W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:10 PM GMT

PDB ID   :   1J3L
Title   :   Structure of the RNA-processing inhibitor RraA from Thermus thermophilis
Authors   :   Rehse, P.H.; Miyano, M.; Tahirov, T.H.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on :   2003-02-04
Resolution :   2.30 Å(reported)

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

MolProbity   :   4.02b-467
Mogul   :   1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)   :   1.9-1692
EDS   :   rb-20026688
Percentile statistics   :   20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac   :   5.8.0135
CCP4   :   6.5.0
Ideal geometry (proteins) :   Engh & Huber (2001)
Ideal geometry (DNA, RNA) :   Parkinson et al. (1996)
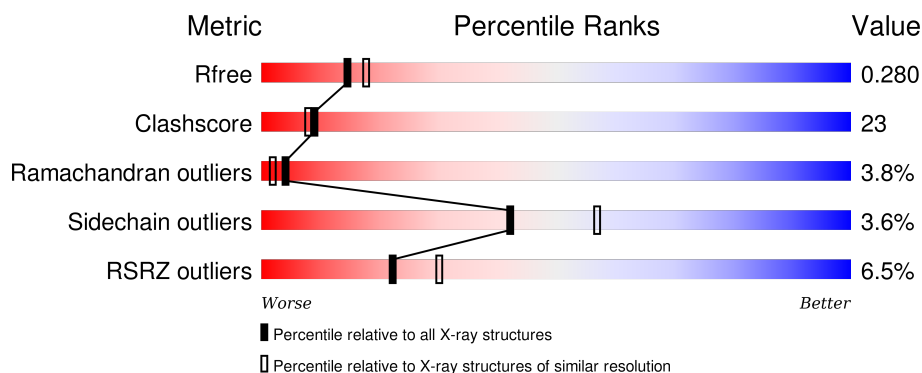Validation Pipeline (wwPDB-VP) :   trunk26865

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 2.30 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	Percentile Ranks	Value
Rfree		0.280
Clashscore		23
Ramachandran outliers		3.8%
Sidechain outliers		3.6%
RSRZ outliers		6.5%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	164	2% 70% 28% •
1	B	164	4% 69% 28% • •
1	C	164	3% 71% 25% • •
1	D	164	10% 46% 48% 6%
1	E	164	10% 45% 46% 9%

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Mol	Chain	Length	Quality of chain
1	F	164	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7692 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 Demethylmenaquinone Methyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	164	Total 1224	C 775	N 218	O 229	S 1	Se 1	0	0	0
1	B	164	Total 1223	C 773	N 218	O 230	S 1	Se 1	0	0	0
1	C	161	Total 1211	C 769	N 215	O 225	S 1	Se 1	0	0	0
1	D	164	Total 1226	C 776	N 218	O 230	S 1	Se 1	0	0	0
1	E	164	Total 1226	C 776	N 218	O 230	S 1	Se 1	0	0	0
1	F	157	Total 1181	C 752	N 208	O 219	S 1	Se 1	0	0	0

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Mg 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Cl 1	0	0
3	A	1	Total 1	Cl 1	0	0

- Molecule 4 is water.

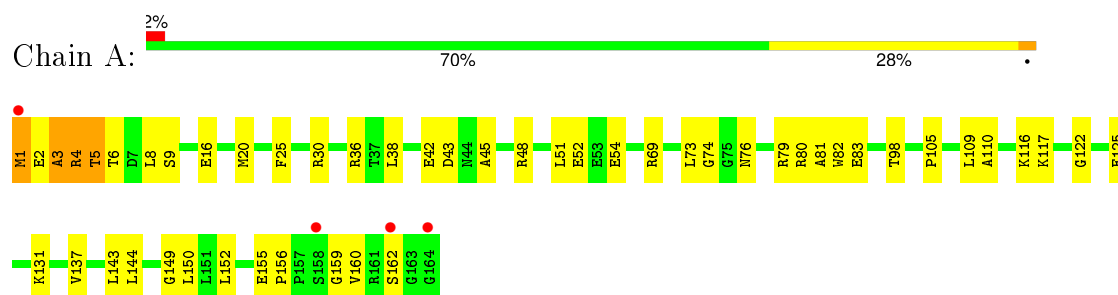| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	90	Total 90	O 90	0	0

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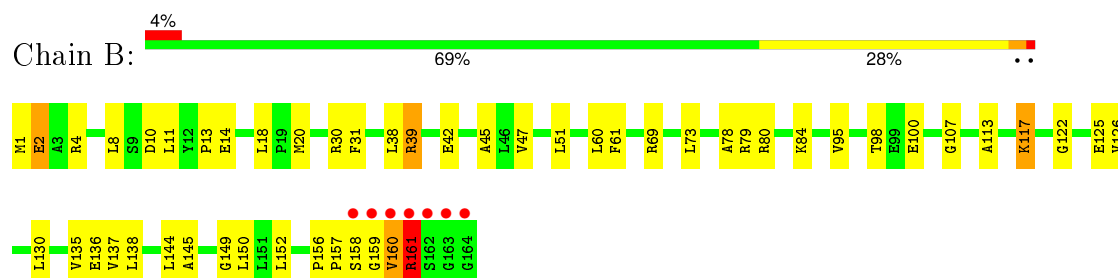| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	116	Total 116	O 116	0	0
4	C	72	Total 72	O 72	0	0
4	D	60	Total 60	O 60	0	0
4	E	28	Total 28	O 28	0	0
4	F	32	Total 32	O 32	0	0

