Full wwPDB X-ray Structure Validation Report (i)

May 15, 2020 – 06:49 pm BST

PDB ID	:	3E0O
Title	:	Crystal structure of MsrB
Authors	:	Park, A.K.; Shin, Y.J.; Kim, Y.K.; Chi, Y.M.; Hwang, K.Y.
Deposited on	:	2008-07-31
Resolution	:	2.60 Å(reported)

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

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

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 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
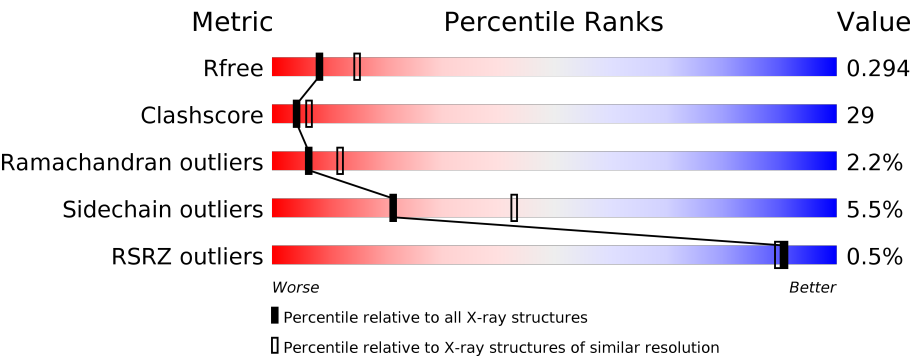
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	144	49% 45% · ··
1	B	144	62% 31% 6% ·
1	C	144	47% 44% 5% ·
1	D	144	47% 46% · ·
1	E	144	% 60% 33% · ··
1	F	144	% 39% 53% 6% ·

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7294 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 Peptide methionine sulfoxide reductase msrB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	142	Total 1161	C 733	N 198	O 224	S 6	0	0	0
1	B	142	Total 1161	C 733	N 198	O 224	S 6	0	0	0
1	C	139	Total 1140	C 720	N 195	O 221	S 4	0	0	0
1	D	139	Total 1140	C 720	N 195	O 221	S 4	0	0	0
1	E	141	Total 1153	C 728	N 197	O 223	S 5	0	0	0
1	F	141	Total 1152	C 728	N 197	O 222	S 5	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	INITIATING METHIONINE	UNP P54155
B	0	MET	-	INITIATING METHIONINE	UNP P54155
C	0	MET	-	INITIATING METHIONINE	UNP P54155
D	0	MET	-	INITIATING METHIONINE	UNP P54155
E	0	MET	-	INITIATING METHIONINE	UNP P54155
F	0	MET	-	INITIATING METHIONINE	UNP P54155

- Molecule 2 is water.

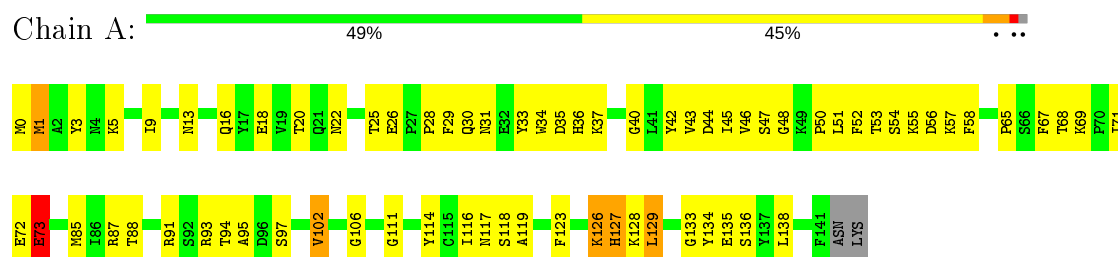| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	75	Total 75	O 75	0	0
2	B	51	Total 51	O 51	0	0
2	C	64	Total 64	O 64	0	0

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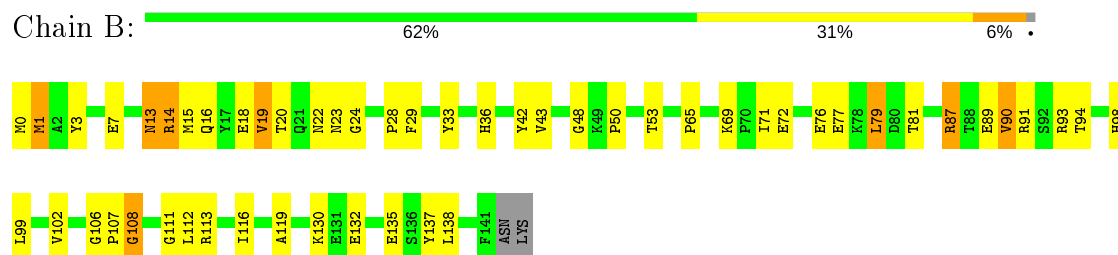| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	61	Total 61	O 61	0	0
2	E	68	Total 68	O 68	0	0
2	F	68	Total 68	O 68	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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.
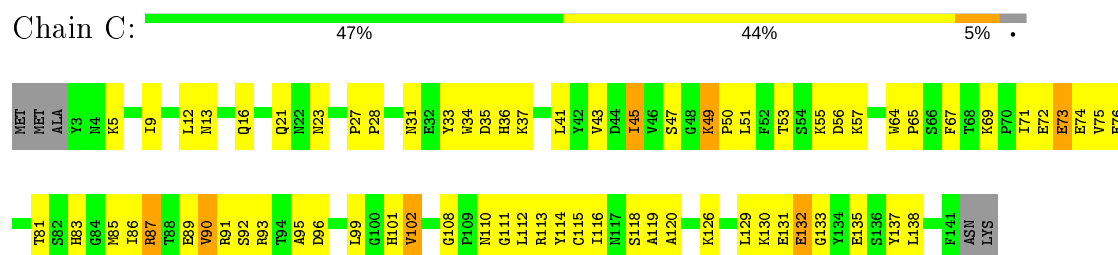
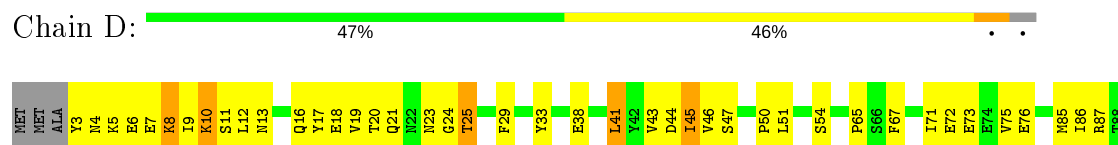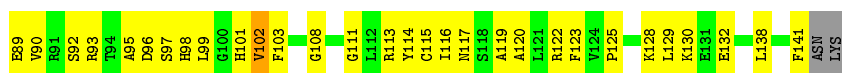- Molecule 1: Peptide methionine sulfoxide reductase msrB

