Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:20 AM GMT

PDB ID	:	3E6M
Title	:	The crystal structure of a MarR family transcriptional regulator from Silicibacter pomeroyi DSS.
Authors	:	Tan, K.; Volkart, L.; Freeman, L.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2008-08-15
Resolution	:	2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

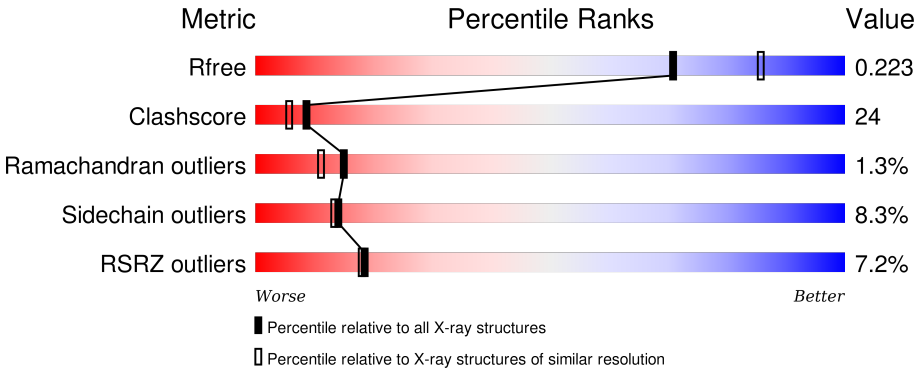
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	161	4% 52% 34% 5% 9%
1	B	161	9% 52% 34% 6% 9%
1	C	161	8% 50% 34% 7% 9%
1	D	161	7% 52% 38% • 7%
1	E	161	6% 52% 35% 5% 9%

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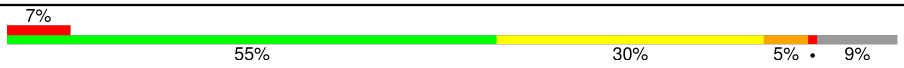
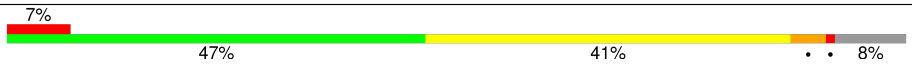
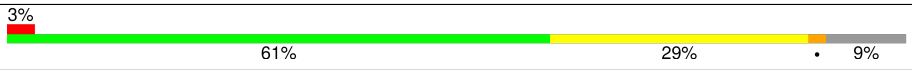
Mol	Chain	Length	Quality of chain
1	F	161	
1	G	161	
1	H	161	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9532 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 MarR family Transcriptional regulator.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	146	Total	C	N	O	S	Se	0	0	0
			1115	708	192	213	1	1			
1	B	147	Total	C	N	O	S	Se	0	0	0
			1132	717	192	221	1	1			
1	C	146	Total	C	N	O	S	Se	0	0	0
			1119	709	192	216	1	1			
1	D	149	Total	C	N	O	S	Se	0	0	0
			1142	723	194	223	1	1			
1	E	147	Total	C	N	O	S	Se	0	0	0
			1135	721	193	219	1	1			
1	F	146	Total	C	N	O	S	Se	0	0	0
			1128	715	192	219	1	1			
1	G	148	Total	C	N	O	S	Se	0	0	0
			1144	726	195	221	1	1			
1	H	147	Total	C	N	O	S	Se	0	0	0
			1132	717	192	221	1	1			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q5LLB9
A	-1	ASN	-	expression tag	UNP Q5LLB9
A	0	ALA	-	expression tag	UNP Q5LLB9
B	-2	SER	-	expression tag	UNP Q5LLB9
B	-1	ASN	-	expression tag	UNP Q5LLB9
B	0	ALA	-	expression tag	UNP Q5LLB9
C	-2	SER	-	expression tag	UNP Q5LLB9
C	-1	ASN	-	expression tag	UNP Q5LLB9
C	0	ALA	-	expression tag	UNP Q5LLB9
D	-2	SER	-	expression tag	UNP Q5LLB9
D	-1	ASN	-	expression tag	UNP Q5LLB9
D	0	ALA	-	expression tag	UNP Q5LLB9
E	-2	SER	-	expression tag	UNP Q5LLB9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	ASN	-	expression tag	UNP Q5LLB9
E	0	ALA	-	expression tag	UNP Q5LLB9
F	-2	SER	-	expression tag	UNP Q5LLB9
F	-1	ASN	-	expression tag	UNP Q5LLB9
F	0	ALA	-	expression tag	UNP Q5LLB9
G	-2	SER	-	expression tag	UNP Q5LLB9
G	-1	ASN	-	expression tag	UNP Q5LLB9
G	0	ALA	-	expression tag	UNP Q5LLB9
H	-2	SER	-	expression tag	UNP Q5LLB9
H	-1	ASN	-	expression tag	UNP Q5LLB9
H	0	ALA	-	expression tag	UNP Q5LLB9

- Molecule 2 is water.

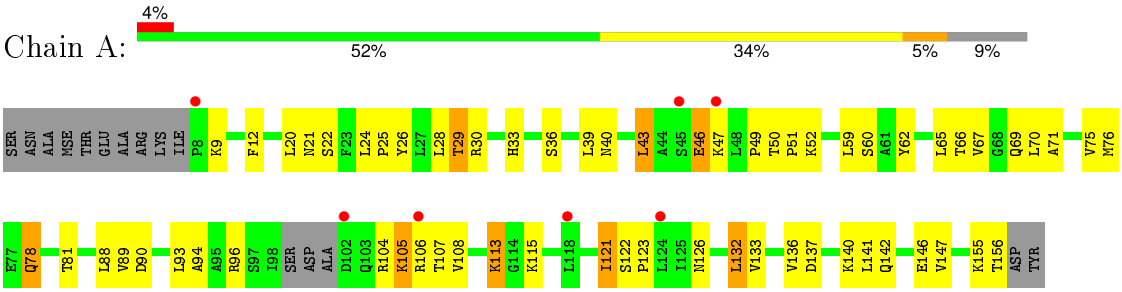
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	65	Total O 65 65	0	0
2	B	57	Total O 57 57	0	0
2	C	59	Total O 59 59	0	0
2	D	50	Total O 50 50	0	0
2	E	69	Total O 69 69	0	0
2	F	58	Total O 58 58	0	0
2	G	62	Total O 62 62	0	0
2	H	65	Total O 65 65	0	0

3 Residue-property plots (i)

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.