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 errors 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.
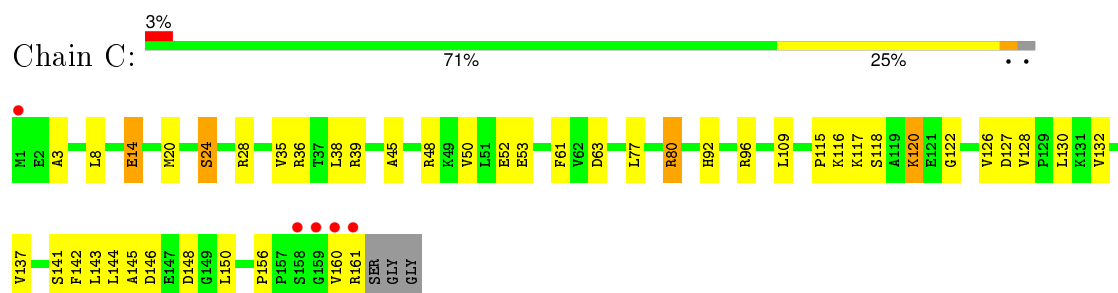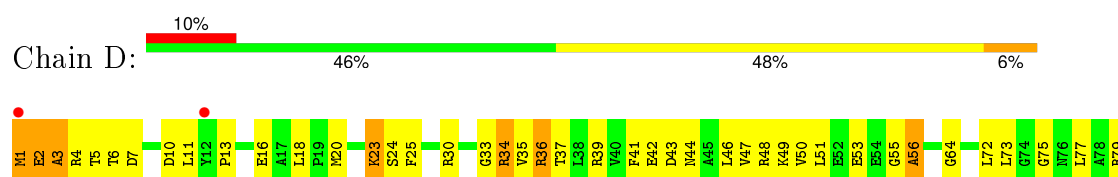
- Molecule 1: Demethylmenaquinone Methyltransferase

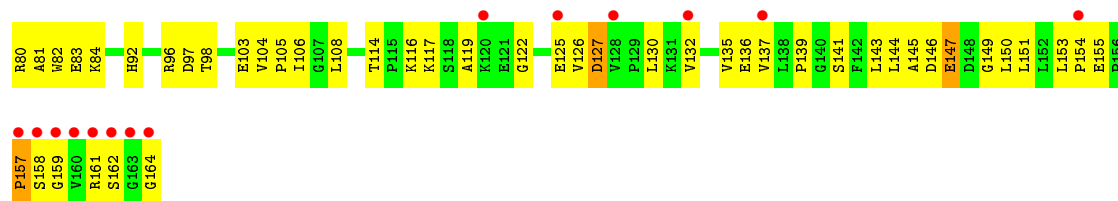Chain A:

- Molecule 1: Demethylmenaquinone Methyltransferase

Chain B:
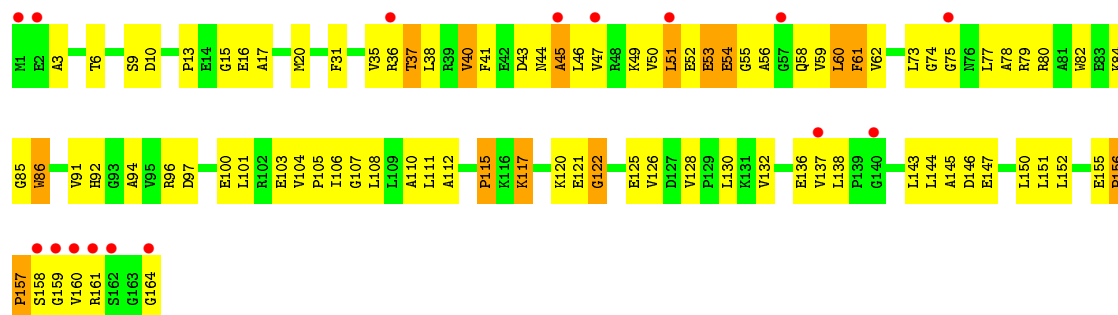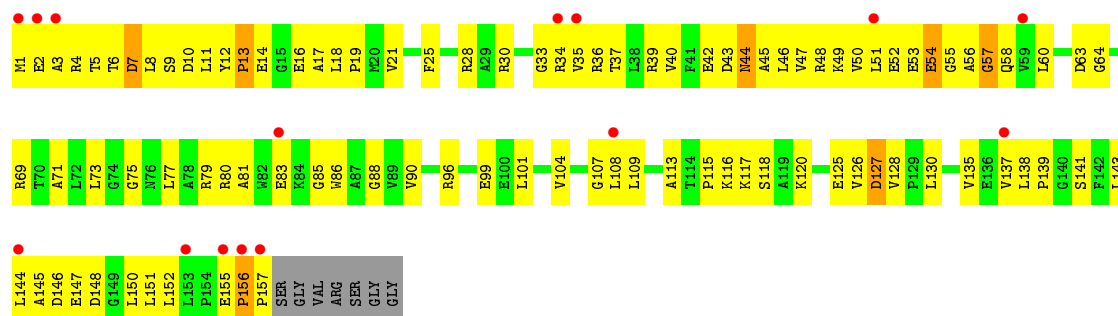
- Molecule 1: Demethylmenaquinone Methyltransferase

Chain C:

- Molecule 1: Demethylmenaquinone Methyltransferase

Chain D:

R80 A81 W82 E83 K84 H92 R96 D97 T98 E103 V104 P105 I106 G107 L108 T114 P115 K116 K117 S118 A119 K120 E121 G122 E125 V126 D127 V128 P129 L130 K131 V132 V135 E136 V137 L138 P139 G140 S141 F142 L143 L144 A145 D146 E147 D148 G149 L150 L151 L152 L153 P154 E155 P156

P157 S158 G159 V160 R161 S162 G163 G164

• Molecule 1: Demethylmenaquinone Methyltransferase

Chain E:

10%

45% 46% 9%

M1 E2 A3 T6 S9 D10 P13 E14 G15 E16 A17 M20 F31 V35 R36 T37 L38 R39 V40 F41 E42 D43 N44 A45 L46 V47 R48 K49 V50 L51 E52 E53 E54 G55 A56 G57 Q58 V59 L60 F61 V62 L73 G74 G75 N76 L77 A78 R79 R80 A81 W82 E83 K84

G85 W86 V91 H92 G93 A94 V95 R96 D97 E100 L101 R102 E103 V104 P105 I106 G107 L108 L109 A110 L111 A112 P115 K116 K117 K120 E121 G122 E125 V126 D127 V128 P129 L130 K131 V132 E136 V137 L138 P139 G140 L143 L144 A145 D146 E147 L150 L151 L152 E155 P156

P157 S158 G159 V160 R161 S162 G163 G164

• Molecule 1: Demethylmenaquinone Methyltransferase

Chain F:

9%

37% 55%

M1 E2 A3 R4 T5 T6 D7 L8 S9 D10 L11 Y12 P13 E14 G15 E16 A17 L18 P19 M20 V21 F25 R28 A29 R30 G33 R34 V35 R36 T37 L38 R39 V40 F41 E42 D43 N44 A45 L46 V47 R48 K49 V50 L51 E52 E53 E54 G55 A56 G57 Q58 V59 L60 D63 G64

