Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 01:31 AM EDT

PDB ID	:	3EUH
Title	:	Crystal Structure of the MukE-MukF Complex
Authors	:	Suh, M.K.; Ku, B.; Ha, N.C.; Woo, J.S.; Oh, B.H.
Deposited on	:	2008-10-10
Resolution	:	2.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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:

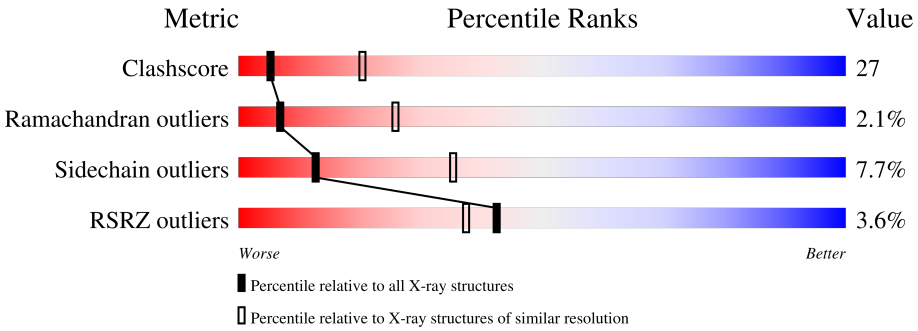
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	440	38% 31% • 28%
1	B	440	2% 40% 29% • 27%
2	C	234	3% 56% 26% 6% 12%
2	D	234	5% 44% 34% • 20%
2	E	234	3% 47% 35% • 14%
2	F	234	6% 31% 42% • 22%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11564 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.

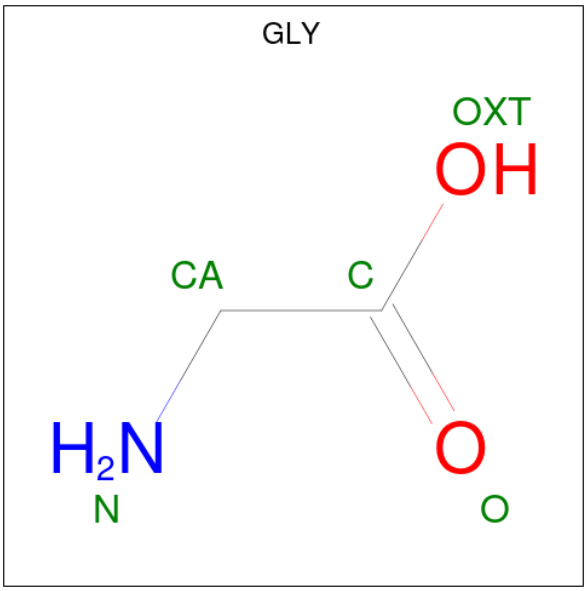
- Molecule 1 is a protein called Chromosome partition protein mukF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	0	0
			2549	1598	454	489	8			
1	B	321	Total	C	N	O	S	0	0	0
			2596	1625	463	500	8			

- Molecule 2 is a protein called MukE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	206	Total	C	N	O	S	0	0	0
			1673	1058	298	309	8			
2	D	188	Total	C	N	O	S	0	0	0
			1542	984	274	277	7			
2	E	201	Total	C	N	O	S	0	0	0
			1629	1035	287	299	8			
2	F	182	Total	C	N	O	S	0	0	0
			1498	960	265	266	7			

- Molecule 3 is GLYCINE (three-letter code: GLY) (formula: $C_2H_5NO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 5 2 1 2	0	0
3	D	1	Total C N O 5 2 1 2	0	0
3	D	1	Total C N O 5 2 1 2	0	0
3	D	1	Total C N O 5 2 1 2	0	0

- Molecule 4 is water.

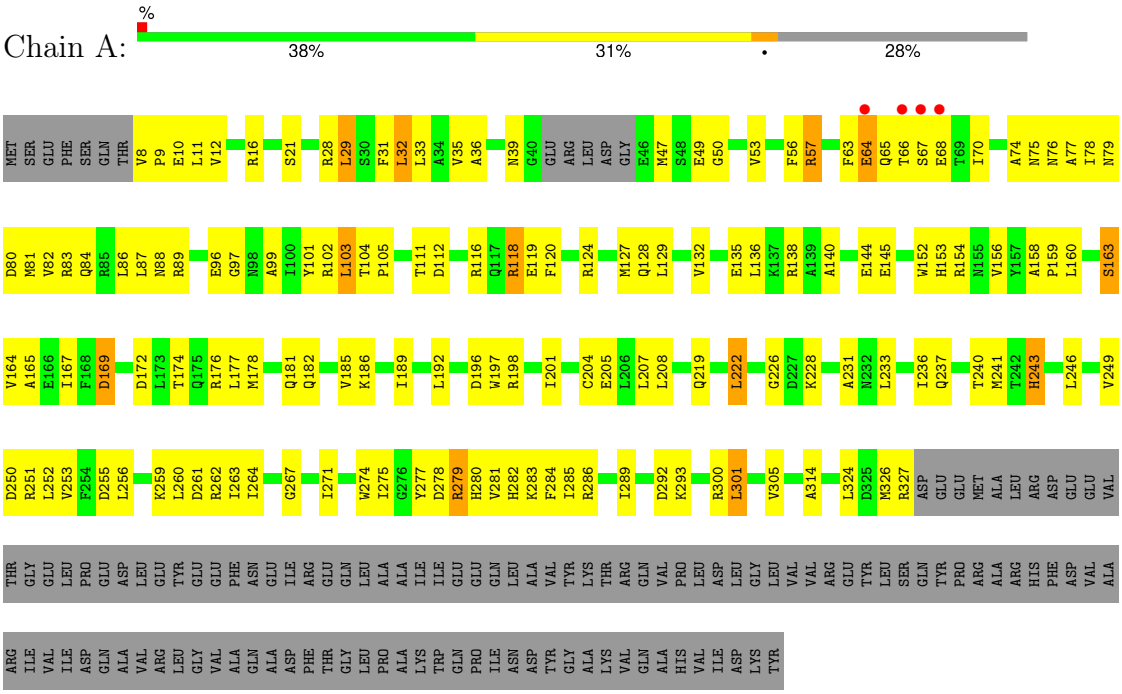
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	14	Total O 14 14	0	0
4	B	11	Total O 11 11	0	0
4	C	12	Total O 12 12	0	0
4	D	10	Total O 10 10	0	0
4	E	6	Total O 6 6	0	0
4	F	4	Total O 4 4	0	0

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.

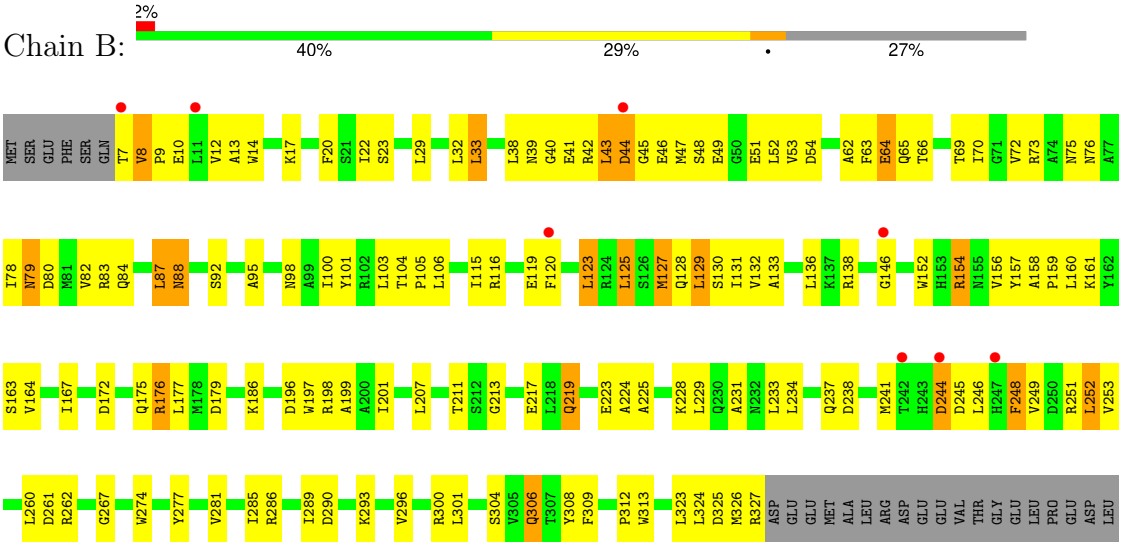
• Molecule 1: Chromosome partition protein mukF

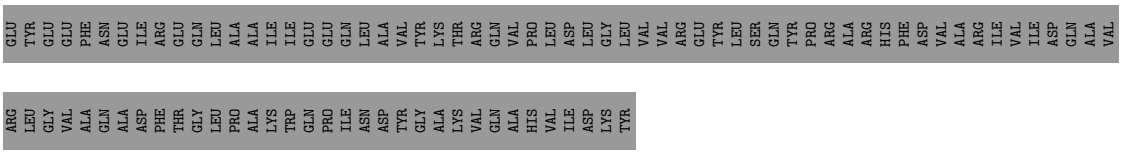
Chain A:



• Molecule 1: Chromosome partition protein mukF

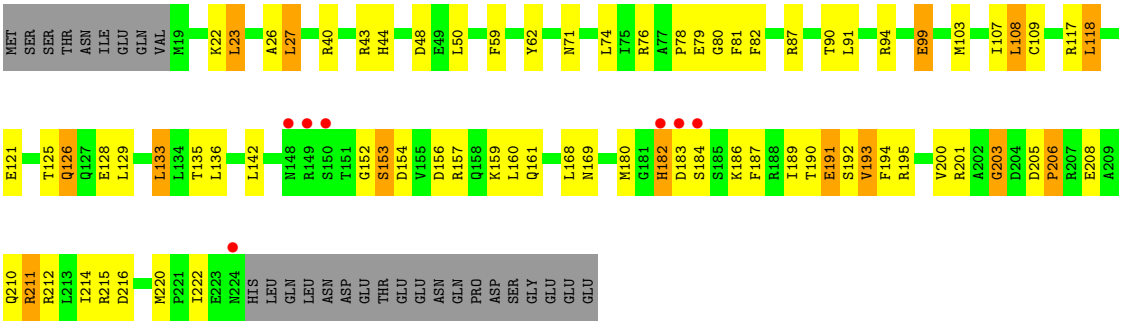
Chain B:





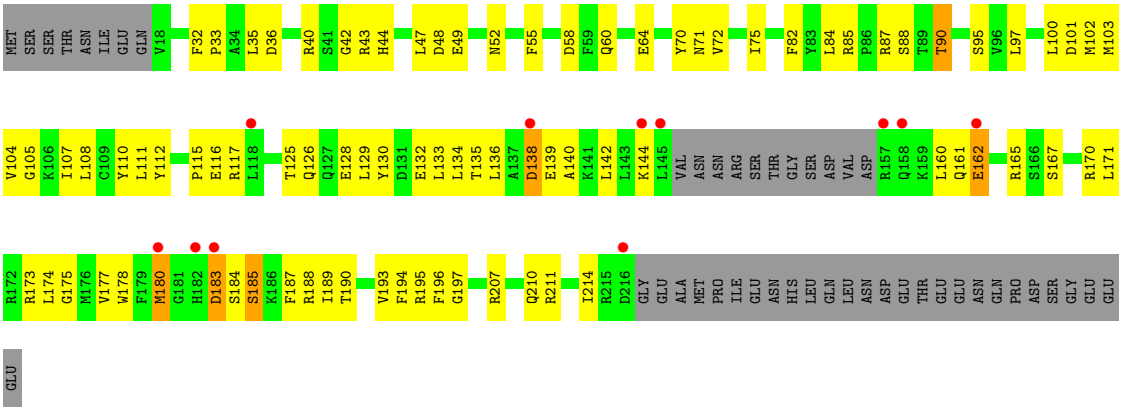
• Molecule 2: MukE

Chain C:



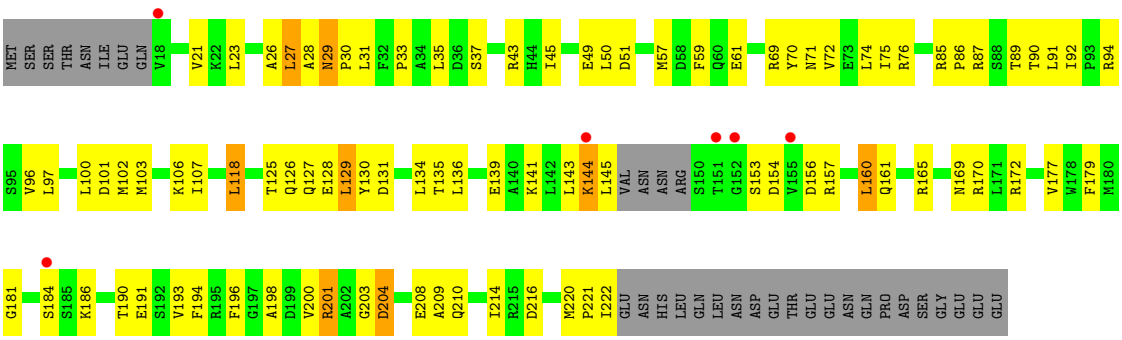
• Molecule 2: MukE

Chain D:



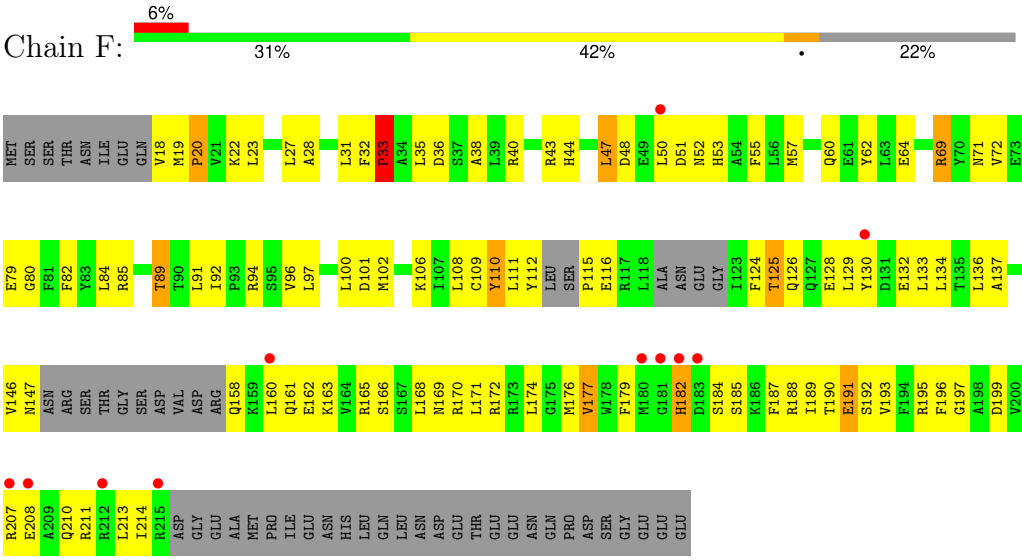
• Molecule 2: MukE

Chain E:



• Molecule 2: MukE

Chain F:


6%
31%
42%
22%
MET SER SER THR ASN ILE GLU GLN V18 M19 P20 V21 K22 L23 L27 A28 L31 F32 P33 A34 L35 D36 S37 A38 L39 R40 R43 H44 L47 D48 E49 L50 D51 N52 H53 A54 F55 L56 M57 Q60 E61 Y62 L63 E64 R69 Y70 N71 V72 E73 L74 I75 R76 A77 P78
E79 G80 F81 F82 Y83 L84 R85 T89 T90 L91 I92 P93 R94 S95 V96 L97 L100 D101 M102 K106 I107 L108 C109 Y110 L111 Y112 LEU SER P115 E116 R117 L118 ALA ASN GLU GLY I123 F124 T125 Q126 Q127 E128 L129 Y130 D131 E132 L133 L134 T135 L136 A137 K141 L142 L143 K144 L145
V146 N147 ASN ARG SER THR GLY SER ASP VAL ASP ARG Q158 K159 L160 Q161 E162 K163 V164 R165 S166 S167 L168 N169 R170 L171 R172 R173 L174 G175 M176 V177 W178 F179 M180 G181 H182 D183 S184 S185 K186 F187 R188 I189 T190 E191 S192 V193 F194 R195 F196 G197 A198 D199 V200 R201 A202 G203 P206
R207 E208 A209 Q210 R211 R212 L213 I214 R215 ASP GLY GLU GLU ALA MET PRO ILE GLU GLU ASN HIS LEU GLN LEU ASN ASP GLU THR GLU GLU ASN GLN PRO ASP SER GLY GLU GLU GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	77.34Å 151.15Å 188.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 29.87 – 2.69	Depositor EDS
% Data completeness (in resolution range)	98.0 (20.00-2.90) 96.5 (29.87-2.69)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.55 (at 2.68Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.225 , 0.274 0.240 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	60.5	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 55.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	11564	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.39	0/2592	0.59	0/3506
1	B	0.37	0/2640	0.59	0/3572
2	C	0.46	0/1704	0.69	1/2296 (0.0%)
2	D	0.47	0/1571	0.70	0/2114
2	E	0.41	0/1659	0.64	0/2234
2	F	0.36	0/1525	0.61	0/2049
All	All	0.41	0/11691	0.63	1/15771 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	80	GLY	N-CA-C	5.18	126.05	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2549	0	2498	169	0
1	B	2596	0	2543	139	0
2	C	1673	0	1672	82	0
2	D	1542	0	1556	67	0
2	E	1629	0	1634	95	0
2	F	1498	0	1517	125	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	5	0	2	0	0
3	D	15	0	9	0	0
4	A	14	0	0	0	0
4	B	11	0	0	0	0
4	C	12	0	0	0	0
4	D	10	0	0	0	0
4	E	6	0	0	1	0
4	F	4	0	0	0	0
All	All	11564	0	11431	609	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 27.