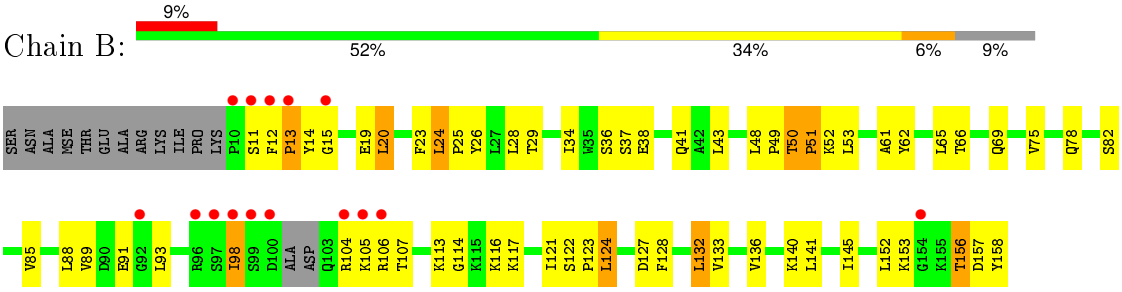
- Molecule 1: MarR family Transcriptional regulator

Chain A:



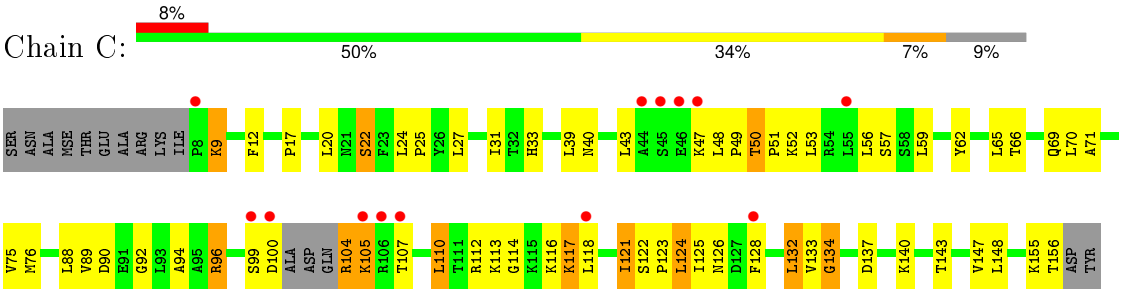
- Molecule 1: MarR family Transcriptional regulator

Chain B:



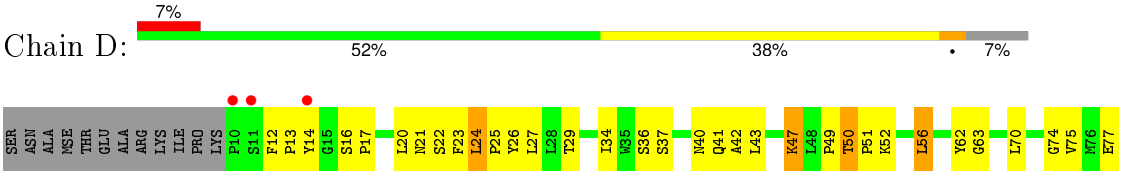
- Molecule 1: MarR family Transcriptional regulator

Chain C:

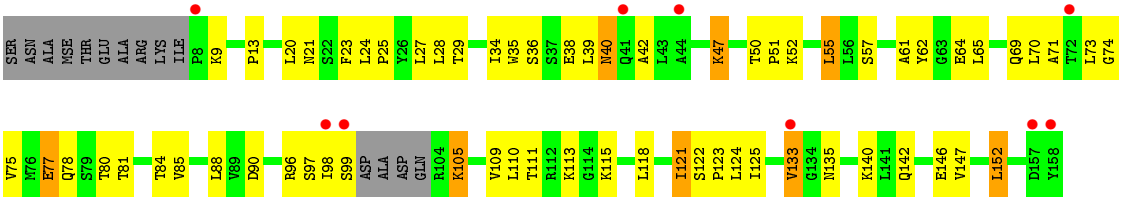


- Molecule 1: MarR family Transcriptional regulator

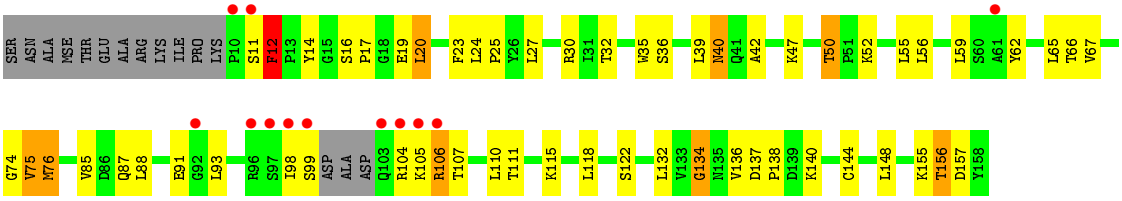
Chain D:



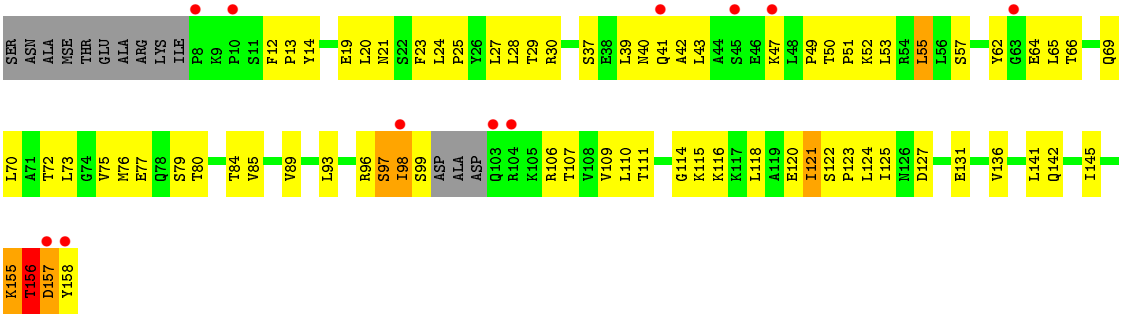
• Molecule 1: MarR family Transcriptional regulator



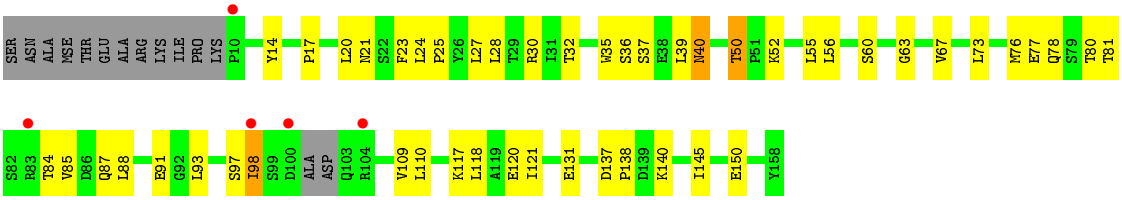
• Molecule 1: MarR family Transcriptional regulator



• Molecule 1: MarR family Transcriptional regulator



• Molecule 1: MarR family Transcriptional regulator



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	75.43Å 93.20Å 101.56Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	39.60 – 2.20 39.64 – 2.19	Depositor EDS
% Data completeness (in resolution range)	96.1 (39.60-2.20) 97.4 (39.64-2.19)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.00 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.185 , 0.230 0.186 , 0.223	Depositor DCC
R_{free} test set	3517 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	39.2	Xtriage
Anisotropy	0.756	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 53.7	EDS
Estimated twinning fraction	0.479 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Outliers	1 of 70328 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9532	wwPDB-VP
Average B, all atoms (Å^2)	61.0	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 54.99 % 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 3.3753e-05.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0/1131	0.59	0/1529
1	B	0.37	0/1148	0.65	0/1551
1	C	0.42	0/1135	0.61	0/1534
1	D	0.39	0/1159	0.60	0/1568
1	E	0.39	0/1152	0.60	0/1556
1	F	0.39	0/1144	0.64	0/1545
1	G	0.39	0/1161	0.58	0/1568
1	H	0.39	0/1148	0.56	0/1551
All	All	0.39	0/9178	0.60	0/12402

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

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	1115	0	1157	64	0
1	B	1132	0	1166	65	0
1	C	1119	0	1162	70	0
1	D	1142	0	1174	71	0
1	E	1135	0	1180	56	0
1	F	1128	0	1168	62	0
1	G	1144	0	1188	74	0
1	H	1132	0	1166	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	65	0	0	6	0
2	B	57	0	0	5	0
2	C	59	0	0	6	0
2	D	50	0	0	5	0
2	E	69	0	0	2	0
2	F	58	0	0	3	0
2	G	62	0	0	0	0
2	H	65	0	0	3	0
All	All	9532	0	9361	436	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 24.