R69 T70 A71 L72 L73 G74 G75 N76 L77 A78 R79 R80 A81 W82 E83 K84 G85 W86 A87 G88 V89 V90 R96 E99 E100 L101 V104 G107 L108 L109 A113 T114 P115 K116 K117 S118 A119 K120 E125 V126 D127 V128 P129 L130 V135 E136 V137 L138 P139 G140 S141 F142 L143

L144 A145 D146 E147 D148 G149 L150 L151 L152 L153 P154 E155 P156 P157 SER GLY VAL ARG SER GLY GLY

4   Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	61.87Å 109.07Å 270.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.40 – 2.30 38.39 – 2.29	Depositor EDS
% Data completeness (in resolution range)	85.3 (38.40-2.30) 88.7 (38.39-2.29)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.50 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.206 , 0.274 0.214 , 0.280	Depositor DCC
R_{free} test set	2164 reflections (6.27%)	DCC
Wilson B-factor (Å^2)	32.8	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 58.5	EDS
Estimated twinning fraction	0.029 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.064 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46, < L^2 > = 0.29$	Xtriage
Outliers	2 of 71048 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7692	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

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

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: MG, CL

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	0.40	0/1243	0.68	0/1676
1	B	0.38	0/1242	0.69	1/1674 (0.1%)
1	C	0.35	0/1230	0.62	0/1661
1	D	0.38	0/1245	0.65	0/1679
1	E	0.28	0/1245	0.57	0/1679
1	F	0.27	0/1200	0.55	0/1621
All	All	0.35	0/7405	0.63	1/9990 (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})
1	B	39	ARG	NE-CZ-NH1	-5.79	117.41	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1224	0	1253	37	0
1	B	1223	0	1249	41	0
1	C	1211	0	1246	33	0
1	D	1226	0	1257	73	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1226	0	1257	90	0
1	F	1181	0	1215	88	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	90	0	0	6	0
4	B	116	0	0	4	0
4	C	72	0	0	1	0
4	D	60	0	0	1	0
4	E	28	0	0	0	0
4	F	32	0	0	2	0
All	All	7692	0	7477	343	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 23.