- Molecule 1: Peptide methionine sulfoxide reductase msrB

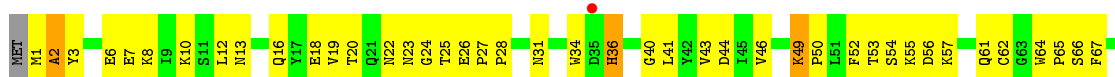- Molecule 1: Peptide methionine sulfoxide reductase msrB

- Molecule 1: Peptide methionine sulfoxide reductase msrB

E89 V90 R91 S92 R93 T94 A95 D96 S97 H98 L99 G100 H101 V102 F103 G108 G111 L112 R113 Y114 C115 I116 N117 S118 A119 A120 L121 R122 F123 V124 P125 K128 L129 K130 E131 E132 L138 F141 ASN LYS

• Molecule 1: Peptide methionine sulfoxide reductase msrB

Chain E:

%

60% 33%

MET M1 A2 Y3 N4 E7 K10 N13 R14 M15 Q16 V19 N23 G24 T25 E26 H36 K37 E38 E39 V43 D44 I45 V46 S47 G48 K49 P50 L51 F52 K55 S60 W64 P65 S66 F67 P70 I71 E72 E73 E74 V75 E89 V90 R91 S92 R93 T94

A95 D96 V102 Y114 C115 I116 N117 R122 K126 K130 E131 E132 E135 S136 Y137 L138 H139 L140 F141 ASN LYS

• Molecule 1: Peptide methionine sulfoxide reductase msrB

Chain F:

%

39% 53% 6%

MET M1 A2 Y3 E6 E7 K8 I9 K10 S11 L12 N13 Q16 Y17 E18 V19 T20 Q21 N22 N23 G24 T25 E26 P27 P28 N31 W34 D35 H36 G40 L41 Y42 V43 D44 I45 V46 K49 P50 L51 F52 T53 S54 K55 D56 K57 Q61 C62 G63 W64 P65 S66 F67

P70 I71 E72 E73 E74 V75 E76 D80 T81 S82 H83 G84 M85 I86 R87 T88 E89 V90 R91 S92 R93 T94 A95 D96 S97 H98 L99 G100 H101 V102 F103 G106 P107 G108 G111 L112 R113 Y114 C115 I116 N117 S118 A119 V124 H127 K128 L129 K130 E131 E132 G133 Y134 E135 S136 Y137

L138 H139 L140 F141 ASN LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α, β, γ	136.11Å 136.11Å 61.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.79 – 2.60 45.80 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.2 (19.79-2.60) 98.3 (45.80-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.51 (at 2.61Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.235 , 0.294 0.235 , 0.294	Depositor DCC
R_{free} test set	3885 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	24.2	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 29.1	EDS
L-test for twinning [2]	$< |L| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.488 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7294	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.67 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0652e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	A	0.41	0/1192	0.64	0/1607
1	B	0.39	0/1192	0.62	0/1607
1	C	0.37	0/1171	0.57	0/1580
1	D	0.39	0/1171	0.61	0/1580
1	E	0.39	0/1184	0.61	0/1597
1	F	0.36	0/1183	0.58	0/1596
All	All	0.38	0/7093	0.61	0/9567

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1161	0	1107	62	0
1	B	1161	0	1107	56	0
1	C	1140	0	1081	64	0
1	D	1140	0	1081	81	0
1	E	1153	0	1098	60	0
1	F	1152	0	1095	78	0
2	A	75	0	0	7	0
2	B	51	0	0	6	0
2	C	64	0	0	3	0
2	D	61	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	68	0	0	8	0
2	F	68	0	0	7	0
All	All	7294	0	6569	392	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 29.

