43
1:B:64:THR:O	1:B:82:THR:CG2	2.66	0.43
1:B:111:MET:HE2	1:B:125:CYS:CB	2.46	0.43
1:C:91:PHE:CE1	1:C:102:LYS:O	2.72	0.43
2:J:227:ARG:HA	2:K:239:LEU:O	2.18	0.43
2:K:182:TYR:O	2:K:247:ILE:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:150:LYS:HG3	2:L:151:ILE:N	2.33	0.43
2:L:196:ILE:H	2:L:196:ILE:HG12	1.58	0.43
1:B:26:GLY:O	1:B:27:LEU:HD23	2.18	0.43
1:C:79:THR:OG1	2:L:253:ASN:ND2	2.52	0.43
1:I:91:PHE:CD2	1:I:92:ARG:O	2.70	0.43
2:L:179:LYS:HB2	2:L:251:LYS:HA	2.00	0.43
2:L:198:GLU:HG3	2:L:199:ASN:N	2.34	0.43
2:E:150:LYS:HA	2:E:259:SER:HB2	2.00	0.43
2:F:280:VAL:CG2	2:F:281:GLY:N	2.79	0.43
1:I:99:MET:HG3	2:L:239:LEU:CD2	2.48	0.43
1:B:52:THR:O	1:B:53:HIS:ND1	2.52	0.42
2:E:264:HIS:C	2:E:265:LEU:HD23	2.39	0.42
1:I:66:CYS:HB3	1:I:70:GLU:HB3	2.01	0.42
2:J:197:LYS:H	2:J:202:ASN:HD21	1.67	0.42
2:J:243:TYR:CD1	2:J:244:GLN:N	2.87	0.42
1:G:53:HIS:CD2	2:L:218:ASP:OD2	2.71	0.42
2:L:243:TYR:CD1	2:L:244:GLN:N	2.88	0.42
1:C:49:ASP:HB2	1:C:60:CYS:HB3	2.01	0.42
1:I:29:PRO:C	1:I:30:PRO:O	2.57	0.42
1:I:67:ASP:C	1:I:68:SER:O	2.58	0.42
2:J:243:TYR:CD1	2:J:243:TYR:C	2.92	0.42
2:D:231:TRP:CD2	2:E:235:ALA:HA	2.53	0.42
2:F:123:ALA:O	2:F:124:ALA:HB2	2.19	0.42
2:L:150:LYS:NZ	2:L:173:GLU:OE2	2.53	0.42
2:L:181:PHE:CD1	2:L:249:GLU:HG3	2.54	0.42
1:A:50:TYR:CE2	1:A:81:ASN:HB2	2.55	0.42
1:B:34:ILE:HG12	1:B:38:GLY:HA2	2.01	0.42
2:F:131:GLY:O	2:F:269:ASP:HA	2.19	0.42
1:I:50:TYR:CZ	1:I:61:LEU:HD12	2.54	0.42
2:L:254:ASP:C	2:L:255:ARG:HG3	2.40	0.42
2:D:194:GLU:HB2	4:D:3088:HOH:O	2.19	0.42
1:G:21:SER:HB2	1:G:41:CYS:HB2	2.00	0.42
1:G:99:MET:HE1	2:J:191:ARG:HD2	1.99	0.42
1:G:108:PRO:O	1:G:109:ARG:C	2.57	0.42
1:G:126:VAL:HG13	1:G:127:HIS:N	2.35	0.42
1:I:102:LYS:HG3	2:L:236:GLU:OE1	2.18	0.42
2:L:169:LEU:HG	2:L:170:ARG:N	2.34	0.42
2:D:192:PHE:CD1	2:D:194:GLU:CG	2.86	0.42
2:F:212:LYS:HG2	2:F:222:LEU:HD21	2.01	0.42
1:G:104:ARG:HB2	1:G:123:ILE:HG12	2.02	0.42
1:H:81:ASN:ND2	1:H:82:THR:H	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:161:HIS:ND1	2:K:270:HIS:CD2	2.88	0.42
2:D:169:LEU:HD12	2:D:169:LEU:HA	1.89	0.42
2:F:208:GLN:O	2:F:224:LYS:HA	2.20	0.42
1:I:50:TYR:CD2	1:I:50:TYR:C	2.93	0.42
2:J:120:GLN:OE1	2:J:120:GLN:CA	2.67	0.42
2:J:214:THR:O	2:J:216:TYR:N	2.53	0.42
2:K:150:LYS:HA	2:K:259:SER:HA	2.02	0.42
2:K:190:PHE:CZ	2:K:266:ILE:HD11	2.55	0.42
2:K:243:TYR:CD1	2:K:243:TYR:C	2.92	0.42
2:L:224:LYS:O	2:L:224:LYS:HG3	2.19	0.42
1:B:59:PHE:CD2	2:E:159:SER:HA	2.55	0.42
2:D:181:PHE:HB2	2:D:280:VAL:HG23	2.02	0.42
2:D:189:TYR:HD2	2:D:272:ALA:HB1	1.85	0.42
2:E:243:TYR:CD1	2:E:244:GLN:N	2.87	0.42
1:I:123:ILE:HD12	1:I:123:ILE:O	2.20	0.42
2:J:173:GLU:HG2	2:J:257:PHE:HB3	2.02	0.42
2:K:175:VAL:HG22	2:K:255:ARG:CG	2.48	0.42
2:K:184:ILE:O	2:K:245:GLY:HA2	2.20	0.42
1:B:92:ARG:HG3	1:B:96:SER:O	2.20	0.41
1:C:76:CYS:H	2:L:170:ARG:CZ	2.33	0.41
2:K:207:VAL:HG13	2:K:226:ALA:HB2	2.01	0.41
2:E:126:ILE:HA	2:E:162:SER:HB2	2.02	0.41
2:E:130:ARG:O	2:E:130:ARG:HG3	2.20	0.41
1:G:73:LEU:HD21	1:G:85:GLN:CD	2.40	0.41
1:G:93:GLU:CG	1:G:94:GLU:N	2.67	0.41