All (343) 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:E:117:LYS:H	1:E:117:LYS:HE2	1.11	1.12
1:E:117:LYS:N	1:E:117:LYS:HE2	1.84	0.91
1:F:138:LEU:HD12	1:F:139:PRO:HD2	1.53	0.88
1:E:117:LYS:CE	1:E:117:LYS:H	1.86	0.88
1:C:8:LEU:HD12	1:C:144:LEU:HD22	1.56	0.86
1:E:36:ARG:HD2	1:E:58:GLN:NE2	1.92	0.85
1:E:160:VAL:HG23	1:E:161:ARG:H	1.41	0.85
1:F:71:ALA:O	1:F:118:SER:HB2	1.79	0.82
1:E:115:PRO:HA	1:F:6:THR:HG22	1.60	0.81
1:C:130:LEU:HB2	1:C:137:VAL:HB	1.61	0.81
1:F:16:GLU:HB3	1:F:135:VAL:HG13	1.63	0.80
4:A:1036:HOH:O	1:C:116:LYS:HE2	1.81	0.79
1:B:14:GLU:HG3	4:B:1069:HOH:O	1.84	0.78
1:D:23:LYS:HE3	1:D:24:SER:N	2.00	0.76
1:D:49:LYS:O	1:D:53:GLU:HG3	1.86	0.76
1:B:156:PRO:HG2	1:B:161:ARG:HB3	1.66	0.76
1:E:161:ARG:N	1:E:161:ARG:HE	1.85	0.75
1:B:45:ALA:HB3	1:B:122:GLY:HA2	1.69	0.75
1:B:1:MET:HA	1:B:30:ARG:HB3	1.68	0.74
1:E:161:ARG:H	1:E:161:ARG:HE	1.37	0.73
1:E:96:ARG:NH1	1:E:117:LYS:HB3	2.04	0.73
1:D:23:LYS:HE3	1:D:24:SER:H	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:35:VAL:HG22	1:E:59:VAL:HB	1.71	0.73
1:C:45:ALA:HB3	1:C:122:GLY:HA2	1.71	0.72
1:F:63:ASP:HB2	1:F:130:LEU:HD13	1.70	0.72
1:E:55:GLY:HA3	1:E:58:GLN:NE2	2.05	0.72
1:E:78:ALA:HB1	1:E:104:VAL:HG21	1.72	0.72
1:A:137:VAL:HG22	1:A:152:LEU:HD11	1.73	0.71
1:A:16:GLU:HG3	4:A:1089:HOH:O	1.90	0.71
1:F:143:LEU:HD23	1:F:144:LEU:N	2.07	0.70
1:C:35:VAL:HG12	1:C:141:SER:O	1.92	0.69
1:C:8:LEU:HD12	1:C:144:LEU:CD2	2.21	0.69
1:D:143:LEU:HD23	1:D:144:LEU:N	2.08	0.68
1:F:44:ASN:HD22	1:F:44:ASN:H	1.39	0.67
1:E:104:VAL:HG12	1:E:106:ILE:HG12	1.76	0.67
1:A:76:ASN:HB3	4:A:1045:HOH:O	1.92	0.67
1:D:104:VAL:HG12	1:D:106:ILE:HG12	1.76	0.67
1:D:5:THR:HG23	1:D:151:LEU:HB2	1.77	0.67
1:A:20:MSE:HE2	1:A:149:GLY:HA2	1.79	0.65
1:F:101:LEU:O	1:F:104:VAL:HG22	1.96	0.65
1:E:160:VAL:CG2	1:E:161:ARG:HH21	2.08	0.65
1:E:36:ARG:HH22	1:E:53:GLU:HG3	1.62	0.65
1:C:14:GLU:H	1:C:14:GLU:CD	2.01	0.65
1:F:88:GLY:HA2	1:F:107:GLY:O	1.97	0.64
1:A:1:MET:HG3	1:A:30:ARG:HH12	1.62	0.64
1:D:116:LYS:HG2	1:E:9:SER:OG	1.99	0.63
1:D:39:ARG:NH1	1:D:130:LEU:HD23	2.13	0.63
1:F:17:ALA:O	1:F:135:VAL:HG21	1.98	0.63
1:F:81:ALA:O	1:F:86:TRP:HB2	1.98	0.63
1:E:143:LEU:HD23	1:E:144:LEU:N	2.14	0.63
1:C:143:LEU:HD23	1:C:143:LEU:C	2.20	0.62
1:F:144:LEU:HD23	1:F:145:ALA:N	2.15	0.62
1:F:127:ASP:O	1:F:139:PRO:HG3	1.99	0.62
1:E:160:VAL:HG23	1:E:161:ARG:N	2.13	0.61
1:E:51:LEU:HD23	1:E:51:LEU:O	1.98	0.61
1:E:136:GLU:OE2	1:E:138:LEU:HD11	2.00	0.61
1:E:97:ASP:HB3	1:E:100:GLU:HB2	1.80	0.61
1:F:2:GLU:HG2	1:F:3:ALA:N	2.16	0.61
1:E:60:LEU:HD12	1:E:86:TRP:HZ3	1.66	0.60
1:D:126:VAL:HG12	1:D:127:ASP:OD1	2.00	0.60
1:C:143:LEU:HD23	1:C:144:LEU:N	2.16	0.60
1:E:96:ARG:HH21	1:F:6:THR:HB	1.66	0.60
1:F:4:ARG:HB2	1:F:7:ASP:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:96:ARG:NH2	1:D:117:LYS:HB3	2.17	0.60
1:F:75:GLY:O	1:F:79:ARG:HG3	2.01	0.60
1:D:25:PHE:HB2	1:D:108:LEU:HD22	1.83	0.60
1:D:146:ASP:HB2	1:D:147:GLU:OE2	2.02	0.59
1:F:96:ARG:CZ	1:F:117:LYS:HB3	2.32	0.59
1:E:52:GLU:C	1:E:54:GLU:H	2.04	0.59
1:F:18:LEU:HD12	1:F:150:LEU:HD12	1.84	0.59
1:D:46:LEU:HD11	1:D:122:GLY:O	2.03	0.59
1:E:155:GLU:HB2	1:E:156:PRO:HD2	1.85	0.58
1:E:143:LEU:HD23	1:E:143:LEU:C	2.24	0.58
1:F:5:THR:HB	1:F:146:ASP:OD1	2.03	0.58
1:F:35:VAL:HG21	1:F:143:LEU:HB2	1.86	0.58
1:D:46:LEU:O	1:D:50:VAL:HG23	2.04	0.58
1:A:160:VAL:HG12	1:A:160:VAL:O	2.04	0.57
1:F:18:LEU:HD21	1:F:135:VAL:HB	1.85	0.57
1:B:51:LEU:HD21	1:B:60:LEU:HD23	1.87	0.57
1:F:30:ARG:HG2	1:F:146:ASP:HB3	1.87	0.57
1:A:4:ARG:HH11	1:A:4:ARG:CG	2.18	0.57
1:E:60:LEU:HD12	1:E:86:TRP:CZ3	2.40	0.57
1:D:48:ARG:HH11	1:D:48:ARG:HG3	1.69	0.57
1:D:16:GLU:O	1:D:151:LEU:HD12	2.05	0.57
1:C:50:VAL:O	1:C:53:GLU:HB2	2.04	0.56
1:B:69:ARG:NH2	1:D:103:GLU:HG3	2.20	0.56
1:F:138:LEU:CD1	1:F:139:PRO:HD2	2.32	0.56
1:D:23:LYS:CE	1:D:24:SER:H	2.18	0.56
1:E:51:LEU:HA	1:E:86:TRP:CH2	2.40	0.56
1:E:130:LEU:HB2	1:E:137:VAL:HB	1.85	0.56
1:C:28:ARG:HG3	1:C:28:ARG:HH11	1.70	0.56
1:B:84:LYS:HD2	4:B:1071:HOH:O	2.05	0.56
1:D:125:GLU:HG3	4:D:184:HOH:O	2.06	0.56
1:B:117:LYS:HD2	4:C:197:HOH:O	2.06	0.55
1:E:20:MSE:HE2	1:E:146:ASP:O	2.05	0.55
1:D:4:ARG:HB2	1:D:7:ASP:OD2	2.07	0.55
1:E:40:VAL:HG21	1:E:43:ASP:O	2.05	0.55
1:E:31:PHE:CD2	1:E:107:GLY:HA3	2.42	0.55
1:B:38:LEU:HD23	1:B:47:VAL:HG22	1.88	0.55
1:D:18:LEU:HD12	1:D:150:LEU:HD12	1.89	0.55
1:F:73:LEU:HD21	1:F:108:LEU:HD22	1.88	0.55
1:A:4:ARG:NH1	1:A:4:ARG:HG3	2.20	0.55
1:D:6:THR:HG21	4:F:168:HOH:O	2.05	0.55
1:F:16:GLU:O	1:F:151:LEU:HD12	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ARG:HG3	1:A:4:ARG:HH11	1.72	0.54
1:D:41:PHE:CE2	1:D:42:GLU:HG3	2.43	0.54
1:D:143:LEU:HD23	1:D:143:LEU:C	2.28	0.54
1:F:96:ARG:NH2	1:F:117:LYS:HB3	2.23	0.54
1:B:69:ARG:CZ	1:D:103:GLU:HG3	2.38	0.54
1:B:98:THR:HB	4:B:1081:HOH:O	2.08	0.53
1:A:42:GLU:OE2	1:A:69:ARG:HD2	2.08	0.53
1:B:137:VAL:HG22	1:B:152:LEU:HD11	1.89	0.53
1:E:50:VAL:O	1:E:53:GLU:HG2	2.08	0.53
1:E:52:GLU:HG2	1:E:80:ARG:HH21	1.72	0.53
1:D:147:GLU:H	1:D:147:GLU:CD	2.12	0.53