All (392) 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:F:53:THR:HG22	1:F:55:LYS:H	1.19	1.02
1:D:128:LYS:O	1:D:132:GLU:HG2	1.65	0.97
1:A:53:THR:HG22	1:A:55:LYS:H	1.26	0.97
1:E:23:ASN:ND2	1:E:91:ARG:HH12	1.64	0.96
1:C:53:THR:HG22	1:C:55:LYS:H	1.31	0.94
1:E:47:SER:HB3	1:E:95:ALA:HB2	1.58	0.86
1:C:47:SER:HB3	1:C:95:ALA:HB2	1.57	0.84
1:D:108:GLY:HA2	1:D:111:GLY:H	1.41	0.84
1:F:28:PRO:HG3	1:F:64:TRP:CZ2	2.15	0.82
1:A:73:GLU:HB3	2:A:170:HOH:O	1.80	0.81
1:F:50:PRO:HB2	1:F:71:ILE:HD11	1.63	0.81
1:C:33:TYR:HA	1:C:36:HIS:HB2	1.65	0.79
1:D:10:LYS:HE2	1:D:11:SER:HB3	1.63	0.79
1:F:31:ASN:HD21	1:F:34:TRP:HB3	1.46	0.79
1:F:49:LYS:HG3	1:F:94:THR:HG21	1.64	0.79
1:E:131:GLU:HG3	2:E:200:HOH:O	1.82	0.78
1:D:113:ARG:HH12	1:D:115:CYS:HB2	1.47	0.78
1:E:93:ARG:HD2	2:E:157:HOH:O	1.83	0.77
1:F:114:TYR:HB3	1:F:116:ILE:HD11	1.66	0.76
1:F:26:GLU:H	1:F:117:ASN:ND2	1.84	0.76
1:D:73:GLU:HG3	2:D:187:HOH:O	1.85	0.75
1:E:71:ILE:HG23	1:E:72:GLU:HG3	1.69	0.75
1:C:45:ILE:O	1:C:45:ILE:HD13	1.87	0.74
1:A:26:GLU:HG2	1:A:117:ASN:HD22	1.53	0.74
1:D:108:GLY:HA2	1:D:111:GLY:N	2.02	0.74
1:B:135:GLU:HB2	2:B:156:HOH:O	1.89	0.72
1:C:90:VAL:HG12	1:C:99:LEU:HB2	1.71	0.72
1:D:41:LEU:HG	1:D:129:LEU:HD21	1.72	0.72
1:D:113:ARG:NH1	1:D:115:CYS:HB2	2.04	0.72
1:E:23:ASN:HD21	1:E:91:ARG:HH12	1.35	0.72
1:C:129:LEU:HD12	1:C:138:LEU:HD23	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:72:GLU:HG2	2:F:167:HOH:O	1.89	0.71
1:E:39:GLU:OE2	1:E:126:LYS:HD2	1.89	0.71
1:D:72:GLU:HB3	1:D:73:GLU:OE2	1.90	0.71
1:F:50:PRO:CB	1:F:71:ILE:HD11	2.21	0.71
1:F:128:LYS:O	1:F:132:GLU:HB2	1.91	0.70
1:C:92:SER:O	1:C:96:ASP:HA	1.92	0.70
1:D:86:ILE:HG13	1:D:86:ILE:O	1.92	0.70
1:E:45:ILE:HD13	1:E:45:ILE:O	1.92	0.69
1:F:101:HIS:CD2	2:F:156:HOH:O	2.44	0.69
1:D:20:THR:HG23	1:D:97:SER:CB	2.23	0.69
1:F:53:THR:HG22	1:F:55:LYS:N	2.02	0.69
1:B:87:ARG:HH11	1:B:87:ARG:HG3	1.58	0.69
1:D:20:THR:HG23	1:D:97:SER:HB2	1.74	0.69
1:A:5:LYS:HE2	1:A:9:ILE:HD11	1.74	0.68
1:D:90:VAL:HG22	1:D:102:VAL:HG22	1.74	0.68
1:C:108:GLY:HA2	1:C:111:GLY:H	1.58	0.66
1:D:4:ASN:O	1:D:8:LYS:HB2	1.95	0.66
1:A:73:GLU:HG3	2:A:171:HOH:O	1.96	0.66
1:B:36:HIS:HD2	1:B:42:TYR:OH	1.77	0.66
1:B:1:MET:HG2	1:B:3:TYR:CZ	2.32	0.65
1:D:7:GLU:O	1:D:10:LYS:HG3	1.96	0.65
1:C:56:ASP:OD2	1:C:69:LYS:HB3	1.96	0.65
1:D:9:ILE:HA	1:D:12:LEU:HG	1.78	0.65
1:B:19:VAL:HA	1:B:24:GLY:H	1.63	0.64
1:A:26:GLU:H	1:A:117:ASN:ND2	1.96	0.64
1:B:15:MET:O	1:B:19:VAL:HG13	1.98	0.64
1:D:45:ILE:CD1	1:D:46:VAL:HG23	2.28	0.64
1:A:91:ARG:HG3	2:A:157:HOH:O	1.96	0.63
1:B:23:ASN:HD21	1:B:91:ARG:HH12	1.44	0.63
1:A:25:THR:HG23	1:A:117:ASN:HD21	1.62	0.63
1:F:23:ASN:OD1	1:F:98:HIS:HB2	1.99	0.63
1:A:56:ASP:OD1	1:A:69:LYS:HE3	1.98	0.62
1:A:53:THR:HG22	1:A:55:LYS:N	2.08	0.62
1:B:89:GLU:OE2	1:B:98:HIS:HD2	1.83	0.62
1:E:3:TYR:O	1:E:7:GLU:HB2	1.99	0.62
1:A:126:LYS:NZ	1:A:126:LYS:HB3	2.15	0.62
1:A:13:ASN:H	1:A:16:GLN:HE21	1.48	0.62
1:F:116:ILE:HD12	1:F:116:ILE:N	2.14	0.62
1:F:6:GLU:O	1:F:10:LYS:HG3	2.00	0.61
1:D:65:PRO:HG2	1:D:116:ILE:O	2.00	0.61
1:C:83:HIS:HB3	1:F:34:TRP:HH2	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:55:LYS:HB3	1:E:55:LYS:NZ	2.15	0.61
1:F:89:GLU:HA	1:F:101:HIS:HD2	1.65	0.61
1:B:13:ASN:HD22	1:B:13:ASN:C	2.01	0.61
1:B:130:LYS:HE2	1:B:135:GLU:OE2	2.01	0.61
1:C:110:ASN:HD22	1:C:112:LEU:HB2	1.67	0.60
1:E:36:HIS:CE1	1:E:38:GLU:HB2	2.37	0.60
1:F:73:GLU:HB2	2:F:153:HOH:O	2.02	0.59
1:E:4:ASN:ND2	2:E:171:HOH:O	2.34	0.59
1:C:28:PRO:HG3	1:C:64:TRP:CH2	2.37	0.59
1:C:75:VAL:HG13	1:C:90:VAL:HG13	1.85	0.59
1:B:65:PRO:HG2	1:B:116:ILE:O	2.03	0.59
1:A:20:THR:HB	1:A:97:SER:HB2	1.84	0.58
1:A:36:HIS:HD2	1:A:42:TYR:OH	1.85	0.58
1:E:25:THR:HG22	2:E:172:HOH:O	2.04	0.58
1:B:13:ASN:HB2	1:B:14:ARG:HH21	1.68	0.58
1:D:45:ILE:HG13	1:D:120:ALA:C	2.24	0.58
1:A:106:GLY:O	1:A:111:GLY:HA2	2.03	0.58
1:C:110:ASN:ND2	1:C:112:LEU:H	2.02	0.58
1:E:71:ILE:CG2	1:E:72:GLU:HG3	2.34	0.58
1:D:138:LEU:O	1:D:141:PHE:HD2	1.86	0.57
1:D:90:VAL:CG2	1:D:102:VAL:HG22	2.34	0.57
1:E:49:LYS:HE3	1:E:74:GLU:OE2	2.05	0.57
1:B:79:LEU:CD1	1:B:81:THR:HG23	2.35	0.57
1:A:65:PRO:HD2	1:A:116:ILE:O	2.05	0.57
1:B:13:ASN:H	1:B:16:GLN:HE21	1.51	0.57
1:C:126:LYS:HD3	1:C:126:LYS:O	2.05	0.57
1:D:43:VAL:HG22	1:D:122:ARG:O	2.05	0.57