2:K:197:LYS:H	2:K:202:ASN:HD21	1.67	0.41
1:A:86:CYS:SG	1:A:92:ARG:CD	3.06	0.41
1:B:106:GLY:O	1:B:123:ILE:HD11	2.20	0.41
1:B:120:TRP:CD2	1:B:120:TRP:N	2.86	0.41
2:F:173:GLU:HG2	2:F:257:PHE:HB3	2.02	0.41
2:J:189:TYR:HD2	2:J:272:ALA:HB1	1.85	0.41
1:C:62:ARG:NH1	2:F:270:HIS:ND1	2.68	0.41
1:C:75:PRO:HB3	2:L:170:ARG:CD	2.22	0.41
1:G:45:LYS:O	1:G:48:GLN:HB2	2.20	0.41
1:G:53:HIS:CD2	2:L:217:PRO:HB2	2.56	0.41
2:K:156:SER:O	2:K:157:SER:O	2.39	0.41
2:K:170:ARG:O	2:K:171:ASN:HB2	2.20	0.41
1:A:44:CYS:O	1:A:78:THR:HG22	2.21	0.41
1:G:107:CYS:HB3	1:G:108:PRO:CD	2.51	0.41
2:K:174:LEU:HB2	2:K:256:ILE:HG13	2.02	0.41
2:K:198:GLU:C	2:K:200:THR:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:GLY:HA2	1:A:78:THR:O	2.21	0.41
2:D:183:TYR:O	2:D:277:ALA:HA	2.21	0.41
2:D:225:SER:HG	2:D:227:ARG:HH12	1.67	0.41
2:E:130:ARG:HG2	2:E:269:ASP:OD1	2.21	0.41
2:F:150:LYS:HG3	2:F:151:ILE:N	2.36	0.41
1:H:63:CYS:HA	1:H:81:ASN:HD21	1.86	0.41
2:J:189:TYR:CD2	2:J:272:ALA:HB1	2.55	0.41
1:C:50:TYR:CZ	1:C:81:ASN:HB2	2.55	0.41
2:F:155:GLU:OE1	2:F:161:HIS:CE1	2.74	0.41
2:F:212:LYS:HE2	4:F:3119:HOH:O	2.19	0.41
2:K:126:ILE:HA	2:K:162:SER:HB2	2.02	0.41
1:B:30:PRO:HD3	1:B:54:TRP:CD1	2.55	0.41
2:F:181:PHE:O	2:F:280:VAL:HG22	2.20	0.41
1:G:85:GLN:CD	1:G:119:PRO:HG3	2.40	0.41
1:H:73:LEU:HD13	1:H:85:GLN:HB3	2.03	0.41
2:L:127:THR:HG23	2:L:162:SER:HB3	2.02	0.41
2:L:155:GLU:OE1	2:L:161:HIS:CE1	2.73	0.41
2:L:189:TYR:HD2	2:L:272:ALA:HB1	1.85	0.41
1:A:96:SER:N	1:A:97:PRO:HD3	2.36	0.41
1:B:64:THR:O	1:B:82:THR:HG21	2.21	0.41
1:C:22:SER:HA	1:C:23:PRO:HD3	1.82	0.41
2:E:174:LEU:HB2	2:E:256:ILE:HG13	2.03	0.41
2:E:190:PHE:CZ	2:E:266:ILE:HD11	2.56	0.41
1:H:86:CYS:SG	1:H:92:ARG:HB2	2.60	0.41
1:H:90:THR:CB	1:H:100:CYS:HB3	2.50	0.41
2:J:196:ILE:H	2:J:196:ILE:HG13	1.41	0.41
2:K:243:TYR:CD1	2:K:244:GLN:N	2.89	0.41
2:L:260:VAL:HG21	2:L:266:ILE:HD11	2.03	0.41
2:J:182:TYR:O	2:J:247:ILE:HA	2.21	0.41
2:K:161:HIS:ND1	2:K:270:HIS:CG	2.89	0.41
1:C:50:TYR:OH	1:C:81:ASN:HB2	2.20	0.40
1:C:77:THR:N	1:C:80:ARG:O	2.54	0.40
2:D:121:ARG:HG2	2:F:281:GLY:HA3	2.03	0.40
2:E:212:LYS:HA	2:E:255:ARG:O	2.21	0.40
2:L:126:ILE:HD12	2:L:154:TRP:CB	2.51	0.40
1:B:52:THR:HB	1:B:79:THR:O	2.22	0.40
2:D:199:ASN:HA	4:D:3157:HOH:O	2.21	0.40
2:D:227:ARG:CZ	2:D:242:ILE:HG12	2.52	0.40
1:H:22:SER:O	1:H:23:PRO:C	2.59	0.40
2:K:252:GLU:HG2	2:K:253:ASN:OD1	2.21	0.40
2:L:209:TYR:CD1	2:L:221:LEU:HD11	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:LEU:HB3	2:F:132:ARG:HH11	1.86	0.40
2:D:186:SER:HB3	2:D:208:GLN:NE2	2.36	0.40
2:D:189:TYR:CD2	2:D:272:ALA:HB1	2.56	0.40
2:E:270:HIS:CD2	2:E:271:GLU:HG3	2.57	0.40
1:I:29:PRO:O	1:I:30:PRO:O	2.40	0.40
1:B:29:PRO:O	1:B:30:PRO:C	2.60	0.40
1:H:42:ILE:HD12	1:H:42:ILE:N	2.29	0.40
1:H:50:TYR:HE1	1:H:81:ASN:ND2	2.20	0.40
2:J:198:GLU:H	2:J:198:GLU:CD	2.24	0.40
2:K:122:VAL:HG13	2:K:167:LEU:CD1	2.52	0.40
1:A:28:CYS:SG	1:A:34:ILE:HA	2.62	0.40
2:E:164:LEU:HD13	2:E:168:HIS:HA	2.04	0.40
1:I:118:THR:HA	1:I:119:PRO:HD3	1.95	0.40