All (436) 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:C:66:THR:HG21	1:C:105:LYS:HE3	1.45	0.97
1:F:40:ASN:HD21	1:F:50:THR:H	1.12	0.95
1:G:156:THR:C	1:G:158:TYR:H	1.70	0.94
1:C:56:LEU:HB3	1:C:118:LEU:HD11	1.52	0.91
1:A:90:ASP:HB3	2:A:176:HOH:O	1.70	0.90
1:G:121:ILE:HD13	1:G:121:ILE:O	1.72	0.88
1:B:24:LEU:O	1:B:28:LEU:HD23	1.75	0.86
1:B:157:ASP:HB3	2:B:169:HOH:O	1.76	0.86
1:B:13:PRO:HG3	2:B:179:HOH:O	1.78	0.83
1:A:49:PRO:HD2	1:A:52:LYS:HE2	1.58	0.82
2:A:187:HOH:O	1:B:14:TYR:HB2	1.81	0.80
1:A:122:SER:HB2	1:B:12:PHE:CE1	2.18	0.79
1:F:66:THR:HG21	1:F:105:LYS:HD3	1.65	0.78
1:B:24:LEU:HG	1:B:28:LEU:CD2	2.15	0.77
1:C:49:PRO:HB2	1:C:51:PRO:HG2	1.65	0.77
2:E:197:HOH:O	1:H:131:GLU:HG2	1.84	0.77
1:C:140:LYS:HD2	2:C:244:HOH:O	1.84	0.76
1:A:75:VAL:HG21	1:B:29:THR:HG22	1.66	0.76
1:C:90:ASP:HB3	2:C:249:HOH:O	1.85	0.76
1:C:126:ASN:HD21	1:D:13:PRO:HD3	1.52	0.75
1:H:40:ASN:HD21	1:H:50:THR:H	1.34	0.75
1:E:152:LEU:HD21	1:F:30:ARG:HG2	1.67	0.74
1:E:57:SER:HB2	1:F:14:TYR:CE2	2.22	0.74
1:E:13:PRO:HG3	1:F:118:LEU:HB3	1.69	0.74
1:B:24:LEU:HG	1:B:28:LEU:HD23	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:93:LEU:HD22	1:G:114:GLY:HA2	1.70	0.74
1:E:25:PRO:O	1:E:29:THR:HG23	1.88	0.73
1:E:105:LYS:HE2	1:H:131:GLU:HG3	1.70	0.73
1:C:122:SER:OG	1:C:123:PRO:HD3	1.89	0.73
1:B:117:LYS:O	1:B:121:ILE:HG12	1.88	0.73
1:D:43:LEU:HD21	1:D:124:LEU:HD22	1.69	0.73
1:D:122:SER:HB2	1:D:123:PRO:HD3	1.71	0.72
1:C:66:THR:HG22	1:C:107:THR:HG22	1.71	0.71
1:B:52:LYS:HB3	1:B:88:LEU:HD21	1.71	0.71
1:B:65:LEU:HA	1:B:69:GLN:HE21	1.56	0.71
1:A:105:LYS:HE2	1:A:105:LYS:N	2.05	0.71
1:C:75:VAL:HG21	1:D:29:THR:HG22	1.73	0.70
1:D:141:LEU:O	1:D:145:ILE:HD12	1.93	0.69
1:F:23:PHE:CZ	1:F:25:PRO:HG2	2.28	0.69
1:B:11:SER:HB2	1:B:19:GLU:OE2	1.93	0.68
1:E:77:GLU:HG2	1:E:80:THR:HG23	1.75	0.68
1:G:75:VAL:O	1:G:75:VAL:HG12	1.93	0.68
1:F:16:SER:HB2	1:F:17:PRO:HD2	1.74	0.68
1:H:150:GLU:HB2	2:H:211:HOH:O	1.94	0.68
1:E:39:LEU:HD21	1:E:125:ILE:HD11	1.76	0.67
1:C:59:LEU:HG	1:C:70:LEU:HD21	1.75	0.67
1:B:65:LEU:HA	1:B:69:GLN:NE2	2.09	0.67
1:F:40:ASN:ND2	1:F:50:THR:H	1.88	0.67
1:G:57:SER:HB2	1:H:14:TYR:CD1	2.30	0.67
1:E:29:THR:HG22	1:F:32:THR:HG23	1.75	0.66
1:F:12:PHE:HB2	1:F:19:GLU:OE1	1.93	0.66
1:G:69:GLN:O	1:G:73:LEU:HB2	1.96	0.66
1:E:152:LEU:HD23	1:F:27:LEU:HD23	1.76	0.66
1:E:42:ALA:HB1	1:E:124:LEU:HD21	1.78	0.66
1:G:110:LEU:HD13	1:G:115:LYS:HG2	1.78	0.66
1:H:76:MSE:HE3	1:H:80:THR:HG22	1.76	0.66
1:G:29:THR:HG22	1:H:32:THR:HG23	1.77	0.65
1:C:50:THR:N	1:C:51:PRO:HD2	2.12	0.64
1:A:126:ASN:HD21	1:B:12:PHE:HB2	1.62	0.64
1:C:57:SER:HB2	1:D:14:TYR:CE1	2.31	0.64
1:G:156:THR:O	1:G:156:THR:CG2	2.46	0.64
1:E:38:GLU:OE2	1:F:155:LYS:NZ	2.30	0.64
1:C:20:LEU:HD23	1:D:62:TYR:HE2	1.62	0.64
1:F:40:ASN:HD21	1:F:50:THR:N	1.90	0.64
1:B:12:PHE:O	1:B:14:TYR:N	2.30	0.64
1:G:55:LEU:HG	1:G:70:LEU:HD22	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:65:LEU:HD22	1:E:69:GLN:HB3	1.78	0.63
1:G:39:LEU:HD21	1:G:125:ILE:HD11	1.81	0.63
1:G:39:LEU:HD21	1:G:125:ILE:CD1	2.29	0.63
1:G:62:TYR:HE1	1:H:20:LEU:HD23	1.64	0.63
1:C:71:ALA:HB1	1:C:76:MSE:O	1.99	0.63
1:G:116:LYS:O	1:G:120:GLU:HG3	1.99	0.63
1:D:56:LEU:HD13	1:D:88:LEU:HD23	1.81	0.63
1:H:24:LEU:HB3	1:H:25:PRO:HD3	1.80	0.62
1:A:142:GLN:O	1:A:146:GLU:HG3	1.99	0.62
1:G:156:THR:C	1:G:158:TYR:N	2.42	0.62
1:A:155:LYS:HG3	1:B:132:LEU:HD23	1.81	0.62
1:G:42:ALA:HB1	1:G:124:LEU:HD11	1.81	0.62
1:G:156:THR:O	1:G:156:THR:HG23	1.98	0.62
1:F:118:LEU:O	1:F:122:SER:HB3	1.99	0.62
1:D:47:LYS:C	1:D:49:PRO:HD3	2.20	0.62
1:G:50:THR:HB	1:G:51:PRO:HD3	1.82	0.61
1:E:133:VAL:O	1:E:133:VAL:HG13	2.00	0.61
1:C:24:LEU:HB3	1:C:25:PRO:HD3	1.80	0.61
1:C:66:THR:CG2	1:C:105:LYS:HE3	2.25	0.61
1:G:20:LEU:O	1:G:23:PHE:HB3	2.00	0.61
1:A:122:SER:OG	1:A:123:PRO:HD3	1.99	0.61
1:C:66:THR:OG1	1:C:69:GLN:HG3	2.01	0.61
1:C:56:LEU:CB	1:C:118:LEU:HD11	2.26	0.61
1:D:12:PHE:CE2	1:D:13:PRO:HB3	2.35	0.61
1:A:47:LYS:O	1:A:49:PRO:HD3	2.01	0.61
1:F:59:LEU:HB3	1:F:110:LEU:HG	1.82	0.60
1:A:133:VAL:O	1:A:136:VAL:HG23	2.01	0.60
1:D:99:SER:O	1:D:103:GLN:HA	2.01	0.60
1:G:24:LEU:HB2	1:H:145:ILE:HD11	1.82	0.60
1:A:49:PRO:CD	1:A:52:LYS:HE2	2.30	0.60
1:H:40:ASN:ND2	1:H:50:THR:H	1.98	0.60
1:B:91:GLU:HB3	2:B:172:HOH:O	2.02	0.59
1:F:35:TRP:O	1:F:39:LEU:HD13	2.02	0.59
1:D:47:LYS:O	1:D:49:PRO:HD3	2.03	0.59
1:B:65:LEU:HB3	1:B:69:GLN:HB2	1.83	0.59
1:G:72:THR:HG1	1:G:158:TYR:HE2	1.50	0.59
1:G:62:TYR:CD1	1:G:73:LEU:HD21	2.38	0.59
1:E:39:LEU:HD21	1:E:125:ILE:CD1	2.33	0.58
1:F:56:LEU:HD21	1:F:88:LEU:HD22	1.84	0.58
1:F:134:GLY:HA2	2:F:188:HOH:O	2.03	0.58
1:A:66:THR:HG22	1:A:107:THR:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:SER:HB2	1:D:14:TYR:CD1	2.38	0.58
1:D:40:ASN:HD22	1:D:50:THR:H	1.50	0.58
1:A:67:VAL:HG21	2:D:182:HOH:O	2.02	0.58