1:F:89:GLU:HA	1:F:101:HIS:CD2	2.39	0.57
1:F:87:ARG:CB	2:F:156:HOH:O	2.52	0.56
1:A:57:LYS:HB2	1:A:67:PHE:CE2	2.40	0.56
1:C:71:ILE:O	1:C:73:GLU:N	2.38	0.56
1:D:128:LYS:HE2	1:D:132:GLU:OE1	2.05	0.56
1:C:87:ARG:HG3	1:C:101:HIS:CD2	2.39	0.56
1:E:114:TYR:HB3	1:E:116:ILE:HD11	1.88	0.56
1:B:14:ARG:NE	2:B:145:HOH:O	2.39	0.56
1:B:23:ASN:ND2	1:B:91:ARG:HH12	2.03	0.56
1:F:65:PRO:HG2	1:F:116:ILE:O	2.05	0.56
1:F:1:MET:O	1:F:2:ALA:HB2	2.05	0.56
1:A:85:MET:CE	1:A:87:ARG:HD2	2.35	0.56
1:B:87:ARG:NH1	1:B:87:ARG:HG3	2.21	0.56
1:F:89:GLU:HG2	1:F:90:VAL:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:ARG:CZ	2:B:145:HOH:O	2.53	0.55
1:B:93:ARG:HH11	1:B:93:ARG:HG3	1.72	0.55
1:D:20:THR:HG22	1:D:21:GLN:OE1	2.06	0.55
1:C:23:ASN:HD22	1:C:23:ASN:N	2.04	0.55
1:C:130:LYS:HG3	1:C:135:GLU:OE1	2.07	0.55
1:A:116:ILE:HD12	1:A:116:ILE:N	2.22	0.55
1:B:14:ARG:H	1:B:14:ARG:HE	1.54	0.55
1:D:18:GLU:OE2	1:D:24:GLY:HA3	2.06	0.55
1:A:114:TYR:HB3	1:A:116:ILE:HD11	1.88	0.54
1:C:83:HIS:HB3	1:F:34:TRP:CH2	2.41	0.54
1:D:89:GLU:HG2	1:D:90:VAL:N	2.22	0.54
1:B:13:ASN:H	1:B:16:GLN:NE2	2.05	0.54
1:E:65:PRO:HD2	1:E:116:ILE:O	2.08	0.54
1:C:81:THR:HG22	1:C:86:ILE:HG12	1.89	0.54
1:A:5:LYS:CE	1:A:9:ILE:HD11	2.36	0.54
1:B:18:GLU:O	1:B:22:ASN:HB2	2.06	0.54
1:F:81:THR:HA	1:F:85:MET:O	2.07	0.54
1:C:28:PRO:HG3	1:C:64:TRP:CZ2	2.42	0.54
1:C:99:LEU:HB3	1:C:116:ILE:HG23	1.90	0.54
1:E:43:VAL:HG22	1:E:122:ARG:O	2.07	0.54
1:E:139:HIS:C	1:E:141:PHE:H	2.11	0.54
1:C:81:THR:HA	1:C:85:MET:O	2.08	0.54
1:F:74:GLU:OE2	1:F:94:THR:HG22	2.07	0.54
1:C:34:TRP:CH2	1:F:83:HIS:HB3	2.42	0.54
1:C:131:GLU:HB2	2:C:158:HOH:O	2.07	0.54
1:E:14:ARG:HD3	1:E:14:ARG:H	1.73	0.54
1:F:26:GLU:H	1:F:117:ASN:HD22	1.53	0.54
1:D:128:LYS:HD2	2:D:159:HOH:O	2.06	0.54
1:E:116:ILE:HD12	1:E:116:ILE:N	2.23	0.54
1:F:87:ARG:HB2	2:F:156:HOH:O	2.08	0.53
1:B:19:VAL:HA	1:B:24:GLY:N	2.23	0.53
1:D:7:GLU:HA	1:D:10:LYS:HG2	1.89	0.53
1:A:40:GLY:HA3	1:A:123:PHE:CZ	2.43	0.53
1:B:13:ASN:ND2	1:B:16:GLN:H	2.07	0.53
1:A:133:GLY:HA3	1:B:3:TYR:HA	1.91	0.53
1:C:35:ASP:O	1:C:37:LYS:HG3	2.09	0.53
1:D:17:TYR:CE1	1:D:21:GLN:HG2	2.44	0.52
1:F:12:LEU:HB3	1:F:16:GLN:HB2	1.91	0.52
1:C:113:ARG:NH1	1:C:115:CYS:HB2	2.24	0.52
1:B:108:GLY:HA2	1:B:111:GLY:H	1.74	0.52
1:D:13:ASN:HB3	1:D:16:GLN:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:70:PRO:HD3	1:F:114:TYR:CZ	2.44	0.52
1:B:106:GLY:HA3	1:B:112:LEU:O	2.09	0.52
1:C:37:LYS:NZ	1:C:37:LYS:HB3	2.24	0.52
1:B:132:GLU:HB3	2:B:176:HOH:O	2.09	0.52
1:B:43:VAL:CG1	1:B:48:GLY:HA2	2.40	0.52
1:F:50:PRO:HG2	1:F:137:TYR:CZ	2.44	0.52
1:A:126:LYS:C	1:A:126:LYS:HD2	2.31	0.51
1:B:33:TYR:HA	1:B:36:HIS:HB2	1.91	0.51
1:A:129:LEU:HB3	1:A:138:LEU:CD2	2.41	0.51
1:C:129:LEU:HD12	1:C:138:LEU:CD2	2.39	0.51
1:D:43:VAL:HG12	1:D:50:PRO:HA	1.92	0.51
1:F:101:HIS:HB2	2:F:157:HOH:O	2.10	0.51
1:C:13:ASN:HB3	1:C:16:GLN:HG3	1.91	0.51
1:D:45:ILE:HD13	1:D:46:VAL:HG23	1.92	0.51
1:C:76:GLU:CD	1:C:93:ARG:HB3	2.31	0.51
1:E:71:ILE:CG2	1:E:72:GLU:N	2.73	0.51
1:F:130:LYS:HG3	1:F:135:GLU:OE2	2.11	0.50
1:B:23:ASN:HD22	1:B:98:HIS:HB2	1.77	0.50
1:E:139:HIS:NE2	2:E:168:HOH:O	2.33	0.50
1:E:15:MET:HE3	1:E:19:VAL:HG23	1.94	0.50
1:E:130:LYS:HE3	1:E:135:GLU:OE1	2.11	0.50
1:A:0:MET:HE1	1:A:46:VAL:HG12	1.94	0.50
1:C:75:VAL:CG1	1:C:90:VAL:HG13	2.41	0.50
1:D:20:THR:HG23	1:D:97:SER:HB3	1.93	0.50
1:E:51:LEU:HB3	1:E:52:PHE:CD1	2.47	0.50
1:D:8:LYS:HE2	1:D:8:LYS:O	2.12	0.49
1:D:51:LEU:O	1:D:71:ILE:HG12	2.12	0.49
1:C:34:TRP:HH2	1:F:83:HIS:HB3	1.76	0.49
1:D:51:LEU:N	1:D:71:ILE:HD11	2.27	0.49
1:B:50:PRO:HG2	1:B:137:TYR:CE2	2.48	0.49
1:D:20:THR:CG2	1:D:21:GLN:OE1	2.60	0.49
1:F:31:ASN:HB2	1:F:118:SER:HB2	1.94	0.49
1:B:13:ASN:C	1:B:13:ASN:ND2	2.66	0.49
1:B:79:LEU:HD13	1:B:81:THR:HG23	1.93	0.49
1:F:40:GLY:H	1:F:54:SER:CB	2.26	0.49
1:D:125:PRO:HG2	1:D:128:LYS:HG3	1.95	0.49
1:D:132:GLU:HA	1:D:132:GLU:OE2	2.13	0.49
1:E:89:GLU:HG2	1:E:90:VAL:N	2.28	0.49
1:E:23:ASN:HD22	1:E:91:ARG:HH12	1.52	0.49
1:A:129:LEU:HB3	1:A:138:LEU:HD21	1.93	0.49
1:D:116:ILE:N	1:D:116:ILE:HD12	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:132:GLU:OE2	1:E:132:GLU:HA	2.13	0.49
1:C:132:GLU:HG2	2:C:177:HOH:O	2.13	0.48
1:D:115:CYS:C	1:D:116:ILE:HD12	2.33	0.48
1:B:16:GLN:HA	1:B:119:ALA:HB1	1.95	0.48