All (4) 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)
4:B:3160:HOH:O	4:H:3078:HOH:O[1_554]	0.57	1.63
4:G:3053:HOH:O	4:I:3050:HOH:O[2_656]	1.19	1.01
4:B:3160:HOH:O	4:H:3105:HOH:O[1_554]	1.82	0.38
1:B:129:GLU:CG	4:H:3079:HOH:O[1_554]	1.85	0.35

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	86/130 (66%)	77 (90%)	6 (7%)	3 (4%)	3 1
1	B	108/130 (83%)	93 (86%)	12 (11%)	3 (3%)	5 2
1	C	86/130 (66%)	61 (71%)	23 (27%)	2 (2%)	6 3
1	G	106/130 (82%)	90 (85%)	14 (13%)	2 (2%)	8 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	86/130 (66%)	75 (87%)	9 (10%)	2 (2%)	6	3
1	I	86/130 (66%)	72 (84%)	10 (12%)	4 (5%)	2	1
2	D	148/168 (88%)	132 (89%)	13 (9%)	3 (2%)	7	4
2	E	148/168 (88%)	131 (88%)	12 (8%)	5 (3%)	3	1
2	F	148/168 (88%)	124 (84%)	20 (14%)	4 (3%)	5	2
2	J	148/168 (88%)	132 (89%)	13 (9%)	3 (2%)	7	4
2	K	148/168 (88%)	130 (88%)	13 (9%)	5 (3%)	3	1
2	L	148/168 (88%)	125 (84%)	19 (13%)	4 (3%)	5	2
All	All	1446/1788 (81%)	1242 (86%)	164 (11%)	40 (3%)	5	2