All (609) 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:B:8:VAL:HB	1:B:9:PRO:HD3	1.28	1.09
2:E:125:THR:HG22	2:E:127:GLN:H	1.27	0.99
1:A:300:ARG:HH22	2:C:203:GLY:HA2	1.26	0.99
2:C:205:ASP:HB3	2:C:208:GLU:HB2	1.44	0.97
1:B:196:ASP:HB3	1:B:199:ALA:HB3	1.45	0.96
1:A:102:ARG:HH12	1:B:262:ARG:HH12	1.04	0.95
1:B:80:ASP:HA	1:B:83:ARG:HG2	1.48	0.95
2:D:100:LEU:O	2:D:104:VAL:HG23	1.67	0.94
2:F:75:ILE:HD11	2:F:85:ARG:CZ	1.99	0.93
1:B:23:SER:H	1:B:84:GLN:HE22	1.19	0.91
1:A:262:ARG:HE	1:B:42:ARG:HH11	1.19	0.91
2:E:90:THR:HG22	2:E:92:ILE:H	1.35	0.89
2:E:29:ASN:HD22	2:E:31:LEU:H	1.20	0.89
2:E:70:TYR:HA	2:E:91:LEU:HD12	1.53	0.89
1:B:23:SER:H	1:B:84:GLN:NE2	1.71	0.88
2:D:190:THR:O	2:D:193:VAL:HG23	1.72	0.88
1:B:125:LEU:HD22	1:B:129:LEU:HD22	1.56	0.87
1:B:198:ARG:HD2	1:B:293:LYS:HE3	1.55	0.87
2:E:141:LYS:O	2:E:144:LYS:HB3	1.74	0.87
2:E:126:GLN:HE22	2:E:165:ARG:HH11	1.18	0.86
2:E:134:LEU:HD22	2:E:139:GLU:HG3	1.56	0.86
1:A:102:ARG:NH1	1:B:262:ARG:HH12	1.72	0.86
2:F:47:LEU:H	2:F:47:LEU:HD12	1.39	0.85
2:E:125:THR:HB	2:E:128:GLU:HG3	1.57	0.85
2:C:44:HIS:HE1	2:C:195:ARG:HH11	1.17	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:176:MET:O	2:F:177:VAL:HG23	1.78	0.84
2:C:44:HIS:CE1	2:C:195:ARG:HH11	1.95	0.83
2:E:29:ASN:ND2	2:E:31:LEU:H	1.77	0.82
1:A:28:ARG:HG2	1:A:28:ARG:HH11	1.43	0.82
2:E:126:GLN:NE2	2:E:165:ARG:HH11	1.76	0.82
2:D:125:THR:OG1	2:D:128:GLU:HG3	1.80	0.81
1:A:118:ARG:HD2	1:A:120:PHE:H	1.43	0.81
1:B:219:GLN:HE21	1:B:267:GLY:HA3	1.43	0.81
2:C:23:LEU:HD22	2:C:27:LEU:HD22	1.62	0.80
1:A:262:ARG:HE	1:B:42:ARG:NH1	1.80	0.80
1:B:306:GLN:HE21	1:B:306:GLN:HA	1.47	0.80
1:B:72:VAL:HG12	1:B:76:ASN:HD21	1.47	0.80
1:A:118:ARG:HD3	1:A:120:PHE:CD2	2.16	0.79
1:A:102:ARG:HH12	1:B:262:ARG:NH1	1.80	0.79
2:C:159:LYS:HE2	2:C:159:LYS:HA	1.64	0.79
2:F:47:LEU:HD12	2:F:47:LEU:N	1.97	0.79
2:D:107:ILE:HD13	2:D:214:ILE:HD13	1.64	0.79
1:A:67:SER:HA	1:A:70:ILE:HG13	1.65	0.79
2:F:125:THR:HG23	2:F:128:GLU:HG3	1.65	0.79
1:A:300:ARG:CB	2:C:200:VAL:HG11	2.13	0.78
2:F:69:ARG:HG2	2:F:69:ARG:HH11	1.47	0.77
1:B:286:ARG:HA	1:B:290:ASP:OD2	1.86	0.76
2:F:197:GLY:HA2	2:F:210:GLN:OE1	1.85	0.76
2:F:32:PHE:HB3	2:F:33:PRO:HD3	1.67	0.76
2:F:146:VAL:HG21	2:F:160:LEU:HG	1.66	0.76
1:B:43:LEU:HD12	1:B:44:ASP:N	2.00	0.76
1:B:198:ARG:HD3	1:B:293:LYS:HG3	1.68	0.75
2:D:105:GLY:HA2	2:D:108:LEU:HD12	1.68	0.74
1:A:222:LEU:HD11	1:A:263:ILE:HG22	1.69	0.74
2:F:44:HIS:CE1	2:F:195:ARG:HH11	2.05	0.74
1:A:300:ARG:HB3	2:C:200:VAL:HG11	1.69	0.73
1:A:57:ARG:HH11	1:A:57:ARG:HB3	1.54	0.73
2:F:168:LEU:HD21	2:F:177:VAL:HG11	1.71	0.73
2:F:146:VAL:HG22	2:F:163:LYS:HD2	1.71	0.71
2:F:47:LEU:H	2:F:47:LEU:CD1	2.03	0.70
1:A:169:ASP:OD1	1:A:259:LYS:HE2	1.91	0.70
1:B:8:VAL:HB	1:B:9:PRO:CD	2.15	0.70
1:A:178:MET:HE1	1:A:181:GLN:HG2	1.73	0.70
1:B:163:SER:O	1:B:167:ILE:HG13	1.92	0.70
1:A:12:VAL:O	1:A:16:ARG:HG3	1.91	0.70
1:B:301:LEU:O	1:B:304:SER:HB3	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:ARG:H	2:F:102:MET:HE3	1.57	0.70
2:C:78:PRO:HG2	2:C:79:GLU:OE2	1.92	0.70
2:F:75:ILE:HG22	2:F:76:ARG:N	2.07	0.70
1:A:89:ARG:NH1	1:A:101:TYR:OH	2.25	0.69
2:C:107:ILE:HD13	2:C:133:LEU:HA	1.72	0.69
2:E:144:LYS:O	2:E:144:LYS:HG2	1.91	0.69
2:F:78:PRO:HG2	2:F:79:GLU:OE2	1.91	0.69
2:D:126:GLN:HG2	2:D:185:SER:O	1.91	0.69
2:E:198:ALA:HA	2:E:201:ARG:HD3	1.74	0.69
2:F:210:GLN:O	2:F:214:ILE:HG12	1.91	0.69
1:B:161:LYS:HB2	1:B:252:LEU:HD11	1.73	0.68
1:B:8:VAL:CB	1:B:9:PRO:HD3	2.15	0.68
1:A:249:VAL:HG12	1:A:249:VAL:O	1.92	0.68
1:A:118:ARG:HD2	1:A:119:GLU:N	2.09	0.68
2:C:157:ARG:O	2:C:161:GLN:HG3	1.94	0.68
2:F:69:ARG:HG2	2:F:69:ARG:NH1	2.09	0.68
1:A:136:LEU:HD13	1:A:164:VAL:HG21	1.77	0.67
1:A:135:GLU:OE1	1:A:163:SER:HB3	1.94	0.67
2:D:197:GLY:HA2	2:D:210:GLN:HE22	1.60	0.67
1:A:300:ARG:NH2	2:C:203:GLY:HA2	2.05	0.67
2:D:44:HIS:CE1	2:D:195:ARG:HH11	2.13	0.67
1:A:66:THR:HG22	1:A:68:GLU:H	1.60	0.67
1:A:118:ARG:CD	1:A:120:PHE:H	2.07	0.66
1:A:152:TRP:CZ3	1:A:246:LEU:HD13	2.30	0.66
1:B:300:ARG:NH1	2:E:203:GLY:HA2	2.11	0.66
1:A:165:ALA:HB2	1:A:256:LEU:HD21	1.77	0.66
2:D:142:LEU:HG	2:D:160:LEU:HD21	1.78	0.66
2:F:57:MET:SD	2:F:76:ARG:NH1	2.69	0.65
2:D:130:TYR:CZ	2:D:161:GLN:HG3	2.31	0.65
2:D:189:ILE:CG2	2:D:193:VAL:HG21	2.26	0.65
2:F:116:GLU:O	2:F:116:GLU:HG2	1.95	0.65
2:F:137:ALA:HB3	2:F:142:LEU:HD22	1.76	0.65
1:A:89:ARG:HG3	1:A:101:TYR:CE1	2.32	0.64
2:E:26:ALA:HB2	2:E:59:PHE:CD2	2.33	0.64
1:A:262:ARG:NE	1:B:42:ARG:HH11	1.92	0.64
2:D:48:ASP:CG	2:D:188:ARG:HH12	2.00	0.64
1:A:324:LEU:HD22	2:D:97:LEU:CD1	2.27	0.64
1:B:225:ALA:O	1:B:229:LEU:HD13	1.98	0.64
2:E:90:THR:HG22	2:E:92:ILE:N	2.11	0.64
2:D:101:ASP:OD2	2:D:170:ARG:NH2	2.31	0.64
1:B:198:ARG:CD	1:B:293:LYS:HE3	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:144:LYS:HG3	2:F:147:ASN:HD22	1.61	0.63
2:F:146:VAL:HA	2:F:163:LYS:HZ2	1.63	0.63
2:E:143:LEU:C	2:E:145:LEU:H	2.00	0.63
2:F:146:VAL:HA	2:F:163:LYS:NZ	2.14	0.63
1:A:324:LEU:HD22	2:D:97:LEU:HD12	1.80	0.63
1:A:35:VAL:HG13	1:A:47:MET:CE	2.28	0.63
1:B:42:ARG:CZ	1:B:46:GLU:OE2	2.47	0.63
1:A:222:LEU:HD13	1:A:264:ILE:HD13	1.80	0.63
1:B:87:LEU:CD1	1:B:103:LEU:HD23	2.29	0.62
1:B:158:ALA:HB3	1:B:159:PRO:HD3	1.80	0.62
2:C:220:MET:HE3	2:C:220:MET:HA	1.81	0.62
2:E:130:TYR:HE1	2:E:160:LEU:HD13	1.65	0.62
1:B:7:THR:HG22	1:B:8:VAL:H	1.64	0.62
1:A:74:ALA:O	1:A:78:ILE:HG13	1.99	0.62