1:F:143:LEU:HD12	1:F:152:LEU:HD21	1.89	0.53
1:C:35:VAL:HG22	1:C:36:ARG:N	2.23	0.53
1:B:80:ARG:O	1:B:84:LYS:HG2	2.08	0.53
1:E:45:ALA:CB	1:E:122:GLY:HA2	2.38	0.53
1:F:39:ARG:HB3	1:F:125:GLU:HG3	1.91	0.52
1:D:41:PHE:CD2	1:D:42:GLU:HG3	2.44	0.52
1:F:55:GLY:O	1:F:58:GLN:HG3	2.10	0.52
1:F:137:VAL:HG22	1:F:152:LEU:HD11	1.92	0.52
1:E:50:VAL:C	1:E:52:GLU:H	2.12	0.52
1:D:39:ARG:HH11	1:D:130:LEU:HD23	1.73	0.52
1:C:142:PHE:CD1	1:C:156:PRO:HG3	2.45	0.52
1:B:130:LEU:HB2	1:B:137:VAL:HB	1.92	0.52
1:F:43:ASP:N	1:F:118:SER:OG	2.42	0.52
1:E:125:GLU:HB3	1:E:128:VAL:HG11	1.92	0.52
1:D:96:ARG:HD2	1:E:6:THR:HG22	1.93	0.51
1:A:38:LEU:HD12	1:A:125:GLU:O	2.09	0.51
1:E:145:ALA:HB2	1:E:150:LEU:HD22	1.92	0.51
1:F:36:ARG:O	1:F:60:LEU:HD12	2.11	0.51
1:A:143:LEU:HD23	1:A:143:LEU:C	2.30	0.51
1:D:135:VAL:HG12	1:D:136:GLU:N	2.26	0.51
1:D:92:HIS:CD2	1:D:132:VAL:HG13	2.45	0.51
1:C:96:ARG:NH2	1:C:117:LYS:HB3	2.26	0.51
1:E:92:HIS:CD2	1:E:111:LEU:HD11	2.46	0.51
1:D:141:SER:HB2	1:D:153:LEU:O	2.11	0.51
1:F:43:ASP:N	1:F:118:SER:HG	2.09	0.51
1:E:73:LEU:HA	1:E:77:LEU:HD12	1.93	0.51
1:E:117:LYS:HZ2	1:F:9:SER:C	2.15	0.50
1:F:12:TYR:N	1:F:13:PRO:HD3	2.25	0.50
1:E:158:SER:O	1:E:160:VAL:N	2.45	0.50
1:D:159:GLY:HA3	1:D:162:SER:OG	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:SER:HA	1:C:109:LEU:HD23	1.93	0.50
1:A:79:ARG:O	1:A:83:GLU:HG3	2.12	0.50
1:D:18:LEU:HD23	1:D:135:VAL:HG21	1.93	0.50
1:F:156:PRO:HB3	1:F:157:PRO:HD2	1.92	0.50
1:B:157:PRO:C	1:B:159:GLY:H	2.15	0.50
1:A:82:TRP:NE1	1:A:105:PRO:HG2	2.27	0.50
1:F:73:LEU:CD2	1:F:108:LEU:HD22	2.41	0.50
1:F:28:ARG:HG3	1:F:28:ARG:HH11	1.77	0.50
1:B:156:PRO:HB3	1:B:161:ARG:HA	1.94	0.50
1:F:8:LEU:O	1:F:12:TYR:HD1	1.94	0.49
1:D:48:ARG:HG3	1:D:48:ARG:NH1	2.27	0.49
1:F:2:GLU:CG	1:F:3:ALA:N	2.75	0.49
1:F:46:LEU:O	1:F:50:VAL:HG23	2.12	0.49
1:D:20:MSE:HE2	1:D:149:GLY:HA2	1.93	0.49
1:F:48:ARG:O	1:F:52:GLU:HG2	2.13	0.49
1:E:60:LEU:HD22	1:E:62:VAL:CG2	2.43	0.49
1:B:125:GLU:OE2	1:D:84:LYS:HA	2.13	0.49
1:E:45:ALA:HB1	1:E:122:GLY:HA2	1.94	0.49
1:E:17:ALA:HB2	1:E:151:LEU:HD12	1.94	0.49
1:E:115:PRO:HA	1:F:6:THR:CG2	2.37	0.48
1:E:44:ASN:HD21	1:E:77:LEU:HD11	1.77	0.48
1:E:10:ASP:O	1:E:13:PRO:HD3	2.13	0.48
1:D:64:GLY:HA3	1:D:72:LEU:HD11	1.95	0.48
1:F:143:LEU:HD23	1:F:143:LEU:C	2.33	0.48
1:B:2:GLU:CD	1:B:2:GLU:N	2.67	0.48
1:C:63:ASP:HA	1:C:92:HIS:HB3	1.96	0.48
1:B:18:LEU:HD21	1:B:135:VAL:HB	1.95	0.48
1:A:9:SER:OG	1:C:116:LYS:HG2	2.13	0.48
1:C:38:LEU:HD12	1:C:39:ARG:N	2.29	0.48
1:D:73:LEU:HD23	1:D:73:LEU:C	2.34	0.48
1:B:156:PRO:CG	1:B:161:ARG:HB3	2.39	0.48
1:A:155:GLU:HB2	1:A:156:PRO:HD2	1.94	0.48
1:A:109:LEU:CD1	1:A:150:LEU:HD21	2.44	0.48
1:F:44:ASN:HB2	1:F:47:VAL:HB	1.95	0.48
1:D:157:PRO:O	1:D:158:SER:HB2	2.13	0.48
1:A:25:PHE:CD1	1:A:98:THR:HG22	2.48	0.48
1:A:117:LYS:HD2	1:B:10:ASP:OD1	2.13	0.48
1:E:36:ARG:HD2	1:E:58:GLN:HE21	1.76	0.48
1:E:143:LEU:HD12	1:E:152:LEU:HD21	1.96	0.48
1:B:157:PRO:O	1:B:159:GLY:N	2.42	0.48
1:D:37:THR:OG1	1:D:127:ASP:HA	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:40:VAL:HG22	1:E:41:PHE:N	2.29	0.47
1:C:20:MSE:HE2	1:C:146:ASP:O	2.14	0.47
1:B:1:MET:HA	1:B:30:ARG:CB	2.39	0.47
1:D:80:ARG:CZ	1:D:84:LYS:HE2	2.44	0.47
1:B:79:ARG:NH2	1:B:100:GLU:OE1	2.47	0.47
1:B:136:GLU:OE2	1:B:138:LEU:HD11	2.15	0.47
1:C:126:VAL:O	1:C:128:VAL:HG13	2.15	0.47
1:D:5:THR:CG2	1:D:151:LEU:HB2	2.45	0.47
1:B:42:GLU:OE2	1:B:69:ARG:HD2	2.15	0.47
1:F:49:LYS:O	1:F:53:GLU:HG3	2.15	0.47
1:F:137:VAL:HG22	1:F:152:LEU:CD1	2.45	0.47
1:F:33:GLY:HA3	1:F:57:GLY:O	2.15	0.47
1:E:16:GLU:O	1:E:151:LEU:HD12	2.15	0.47
1:E:160:VAL:HG21	1:E:164:GLY:C	2.35	0.46
1:F:53:GLU:O	1:F:54:GLU:HB2	2.15	0.46
1:E:101:LEU:HD22	1:E:108:LEU:HD13	1.97	0.46
1:E:160:VAL:HG23	1:E:161:ARG:HH21	1.79	0.46
1:E:37:THR:HB	1:E:130:LEU:HG	1.98	0.46
1:B:38:LEU:HD13	1:B:126:VAL:HG22	1.96	0.46
1:F:12:TYR:O	1:F:14:GLU:N	2.48	0.46
1:F:42:GLU:CD	1:F:69:ARG:HH21	2.17	0.46
1:F:90:VAL:HG22	1:F:109:LEU:HD12	1.96	0.46
1:C:145:ALA:HB2	1:C:150:LEU:HD22	1.98	0.46
1:F:5:THR:O	1:F:151:LEU:HD22	2.16	0.46
1:A:137:VAL:HG22	1:A:152:LEU:CD1	2.45	0.46
1:A:143:LEU:HD23	1:A:144:LEU:N	2.31	0.46
1:A:80:ARG:HA	1:A:80:ARG:HD2	1.78	0.46
1:A:116:LYS:HE2	4:B:1027:HOH:O	2.15	0.46
1:D:44:ASN:O	1:D:47:VAL:N	2.49	0.46
1:E:120:LYS:HD2	1:E:120:LYS:N	2.30	0.46
1:F:37:THR:CG2	1:F:137:VAL:HG12	2.45	0.46
1:E:38:LEU:O	1:E:62:VAL:HA	2.16	0.46
1:F:51:LEU:HD13	1:F:81:ALA:HB2	1.98	0.46
1:C:3:ALA:HB3	1:C:8:LEU:HD11	1.98	0.46
1:F:2:GLU:CG	1:F:3:ALA:H	2.29	0.46
1:D:2:GLU:HG3	1:D:3:ALA:H	1.80	0.46
1:F:19:PRO:HB2	1:F:21:VAL:HG13	1.97	0.45
1:E:104:VAL:CG1	1:E:106:ILE:HG12	2.46	0.45
1:D:96:ARG:O	1:D:97:ASP:HB2	2.15	0.45
1:F:16:GLU:HB3	1:F:135:VAL:CG1	2.39	0.45
1:F:126:VAL:HG12	1:F:127:ASP:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:44:ASN:N	1:F:44:ASN:HD22	2.03	0.45
1:F:7:ASP:O	1:F:11:LEU:HG	2.17	0.45
1:E:155:GLU:HB2	1:E:156:PRO:CD	2.45	0.45
1:A:51:LEU:HD13	1:A:81:ALA:HB2	1.98	0.45
1:F:9:SER:HB2	1:F:151:LEU:HD13	1.99	0.45
1:E:54:GLU:CD	1:E:84:LYS:HB3	2.37	0.45