1:E:55:LEU:HG	1:E:70:LEU:HD22	1.86	0.58
1:A:25:PRO:O	1:A:29:THR:HG22	2.03	0.58
1:E:24:LEU:HB3	1:E:25:PRO:HD3	1.83	0.58
1:A:155:LYS:O	1:A:156:THR:HB	2.04	0.58
1:C:33:HIS:CG	1:D:75:VAL:HB	2.39	0.58
1:A:137:ASP:OD2	1:A:140:LYS:HG3	2.03	0.58
1:A:96:ARG:HH22	1:A:106:ARG:NH1	2.02	0.57
1:F:91:GLU:HB3	2:F:210:HOH:O	2.03	0.57
1:D:116:LYS:CD	1:E:135:ASN:HB3	2.34	0.57
1:C:110:LEU:CD2	1:C:114:GLY:HA3	2.34	0.57
1:B:41:GLN:HG2	2:B:208:HOH:O	2.03	0.57
1:H:76:MSE:HE1	1:H:84:THR:OG1	2.05	0.57
1:A:59:LEU:HG	1:A:70:LEU:HD21	1.86	0.57
1:C:66:THR:HG22	1:C:107:THR:CG2	2.34	0.57
1:A:76:MSE:HE2	1:A:81:THR:HA	1.87	0.57
1:C:40:ASN:ND2	1:C:50:THR:OG1	2.38	0.56
1:E:9:LYS:H	1:E:9:LYS:HD2	1.70	0.56
1:A:39:LEU:O	1:A:43:LEU:HB2	2.05	0.56
1:F:98:ILE:HD12	1:F:104:ARG:NH1	2.21	0.56
1:C:137:ASP:HB3	1:C:140:LYS:HB2	1.88	0.56
1:A:89:VAL:HG21	1:A:96:ARG:HD3	1.88	0.56
1:D:77:GLU:H	1:D:77:GLU:CD	2.09	0.56
1:C:132:LEU:C	1:C:134:GLY:H	2.07	0.56
1:B:24:LEU:HG	1:B:28:LEU:HD21	1.87	0.56
1:G:62:TYR:CE1	1:G:73:LEU:HD11	2.41	0.55
1:E:24:LEU:O	1:E:28:LEU:HD13	2.07	0.55
1:C:121:ILE:O	1:C:121:ILE:HD13	2.06	0.55
1:C:110:LEU:HD11	1:C:118:LEU:HD22	1.88	0.55
1:G:62:TYR:CE1	1:H:20:LEU:HD23	2.40	0.55
1:C:89:VAL:HA	1:C:94:ALA:O	2.07	0.55
1:E:57:SER:HB2	1:F:14:TYR:CD2	2.41	0.54
1:F:23:PHE:CE1	1:F:25:PRO:HG2	2.41	0.54
1:B:36:SER:HB2	1:B:50:THR:HG21	1.87	0.54
1:H:35:TRP:O	1:H:39:LEU:HD13	2.07	0.54
2:A:177:HOH:O	1:B:75:VAL:HG12	2.06	0.54
1:D:52:LYS:HG2	1:D:88:LEU:HD11	1.89	0.54
1:G:47:LYS:O	1:G:47:LYS:HG3	2.07	0.54
1:D:52:LYS:CG	1:D:88:LEU:HD11	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:LEU:HD23	1:B:128:PHE:HE2	1.73	0.54
1:F:111:THR:O	1:F:115:LYS:HG3	2.08	0.54
1:B:24:LEU:HB3	1:B:25:PRO:HD3	1.90	0.53
1:G:55:LEU:HD22	1:G:84:THR:CG2	2.38	0.53
1:C:31:ILE:HD11	1:D:148:LEU:O	2.08	0.53
1:B:23:PHE:CD1	1:B:25:PRO:HD2	2.43	0.53
1:G:75:VAL:CG2	1:H:30:ARG:HD2	2.38	0.53
1:A:78:GLN:HB2	1:D:42:ALA:CB	2.39	0.53
1:A:133:VAL:HG21	1:A:141:LEU:HD21	1.90	0.53
1:D:63:GLY:O	1:D:109:VAL:HG23	2.09	0.53
1:F:16:SER:HB2	1:F:17:PRO:CD	2.37	0.53
1:G:99:SER:HB2	1:G:107:THR:HG21	1.91	0.53
1:B:49:PRO:HB2	1:B:51:PRO:HD2	1.89	0.53
1:D:109:VAL:HG22	2:D:173:HOH:O	2.09	0.53
1:B:34:ILE:O	1:B:38:GLU:HG3	2.09	0.53
1:F:88:LEU:HD23	1:F:93:LEU:HD12	1.91	0.52
1:E:21:ASN:O	1:E:27:LEU:HD21	2.10	0.52
1:A:147:VAL:HG13	1:B:136:VAL:HG11	1.92	0.52
1:A:126:ASN:ND2	1:B:12:PHE:HB2	2.24	0.52
1:G:40:ASN:ND2	1:G:50:THR:OG1	2.43	0.52
1:A:30:ARG:HD2	1:B:75:VAL:HG13	1.91	0.52
1:B:124:LEU:HD23	1:B:128:PHE:CE2	2.45	0.52
1:C:105:LYS:HB2	1:C:105:LYS:NZ	2.25	0.52
1:F:24:LEU:HB3	1:F:25:PRO:HD3	1.91	0.52
1:A:67:VAL:CG2	2:D:182:HOH:O	2.57	0.52
1:C:117:LYS:NZ	2:C:256:HOH:O	2.43	0.52
1:B:48:LEU:HD11	1:B:117:LYS:HE2	1.92	0.52
1:B:37:SER:O	1:B:41:GLN:HB2	2.08	0.52
1:C:49:PRO:HG2	1:C:52:LYS:HE3	1.92	0.51
1:E:133:VAL:CG1	1:E:133:VAL:O	2.58	0.51
1:A:40:ASN:N	1:A:40:ASN:HD22	2.08	0.51
1:B:105:LYS:O	1:B:107:THR:HG23	2.11	0.51
1:A:47:LYS:O	1:A:47:LYS:HG3	2.10	0.51
1:C:124:LEU:O	1:C:128:PHE:HD1	1.93	0.51
1:C:143:THR:O	1:C:147:VAL:HG23	2.11	0.51
1:G:21:ASN:O	1:G:27:LEU:HD21	2.10	0.51
1:H:117:LYS:HG3	1:H:117:LYS:O	2.11	0.51
1:C:75:VAL:O	1:C:75:VAL:HG12	2.11	0.51
1:C:147:VAL:HG21	1:D:140:LYS:O	2.10	0.51
1:E:121:ILE:O	1:E:121:ILE:HD13	2.10	0.51
1:D:52:LYS:HE2	1:D:87:GLN:OE1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:63:GLY:O	1:H:109:VAL:HG23	2.10	0.50
1:D:16:SER:HB2	1:D:17:PRO:HD2	1.94	0.50
1:E:98:ILE:O	1:E:99:SER:C	2.50	0.50
1:C:96:ARG:NH2	2:C:229:HOH:O	2.45	0.50
1:B:66:THR:OG1	1:B:69:GLN:HG3	2.12	0.50
1:G:64:GLU:HG3	1:G:109:VAL:HG23	1.94	0.50
1:A:71:ALA:HB1	1:A:76:MSE:O	2.12	0.50
1:H:52:LYS:HE2	1:H:87:GLN:OE1	2.12	0.50
1:B:85:VAL:O	1:B:89:VAL:HG23	2.12	0.50
1:H:91:GLU:HB3	2:H:216:HOH:O	2.11	0.50
1:G:29:THR:HG22	1:H:32:THR:CG2	2.41	0.49
1:D:40:ASN:HD21	1:D:49:PRO:HB3	1.76	0.49
1:E:142:GLN:O	1:E:146:GLU:HG3	2.12	0.49
1:H:40:ASN:HD21	1:H:50:THR:N	2.07	0.49
1:F:59:LEU:HD23	1:F:65:LEU:HD12	1.94	0.49
1:H:137:ASP:HB3	1:H:140:LYS:HB2	1.95	0.49
1:G:122:SER:OG	1:G:123:PRO:HD3	2.12	0.49
1:B:98:ILE:HD11	1:B:104:ARG:NE	2.27	0.49
1:C:126:ASN:ND2	1:D:13:PRO:HD3	2.24	0.49
1:H:36:SER:O	1:H:40:ASN:HB2	2.13	0.49
1:A:66:THR:OG1	1:A:69:GLN:HG3	2.13	0.49
1:G:75:VAL:HG23	1:H:30:ARG:HD2	1.93	0.49
1:C:69:GLN:HG3	2:C:231:HOH:O	2.12	0.49
1:D:16:SER:HB2	1:D:17:PRO:CD	2.43	0.49
1:G:13:PRO:CG	1:H:118:LEU:HB3	2.43	0.49
1:C:112:ARG:NH1	1:C:112:ARG:HB3	2.28	0.49
1:D:23:PHE:CG	1:D:25:PRO:HD2	2.47	0.49
1:G:55:LEU:HD22	1:G:84:THR:HG21	1.95	0.49
1:B:113:LYS:HE2	2:B:168:HOH:O	2.13	0.49
1:H:137:ASP:OD1	1:H:138:PRO:HD2	2.13	0.48
1:E:47:LYS:HE2	2:E:173:HOH:O	2.13	0.48
1:B:156:THR:HB	1:B:158:TYR:H	1.77	0.48
1:B:43:LEU:HD12	1:B:53:LEU:HD22	1.95	0.48
1:G:13:PRO:HG3	1:H:118:LEU:HB3	1.95	0.48