1:A:262:ARG:HG3	1:B:42:ARG:CZ	2.29	0.62
1:B:72:VAL:HG12	1:B:76:ASN:ND2	2.13	0.62
2:C:211:ARG:HG3	2:C:211:ARG:HH11	1.64	0.62
1:A:32:LEU:HG	1:A:81:MET:CE	2.30	0.61
2:F:75:ILE:HD11	2:F:85:ARG:NH1	2.14	0.61
1:A:240:THR:CG2	1:A:250:ASP:HB2	2.29	0.61
1:A:49:GLU:O	1:A:53:VAL:HG23	2.00	0.61
2:F:71:ASN:HB3	2:F:89:THR:HG22	1.82	0.61
2:F:72:VAL:HG21	2:F:92:ILE:HD12	1.83	0.61
1:A:160:LEU:HB2	1:A:252:LEU:HD21	1.81	0.61
1:B:63:PHE:O	1:B:65:GLN:HG3	2.01	0.61
1:A:36:ALA:HB2	1:A:111:THR:HG21	1.83	0.61
1:A:300:ARG:HB2	2:C:200:VAL:HG11	1.81	0.61
2:C:125:THR:HG22	2:C:186:LYS:HG2	1.82	0.61
1:A:12:VAL:HG11	1:B:62:ALA:HB1	1.81	0.61
1:A:219:GLN:NE2	1:A:267:GLY:HA3	2.16	0.61
1:B:42:ARG:NH1	1:B:46:GLU:OE2	2.34	0.61
2:E:126:GLN:NE2	2:E:165:ARG:NH1	2.48	0.61
2:D:130:TYR:CE1	2:D:161:GLN:HG3	2.36	0.61
2:F:129:LEU:O	2:F:133:LEU:HB2	2.00	0.61
2:F:176:MET:SD	2:F:196:PHE:HE2	2.24	0.60
2:C:182:HIS:CD2	2:C:182:HIS:H	2.18	0.60
2:C:190:THR:HG22	2:C:191:GLU:N	2.15	0.60
1:B:23:SER:N	1:B:84:GLN:NE2	2.45	0.60
2:E:96:VAL:HG11	2:E:220:MET:HB2	1.82	0.60
1:A:28:ARG:O	1:A:31:PHE:HB3	2.02	0.60
2:D:32:PHE:HB3	2:D:33:PRO:HD3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:69:ARG:HH12	2:F:28:ALA:HA	1.65	0.60
2:D:125:THR:HG23	2:D:128:GLU:OE2	2.02	0.60
1:A:176:ARG:HH22	1:A:262:ARG:NH2	1.99	0.59
2:E:33:PRO:HG2	4:E:245:HOH:O	2.02	0.59
2:F:158:GLN:HA	2:F:161:GLN:HB2	1.84	0.59
2:C:23:LEU:CD2	2:C:27:LEU:HD22	2.32	0.59
2:E:154:ASP:HA	2:E:157:ARG:HB2	1.83	0.59
2:F:72:VAL:CG1	2:F:84:LEU:HG	2.32	0.59
1:A:189:ILE:HG23	1:A:204:CYS:SG	2.42	0.59
1:B:23:SER:N	1:B:84:GLN:HE22	1.95	0.59
2:C:201:ARG:HG2	2:C:201:ARG:HH11	1.67	0.59
2:F:189:ILE:HG23	2:F:193:VAL:HG21	1.85	0.59
1:A:105:PRO:HG2	1:B:177:LEU:HD12	1.84	0.58
1:B:246:LEU:HD12	1:B:248:PHE:HE2	1.67	0.58
2:C:125:THR:OG1	2:C:128:GLU:HG3	2.02	0.58
2:D:72:VAL:CG1	2:D:84:LEU:HB3	2.34	0.58
2:D:47:LEU:C	2:D:49:GLU:H	2.06	0.58
1:A:104:THR:HB	1:A:105:PRO:CD	2.34	0.58
1:B:207:LEU:O	1:B:211:THR:HG23	2.03	0.58
2:F:71:ASN:ND2	2:F:89:THR:HG23	2.18	0.58
2:F:72:VAL:HG11	2:F:84:LEU:HG	1.85	0.58
1:B:213:GLY:O	1:B:217:GLU:HG3	2.03	0.58
2:F:111:LEU:HD21	2:F:132:GLU:HG3	1.86	0.58
1:A:28:ARG:HG2	1:A:28:ARG:NH1	2.12	0.58
1:A:32:LEU:HG	1:A:81:MET:HE1	1.86	0.58
1:B:219:GLN:HE21	1:B:267:GLY:CA	2.12	0.58
2:C:108:LEU:HB3	2:C:193:VAL:HG21	1.86	0.58
1:A:35:VAL:HG13	1:A:47:MET:HE3	1.85	0.57
1:A:50:GLY:HA3	1:A:96:GLU:HG2	1.86	0.57
2:E:210:GLN:O	2:E:214:ILE:HG13	2.05	0.57
1:B:43:LEU:HD12	1:B:44:ASP:H	1.69	0.57
2:D:87:ARG:O	2:D:90:THR:HG22	2.05	0.57
2:E:71:ASN:ND2	2:E:89:THR:O	2.36	0.57
2:E:86:PRO:CG	2:E:94:ARG:HB2	2.35	0.57
2:F:190:THR:O	2:F:193:VAL:HG23	2.04	0.57
1:B:49:GLU:O	1:B:53:VAL:HG23	2.04	0.56
2:E:31:LEU:HD11	2:E:51:ASP:HB3	1.86	0.56
2:E:200:VAL:HG12	2:E:200:VAL:O	2.04	0.56
1:B:286:ARG:O	1:B:286:ARG:HG2	2.05	0.56
1:B:38:LEU:O	1:B:41:GLU:HG2	2.06	0.56
2:C:200:VAL:HG12	2:C:200:VAL:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:VAL:O	1:B:159:PRO:HD2	2.05	0.56
2:E:86:PRO:HG3	2:E:94:ARG:HB2	1.86	0.56
2:F:108:LEU:O	2:F:189:ILE:HD13	2.05	0.56
1:B:327:ARG:HG2	2:F:96:VAL:HG12	1.87	0.56
2:F:168:LEU:CD2	2:F:177:VAL:HG11	2.35	0.56
1:A:153:HIS:HD2	1:B:127:MET:SD	2.29	0.56
2:C:182:HIS:CD2	2:C:182:HIS:N	2.74	0.56
1:A:67:SER:HA	1:A:70:ILE:CG1	2.36	0.56
1:A:241:MET:CE	1:A:241:MET:HA	2.36	0.56
1:A:260:LEU:O	1:A:264:ILE:HG12	2.05	0.56
1:B:48:SER:OG	1:B:51:GLU:HG3	2.06	0.56
1:A:57:ARG:HB3	1:A:57:ARG:NH1	2.21	0.55
1:A:136:LEU:HD21	1:A:233:LEU:HG	1.86	0.55
1:B:327:ARG:HG2	2:F:96:VAL:CG1	2.35	0.55
1:A:178:MET:HE1	1:A:181:GLN:CG	2.36	0.55
1:B:325:ASP:OD1	2:F:94:ARG:NH1	2.39	0.55
2:C:117:ARG:HG2	2:C:117:ARG:HH11	1.70	0.55
1:A:8:VAL:N	1:A:9:PRO:CD	2.69	0.55
1:A:198:ARG:HD2	1:A:293:LYS:HG2	1.87	0.55
1:A:140:ALA:O	1:A:144:GLU:HB2	2.06	0.55
1:B:326:MET:HA	2:F:102:MET:HE1	1.89	0.55
2:C:107:ILE:CD1	2:C:133:LEU:HA	2.36	0.55
2:E:125:THR:HG22	2:E:127:GLN:N	2.10	0.55
1:B:42:ARG:HG3	1:B:45:GLY:O	2.07	0.55
1:B:136:LEU:HD11	1:B:233:LEU:HD23	1.89	0.55
2:C:205:ASP:HB3	2:C:208:GLU:CB	2.27	0.55
1:A:240:THR:HG23	1:A:246:LEU:O	2.07	0.54
1:B:115:ILE:HG13	1:B:116:ARG:N	2.22	0.54
2:D:134:LEU:HD23	2:D:142:LEU:CD2	2.36	0.54
2:E:29:ASN:HD22	2:E:29:ASN:C	2.09	0.54
1:A:198:ARG:HG3	1:A:289:ILE:HG22	1.88	0.54
1:B:324:LEU:HB2	2:F:174:LEU:HD21	1.88	0.54
2:D:60:GLN:O	2:D:64:GLU:HB2	2.08	0.54
1:A:152:TRP:CE3	1:A:246:LEU:HD13	2.43	0.54
1:A:240:THR:HG21	1:A:250:ASP:HB2	1.89	0.54
1:B:152:TRP:CE3	1:B:246:LEU:HD21	2.43	0.54
2:F:38:ALA:O	2:F:43:ARG:HB3	2.08	0.54
1:A:102:ARG:HG2	1:A:102:ARG:HH11	1.73	0.54
2:D:126:GLN:NE2	2:D:184:SER:HB3	2.23	0.54
2:E:29:ASN:HD22	2:E:30:PRO:N	2.06	0.53
2:F:32:PHE:HB3	2:F:33:PRO:CD	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:GLU:HG3	1:A:174:THR:OG1	2.09	0.53
2:C:126:GLN:OE1	2:C:168:LEU:HD23	2.09	0.53
2:F:36:ASP:O	2:F:40:ARG:HG3	2.09	0.53
1:A:283:LYS:HA	1:A:286:ARG:NH2	2.23	0.53
2:D:177:VAL:HG12	2:D:178:TRP:N	2.22	0.53
2:F:71:ASN:ND2	2:F:89:THR:CG2	2.71	0.53
1:A:78:ILE:O	1:A:82:VAL:HG23	2.08	0.53
1:A:120:PHE:CE1	1:A:178:MET:HE2	2.44	0.53
1:A:156:VAL:O	1:A:160:LEU:HG	2.07	0.53
1:A:178:MET:HA	1:A:178:MET:CE	2.39	0.53
1:A:118:ARG:HD2	1:A:120:PHE:N	2.20	0.53
1:A:120:PHE:CE1	1:A:177:LEU:HB3	2.43	0.53
2:F:38:ALA:HB1	2:F:43:ARG:HD3	1.90	0.53
2:F:166:SER:O	2:F:169:ASN:HB3	2.08	0.53
1:A:49:GLU:CD	2:E:186:LYS:HZ1	2.12	0.53