1:E:116:ILE:HG22	1:E:117:ASN:N	2.28	0.48
1:F:19:VAL:HG22	1:F:24:GLY:O	2.12	0.48
1:E:55:LYS:HD2	1:E:140:LEU:O	2.12	0.48
1:D:43:VAL:HG23	1:D:122:ARG:HB3	1.95	0.48
1:C:90:VAL:HG23	1:C:102:VAL:CG2	2.43	0.48
1:A:55:LYS:HE2	2:A:146:HOH:O	2.12	0.48
1:B:53:THR:CG2	1:B:71:ILE:HD11	2.44	0.48
1:F:25:THR:HA	1:F:117:ASN:HD21	1.79	0.48
1:C:43:VAL:HA	1:C:50:PRO:HA	1.94	0.48
1:D:73:GLU:O	1:D:93:ARG:HD3	2.13	0.48
1:D:90:VAL:O	1:D:99:LEU:HB2	2.14	0.48
1:E:50:PRO:HG2	1:E:137:TYR:CZ	2.49	0.48
1:F:106:GLY:HA3	1:F:113:ARG:HB2	1.94	0.48
1:A:1:MET:HG2	1:A:3:TYR:CZ	2.48	0.48
1:A:16:GLN:HA	1:A:119:ALA:HB1	1.95	0.48
1:A:47:SER:HB3	1:A:95:ALA:HB2	1.95	0.48
1:C:12:LEU:CD2	1:C:45:ILE:HD12	2.43	0.48
1:B:0:MET:HG3	1:B:94:THR:HG22	1.95	0.47
1:D:85:MET:HG3	1:D:87:ARG:HD3	1.95	0.47
1:E:72:GLU:OE2	1:E:137:TYR:HE2	1.97	0.47
1:B:0:MET:HG3	1:B:94:THR:CG2	2.44	0.47
1:A:31:ASN:HD21	1:A:34:TRP:HB3	1.79	0.47
1:A:85:MET:HE1	1:A:87:ARG:HD2	1.95	0.47
1:E:55:LYS:HE3	2:E:152:HOH:O	2.14	0.47
1:A:116:ILE:HG22	1:A:117:ASN:O	2.14	0.47
1:F:50:PRO:HG2	1:F:137:TYR:CE2	2.49	0.47
1:E:14:ARG:H	1:E:14:ARG:CD	2.28	0.47
1:C:93:ARG:HB2	1:C:93:ARG:NH1	2.29	0.47
1:D:128:LYS:O	1:D:132:GLU:CG	2.51	0.47
1:D:23:ASN:HA	1:D:98:HIS:CG	2.50	0.47
1:B:19:VAL:CG2	1:B:20:THR:N	2.78	0.47
1:D:45:ILE:HD12	1:D:46:VAL:N	2.29	0.47
1:A:134:TYR:O	1:A:135:GLU:C	2.54	0.46
1:F:31:ASN:HB2	1:F:118:SER:CB	2.46	0.46
1:F:66:SER:HA	1:F:114:TYR:O	2.15	0.46
1:A:0:MET:HB2	1:A:94:THR:HG22	1.97	0.46
1:D:76:GLU:OE2	1:D:93:ARG:HD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ASN:ND2	1:A:118:SER:OG	2.43	0.46
1:E:55:LYS:HB3	1:E:55:LYS:HZ2	1.80	0.46
1:A:126:LYS:HZ3	1:A:126:LYS:HB3	1.80	0.46
1:F:62:CYS:SG	1:F:113:ARG:NH2	2.88	0.46
1:D:51:LEU:C	1:D:71:ILE:HG12	2.36	0.46
1:F:26:GLU:CD	1:F:118:SER:H	2.17	0.46
1:A:85:MET:HE3	1:A:85:MET:HB2	1.69	0.46
1:F:13:ASN:OD1	1:F:16:GLN:HG3	2.15	0.46
1:F:20:THR:HB	1:F:97:SER:HB2	1.98	0.46
1:A:30:GLN:HE22	1:D:25:THR:H	1.64	0.45
1:A:43:VAL:HG12	1:A:50:PRO:HA	1.97	0.45
1:A:58:PHE:CD2	1:A:68:THR:HG23	2.51	0.45
1:A:33:TYR:HA	1:A:36:HIS:HB2	1.97	0.45
1:D:43:VAL:CG2	1:D:122:ARG:HB3	2.46	0.45
1:F:16:GLN:HA	1:F:119:ALA:HB1	1.97	0.45
1:F:52:PHE:HB3	1:F:67:PHE:CD2	2.51	0.45
1:B:107:PRO:O	1:B:108:GLY:O	2.35	0.45
1:C:90:VAL:CG2	1:C:102:VAL:HG22	2.46	0.45
1:E:26:GLU:HG2	1:E:117:ASN:OD1	2.17	0.45
1:D:129:LEU:HD12	1:D:138:LEU:HD13	1.98	0.45
1:F:43:VAL:CG1	1:F:44:ASP:N	2.78	0.45
1:D:19:VAL:HG21	1:D:119:ALA:HB3	1.98	0.45
1:C:31:ASN:HB3	1:C:118:SER:OG	2.17	0.45
1:D:90:VAL:HG23	1:D:101:HIS:HA	1.99	0.45
1:E:70:PRO:HG3	1:E:114:TYR:CZ	2.52	0.45
1:D:47:SER:HB3	1:D:95:ALA:HB2	1.99	0.45
1:A:127:HIS:HE1	2:A:153:HOH:O	2.00	0.44
1:C:33:TYR:O	1:C:65:PRO:HB3	2.17	0.44
1:E:90:VAL:HG23	1:E:102:VAL:HG22	1.99	0.44
1:A:1:MET:CG	1:A:3:TYR:CZ	3.00	0.44
1:A:54:SER:HB2	2:A:155:HOH:O	2.16	0.44
1:D:113:ARG:HH11	1:D:113:ARG:HG2	1.82	0.44
1:D:38:GLU:HA	1:D:38:GLU:OE2	2.17	0.44
1:E:26:GLU:HG3	1:E:64:TRP:HE1	1.82	0.44
1:F:85:MET:HE3	1:F:85:MET:HB2	1.82	0.44
1:A:28:PRO:O	1:A:29:PHE:HB2	2.17	0.44
1:C:89:GLU:HG2	1:C:90:VAL:N	2.30	0.44
1:D:13:ASN:H	1:D:16:GLN:HB2	1.82	0.44
1:E:116:ILE:CG2	1:E:117:ASN:N	2.79	0.44
1:E:15:MET:CE	1:E:19:VAL:HG23	2.47	0.44
1:C:76:GLU:OE2	1:C:93:ARG:NH1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:HIS:HB2	1:D:103:PHE:CZ	2.53	0.44
1:F:90:VAL:HG13	1:F:102:VAL:HG23	1.99	0.44
1:B:90:VAL:HG13	1:B:102:VAL:CG2	2.47	0.44
1:C:47:SER:OG	1:C:49:LYS:HB2	2.18	0.44
1:D:114:TYR:HB3	1:D:116:ILE:HD11	2.00	0.44
1:E:13:ASN:O	1:E:14:ARG:C	2.56	0.44
1:E:75:VAL:CG1	1:E:90:VAL:HG13	2.47	0.44
1:D:92:SER:O	1:D:96:ASP:HA	2.18	0.44
1:D:3:TYR:HE1	1:D:8:LYS:HG3	1.83	0.43
1:D:103:PHE:CD1	1:D:113:ARG:NH2	2.87	0.43
1:E:70:PRO:HD2	2:E:155:HOH:O	2.17	0.43
1:E:89:GLU:OE2	1:E:91:ARG:NH1	2.50	0.43
1:C:27:PRO:HA	1:C:28:PRO:HD3	1.76	0.43
1:F:80:ASP:HB2	1:F:89:GLU:HB2	2.00	0.43
1:F:7:GLU:HG3	1:F:8:LYS:N	2.33	0.43
1:C:23:ASN:N	1:C:23:ASN:ND2	2.65	0.43
1:D:33:TYR:CE2	1:D:123:PHE:HB2	2.53	0.43
1:D:75:VAL:HG13	1:D:90:VAL:HG12	2.00	0.43
1:B:69:LYS:HE2	1:B:69:LYS:HB3	1.82	0.43
1:D:45:ILE:HD12	1:D:46:VAL:H	1.84	0.43
1:A:55:LYS:HB2	2:A:166:HOH:O	2.19	0.43
1:D:114:TYR:HB3	1:D:116:ILE:CD1	2.48	0.43
1:F:94:THR:HG23	1:F:95:ALA:N	2.33	0.43