1:F:137:ASP:HB3	1:F:140:LYS:HB2	1.96	0.48
1:F:66:THR:HG22	1:F:107:THR:HG22	1.96	0.48
1:C:137:ASP:HB3	1:C:140:LYS:HD3	1.95	0.48
1:D:43:LEU:CD2	1:D:124:LEU:HD22	2.41	0.48
1:D:49:PRO:HB2	1:D:51:PRO:HD2	1.96	0.48
1:B:141:LEU:O	1:B:145:ILE:HG13	2.14	0.48
1:C:66:THR:HG23	1:C:69:GLN:OE1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:LEU:HD13	1:C:48:LEU:O	2.13	0.48
1:B:65:LEU:CA	1:B:69:GLN:HE21	2.26	0.48
1:E:34:ILE:O	1:E:38:GLU:HG3	2.13	0.48
1:C:62:TYR:HB3	1:C:65:LEU:HD21	1.95	0.48
1:A:47:LYS:C	1:A:49:PRO:HD3	2.34	0.48
1:A:49:PRO:CB	1:A:51:PRO:HD2	2.44	0.48
1:H:14:TYR:HD2	2:H:197:HOH:O	1.97	0.48
1:G:66:THR:OG1	1:G:69:GLN:HG3	2.14	0.48
1:E:13:PRO:CG	1:F:118:LEU:HB3	2.41	0.47
1:E:111:THR:O	1:E:115:LYS:HG3	2.14	0.47
1:D:23:PHE:CD1	1:D:25:PRO:HD2	2.49	0.47
1:D:84:THR:O	1:D:88:LEU:HD13	2.13	0.47
1:G:28:LEU:HD22	1:H:28:LEU:HD22	1.96	0.47
1:C:56:LEU:CD2	1:C:88:LEU:HD13	2.45	0.47
1:E:62:TYR:CD2	1:E:73:LEU:HD13	2.50	0.47
1:F:99:SER:HB2	1:F:104:ARG:HA	1.96	0.47
1:D:34:ILE:O	1:D:37:SER:HB2	2.14	0.47
1:E:40:ASN:ND2	1:E:50:THR:OG1	2.48	0.47
1:D:78:GLN:O	1:D:82:SER:HB2	2.13	0.47
1:B:123:PRO:O	1:B:127:ASP:HB2	2.15	0.47
1:A:78:GLN:HB2	1:D:42:ALA:HB1	1.97	0.47
1:A:96:ARG:HG2	2:A:159:HOH:O	2.15	0.47
1:A:46:GLU:HG2	1:A:46:GLU:H	1.50	0.46
1:C:56:LEU:HD21	1:C:88:LEU:HD13	1.97	0.46
1:C:147:VAL:HG13	1:D:136:VAL:HG11	1.98	0.46
1:B:23:PHE:CE1	1:B:25:PRO:HD2	2.50	0.46
1:G:23:PHE:CE1	1:G:25:PRO:HD2	2.51	0.46
1:G:14:TYR:HD1	1:G:19:GLU:HB3	1.81	0.46
1:G:76:MSE:HE3	1:G:80:THR:HG22	1.98	0.46
1:F:75:VAL:HG23	1:F:75:VAL:O	2.15	0.46
1:C:121:ILE:CG2	1:C:122:SER:N	2.78	0.46
1:G:75:VAL:O	1:G:75:VAL:CG1	2.64	0.46
1:G:136:VAL:CG1	1:G:141:LEU:HB2	2.46	0.46
1:D:56:LEU:HB3	1:D:118:LEU:HD21	1.98	0.46
1:F:134:GLY:N	2:F:216:HOH:O	2.49	0.46
1:A:62:TYR:HB3	1:A:65:LEU:HD21	1.98	0.46
1:A:126:ASN:OD1	1:B:12:PHE:HB2	2.15	0.46
1:G:65:LEU:HD22	1:G:69:GLN:CB	2.46	0.46
1:G:111:THR:O	1:G:115:LYS:HG3	2.16	0.46
1:E:71:ALA:CB	1:E:78:GLN:HG2	2.46	0.46
1:F:40:ASN:ND2	1:F:50:THR:N	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:TYR:HB3	1:B:65:LEU:HD21	1.98	0.46
1:A:33:HIS:CG	1:B:75:VAL:HB	2.50	0.46
1:D:21:ASN:HA	1:D:26:TYR:CE2	2.51	0.46
1:E:29:THR:HG22	1:F:32:THR:CG2	2.44	0.45
1:C:39:LEU:HD11	1:C:125:ILE:HD13	1.98	0.45
1:B:12:PHE:O	1:B:13:PRO:C	2.53	0.45
1:A:142:GLN:NE2	1:A:146:GLU:OE2	2.45	0.45
1:G:125:ILE:HG13	1:H:14:TYR:OH	2.17	0.45
1:D:109:VAL:CG2	2:D:173:HOH:O	2.64	0.45
1:H:21:ASN:O	1:H:27:LEU:HD11	2.17	0.45
1:D:123:PRO:O	1:D:127:ASP:HB2	2.17	0.45
1:D:141:LEU:HG	1:D:145:ILE:CD1	2.46	0.45
1:H:76:MSE:CE	1:H:80:THR:HG22	2.44	0.45
1:G:12:PHE:CG	1:G:13:PRO:HA	2.50	0.45
1:H:56:LEU:HD22	1:H:110:LEU:HD21	1.99	0.45
1:A:62:TYR:CB	1:A:65:LEU:HD21	2.47	0.45
1:H:23:PHE:CZ	1:H:25:PRO:HG2	2.52	0.45
1:E:147:VAL:HG13	1:F:136:VAL:HG11	1.98	0.45
1:A:89:VAL:HA	1:A:94:ALA:O	2.17	0.45
1:E:122:SER:OG	1:E:123:PRO:HD3	2.16	0.45
1:E:35:TRP:NE1	1:F:25:PRO:HB3	2.31	0.45
1:G:156:THR:O	1:G:158:TYR:N	2.50	0.45
1:C:17:PRO:HB3	1:D:62:TYR:CE1	2.52	0.45
1:F:156:THR:HG22	1:F:157:ASP:H	1.82	0.45
1:G:118:LEU:HA	1:G:121:ILE:HG22	1.98	0.44
1:G:145:ILE:HG23	1:H:27:LEU:CD1	2.47	0.44
1:F:52:LYS:HE2	1:F:87:GLN:OE1	2.17	0.44
1:C:50:THR:HG21	2:C:255:HOH:O	2.17	0.44
1:G:23:PHE:CD1	1:G:25:PRO:HD2	2.52	0.44
1:G:28:LEU:N	1:G:28:LEU:HD23	2.32	0.44
1:F:118:LEU:HA	1:F:118:LEU:HD23	1.79	0.44
1:A:115:LYS:HD2	2:A:200:HOH:O	2.16	0.44
1:B:93:LEU:HD22	1:B:114:GLY:HA2	1.99	0.44
1:B:52:LYS:HD2	1:B:88:LEU:CD2	2.47	0.44
1:F:99:SER:O	1:F:104:ARG:HG3	2.17	0.44
1:G:122:SER:N	1:G:123:PRO:CD	2.81	0.44
1:F:144:CYS:O	1:F:148:LEU:HG	2.17	0.44
1:C:104:ARG:O	1:C:104:ARG:CG	2.66	0.44
1:E:96:ARG:HA	1:E:96:ARG:HD2	1.80	0.44
1:E:40:ASN:HA	1:E:40:ASN:HD22	1.52	0.44
1:C:50:THR:HA	1:C:53:LEU:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:VAL:HG21	1:D:29:THR:CG2	2.44	0.44
1:D:137:ASP:HB3	1:D:140:LYS:HE2	2.00	0.44
1:D:156:THR:O	1:D:157:ASP:HB2	2.18	0.44
1:D:133:VAL:O	1:D:133:VAL:HG23	2.17	0.44
1:F:66:THR:CG2	1:F:107:THR:HG22	2.47	0.44
1:D:74:GLY:O	1:D:75:VAL:HG22	2.17	0.44
1:C:112:ARG:HH11	1:C:112:ARG:HB3	1.81	0.44
1:C:104:ARG:O	1:C:104:ARG:HG2	2.18	0.44
1:A:60:SER:O	1:B:15:GLY:HA2	2.18	0.43
1:A:12:PHE:O	1:B:122:SER:HB2	2.18	0.43
1:G:72:THR:OG1	1:G:158:TYR:HE2	2.01	0.43
1:E:35:TRP:CE2	1:F:25:PRO:HB3	2.53	0.43
1:E:61:ALA:O	1:F:17:PRO:HD3	2.18	0.43
1:E:55:LEU:HD12	1:E:55:LEU:HA	1.75	0.43
1:C:92:GLY:O	1:C:113:LYS:HB3	2.17	0.43
1:E:75:VAL:HG12	1:E:75:VAL:O	2.18	0.43
1:G:155:LYS:HA	1:G:155:LYS:HD2	1.80	0.43
1:A:52:LYS:HB3	1:A:88:LEU:HD21	2.00	0.43
1:E:62:TYR:CE1	1:F:17:PRO:HB3	2.53	0.43
1:G:62:TYR:CE2	1:H:17:PRO:HB3	2.53	0.43
1:A:50:THR:N	1:A:51:PRO:HD2	2.33	0.43
1:G:64:GLU:HG2	1:G:107:THR:HB	2.01	0.43
1:F:62:TYR:CB	1:F:65:LEU:HD21	2.48	0.43
1:B:50:THR:N	1:B:51:PRO:CD	2.82	0.43