1:D:73:LEU:HG	1:D:77:LEU:HB3	1.99	0.45
1:D:55:GLY:O	1:D:56:ALA:C	2.55	0.45
1:E:117:LYS:NZ	1:F:10:ASP:HA	2.31	0.45
1:F:2:GLU:HG2	1:F:3:ALA:H	1.80	0.45
1:B:98:THR:HG23	1:C:148:ASP:OD1	2.17	0.45
1:E:52:GLU:OE2	1:E:84:LYS:HD3	2.17	0.45
1:A:45:ALA:HB3	1:A:122:GLY:HA2	1.99	0.45
1:A:36:ARG:HH11	1:A:36:ARG:HG2	1.80	0.45
1:E:91:VAL:O	1:E:110:ALA:HA	2.17	0.45
1:E:73:LEU:HD23	1:E:73:LEU:C	2.37	0.44
1:E:52:GLU:HB2	1:E:80:ARG:HE	1.82	0.44
1:F:28:ARG:HG3	1:F:28:ARG:NH1	2.32	0.44
1:A:52:GLU:OE2	1:A:80:ARG:NE	2.47	0.44
1:D:79:ARG:O	1:D:83:GLU:HG3	2.16	0.44
1:F:36:ARG:HG3	1:F:58:GLN:OE1	2.18	0.44
1:B:73:LEU:HD21	1:B:78:ALA:HB2	1.99	0.44
1:E:82:TRP:CD2	1:E:105:PRO:HD2	2.53	0.44
1:C:77:LEU:HA	1:C:77:LEU:HD12	1.79	0.44
1:F:18:LEU:CD2	1:F:135:VAL:HB	2.48	0.44
1:F:145:ALA:HB2	1:F:150:LEU:HD22	2.00	0.44
1:E:52:GLU:HG2	1:E:80:ARG:NH2	2.33	0.44
1:C:126:VAL:HG12	1:C:127:ASP:N	2.33	0.44
1:E:47:VAL:O	1:E:51:LEU:HB2	2.18	0.44
1:A:25:PHE:CE2	1:A:110:ALA:HB3	2.52	0.44
1:E:160:VAL:CG2	1:E:161:ARG:H	2.22	0.43
1:B:39:ARG:HG3	1:D:82:TRP:CH2	2.53	0.43
1:C:48:ARG:HA	1:C:77:LEU:HD11	2.00	0.43
1:C:118:SER:O	1:C:120:LYS:HE3	2.18	0.43
1:E:94:ALA:HA	1:E:112:ALA:O	2.18	0.43
1:D:154:PRO:O	1:D:155:GLU:HG3	2.18	0.43
1:F:1:MET:HG2	1:F:1:MET:O	2.18	0.43
1:D:161:ARG:O	1:D:161:ARG:HG3	2.18	0.43
1:D:51:LEU:HD13	1:D:81:ALA:HB2	2.00	0.43
1:E:36:ARG:HD2	1:E:58:GLN:HE22	1.75	0.43
1:E:53:GLU:O	1:E:54:GLU:O	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:48:ARG:HG3	1:F:77:LEU:HD21	2.00	0.43
1:D:98:THR:HB	1:E:147:GLU:HG3	2.01	0.43
1:F:25:PHE:HE2	1:F:113:ALA:HB2	1.83	0.43
1:D:35:VAL:O	1:D:139:PRO:HA	2.18	0.43
1:F:5:THR:CG2	1:F:148:ASP:HB2	2.49	0.43
1:A:5:THR:CG2	1:A:6:THR:N	2.82	0.43
1:D:43:ASP:HA	1:D:119:ALA:O	2.18	0.43
1:E:160:VAL:HG22	1:E:161:ARG:HH21	1.82	0.43
1:F:79:ARG:O	1:F:83:GLU:N	2.49	0.43
1:E:52:GLU:C	1:E:54:GLU:N	2.70	0.43
1:E:49:LYS:HD3	1:E:49:LYS:C	2.38	0.43
1:B:4:ARG:O	1:B:8:LEU:HG	2.18	0.43
1:B:45:ALA:HB3	1:B:122:GLY:CA	2.46	0.43
1:A:48:ARG:HG2	4:A:1056:HOH:O	2.19	0.43
1:E:161:ARG:N	1:E:161:ARG:NE	2.61	0.43
1:B:160:VAL:C	1:B:161:ARG:HD2	2.39	0.43
1:E:73:LEU:HD23	1:E:74:GLY:N	2.34	0.43
1:F:130:LEU:HB2	1:F:137:VAL:HB	2.00	0.43
1:F:85:GLY:O	1:F:86:TRP:C	2.57	0.43
1:A:43:ASP:OD2	1:D:164:GLY:OXT	2.37	0.43
1:D:104:VAL:HA	1:D:105:PRO:HD3	1.87	0.42
1:F:104:VAL:HG23	1:F:104:VAL:O	2.19	0.42
1:E:17:ALA:HB2	1:E:151:LEU:CD1	2.49	0.42
1:F:9:SER:HB2	1:F:151:LEU:CD1	2.49	0.42
1:B:39:ARG:NE	1:D:83:GLU:O	2.43	0.42
1:B:20:MSE:HE2	1:B:149:GLY:HA2	2.01	0.42
1:D:5:THR:HG23	1:D:151:LEU:CB	2.49	0.42
1:D:39:ARG:HB2	1:D:130:LEU:CD2	2.49	0.42
1:F:45:ALA:HB2	1:F:120:LYS:HA	2.02	0.42
1:B:161:ARG:HD2	1:B:161:ARG:N	2.35	0.42
1:F:56:ALA:C	1:F:58:GLN:H	2.23	0.42
1:C:61:PHE:CE1	1:C:132:VAL:HG21	2.54	0.42
1:F:35:VAL:N	1:F:141:SER:O	2.53	0.42
1:D:116:LYS:HE3	1:D:116:LYS:HB3	1.93	0.42
1:D:1:MET:O	1:D:2:GLU:HB2	2.20	0.42
1:D:2:GLU:HG3	1:D:3:ALA:N	2.35	0.42
1:A:2:GLU:O	1:A:3:ALA:C	2.57	0.42
1:B:145:ALA:HB2	1:B:150:LEU:CD2	2.50	0.42
1:F:155:GLU:HG3	1:F:156:PRO:HD2	2.02	0.42
1:D:30:ARG:HA	1:D:145:ALA:O	2.19	0.42
1:D:36:ARG:NH2	1:D:53:GLU:OE1	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:ARG:HG2	1:C:161:ARG:HH11	1.85	0.42
1:C:52:GLU:OE2	1:C:80:ARG:NH1	2.49	0.42
1:F:40:VAL:O	1:F:64:GLY:HA2	2.20	0.42
1:A:4:ARG:NH2	4:A:1015:HOH:O	2.50	0.41
1:E:75:GLY:O	1:E:79:ARG:NE	2.53	0.41
1:D:33:GLY:O	1:D:34:ARG:C	2.58	0.41
1:E:46:LEU:HD13	1:E:126:VAL:HG23	2.02	0.41
1:E:158:SER:O	1:E:161:ARG:HG2	2.20	0.41
1:D:80:ARG:NH2	1:D:84:LYS:HE2	2.35	0.41
1:F:37:THR:HG22	1:F:137:VAL:HG12	2.02	0.41
1:A:8:LEU:HD12	1:A:144:LEU:HD13	2.02	0.41
1:E:61:PHE:CE1	1:E:132:VAL:HG21	2.56	0.41
1:A:73:LEU:HD23	1:A:74:GLY:O	2.20	0.41
1:E:40:VAL:CG2	1:E:43:ASP:HB3	2.50	0.41
1:D:75:GLY:O	1:D:79:ARG:HG3	2.20	0.41
1:A:131:LYS:HE3	4:A:1054:HOH:O	2.19	0.41
1:E:54:GLU:HA	1:E:54:GLU:OE1	2.20	0.41
1:C:35:VAL:CG2	1:C:36:ARG:N	2.83	0.41
1:D:4:ARG:NH2	1:F:99:GLU:OE1	2.54	0.41
1:A:117:LYS:HE3	1:A:117:LYS:HB2	1.86	0.41
1:B:31:PHE:CD1	1:B:107:GLY:HA3	2.55	0.41
1:B:8:LEU:HD12	1:B:144:LEU:HD22	2.01	0.41
1:D:11:LEU:C	1:D:13:PRO:HD3	2.41	0.41
1:F:116:LYS:NZ	4:F:182:HOH:O	2.53	0.41
1:B:11:LEU:C	1:B:13:PRO:HD3	2.40	0.41
1:C:36:ARG:HH21	1:C:127:ASP:CG	2.24	0.41
1:E:60:LEU:HD22	1:E:62:VAL:HG23	2.03	0.41
1:F:125:GLU:OE1	1:F:128:VAL:HG11	2.21	0.41
1:B:95:VAL:O	1:B:113:ALA:HA	2.20	0.41
1:D:23:LYS:HA	1:D:23:LYS:HD2	1.80	0.40
1:E:157:PRO:HB2	1:E:161:ARG:CG	2.51	0.40
1:D:130:LEU:HB2	1:D:137:VAL:HB	2.03	0.40
1:C:28:ARG:HG3	1:C:28:ARG:NH1	2.37	0.40
1:E:117:LYS:NZ	1:F:9:SER:C	2.74	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	162/164 (99%)	153 (94%)	6 (4%)	3 (2%)	10	8
1	B	162/164 (99%)	153 (94%)	5 (3%)	4 (2%)	7	5
1	C	159/164 (97%)	147 (92%)	10 (6%)	2 (1%)	15	15
1	D	162/164 (99%)	140 (86%)	17 (10%)	5 (3%)	5	3
1	E	162/164 (99%)	127 (78%)	19 (12%)	16 (10%)	1	0
1	F	155/164 (94%)	129 (83%)	19 (12%)	7 (4%)	3	1
All	All	962/984 (98%)	849 (88%)	76 (8%)	37 (4%)	4	2