1:A:33:TYR:CE2	1:A:123:PHE:HB2	2.54	0.43
1:C:50:PRO:O	1:C:51:LEU:HD12	2.19	0.43
1:D:7:GLU:HA	1:D:10:LYS:CG	2.48	0.43
1:C:57:LYS:HB2	1:C:67:PHE:CE2	2.54	0.43
1:E:67:PHE:N	1:E:67:PHE:CD1	2.86	0.43
1:F:8:LYS:HG2	1:F:46:VAL:O	2.18	0.43
1:C:129:LEU:HB2	1:C:138:LEU:HD21	2.00	0.43
1:F:40:GLY:H	1:F:54:SER:HB3	1.84	0.43
1:C:85:MET:HE1	1:F:61:GLN:HB3	2.00	0.42
1:B:76:GLU:O	1:B:90:VAL:HA	2.20	0.42
1:D:17:TYR:O	1:D:21:GLN:HB2	2.18	0.42
1:C:27:PRO:HB3	1:F:25:THR:O	2.19	0.42
1:D:23:ASN:HA	1:D:98:HIS:CD2	2.54	0.42
1:F:43:VAL:HG21	1:F:134:TYR:CZ	2.54	0.42
1:A:85:MET:HE2	1:D:29:PHE:CE2	2.54	0.42
1:A:88:THR:HB	1:A:102:VAL:HG23	2.01	0.42
1:B:15:MET:HB3	2:B:185:HOH:O	2.18	0.42
1:D:73:GLU:N	1:D:73:GLU:OE2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:PRO:HG2	1:C:137:TYR:CE2	2.54	0.42
1:E:13:ASN:ND2	1:E:16:GLN:CD	2.72	0.42
1:F:87:ARG:HB3	2:F:156:HOH:O	2.18	0.42
1:C:133:GLY:HA2	2:C:144:HOH:O	2.18	0.42
1:D:73:GLU:CD	1:D:73:GLU:N	2.73	0.42
1:F:18:GLU:O	1:F:22:ASN:HB2	2.19	0.42
1:B:23:ASN:ND2	1:B:91:ARG:NH1	2.66	0.42
1:C:50:PRO:O	1:C:74:GLU:HG2	2.19	0.42
1:D:5:LYS:HB3	2:D:177:HOH:O	2.19	0.42
1:D:50:PRO:C	1:D:71:ILE:HD11	2.39	0.42
1:A:18:GLU:O	1:A:22:ASN:HB2	2.19	0.42
1:A:44:ASP:O	1:A:48:GLY:HA2	2.19	0.42
1:A:51:LEU:HB3	1:A:52:PHE:CD1	2.54	0.42
1:B:7:GLU:HG2	2:B:170:HOH:O	2.20	0.42
1:A:45:ILE:O	1:A:45:ILE:HG12	2.20	0.42
1:B:19:VAL:HB	1:B:24:GLY:O	2.19	0.42
1:C:90:VAL:HG23	1:C:102:VAL:HG22	2.01	0.42
1:E:71:ILE:HG22	1:E:72:GLU:N	2.34	0.42
1:F:57:LYS:HB2	1:F:67:PHE:CE2	2.55	0.42
1:F:95:ALA:O	1:F:96:ASP:HB3	2.19	0.42
1:A:50:PRO:HB2	1:A:71:ILE:HD11	2.01	0.42
1:B:99:LEU:HB3	1:B:116:ILE:HG23	2.01	0.42
1:F:102:VAL:C	1:F:103:PHE:CD1	2.93	0.42
1:D:13:ASN:HB2	1:D:16:GLN:OE1	2.20	0.41
1:A:31:ASN:HB2	1:A:118:SER:HB2	2.02	0.41
1:D:45:ILE:HD12	1:D:46:VAL:HG23	2.01	0.41
1:E:93:ARG:HG2	1:E:93:ARG:HH11	1.85	0.41
1:F:139:HIS:C	1:F:141:PHE:H	2.24	0.41
1:E:10:LYS:HB3	1:E:10:LYS:HE3	1.91	0.41
1:E:139:HIS:C	1:E:141:PHE:N	2.73	0.41
1:A:126:LYS:C	1:A:128:LYS:H	2.24	0.41
1:E:126:LYS:HE2	1:E:141:PHE:HB2	2.03	0.41
1:E:50:PRO:HG2	1:E:137:TYR:CE1	2.55	0.41
1:F:53:THR:CG2	1:F:54:SER:N	2.83	0.41
1:A:35:ASP:O	1:A:37:LYS:HD3	2.20	0.41
1:B:43:VAL:HG13	1:B:48:GLY:HA2	2.02	0.41
1:B:93:ARG:NH1	1:B:93:ARG:HG3	2.34	0.41
1:C:37:LYS:HZ3	1:C:37:LYS:HB3	1.83	0.41
1:E:92:SER:O	1:E:96:ASP:HA	2.20	0.41
1:F:108:GLY:HA2	1:F:111:GLY:H	1.85	0.41
1:B:16:GLN:HG2	1:B:119:ALA:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:ASN:HD22	1:B:98:HIS:CB	2.34	0.41
1:C:102:VAL:HG13	1:C:114:TYR:CG	2.55	0.41
1:C:91:ARG:HA	1:C:99:LEU:HG	2.02	0.41
1:F:89:GLU:OE1	1:F:91:ARG:HD2	2.21	0.41
1:C:12:LEU:HD22	1:C:45:ILE:HD12	2.01	0.41
1:E:43:VAL:CG2	1:E:122:ARG:HB3	2.50	0.41
1:F:41:LEU:HD11	1:F:50:PRO:HB3	2.02	0.41
1:D:116:ILE:CG2	1:D:117:ASN:N	2.83	0.41
1:F:97:SER:O	1:F:99:LEU:HD13	2.21	0.41
1:B:91:ARG:NH1	1:B:98:HIS:HB2	2.36	0.41
1:C:5:LYS:O	1:C:9:ILE:HG13	2.21	0.41
1:D:44:ASP:OD1	1:D:46:VAL:HB	2.21	0.41
1:F:124:VAL:HG13	1:F:132:GLU:OE1	2.20	0.41
1:F:74:GLU:OE1	1:F:94:THR:HG22	2.20	0.41
1:F:81:THR:HG22	1:F:81:THR:O	2.21	0.41
1:A:134:TYR:C	1:A:136:SER:N	2.72	0.41
1:A:135:GLU:HA	1:A:138:LEU:HD23	2.02	0.41
1:E:39:GLU:CD	1:E:126:LYS:HD2	2.41	0.41
1:E:72:GLU:O	1:E:73:GLU:C	2.60	0.41
1:F:74:GLU:CD	1:F:94:THR:HG22	2.41	0.41
1:B:28:PRO:O	1:B:29:PHE:HB2	2.21	0.40
1:E:114:TYR:HB3	1:E:116:ILE:CD1	2.51	0.40
1:F:27:PRO:HA	1:F:28:PRO:HD3	1.64	0.40
1:E:60:SER:HB2	2:E:174:HOH:O	2.20	0.40
1:B:13:ASN:HD21	1:B:16:GLN:H	1.69	0.40
1:B:53:THR:HG22	1:B:71:ILE:HD11	2.03	0.40
1:C:36:HIS:HB3	1:C:57:LYS:NZ	2.36	0.40
1:A:34:TRP:CG	1:A:35:ASP:N	2.89	0.40
1:C:118:SER:C	1:C:120:ALA:H	2.25	0.40
1:C:41:LEU:HD11	1:C:137:TYR:CB	2.51	0.40
1:D:67:PHE:CD1	1:D:67:PHE:N	2.90	0.40
1:F:76:GLU:CD	1:F:93:ARG:HB2	2.41	0.40
1:F:56:ASP:O	1:F:67:PHE:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	140/144 (97%)	125 (89%)	12 (9%)	3 (2%)	7	13
1	B	140/144 (97%)	127 (91%)	11 (8%)	2 (1%)	11	22
1	C	137/144 (95%)	117 (85%)	17 (12%)	3 (2%)	6	12
1	D	137/144 (95%)	115 (84%)	22 (16%)	0	100	100
1	E	139/144 (96%)	125 (90%)	9 (6%)	5 (4%)	3	4
1	F	139/144 (96%)	126 (91%)	8 (6%)	5 (4%)	3	4
All	All	832/864 (96%)	735 (88%)	79 (10%)	18 (2%)	6	12