2:F:75:ILE:CG2	2:F:76:ARG:N	2.71	0.53
2:E:27:LEU:O	2:F:69:ARG:NH2	2.39	0.53
2:F:89:THR:HG23	2:F:89:THR:O	2.08	0.52
1:A:29:LEU:HD22	1:A:33:LEU:HD11	1.90	0.52
1:B:244:ASP:O	1:B:246:LEU:N	2.42	0.52
2:C:180:MET:HA	2:C:180:MET:CE	2.40	0.52
2:F:71:ASN:CB	2:F:89:THR:HG22	2.39	0.52
2:F:208:GLU:HA	2:F:211:ARG:HB3	1.90	0.52
2:D:44:HIS:HE1	2:D:195:ARG:HH11	1.56	0.52
2:F:60:GLN:O	2:F:64:GLU:HB2	2.09	0.52
1:A:208:LEU:HD13	1:A:278:ASP:OD2	2.09	0.52
1:B:75:ASN:O	1:B:79:ASN:HB2	2.10	0.52
2:C:71:ASN:HB2	2:C:90:THR:HA	1.92	0.52
2:F:89:THR:CG2	2:F:89:THR:O	2.57	0.52
2:D:180:MET:CE	2:D:180:MET:HA	2.40	0.52
1:A:279:ARG:NH1	1:A:279:ARG:HG2	2.25	0.52
1:B:327:ARG:H	2:F:102:MET:CE	2.23	0.52
2:E:130:TYR:CZ	2:E:161:GLN:HG3	2.45	0.52
1:A:281:VAL:O	1:A:285:ILE:HG13	2.10	0.52
1:A:31:PHE:O	1:A:35:VAL:HG23	2.10	0.51
1:A:301:LEU:O	1:A:305:VAL:HG23	2.09	0.51
2:E:69:ARG:HH21	2:F:33:PRO:CD	2.23	0.51
1:B:128:GLN:O	1:B:132:VAL:HG23	2.10	0.51
2:E:193:VAL:O	2:E:196:PHE:HB2	2.09	0.51
1:A:158:ALA:HB3	1:A:159:PRO:HD3	1.93	0.51
1:B:313:TRP:C	2:E:222:ILE:HD11	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:112:TYR:HA	2:D:117:ARG:HG3	1.93	0.51
1:B:160:LEU:O	1:B:164:VAL:HB	2.11	0.51
2:F:44:HIS:HE1	2:F:195:ARG:HH11	1.57	0.51
1:A:197:TRP:CZ2	1:A:289:ILE:HG12	2.46	0.51
1:A:300:ARG:NE	2:C:200:VAL:HG13	2.24	0.51
1:A:314:ALA:HB2	2:C:222:ILE:HD11	1.93	0.51
1:A:104:THR:HB	1:A:105:PRO:HD2	1.92	0.51
1:A:198:ARG:HG2	1:A:198:ARG:HH11	1.76	0.51
1:B:309:PHE:HA	1:B:312:PRO:HG3	1.93	0.51
2:C:168:LEU:HD21	2:C:187:PHE:CD1	2.46	0.51
2:F:22:LYS:HB2	2:F:62:TYR:CE2	2.45	0.51
1:B:248:PHE:CE2	1:B:249:VAL:HG23	2.45	0.51
2:C:44:HIS:CE1	2:C:195:ARG:NH1	2.74	0.51
2:F:172:ARG:HG2	2:F:177:VAL:O	2.11	0.51
1:A:262:ARG:NE	1:B:42:ARG:NH1	2.54	0.50
1:B:304:SER:OG	2:E:106:LYS:HE3	2.11	0.50
2:C:211:ARG:HG3	2:C:211:ARG:NH1	2.25	0.50
2:F:20:PRO:O	2:F:23:LEU:HB3	2.12	0.50
1:A:186:LYS:HG2	1:A:277:TYR:CZ	2.46	0.50
1:A:222:LEU:HD11	1:A:263:ILE:CG2	2.39	0.50
2:D:107:ILE:HD13	2:D:214:ILE:CD1	2.38	0.50
1:A:279:ARG:HG2	1:A:279:ARG:HH11	1.77	0.50
2:D:36:ASP:O	2:D:40:ARG:HG3	2.12	0.50
1:A:156:VAL:O	1:A:159:PRO:HD2	2.12	0.50
1:A:241:MET:HA	1:A:241:MET:HE3	1.92	0.50
1:A:327:ARG:H	2:D:102:MET:CE	2.25	0.50
2:C:189:ILE:HG22	2:C:190:THR:N	2.26	0.50
2:F:137:ALA:CB	2:F:142:LEU:HD22	2.41	0.50
2:F:165:ARG:NH2	2:F:184:SER:HA	2.26	0.50
2:E:69:ARG:NH2	2:F:33:PRO:HD3	2.27	0.50
1:A:237:GLN:HB2	1:A:253:VAL:HG11	1.93	0.50
1:A:326:MET:HE3	2:D:196:PHE:CE1	2.47	0.49
2:E:43:ARG:NH1	2:E:49:GLU:OE2	2.44	0.49
2:E:201:ARG:CG	2:E:201:ARG:HH11	2.24	0.49
1:B:327:ARG:N	2:F:102:MET:HE3	2.25	0.49
2:F:100:LEU:HD23	2:F:100:LEU:C	2.33	0.49
1:A:112:ASP:HB3	1:A:116:ARG:HG3	1.95	0.49
1:A:178:MET:HE1	1:A:181:GLN:CB	2.42	0.49
1:B:296:VAL:HG12	1:B:300:ARG:HH21	1.77	0.49
1:B:323:LEU:C	1:B:323:LEU:HD23	2.33	0.49
2:F:134:LEU:HD23	2:F:142:LEU:HD21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ARG:HH11	1:A:279:ARG:CG	2.25	0.49
1:A:284:PHE:CG	2:C:118:LEU:HD21	2.47	0.49
1:B:224:ALA:O	1:B:228:LYS:HE2	2.12	0.49
2:C:22:LYS:HD3	2:C:62:TYR:CE1	2.48	0.49
2:D:70:TYR:O	2:D:71:ASN:HB2	2.12	0.49
2:E:72:VAL:CG2	2:E:90:THR:HG23	2.43	0.49
2:E:143:LEU:C	2:E:145:LEU:N	2.65	0.49
2:C:133:LEU:HD22	2:C:142:LEU:HD21	1.94	0.49
2:E:198:ALA:HA	2:E:201:ARG:CD	2.41	0.49
2:F:162:GLU:N	2:F:162:GLU:OE2	2.46	0.49
2:F:168:LEU:HD23	2:F:168:LEU:O	2.13	0.49
2:F:191:GLU:CD	2:F:191:GLU:H	2.15	0.49
1:B:104:THR:HB	1:B:105:PRO:CD	2.43	0.49
1:A:326:MET:O	1:A:327:ARG:HB2	2.12	0.49
2:D:126:GLN:CD	2:D:184:SER:HB3	2.33	0.49
2:E:181:GLY:O	2:E:184:SER:HB3	2.13	0.49
1:A:83:ARG:HB2	1:A:83:ARG:CZ	2.42	0.49
1:A:251:ARG:O	1:A:255:ASP:HB2	2.12	0.49
1:A:36:ALA:CB	1:A:111:THR:HG21	2.43	0.48
2:D:110:TYR:CE2	2:D:207:ARG:NH2	2.81	0.48
2:D:184:SER:O	2:D:185:SER:C	2.51	0.48
2:F:18:VAL:HG12	2:F:19:MET:N	2.28	0.48
2:F:146:VAL:HG21	2:F:160:LEU:CG	2.42	0.48
1:B:300:ARG:NH1	2:E:203:GLY:CA	2.75	0.48
2:D:177:VAL:CG1	2:D:178:TRP:N	2.76	0.48
1:B:238:ASP:HA	1:B:241:MET:HG2	1.95	0.48
1:B:308:TYR:CD2	2:E:103:MET:CE	2.96	0.48
1:A:236:ILE:HG22	1:A:253:VAL:HG21	1.96	0.48
1:A:66:THR:HG22	1:A:68:GLU:N	2.28	0.48
1:A:128:GLN:O	1:A:132:VAL:HG23	2.13	0.48
2:C:201:ARG:HG2	2:C:201:ARG:NH1	2.28	0.48
2:E:87:ARG:N	2:E:90:THR:OG1	2.46	0.48
2:E:191:GLU:O	2:E:194:PHE:HD1	1.97	0.48
2:F:48:ASP:OD1	2:F:188:ARG:NH2	2.47	0.48
2:F:75:ILE:CD1	2:F:85:ARG:CZ	2.82	0.48
2:F:126:GLN:NE2	2:F:165:ARG:HB2	2.28	0.48
1:A:243:HIS:ND1	1:A:243:HIS:N	2.60	0.48
2:C:133:LEU:CD2	2:C:142:LEU:HD21	2.44	0.48
1:A:77:ALA:O	1:A:80:ASP:HB2	2.13	0.48
2:F:101:ASP:OD1	2:F:170:ARG:NH2	2.39	0.48
1:A:49:GLU:HB2	1:A:99:ALA:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:HIS:CD2	1:B:127:MET:SD	3.07	0.48
1:B:176:ARG:O	1:B:179:ASP:HB2	2.14	0.48
2:D:48:ASP:HB2	2:D:178:TRP:HE1	1.78	0.48
2:E:200:VAL:O	2:E:200:VAL:CG1	2.61	0.48
2:E:220:MET:CE	2:E:221:PRO:HD2	2.43	0.48
2:D:110:TYR:CE2	2:D:136:LEU:HD21	2.50	0.47
1:A:29:LEU:HD22	1:A:33:LEU:CD1	2.44	0.47
2:D:103:MET:O	2:D:107:ILE:HG12	2.15	0.47
2:C:103:MET:HA	2:C:103:MET:HE2	1.95	0.47
2:D:207:ARG:O	2:D:211:ARG:HG2	2.13	0.47
2:F:168:LEU:HD22	2:F:179:PHE:HE2	1.79	0.47
2:C:44:HIS:HE1	2:C:195:ARG:NH1	1.98	0.47
2:F:50:LEU:HD12	2:F:50:LEU:H	1.80	0.47
2:F:168:LEU:HD11	2:F:187:PHE:CE1	2.49	0.47
2:F:76:ARG:HE	2:F:80:GLY:HA2	1.79	0.47
1:B:13:ALA:O	1:B:17:LYS:N	2.48	0.47
2:C:200:VAL:O	2:C:200:VAL:CG1	2.63	0.47