1:C:9:LYS:HD3	1:C:9:LYS:H	1.84	0.43
1:A:132:LEU:HD21	1:B:24:LEU:HD23	2.01	0.43
1:A:126:ASN:OD1	1:B:12:PHE:CB	2.67	0.43
1:A:88:LEU:HD22	1:A:93:LEU:HD12	1.99	0.43
1:A:75:VAL:HG21	1:B:29:THR:CG2	2.42	0.43
1:D:13:PRO:HG3	1:D:23:PHE:CD1	2.54	0.43
1:D:42:ALA:HB1	1:D:124:LEU:HD21	2.00	0.43
1:G:43:LEU:HD11	1:G:53:LEU:HD22	2.01	0.43
1:F:110:LEU:HD23	1:F:110:LEU:HA	1.86	0.43
1:F:55:LEU:HD13	1:F:85:VAL:HG22	2.00	0.43
1:B:20:LEU:HD22	1:B:26:TYR:CG	2.54	0.43
1:D:20:LEU:C	1:D:22:SER:H	2.22	0.43
1:E:64:GLU:HG3	1:E:109:VAL:CG1	2.48	0.43
1:G:127:ASP:O	1:G:131:GLU:HG2	2.19	0.43
1:F:155:LYS:HA	1:F:155:LYS:HD3	1.77	0.43
1:D:27:LEU:HA	1:D:27:LEU:HD23	1.67	0.43
1:B:78:GLN:O	1:B:82:SER:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50:THR:N	1:D:51:PRO:CD	2.82	0.42
1:E:110:LEU:HD12	1:E:110:LEU:HA	1.90	0.42
1:B:152:LEU:O	1:B:153:LYS:C	2.58	0.42
1:E:105:LYS:HE2	1:H:131:GLU:CG	2.45	0.42
1:F:59:LEU:HD23	1:F:59:LEU:HA	1.90	0.42
1:D:77:GLU:N	1:D:77:GLU:CD	2.72	0.42
1:C:43:LEU:O	1:C:47:LYS:N	2.52	0.42
1:E:74:GLY:O	1:E:75:VAL:C	2.57	0.42
1:D:99:SER:HB3	1:D:105:LYS:HB2	2.00	0.42
1:E:81:THR:O	1:E:85:VAL:HG23	2.20	0.42
1:H:97:SER:OG	1:H:98:ILE:N	2.51	0.42
1:A:66:THR:HG21	1:A:105:LYS:HD2	2.00	0.42
1:G:39:LEU:O	1:G:43:LEU:HG	2.19	0.42
1:D:112:ARG:HB2	2:D:186:HOH:O	2.18	0.42
1:A:106:ARG:CD	1:D:123:PRO:HB3	2.50	0.42
1:A:24:LEU:HB3	1:A:25:PRO:HD3	2.01	0.42
1:D:116:LYS:HD2	1:E:135:ASN:HB3	2.00	0.42
1:F:42:ALA:O	1:G:79:SER:HB3	2.19	0.42
1:D:86:ASP:OD1	1:D:96:ARG:NH1	2.52	0.42
1:G:49:PRO:HG2	1:G:52:LYS:HD2	2.02	0.42
1:D:116:LYS:O	1:D:119:ALA:HB3	2.19	0.42
1:C:62:TYR:CB	1:C:65:LEU:HD21	2.49	0.42
1:E:20:LEU:O	1:E:23:PHE:HB3	2.19	0.42
1:D:70:LEU:HD11	1:D:108:VAL:HB	2.02	0.42
1:C:110:LEU:HD22	1:C:114:GLY:HA3	1.99	0.42
1:A:88:LEU:CD2	1:A:93:LEU:HD12	2.50	0.42
1:A:20:LEU:HD22	1:B:61:ALA:HB3	2.02	0.42
1:G:13:PRO:HB2	1:H:60:SER:OG	2.20	0.42
1:G:85:VAL:O	1:G:89:VAL:HG23	2.19	0.42
1:G:65:LEU:HD22	1:G:69:GLN:HB2	2.02	0.42
1:E:55:LEU:HD22	1:E:84:THR:HG21	2.00	0.42
1:A:25:PRO:O	1:A:29:THR:CG2	2.66	0.42
1:C:148:LEU:HA	1:C:148:LEU:HD23	1.80	0.42
1:H:81:THR:O	1:H:85:VAL:HG23	2.20	0.42
1:G:65:LEU:HD11	1:G:73:LEU:HD23	2.02	0.42
1:F:74:GLY:O	1:F:76:MSE:HE2	2.20	0.42
1:A:113:LYS:HD3	2:A:186:HOH:O	2.19	0.42
1:D:13:PRO:HG3	1:D:23:PHE:CE1	2.54	0.41
1:A:28:LEU:CD2	1:B:28:LEU:HD13	2.49	0.41
1:F:98:ILE:HD12	1:F:104:ARG:CZ	2.50	0.41
1:B:132:LEU:HB3	1:B:133:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:132:LEU:C	1:F:134:GLY:H	2.24	0.41
1:A:96:ARG:HH22	1:A:106:ARG:CZ	2.32	0.41
1:E:62:TYR:HE2	1:F:20:LEU:HD12	1.85	0.41
1:H:77:GLU:HB2	1:H:80:THR:OG1	2.20	0.41
1:D:40:ASN:ND2	1:D:49:PRO:HA	2.35	0.41
1:E:52:LYS:HD3	1:E:88:LEU:CD2	2.50	0.41
1:C:105:LYS:HZ3	1:C:105:LYS:HB2	1.84	0.41
1:D:12:PHE:CD2	1:D:13:PRO:HB3	2.56	0.41
1:C:27:LEU:O	1:C:31:ILE:HG13	2.21	0.41
1:E:140:LYS:HB3	1:E:140:LYS:HE2	1.88	0.41
1:G:24:LEU:HB3	1:G:25:PRO:HD3	2.02	0.41
1:D:105:LYS:O	1:D:107:THR:HG23	2.21	0.41
1:H:118:LEU:HD23	1:H:118:LEU:HA	1.80	0.41
1:C:12:PHE:CD1	1:D:125:ILE:HG21	2.55	0.41
1:G:142:GLN:OE1	1:G:142:GLN:HA	2.20	0.41
1:F:106:ARG:HG3	1:F:106:ARG:H	1.74	0.41
1:G:97:SER:OG	1:G:98:ILE:N	2.52	0.41
1:F:40:ASN:HD22	1:F:40:ASN:HA	1.61	0.41
1:C:20:LEU:C	1:C:22:SER:H	2.23	0.41
1:D:23:PHE:CZ	1:D:25:PRO:HG2	2.56	0.41
1:C:117:LYS:HD3	1:C:117:LYS:HA	1.79	0.41
1:G:96:ARG:NH2	1:G:106:ARG:HD3	2.35	0.41
1:F:36:SER:O	1:F:40:ASN:HB2	2.21	0.40
1:C:125:ILE:O	1:C:128:PHE:HB2	2.21	0.40
1:G:156:THR:OG1	1:G:158:TYR:HB3	2.21	0.40
1:C:50:THR:N	1:C:51:PRO:CD	2.83	0.40
1:D:56:LEU:HD13	1:D:88:LEU:CD2	2.50	0.40
1:F:98:ILE:HG23	1:F:104:ARG:NE	2.35	0.40
1:B:12:PHE:C	1:B:12:PHE:CD1	2.90	0.40
1:D:24:LEU:N	1:D:25:PRO:CD	2.85	0.40
1:A:20:LEU:HD23	1:B:62:TYR:HE1	1.85	0.40
1:F:23:PHE:CD1	1:F:25:PRO:HD2	2.56	0.40
1:E:125:ILE:HA	1:E:125:ILE:HD13	1.90	0.40
1:G:109:VAL:HG12	1:G:110:LEU:O	2.21	0.40
1:D:56:LEU:HA	1:D:56:LEU:HD12	1.87	0.40
1:A:121:ILE:CG2	1:A:122:SER:N	2.85	0.40
1:F:137:ASP:HA	1:F:138:PRO:HD3	1.84	0.40
1:E:50:THR:HB	1:E:51:PRO:HD3	2.03	0.40
1:G:30:ARG:NH1	1:H:73:LEU:HD23	2.36	0.40
1:A:147:VAL:HG21	1:B:140:LYS:O	2.21	0.40
1:C:124:LEU:HD23	1:C:124:LEU:HA	1.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:120:GLU:HG3	1:H:121:ILE:N	2.36	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	142/161 (88%)	131 (92%)	10 (7%)	1 (1%)	26	25
1	B	143/161 (89%)	124 (87%)	17 (12%)	2 (1%)	14	10
1	C	142/161 (88%)	126 (89%)	13 (9%)	3 (2%)	9	5
1	D	147/161 (91%)	122 (83%)	23 (16%)	2 (1%)	14	10
1	E	143/161 (89%)	134 (94%)	8 (6%)	1 (1%)	26	25
1	F	142/161 (88%)	134 (94%)	4 (3%)	4 (3%)	6	3
1	G	144/161 (89%)	132 (92%)	10 (7%)	2 (1%)	14	10
1	H	143/161 (89%)	134 (94%)	9 (6%)	0	100	100
All	All	1146/1288 (89%)	1037 (90%)	94 (8%)	15 (1%)	15	11