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	72	GLU
1	E	72	GLU
1	F	2	ALA
1	F	36	HIS
1	A	72	GLU
1	B	72	GLU
1	B	108	GLY
1	C	73	GLU
1	C	119	ALA
1	E	14	ARG
1	A	127	HIS
1	E	140	LEU
1	F	72	GLU
1	A	73	GLU
1	F	140	LEU
1	E	19	VAL
1	E	70	PRO
1	F	108	GLY

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	128/130 (98%)	122 (95%)	6 (5%)	26	50
1	B	128/130 (98%)	118 (92%)	10 (8%)	12	25
1	C	126/130 (97%)	119 (94%)	7 (6%)	21	42
1	D	126/130 (97%)	117 (93%)	9 (7%)	14	29
1	E	127/130 (98%)	123 (97%)	4 (3%)	40	66
1	F	126/130 (97%)	120 (95%)	6 (5%)	25	49
All	All	761/780 (98%)	719 (94%)	42 (6%)	21	43

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	73	GLU
1	A	93	ARG
1	A	102	VAL
1	A	126	LYS
1	A	129	LEU
1	B	1	MET
1	B	13	ASN
1	B	14	ARG
1	B	19	VAL
1	B	77	GLU
1	B	79	LEU
1	B	87	ARG
1	B	90	VAL
1	B	113	ARG
1	B	138	LEU
1	C	21	GLN
1	C	45	ILE
1	C	49	LYS
1	C	87	ARG
1	C	90	VAL
1	C	102	VAL