2:D:107:ILE:CD1	2:D:214:ILE:HD13	2.37	0.47
2:E:126:GLN:HE22	2:E:165:ARG:NH1	1.99	0.47
2:E:204:ASP:HB2	2:E:208:GLU:OE2	2.15	0.47
1:B:9:PRO:HA	1:B:12:VAL:HG23	1.96	0.47
1:B:219:GLN:O	1:B:223:GLU:HG3	2.15	0.47
2:C:152:GLY:O	2:C:153:SER:C	2.53	0.47
2:D:138:ASP:OD1	2:D:140:ALA:HB3	2.14	0.47
1:B:104:THR:HB	1:B:105:PRO:HD2	1.96	0.47
1:B:172:ASP:O	1:B:175:GLN:HB2	2.15	0.47
2:C:79:GLU:HG2	2:C:81:PHE:CE1	2.50	0.47
2:C:108:LEU:HD13	2:C:129:LEU:HD13	1.97	0.47
2:C:117:ARG:HH11	2:C:117:ARG:CG	2.28	0.47
2:F:109:CYS:O	2:F:112:TYR:HB3	2.15	0.47
1:A:138:ARG:NH2	1:B:138:ARG:HH11	2.12	0.46
1:B:7:THR:HB	1:B:10:GLU:HB3	1.97	0.46
1:B:14:TRP:CH2	1:B:20:PHE:HE1	2.33	0.46
1:A:84:GLN:HB3	1:A:86:LEU:CD2	2.45	0.46
1:A:160:LEU:HB2	1:A:252:LEU:CD2	2.43	0.46
2:C:76:ARG:HB2	2:C:82:PHE:CE2	2.51	0.46
2:C:81:PHE:CE2	2:C:192:SER:HA	2.50	0.46
2:D:75:ILE:O	2:D:82:PHE:HA	2.15	0.46
2:E:190:THR:O	2:E:193:VAL:HG22	2.15	0.46
2:E:203:GLY:O	2:E:204:ASP:HB3	2.14	0.46
2:D:197:GLY:HA2	2:D:210:GLN:NE2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:ASP:OD2	1:A:282:HIS:CD2	2.69	0.46
1:B:136:LEU:HD11	1:B:233:LEU:CD2	2.44	0.46
2:F:94:ARG:NH2	2:F:96:VAL:HG22	2.31	0.46
1:A:271:ILE:O	1:A:275:ILE:HG13	2.15	0.46
1:B:308:TYR:CD2	2:E:103:MET:HE2	2.50	0.46
2:C:79:GLU:HG2	2:C:81:PHE:HE1	1.79	0.46
1:A:262:ARG:NE	1:B:42:ARG:HD3	2.30	0.46
1:B:47:MET:O	1:B:100:ILE:HA	2.15	0.46
1:B:300:ARG:HB3	2:E:200:VAL:CG1	2.46	0.46
2:C:210:GLN:O	2:C:214:ILE:HG13	2.15	0.46
2:F:76:ARG:HB2	2:F:82:PHE:CE1	2.51	0.46
2:F:125:THR:CG2	2:F:128:GLU:HG3	2.41	0.46
1:A:259:LYS:O	1:A:263:ILE:HG13	2.16	0.46
2:F:158:GLN:HG2	2:F:161:GLN:OE1	2.16	0.46
1:A:49:GLU:HB3	1:A:97:GLY:HA3	1.97	0.46
1:A:75:ASN:O	1:A:79:ASN:ND2	2.49	0.46
1:B:120:PHE:HD1	1:B:120:PHE:O	1.99	0.46
2:D:194:PHE:C	2:D:196:PHE:N	2.67	0.46
2:E:201:ARG:HH11	2:E:201:ARG:HG3	1.81	0.46
1:A:63:PHE:O	1:A:64:GLU:C	2.54	0.45
1:A:178:MET:HE2	1:A:178:MET:HA	1.98	0.45
1:B:172:ASP:OD1	1:B:176:ARG:NH1	2.49	0.45
2:E:57:MET:HE1	2:E:76:ARG:NH2	2.31	0.45
2:F:52:ASN:O	2:F:55:PHE:HB3	2.16	0.45
2:F:53:HIS:HE1	2:F:80:GLY:O	2.00	0.45
2:F:74:LEU:HG	2:F:74:LEU:O	2.16	0.45
1:A:33:LEU:HD23	1:A:111:THR:HG22	1.98	0.45
1:A:39:ASN:OD1	1:B:262:ARG:NH2	2.48	0.45
2:C:152:GLY:O	2:C:154:ASP:N	2.49	0.45
2:D:189:ILE:HG22	2:D:193:VAL:HG21	1.98	0.45
2:E:28:ALA:HA	2:F:69:ARG:NH2	2.31	0.45
2:F:171:LEU:HD23	2:F:174:LEU:HD12	1.98	0.45
2:F:190:THR:HG22	2:F:191:GLU:CD	2.36	0.45
1:A:219:GLN:NE2	1:A:219:GLN:HA	2.31	0.45
1:B:123:LEU:O	1:B:127:MET:HB2	2.16	0.45
2:F:94:ARG:CZ	2:F:96:VAL:HG22	2.46	0.45
2:E:154:ASP:C	2:E:156:ASP:N	2.70	0.45
2:F:71:ASN:CG	2:F:89:THR:CG2	2.85	0.45
2:F:168:LEU:HD22	2:F:179:PHE:CE2	2.52	0.45
2:C:201:ARG:O	2:C:201:ARG:HD3	2.17	0.45
2:F:97:LEU:HB3	2:F:101:ASP:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:190:THR:O	2:D:193:VAL:CG2	2.56	0.45
1:B:152:TRP:CD2	1:B:246:LEU:HD21	2.52	0.45
1:B:29:LEU:CD1	1:B:33:LEU:HD22	2.47	0.45
1:B:40:GLY:C	1:B:42:ARG:H	2.19	0.45
2:D:47:LEU:C	2:D:49:GLU:N	2.69	0.45
1:A:21:SER:O	1:A:84:GLN:HG2	2.17	0.45
1:A:56:PHE:O	1:A:56:PHE:CD1	2.70	0.45
1:A:197:TRP:CE2	1:A:289:ILE:HG12	2.52	0.45
2:C:99:GLU:H	2:C:99:GLU:HG2	1.49	0.45
2:E:85:ARG:HD3	2:E:216:ASP:O	2.17	0.45
2:E:97:LEU:HB3	2:E:101:ASP:CB	2.47	0.45
2:E:165:ARG:HH11	2:E:165:ARG:HG3	1.81	0.45
2:E:172:ARG:HD3	2:E:179:PHE:CG	2.52	0.45
2:F:115:PRO:HD3	2:F:207:ARG:NH1	2.32	0.45
2:C:81:PHE:CZ	2:C:192:SER:HA	2.52	0.44
2:F:71:ASN:CG	2:F:89:THR:HG22	2.36	0.44
1:A:56:PHE:CD1	1:A:56:PHE:C	2.91	0.44
1:A:127:MET:SD	1:B:154:ARG:HD2	2.57	0.44
1:A:262:ARG:NH2	1:B:39:ASN:HD21	2.15	0.44
2:D:52:ASN:O	2:D:55:PHE:HB3	2.17	0.44
2:E:29:ASN:ND2	2:E:30:PRO:N	2.65	0.44
2:E:75:ILE:CD1	2:E:85:ARG:CZ	2.95	0.44
2:F:176:MET:SD	2:F:196:PHE:CE2	3.07	0.44
1:B:95:ALA:O	1:B:98:ASN:N	2.39	0.44
2:E:71:ASN:HB2	2:E:90:THR:HA	1.99	0.44
1:A:222:LEU:CD1	1:A:263:ILE:HG22	2.43	0.44
1:B:231:ALA:O	1:B:234:LEU:HB3	2.17	0.44
2:C:212:ARG:NH1	2:C:212:ARG:HG2	2.33	0.44
2:E:135:THR:HG22	2:E:136:LEU:HD12	2.00	0.44
1:A:132:VAL:CG2	1:A:167:ILE:HG21	2.47	0.44
1:B:63:PHE:O	1:B:64:GLU:C	2.55	0.44
2:C:103:MET:HA	2:C:103:MET:CE	2.47	0.44
2:E:43:ARG:HG2	2:E:45:ILE:HD13	2.00	0.44
1:A:283:LYS:HA	1:A:286:ARG:CZ	2.47	0.44
2:C:71:ASN:O	2:C:87:ARG:HG3	2.17	0.44
2:D:136:LEU:N	2:D:136:LEU:HD12	2.33	0.44
2:F:32:PHE:O	2:F:33:PRO:C	2.55	0.44
1:A:158:ALA:HB1	1:B:131:ILE:HD11	2.00	0.44
1:B:300:ARG:HB3	2:E:200:VAL:HG11	1.98	0.44
2:C:135:THR:HG22	2:C:136:LEU:HD23	2.00	0.44
2:F:52:ASN:O	2:F:55:PHE:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:LEU:HD23	1:B:52:LEU:HA	1.80	0.44
2:C:205:ASP:CB	2:C:208:GLU:HB2	2.32	0.44
2:D:42:GLY:O	2:D:174:LEU:HD22	2.18	0.44
2:E:107:ILE:HG21	2:E:129:LEU:HD23	1.99	0.44
2:C:190:THR:CG2	2:C:191:GLU:N	2.81	0.44
2:D:48:ASP:OD2	2:D:190:THR:HG22	2.17	0.44
2:F:106:LYS:HE2	2:F:213:LEU:HD21	2.00	0.44
1:A:301:LEU:HD11	2:C:109:CYS:SG	2.58	0.43
1:B:92:SER:O	1:B:98:ASN:HA	2.18	0.43
1:B:127:MET:HA	1:B:127:MET:HE2	2.00	0.43
1:B:300:ARG:HH11	2:E:203:GLY:HA2	1.82	0.43
1:B:325:ASP:HB3	2:F:94:ARG:NH1	2.33	0.43
2:D:111:LEU:HD11	2:D:132:GLU:HG3	1.99	0.43
1:A:8:VAL:C	1:A:10:GLU:H	2.21	0.43
2:C:125:THR:HG22	2:C:186:LYS:HE2	2.00	0.43
2:D:170:ARG:HG3	2:D:173:ARG:NH2	2.33	0.43
2:E:169:ASN:O	2:E:172:ARG:HB3	2.18	0.43
2:D:115:PRO:HG2	2:D:116:GLU:OE1	2.18	0.43
2:F:31:LEU:HD21	2:F:51:ASP:HB3	2.01	0.43