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	75	VAL
1	C	134	GLY
1	F	11	SER
1	F	134	GLY
1	G	157	ASP
1	A	132	LEU
1	B	13	PRO
1	C	132	LEU
1	D	41	GLN

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Mol	Chain	Res	Type
1	E	47	LYS
1	F	12	PHE
1	C	133	VAL
1	G	156	THR
1	D	134	GLY
1	B	51	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	125/138 (91%)	111 (89%)	14 (11%)	7 6
1	B	128/138 (93%)	119 (93%)	9 (7%)	19 19
1	C	127/138 (92%)	112 (88%)	15 (12%)	6 5
1	D	128/138 (93%)	121 (94%)	7 (6%)	27 30
1	E	129/138 (94%)	117 (91%)	12 (9%)	11 10
1	F	128/138 (93%)	119 (93%)	9 (7%)	19 19
1	G	130/138 (94%)	120 (92%)	10 (8%)	16 16
1	H	128/138 (93%)	119 (93%)	9 (7%)	19 19
All	All	1023/1104 (93%)	938 (92%)	85 (8%)	14 13

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	21	ASN
1	A	22	SER
1	A	26	TYR
1	A	29	THR
1	A	36	SER
1	A	43	LEU
1	A	46	GLU
1	A	78	GLN

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Mol	Chain	Res	Type
1	A	104	ARG
1	A	105	LYS
1	A	108	VAL
1	A	113	LYS
1	A	121	ILE
1	B	20	LEU
1	B	24	LEU
1	B	50	THR
1	B	98	ILE
1	B	106	ARG
1	B	116	LYS
1	B	124	LEU
1	B	132	LEU
1	B	156	THR
1	C	9	LYS
1	C	22	SER
1	C	50	THR
1	C	96	ARG
1	C	99	SER
1	C	100	ASP
1	C	104	ARG
1	C	105	LYS
1	C	110	LEU
1	C	116	LYS
1	C	117	LYS
1	C	121	ILE
1	C	124	LEU
1	C	155	LYS
1	C	156	THR
1	D	24	LEU
1	D	36	SER
1	D	47	LYS
1	D	50	THR
1	D	56	LEU
1	D	93	LEU
1	D	124	LEU
1	E	36	SER
1	E	40	ASN
1	E	55	LEU
1	E	77	GLU
1	E	90	ASP
1	E	97	SER