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Mol	Chain	Res	Type
1	C	132	GLU
1	D	6	GLU
1	D	8	LYS
1	D	10	LYS
1	D	25	THR
1	D	41	LEU
1	D	45	ILE
1	D	54	SER
1	D	102	VAL
1	D	130	LYS
1	E	14	ARG
1	E	45	ILE
1	E	72	GLU
1	E	102	VAL
1	F	3	TYR
1	F	36	HIS
1	F	49	LYS
1	F	73	GLU
1	F	90	VAL
1	F	99	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	30	GLN
1	A	31	ASN
1	A	36	HIS
1	A	61	GLN
1	A	117	ASN
1	B	13	ASN
1	B	16	GLN
1	B	21	GLN
1	B	23	ASN
1	B	31	ASN
1	B	36	HIS
1	B	98	HIS
1	C	23	ASN
1	C	110	ASN
1	E	4	ASN
1	E	13	ASN
1	E	23	ASN

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Mol	Chain	Res	Type
1	E	61	GLN
1	E	83	HIS
1	F	21	GLN
1	F	30	GLN
1	F	31	ASN
1	F	101	HIS
1	F	117	ASN

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 carbohydrates in this entry.

5.6   Ligand geometry (i)

There are no ligands in this entry.

5.7   Other polymers (i)

There are no such residues in this entry.

5.8   Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	142/144 (98%)	-0.36	0	100	100	11, 26, 41, 49	0
1	B	142/144 (98%)	-0.45	0	100	100	6, 21, 38, 50	0
1	C	139/144 (96%)	-0.04	0	100	100	27, 44, 61, 64	0
1	D	139/144 (96%)	-0.26	0	100	100	18, 31, 56, 62	0
1	E	141/144 (97%)	-0.36	2 (1%)	75	71	10, 23, 48, 86	0
1	F	141/144 (97%)	-0.08	2 (1%)	75	71	27, 44, 68, 72	0
All	All	844/864 (97%)	-0.26	4 (0%)	91	89	6, 32, 59, 86	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	3	TYR	2.6
1	F	127	HIS	2.5
1	E	1	MET	2.1
1	F	35	ASP	2.1

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.