2:F:146:VAL:HG12	2:F:146:VAL:O	2.19	0.43
2:C:26:ALA:HB2	2:C:59:PHE:CD2	2.54	0.43
1:B:313:TRP:O	2:E:102:MET:HG3	2.19	0.43
1:A:89:ARG:HG3	1:A:101:TYR:CZ	2.54	0.43
1:A:198:ARG:HG3	1:A:289:ILE:CG2	2.49	0.43
2:C:43:ARG:HG3	2:C:43:ARG:HH11	1.84	0.43
2:F:44:HIS:HE1	2:F:195:ARG:HD2	1.83	0.43
2:C:212:ARG:NH1	2:C:216:ASP:OD1	2.52	0.43
2:C:212:ARG:HG2	2:C:212:ARG:HH11	1.84	0.43
2:E:204:ASP:OD2	2:E:209:ALA:N	2.50	0.43
1:B:281:VAL:O	1:B:285:ILE:HG13	2.18	0.42
1:A:12:VAL:HG11	1:B:62:ALA:CB	2.45	0.42
1:A:262:ARG:CG	1:B:42:ARG:NH1	2.82	0.42
1:B:29:LEU:HD13	1:B:33:LEU:HD22	2.01	0.42
1:B:300:ARG:HH12	2:E:203:GLY:CA	2.32	0.42
1:A:102:ARG:NH1	1:A:102:ARG:HG2	2.35	0.42
2:C:194:PHE:CD2	2:C:201:ARG:NH2	2.88	0.42
2:E:94:ARG:NH2	2:E:220:MET:SD	2.93	0.42
1:A:182:GLN:HG3	1:A:274:TRP:CE3	2.55	0.42
1:B:237:GLN:HB2	1:B:253:VAL:HG11	2.01	0.42
2:E:31:LEU:CD1	2:E:51:ASP:HB3	2.49	0.42
2:E:130:TYR:HE1	2:E:160:LEU:CD1	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:115:PRO:CD	2:F:207:ARG:NH1	2.82	0.42
1:A:249:VAL:O	1:A:249:VAL:CG1	2.63	0.42
2:F:177:VAL:HG13	2:F:187:PHE:HB2	2.02	0.42
1:A:324:LEU:HD22	2:D:97:LEU:HD13	1.98	0.42
1:B:129:LEU:HD12	1:B:129:LEU:HA	1.85	0.42
2:E:29:ASN:ND2	2:E:30:PRO:HD2	2.35	0.42
2:E:61:GLU:H	2:E:61:GLU:HG2	1.65	0.42
2:E:204:ASP:OD2	2:E:209:ALA:HB2	2.20	0.42
2:F:75:ILE:HD11	2:F:85:ARG:NE	2.32	0.42
1:A:201:ILE:O	1:A:205:GLU:HG3	2.19	0.42
1:B:80:ASP:HB2	1:B:83:ARG:HE	1.83	0.42
1:B:211:THR:OG1	1:B:274:TRP:CE2	2.73	0.42
1:A:185:VAL:HG13	1:A:207:LEU:HB3	2.01	0.42
1:A:240:THR:HG22	1:A:250:ASP:HB2	1.99	0.42
1:A:262:ARG:HG3	1:B:42:ARG:NH1	2.34	0.42
2:F:201:ARG:C	2:F:201:ARG:HD3	2.40	0.42
1:A:228:LYS:O	1:A:231:ALA:HB3	2.19	0.42
1:A:280:HIS:CD2	2:C:121:GLU:HA	2.55	0.42
1:A:300:ARG:HB3	2:C:200:VAL:CG1	2.43	0.42
1:B:249:VAL:O	1:B:249:VAL:HG12	2.19	0.42
2:D:135:THR:HB	2:D:136:LEU:HD12	2.02	0.42
2:F:44:HIS:HE1	2:F:195:ARG:CD	2.33	0.42
2:F:126:GLN:HB2	2:F:185:SER:HB3	2.00	0.42
2:F:130:TYR:CZ	2:F:161:GLN:HG3	2.55	0.42
1:A:182:GLN:HE21	1:A:182:GLN:HB2	1.60	0.41
2:C:220:MET:HA	2:C:220:MET:CE	2.49	0.41
1:A:84:GLN:HB3	1:A:86:LEU:HD21	2.02	0.41
1:B:98:ASN:HD21	2:C:180:MET:HB3	1.85	0.41
2:F:146:VAL:CG2	2:F:160:LEU:HG	2.43	0.41
1:B:78:ILE:O	1:B:82:VAL:HG23	2.20	0.41
1:B:130:SER:O	1:B:133:ALA:HB3	2.21	0.41
2:E:126:GLN:NE2	2:E:165:ARG:HG3	2.35	0.41
2:F:111:LEU:HB3	2:F:124:PHE:CE2	2.56	0.41
1:A:11:LEU:HD21	1:B:33:LEU:HB3	2.01	0.41
1:A:300:ARG:NH1	1:A:300:ARG:HG3	2.35	0.41
2:E:153:SER:OG	2:E:156:ASP:HB2	2.20	0.41
1:B:197:TRP:CE2	1:B:289:ILE:HG12	2.55	0.41
2:C:48:ASP:OD2	2:C:190:THR:HG23	2.19	0.41
2:C:190:THR:HG22	2:C:191:GLU:H	1.82	0.41
2:D:126:GLN:OE1	2:D:184:SER:HB3	2.21	0.41
2:E:127:GLN:NE2	2:E:131:ASP:OD1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:94:ARG:NH2	2:F:96:VAL:CG2	2.84	0.41
1:A:119:GLU:HB2	1:A:124:ARG:CZ	2.51	0.41
1:B:73:ARG:HA	1:B:76:ASN:HD22	1.85	0.41
1:B:186:LYS:HG2	1:B:277:TYR:CZ	2.55	0.41
2:C:40:ARG:NH1	2:D:40:ARG:CZ	2.84	0.41
2:D:162:GLU:O	2:D:165:ARG:HB2	2.20	0.41
1:B:88:ASN:HD22	1:B:88:ASN:HA	1.57	0.41
2:C:205:ASP:O	2:C:208:GLU:N	2.35	0.41
2:E:154:ASP:HA	2:E:157:ARG:CB	2.49	0.41
1:A:84:GLN:HE21	1:A:84:GLN:HB2	1.71	0.41
2:F:176:MET:HG2	2:F:192:SER:HB2	2.03	0.41
1:A:86:LEU:N	1:A:86:LEU:HD22	2.36	0.41
1:B:22:ILE:HA	1:B:84:GLN:HE21	1.86	0.41
1:B:88:ASN:O	1:B:101:TYR:HA	2.21	0.41
1:B:306:GLN:HE21	1:B:306:GLN:CA	2.18	0.41
1:B:324:LEU:CB	2:F:174:LEU:HD21	2.51	0.41
2:C:79:GLU:HG3	2:C:194:PHE:CD1	2.56	0.41
2:C:91:LEU:HD13	2:D:33:PRO:HB2	2.03	0.41
2:C:183:ASP:CG	2:C:184:SER:H	2.24	0.41
2:E:29:ASN:HD22	2:E:31:LEU:N	2.01	0.41
2:E:75:ILE:HD13	2:E:85:ARG:CZ	2.50	0.41
2:F:36:ASP:OD1	2:F:40:ARG:NE	2.53	0.41
2:F:75:ILE:HG22	2:F:76:ARG:H	1.85	0.41
1:A:83:ARG:HB2	1:A:83:ARG:NH1	2.36	0.41
1:A:196:ASP:O	1:A:197:TRP:C	2.59	0.41
2:D:43:ARG:NH2	2:D:175:GLY:HA2	2.35	0.41
2:E:144:LYS:O	2:E:145:LEU:HG	2.20	0.41
1:A:36:ALA:HB2	1:A:103:LEU:HD21	2.02	0.40
2:F:19:MET:CG	2:F:23:LEU:HD23	2.50	0.40
2:F:136:LEU:CD1	2:F:211:ARG:HG3	2.51	0.40
1:B:198:ARG:O	1:B:201:ILE:HG13	2.21	0.40
2:C:205:ASP:O	2:C:206:PRO:C	2.59	0.40
2:D:167:SER:O	2:D:171:LEU:HG	2.20	0.40
2:E:198:ALA:C	2:E:200:VAL:H	2.25	0.40
1:A:120:PHE:CZ	1:A:177:LEU:HB3	2.56	0.40
1:A:198:ARG:HG2	1:A:198:ARG:NH1	2.36	0.40
2:D:134:LEU:HD23	2:D:142:LEU:HD21	2.01	0.40
2:D:177:VAL:CG1	2:D:187:PHE:HB2	2.51	0.40
2:E:201:ARG:CG	2:E:201:ARG:NH1	2.83	0.40
2:F:190:THR:HG22	2:F:191:GLU:OE2	2.20	0.40
1:A:177:LEU:HD23	1:A:177:LEU:HA	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:LEU:HD23	1:A:192:LEU:HA	1.94	0.40
1:B:87:LEU:HD12	1:B:103:LEU:HA	2.04	0.40
2:C:212:ARG:HG3	2:C:215:ARG:HH21	1.85	0.40
2:D:75:ILE:HD11	2:D:85:ARG:CZ	2.52	0.40
2:E:29:ASN:ND2	2:E:29:ASN:C	2.74	0.40
2:E:154:ASP:C	2:E:156:ASP:H	2.25	0.40
2:F:110:TYR:CB	2:F:210:GLN:HG2	2.52	0.40
1:A:129:LEU:HD23	1:A:129:LEU:HA	1.94	0.40
1:B:251:ARG:HD3	1:B:251:ARG:HA	1.86	0.40
2:E:204:ASP:OD1	2:E:209:ALA:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	311/440 (71%)	287 (92%)	20 (6%)	4 (1%)	12 37
1	B	319/440 (72%)	282 (88%)	30 (9%)	7 (2%)	6 24
2	C	204/234 (87%)	186 (91%)	15 (7%)	3 (2%)	10 34
2	D	184/234 (79%)	171 (93%)	8 (4%)	5 (3%)	5 19
2	E	197/234 (84%)	176 (89%)	15 (8%)	6 (3%)	4 17
2	F	174/234 (74%)	144 (83%)	26 (15%)	4 (2%)	6 23
All	All	1389/1816 (76%)	1246 (90%)	114 (8%)	29 (2%)	7 26