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	130	ARG
2	E	157	SER
2	E	197	LYS
2	E	280	VAL
1	H	25	GLU
1	I	118	THR
2	K	130	ARG
2	K	157	SER
2	K	197	LYS
2	K	280	VAL
2	L	197	LYS
1	A	68	SER
1	C	80	ARG
2	D	130	ARG
2	F	280	VAL
1	H	23	PRO
2	J	130	ARG
2	L	280	VAL
1	A	82	THR
1	B	30	PRO
1	C	50	TYR
2	F	134	ASN
1	I	119	PRO
2	L	134	ASN
1	A	51	SER
2	D	215	SER

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Mol	Chain	Res	Type
1	G	109	ARG
2	J	200	THR
1	B	113	LYS
2	D	198	GLU
1	I	68	SER
2	J	215	SER
2	L	153	SER
2	F	153	SER
2	F	196	ILE
1	B	96	SER
2	E	148	GLY
1	G	119	PRO
1	I	30	PRO
2	K	196	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	84/117 (72%)	64 (76%)	20 (24%)	0	0
1	B	97/117 (83%)	76 (78%)	21 (22%)	1	1
1	C	83/117 (71%)	62 (75%)	21 (25%)	0	0
1	G	99/117 (85%)	78 (79%)	21 (21%)	1	1
1	H	82/117 (70%)	61 (74%)	21 (26%)	0	0
1	I	84/117 (72%)	60 (71%)	24 (29%)	0	0
2	D	134/149 (90%)	117 (87%)	17 (13%)	4	3
2	E	134/149 (90%)	111 (83%)	23 (17%)	2	1
2	F	133/149 (89%)	119 (90%)	14 (10%)	7	6
2	J	133/149 (89%)	113 (85%)	20 (15%)	3	2
2	K	134/149 (90%)	114 (85%)	20 (15%)	3	2
2	L	131/149 (88%)	113 (86%)	18 (14%)	3	3
All	All	1328/1596 (83%)	1088 (82%)	240 (18%)	1	1

All (240) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	SER
1	A	24	SER
1	A	39	ARG
1	A	40	ASP
1	A	45	LYS
1	A	48	GLN
1	A	49	ASP
1	A	52	THR
1	A	58	LEU
1	A	65	ARG
1	A	66	CYS
1	A	71	VAL
1	A	73	LEU
1	A	74	SER
1	A	76	CYS
1	A	80	ARG
1	A	81	ASN
1	A	87	GLU
1	A	102	LYS
1	A	123	ILE
1	B	22	SER
1	B	24	SER
1	B	27	LEU
1	B	36	GLU
1	B	48	GLN
1	B	52	THR
1	B	58	LEU
1	B	65	ARG
1	B	68	SER
1	B	72	GLU
1	B	74	SER
1	B	82	THR
1	B	93	GLU
1	B	101	ARG
1	B	104	ARG
1	B	109	ARG
1	B	111	MET
1	B	114	VAL
1	B	118	THR
1	B	120	TRP
1	B	121	SER
1	C	22	SER

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Mol	Chain	Res	Type
1	C	34	ILE
1	C	39	ARG
1	C	40	ASP
1	C	49	ASP
1	C	51	SER
1	C	57	LEU
1	C	58	LEU
1	C	62	ARG
1	C	67	ASP
1	C	68	SER
1	C	73	LEU
1	C	74	SER
1	C	80	ARG
1	C	82	THR
1	C	83	VAL
1	C	92	ARG
1	C	101	ARG
1	C	116	ASP
1	C	118	THR
1	C	120	TRP
2	D	120	GLN
2	D	126	ILE
2	D	127	THR
2	D	130	ARG
2	D	132	ARG
2	D	153	SER
2	D	158	ARG
2	D	167	LEU
2	D	178	GLU
2	D	179	LYS
2	D	195	GLU
2	D	196	ILE
2	D	218	ASP
2	D	233	LYS
2	D	251	LYS
2	D	256	ILE
2	D	263	GLU
2	E	121	ARG
2	E	130	ARG
2	E	149	ARG
2	E	156	SER
2	E	157	SER

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Mol	Chain	Res	Type
2	E	158	ARG
2	E	161	HIS
2	E	167	LEU
2	E	179	LYS
2	E	194	GLU
2	E	197	LYS
2	E	201	LYS
2	E	212	LYS
2	E	215	SER
2	E	228	ASN
2	E	230	CYS
2	E	233	LYS
2	E	241	SER
2	E	244	GLN
2	E	251	LYS
2	E	259	SER
2	E	274	PHE
2	E	280	VAL
2	F	127	THR
2	F	130	ARG
2	F	133	SER
2	F	158	ARG
2	F	195	GLU
2	F	215	SER
2	F	218	ASP
2	F	233	LYS
2	F	234	ASP
2	F	244	GLN
2	F	251	LYS
2	F	256	ILE
2	F	263	GLU
2	F	266	ILE
1	G	34	ILE
1	G	45	LYS
1	G	52	THR
1	G	58	LEU
1	G	62	ARG
1	G	67	ASP
1	G	68	SER
1	G	77	THR
1	G	80	ARG
1	G	88	GLU