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Mol	Chain	Res	Type
1	E	105	LYS
1	E	113	LYS
1	E	118	LEU
1	E	121	ILE
1	E	133	VAL
1	E	152	LEU
1	F	12	PHE
1	F	20	LEU
1	F	40	ASN
1	F	47	LYS
1	F	50	THR
1	F	67	VAL
1	F	76	MSE
1	F	106	ARG
1	F	156	THR
1	G	37	SER
1	G	41	GLN
1	G	55	LEU
1	G	77	GLU
1	G	97	SER
1	G	98	ILE
1	G	121	ILE
1	G	155	LYS
1	G	156	THR
1	G	157	ASP
1	H	37	SER
1	H	40	ASN
1	H	50	THR
1	H	55	LEU
1	H	67	VAL
1	H	78	GLN
1	H	88	LEU
1	H	93	LEU
1	H	98	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	40	ASN
1	A	78	GLN
1	B	21	ASN

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Mol	Chain	Res	Type
1	B	69	GLN
1	C	40	ASN
1	C	78	GLN
1	C	126	ASN
1	D	21	ASN
1	D	40	ASN
1	E	40	ASN
1	E	78	GLN
1	E	126	ASN
1	F	40	ASN
1	F	129	HIS
1	G	40	ASN
1	G	129	HIS
1	H	40	ASN
1	H	78	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	145/161 (90%)	0.51	7 (4%) 34 34	42, 56, 90, 112	0
1	B	146/161 (90%)	0.80	15 (10%) 9 8	38, 62, 102, 129	0
1	C	145/161 (90%)	0.64	13 (8%) 12 11	27, 56, 89, 111	0
1	D	148/161 (91%)	0.56	12 (8%) 15 14	27, 59, 98, 120	0
1	E	146/161 (90%)	0.53	9 (6%) 24 23	37, 55, 90, 142	0
1	F	145/161 (90%)	0.77	12 (8%) 14 13	40, 60, 106, 154	0
1	G	147/161 (91%)	0.68	11 (7%) 17 17	34, 54, 98, 138	0
1	H	146/161 (90%)	0.53	5 (3%) 49 47	41, 58, 96, 146	0
All	All	1168/1288 (90%)	0.63	84 (7%) 18 18	27, 58, 98, 154	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	158	TYR	11.9
1	F	104	ARG	9.3
1	A	8	PRO	8.9
1	C	100	ASP	8.4
1	E	8	PRO	7.7
1	F	99	SER	7.6
1	D	10	PRO	7.4
1	G	103	GLN	7.0
1	H	10	PRO	6.7
1	B	104	ARG	6.7
1	F	11	SER	6.6
1	C	106	ARG	6.4
1	C	8	PRO	5.0
1	B	10	PRO	4.6
1	D	14	TYR	4.4
1	G	98	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	11	SER	4.4
1	B	13	PRO	4.4
1	C	45	SER	4.3
1	F	103	GLN	4.3
1	F	105	LYS	4.2
1	A	47	LYS	4.2
1	E	157	ASP	4.1
1	B	12	PHE	4.1
1	A	118	LEU	4.0
1	B	97	SER	3.8
1	B	99	SER	3.7
1	A	45	SER	3.6
1	F	10	PRO	3.6
1	B	98	ILE	3.4
1	D	100	ASP	3.4
1	C	47	LYS	3.4
1	E	158	TYR	3.4
1	C	99	SER	3.3
1	B	92	GLY	3.3
1	C	44	ALA	3.3
1	A	102	ASP	3.2
1	B	15	GLY	3.2
1	D	99	SER	3.1
1	G	8	PRO	3.1
1	B	96	ARG	3.1
1	B	105	LYS	3.0
1	G	47	LYS	3.0
1	F	106	ARG	3.0
1	D	102	ASP	3.0
1	D	106	ARG	2.9
1	E	44	ALA	2.9
1	H	98	ILE	2.9
1	C	118	LEU	2.7
1	E	99	SER	2.7
1	D	97	SER	2.6
1	B	100	ASP	2.6
1	D	104	ARG	2.6
1	A	106	ARG	2.6
1	C	107	THR	2.5
1	B	154	GLY	2.5
1	D	105	LYS	2.4
1	H	100	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	133	VAL	2.4
1	G	45	SER	2.4
1	C	46	GLU	2.3
1	G	157	ASP	2.3
1	C	128	PHE	2.3
1	H	104	ARG	2.3
1	G	63	GLY	2.3
1	G	104	ARG	2.3
1	B	106	ARG	2.3
1	F	98	ILE	2.3
1	H	83	ARG	2.3
1	D	157	ASP	2.3
1	F	96	ARG	2.3
1	D	101	ALA	2.2
1	F	97	SER	2.2
1	C	105	LYS	2.2
1	C	55	LEU	2.2
1	F	61	ALA	2.2
1	A	124	LEU	2.1
1	G	41	GLN	2.1
1	E	98	ILE	2.1
1	F	92	GLY	2.0
1	E	41	GLN	2.0
1	D	11	SER	2.0
1	G	10	PRO	2.0
1	E	72	THR	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.