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	185	SER
1	A	64	GLU

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Mol	Chain	Res	Type
1	A	145	GLU
1	A	292	ASP
1	B	146	GLY
1	B	245	ASP
2	C	153	SER
2	D	139	GLU
2	E	118	LEU
2	F	177	VAL
2	F	206	PRO
1	B	8	VAL
1	B	64	GLU
2	D	144	LYS
2	D	183	ASP
2	E	204	ASP
1	B	66	THR
2	C	118	LEU
2	E	27	LEU
2	E	50	LEU
2	E	144	LYS
1	B	157	TYR
2	D	138	ASP
2	F	182	HIS
2	C	203	GLY
1	A	226	GLY
1	B	70	ILE
2	E	21	VAL
2	F	33	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	273/380 (72%)	255 (93%)	18 (7%)	16 44
1	B	278/380 (73%)	254 (91%)	24 (9%)	10 30
2	C	180/207 (87%)	163 (91%)	17 (9%)	8 26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	165/207 (80%)	155 (94%)	10 (6%)	18 48
2	E	175/207 (84%)	163 (93%)	12 (7%)	15 41
2	F	161/207 (78%)	147 (91%)	14 (9%)	10 30
All	All	1232/1588 (78%)	1137 (92%)	95 (8%)	13 35

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	32	LEU
1	A	57	ARG
1	A	65	GLN
1	A	76	ASN
1	A	87	LEU
1	A	88	ASN
1	A	103	LEU
1	A	118	ARG
1	A	154	ARG
1	A	163	SER
1	A	169	ASP
1	A	172	ASP
1	A	222	LEU
1	A	243	HIS
1	A	261	ASP
1	A	279	ARG
1	A	301	LEU
1	B	32	LEU
1	B	33	LEU
1	B	43	LEU
1	B	44	ASP
1	B	54	ASP
1	B	69	THR
1	B	79	ASN
1	B	87	LEU
1	B	88	ASN
1	B	106	LEU
1	B	119	GLU
1	B	123	LEU
1	B	125	LEU
1	B	127	MET
1	B	129	LEU

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Mol	Chain	Res	Type
1	B	154	ARG
1	B	176	ARG
1	B	219	GLN
1	B	244	ASP
1	B	248	PHE
1	B	252	LEU
1	B	260	LEU
1	B	261	ASP
1	B	306	GLN
2	C	23	LEU
2	C	27	LEU
2	C	50	LEU
2	C	74	LEU
2	C	94	ARG
2	C	99	GLU
2	C	108	LEU
2	C	126	GLN
2	C	133	LEU
2	C	156	ASP
2	C	160	LEU
2	C	169	ASN
2	C	182	HIS
2	C	191	GLU
2	C	193	VAL
2	C	206	PRO
2	C	211	ARG
2	D	35	LEU
2	D	58	ASP
2	D	88	SER
2	D	90	THR
2	D	95	SER
2	D	129	LEU
2	D	133	LEU
2	D	162	GLU
2	D	180	MET
2	D	183	ASP
2	E	23	LEU
2	E	29	ASN
2	E	35	LEU
2	E	37	SER
2	E	74	LEU
2	E	100	LEU

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Mol	Chain	Res	Type
2	E	118	LEU
2	E	129	LEU
2	E	160	LEU
2	E	170	ARG
2	E	177	VAL
2	E	201	ARG
2	F	20	PRO
2	F	27	LEU
2	F	33	PRO
2	F	35	LEU
2	F	47	LEU
2	F	69	ARG
2	F	89	THR
2	F	91	LEU
2	F	110	TYR
2	F	125	THR
2	F	182	HIS
2	F	191	GLU
2	F	199	ASP
2	F	201	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	79	ASN
1	A	153	HIS
1	A	155	ASN
1	A	182	GLN
1	A	184	GLN
1	A	219	GLN
1	A	230	GLN
1	A	257	GLN
1	A	268	GLN
1	A	280	HIS
1	A	282	HIS
1	A	319	ASN
1	B	18	ASN
1	B	39	ASN
1	B	76	ASN
1	B	84	GLN
1	B	88	ASN

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Mol	Chain	Res	Type
1	B	94	GLN
1	B	98	ASN
1	B	219	GLN
1	B	230	GLN
1	B	257	GLN
1	B	269	GLN
1	B	299	GLN
1	B	306	GLN
2	C	44	HIS
2	C	52	ASN
2	C	182	HIS
2	D	25	GLN
2	D	44	HIS
2	D	60	GLN
2	D	210	GLN
2	E	25	GLN
2	E	29	ASN
2	E	52	ASN
2	E	60	GLN
2	E	126	GLN
2	E	127	GLN
2	F	25	GLN
2	F	44	HIS
2	F	126	GLN
2	F	147	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GLY	A	441	-	4,4,4	0.96	0	3,4,4	0.93	0
3	GLY	D	1	-	4,4,4	1.00	0	3,4,4	0.88	0
3	GLY	D	245	-	4,4,4	0.97	0	3,4,4	0.96	0
3	GLY	D	244	-	4,4,4	0.92	0	3,4,4	1.00	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLY	A	441	-	-	2/2/2/2	-
3	GLY	D	1	-	-	2/2/2/2	-
3	GLY	D	245	-	-	2/2/2/2	-
3	GLY	D	244	-	-	1/2/2/2	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1	GLY	O-C-CA-N
3	D	1	GLY	OXT-C-CA-N
3	D	245	GLY	O-C-CA-N
3	D	245	GLY	OXT-C-CA-N
3	A	441	GLY	OXT-C-CA-N
3	A	441	GLY	O-C-CA-N
3	D	244	GLY	OXT-C-CA-N

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)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	315/440 (71%)	-0.22	4 (1%)	77	77	27, 60, 105, 132	0
1	B	321/440 (72%)	-0.05	8 (2%)	57	55	42, 68, 113, 127	0
2	C	206/234 (88%)	-0.26	7 (3%)	45	40	26, 48, 94, 119	0
2	D	188/234 (80%)	-0.18	11 (5%)	22	18	27, 51, 115, 152	0
2	E	201/234 (85%)	-0.15	6 (2%)	50	45	34, 56, 105, 119	0
2	F	182/234 (77%)	0.31	15 (8%)	11	9	40, 94, 143, 153	0
All	All	1413/1816 (77%)	-0.10	51 (3%)	42	37	26, 63, 122, 153	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	68	GLU	6.5
2	D	145	LEU	4.6
2	F	181	GLY	4.5
2	F	182	HIS	4.5
2	C	182	HIS	4.4
2	D	183	ASP	4.3
2	C	183	ASP	4.0
1	A	66	THR	3.9
1	B	242	THR	3.6
2	C	148	ASN	3.5
2	D	182	HIS	3.4
2	F	201	ARG	3.3
2	C	224	ASN	3.2
1	B	44	ASP	3.2
1	B	120	PHE	3.2
1	A	64	GLU	3.1
2	F	141	LYS	3.1
2	F	180	MET	3.0
2	E	155	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
2	F	130	TYR	2.8
2	C	184	SER	2.8
2	F	145	LEU	2.8
1	B	7	THR	2.7
1	B	146	GLY	2.7
2	F	183	ASP	2.6
2	D	158	GLN	2.6
1	B	11	LEU	2.6
2	D	157	ARG	2.6
1	B	247	HIS	2.5
2	F	208	GLU	2.4
2	E	18	VAL	2.4
2	C	149	ARG	2.4
2	F	215	ARG	2.4
1	A	67	SER	2.4
2	D	216	ASP	2.3
2	E	144	LYS	2.3
2	E	184	SER	2.3
2	D	144	LYS	2.2
1	B	244	ASP	2.2
2	E	152	GLY	2.2
2	F	160	LEU	2.2
2	D	180	MET	2.2
2	D	138	ASP	2.2
2	E	151	THR	2.1
2	D	118	LEU	2.1
2	D	162	GLU	2.1
2	C	150	SER	2.1
2	F	50	LEU	2.1
2	F	207	ARG	2.1
2	F	203	GLY	2.1
2	F	212	ARG	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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GLY	D	244	5/5	0.77	0.30	78,80,80,80	0
3	GLY	D	1	5/5	0.93	0.24	73,74,74,75	0
3	GLY	A	441	5/5	0.93	0.17	76,78,78,79	0
3	GLY	D	245	5/5	0.93	0.21	83,84,84,85	0

6.5 Other polymers

There are no such residues in this entry.