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	SER
1	B	160	VAL
1	B	161	ARG
1	D	2	GLU
1	D	157	PRO
1	E	54	GLU
1	E	85	GLY
1	A	3	ALA
1	B	158	SER
1	D	3	ALA
1	D	56	ALA
1	D	147	GLU
1	E	56	ALA
1	E	121	GLU
1	E	157	PRO
1	E	159	GLY
1	F	127	ASP
1	F	156	PRO
1	E	156	PRO
1	F	54	GLU

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Mol	Chain	Res	Type
1	F	57	GLY
1	F	115	PRO
1	B	2	GLU
1	E	3	ALA
1	E	37	THR
1	E	51	LEU
1	F	147	GLU
1	A	159	GLY
1	E	45	ALA
1	E	53	GLU
1	E	115	PRO
1	F	13	PRO
1	C	160	VAL
1	E	15	GLY
1	E	122	GLY
1	E	40	VAL
1	C	115	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	124/124 (100%)	120 (97%)	4 (3%)	46	62
1	B	124/124 (100%)	121 (98%)	3 (2%)	57	74
1	C	124/124 (100%)	120 (97%)	4 (3%)	46	62
1	D	125/124 (101%)	118 (94%)	7 (6%)	26	35
1	E	125/124 (101%)	120 (96%)	5 (4%)	38	52
1	F	121/124 (98%)	117 (97%)	4 (3%)	45	61
All	All	743/744 (100%)	716 (96%)	27 (4%)	42	57