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Mol	Chain	Res	Type
1	G	93	GLU
1	G	102	LYS
1	G	105	THR
1	G	111	MET
1	G	116	ASP
1	G	117	CYS
1	G	118	THR
1	G	121	SER
1	G	124	GLU
1	G	126	VAL
1	G	128	LYS
1	H	24	SER
1	H	25	GLU
1	H	39	ARG
1	H	43	SER
1	H	45	LYS
1	H	49	ASP
1	H	51	SER
1	H	52	THR
1	H	56	ASP
1	H	62	ARG
1	H	67	ASP
1	H	73	LEU
1	H	74	SER
1	H	81	ASN
1	H	82	THR
1	H	88	GLU
1	H	93	GLU
1	H	116	ASP
1	H	117	CYS
1	H	120	TRP
1	H	121	SER
1	I	21	SER
1	I	22	SER
1	I	34	ILE
1	I	37	ASP
1	I	39	ARG
1	I	40	ASP
1	I	42	ILE
1	I	43	SER
1	I	45	LYS
1	I	52	THR

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Mol	Chain	Res	Type
1	I	58	LEU
1	I	62	ARG
1	I	65	ARG
1	I	67	ASP
1	I	68	SER
1	I	71	VAL
1	I	80	ARG
1	I	82	THR
1	I	88	GLU
1	I	92	ARG
1	I	99	MET
1	I	116	ASP
1	I	118	THR
1	I	123	ILE
2	J	120	GLN
2	J	126	ILE
2	J	127	THR
2	J	130	ARG
2	J	132	ARG
2	J	153	SER
2	J	158	ARG
2	J	167	LEU
2	J	178	GLU
2	J	179	LYS
2	J	196	ILE
2	J	199	ASN
2	J	200	THR
2	J	218	ASP
2	J	224	LYS
2	J	233	LYS
2	J	239	LEU
2	J	251	LYS
2	J	256	ILE
2	J	263	GLU
2	K	121	ARG
2	K	130	ARG
2	K	149	ARG
2	K	156	SER
2	K	157	SER
2	K	158	ARG
2	K	161	HIS
2	K	179	LYS

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Mol	Chain	Res	Type
2	K	194	GLU
2	K	197	LYS
2	K	201	LYS
2	K	212	LYS
2	K	215	SER
2	K	233	LYS
2	K	241	SER
2	K	244	GLN
2	K	251	LYS
2	K	259	SER
2	K	274	PHE
2	K	280	VAL
2	L	130	ARG
2	L	133	SER
2	L	152	ASN
2	L	156	SER
2	L	158	ARG
2	L	194	GLU
2	L	195	GLU
2	L	196	ILE
2	L	215	SER
2	L	218	ASP
2	L	225	SER
2	L	233	LYS
2	L	234	ASP
2	L	244	GLN
2	L	251	LYS
2	L	256	ILE
2	L	263	GLU
2	L	266	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	48	GLN
1	A	81	ASN
1	B	32	HIS
1	B	33	HIS
1	B	81	ASN
1	C	33	HIS
2	D	134	ASN

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Mol	Chain	Res	Type
2	D	208	GLN
2	D	228	ASN
2	D	270	HIS
2	E	134	ASN
2	E	171	ASN
2	E	202	ASN
2	E	228	ASN
2	F	161	HIS
2	F	208	GLN
2	F	270	HIS
1	G	32	HIS
1	H	32	HIS
1	H	33	HIS
1	H	81	ASN
1	I	32	HIS
1	I	33	HIS
1	I	48	GLN
1	I	53	HIS
2	J	202	ASN
2	J	208	GLN
2	J	228	ASN
2	J	270	HIS
2	K	134	ASN
2	K	171	ASN
2	K	202	ASN
2	K	228	ASN
2	K	270	HIS
2	L	161	HIS
2	L	208	GLN
2	L	253	ASN
2	L	270	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)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	I	1
2	D	1
2	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	117:CYS	C	118:THR	N	1.82
1	D	191:ARG	C	192:PHE	N	1.20
1	F	191:ARG	C	192:PHE	N	1.12

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.