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET

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Mol	Chain	Res	Type
1	A	4	ARG
1	A	5	THR
1	A	54	GLU
1	B	61	PHE
1	B	117	LYS
1	B	161	ARG
1	C	14	GLU
1	C	24	SER
1	C	80	ARG
1	C	120	LYS
1	D	1	MET
1	D	10	ASP
1	D	23	LYS
1	D	34	ARG
1	D	36	ARG
1	D	114	THR
1	D	127	ASP
1	E	60	LEU
1	E	61	PHE
1	E	86	TRP
1	E	103	GLU
1	E	117	LYS
1	F	7	ASP
1	F	34	ARG
1	F	44	ASN
1	F	80	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	E	44	ASN
1	E	58	GLN
1	F	44	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)

Of 3 ligands modelled in this entry, 3 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)

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(Å²)	Q<0.9
1	A	163/164 (99%)	-0.25	4 (2%)	61	70	13, 29, 64, 103	0
1	B	163/164 (99%)	-0.22	7 (4%)	39	48	15, 26, 53, 107	0
1	C	160/164 (97%)	-0.32	5 (3%)	52	62	21, 34, 59, 98	0
1	D	163/164 (99%)	0.40	16 (9%)	10	14	23, 50, 94, 110	0
1	E	163/164 (99%)	0.65	16 (9%)	10	14	36, 66, 98, 117	0
1	F	156/164 (95%)	0.60	15 (9%)	10	15	39, 73, 94, 107	0
All	All	968/984 (98%)	0.14	63 (6%)	22	30	13, 44, 92, 117	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	160	VAL	12.1
1	D	163	GLY	11.5
1	E	160	VAL	8.5
1	E	159	GLY	7.0
1	B	159	GLY	6.4
1	E	158	SER	6.3
1	D	164	GLY	5.9
1	F	155	GLU	5.7
1	D	162	SER	5.7
1	C	158	SER	5.3
1	A	162	SER	5.2
1	B	163	GLY	5.2
1	F	2	GLU	5.1
1	E	162	SER	4.9
1	A	1	MET	4.8
1	C	1	MET	4.8
1	D	159	GLY	4.8
1	F	1	MET	4.5
1	C	160	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	1	MET	4.3
1	C	159	GLY	4.2
1	E	164	GLY	4.2
1	B	162	SER	4.1
1	B	161	ARG	4.0
1	B	164	GLY	4.0
1	E	1	MET	4.0
1	D	160	VAL	3.8
1	F	144	LEU	3.6
1	E	51	LEU	3.6
1	F	156	PRO	3.5
1	F	59	VAL	3.5
1	D	161	ARG	3.3
1	F	108	LEU	3.2
1	F	34	ARG	3.1
1	D	158	SER	3.1
1	B	158	SER	3.1
1	F	157	PRO	3.0
1	E	137	VAL	3.0
1	F	83	GLU	3.0
1	F	35	VAL	2.9
1	E	47	VAL	2.8
1	E	57	GLY	2.8
1	E	36	ARG	2.7
1	F	137	VAL	2.7
1	A	158	SER	2.6
1	E	161	ARG	2.6
1	D	12	TYR	2.6
1	F	51	LEU	2.6
1	D	154	PRO	2.4
1	D	132	VAL	2.4
1	D	137	VAL	2.4
1	E	75	GLY	2.4
1	A	164	GLY	2.4
1	E	140	GLY	2.3
1	D	128	VAL	2.3
1	C	161	ARG	2.3
1	D	157	PRO	2.3
1	F	3	ALA	2.3
1	D	125	GLU	2.1
1	F	153	LEU	2.1
1	E	45	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	120	LYS	2.1
1	E	2	GLU	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 carbohydrates in this entry.

6.4   Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	CL	A	1002	1/1	0.98	0.07	-2.88	30,30,30,30	0
2	MG	A	1001	1/1	0.96	0.10	-	34,34,34,34	0
3	CL	B	1003	1/1	0.98	0.05	-	27,27,27,27	0

6.5   Other polymers (i)

There are no such residues in this entry.