Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 01:00 am BST

PDB ID	:	2ETN
Title	:	Crystal structure of Thermus aquaticus Gfh1
Authors	:	Lamour, V.; Hogan, B.P.; Erie, D.A.; Darst, S.A.
Deposited on	:	2005-10-27
Resolution	:	3.30 Å(reported)

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

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

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

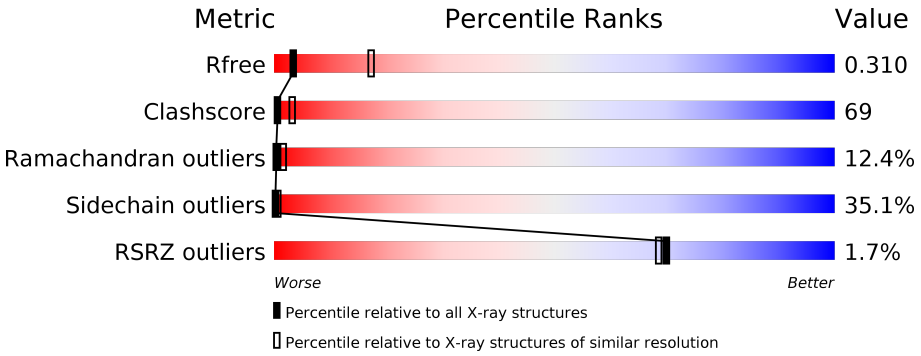
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.30 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	157	3% 13% 52% 27% 6%
1	B	157	21% 45% 25% 8%
1	C	157	2% 24% 39% 25% 11%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3550 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 anti-cleavage anti-GreA transcription factor Gfh1.

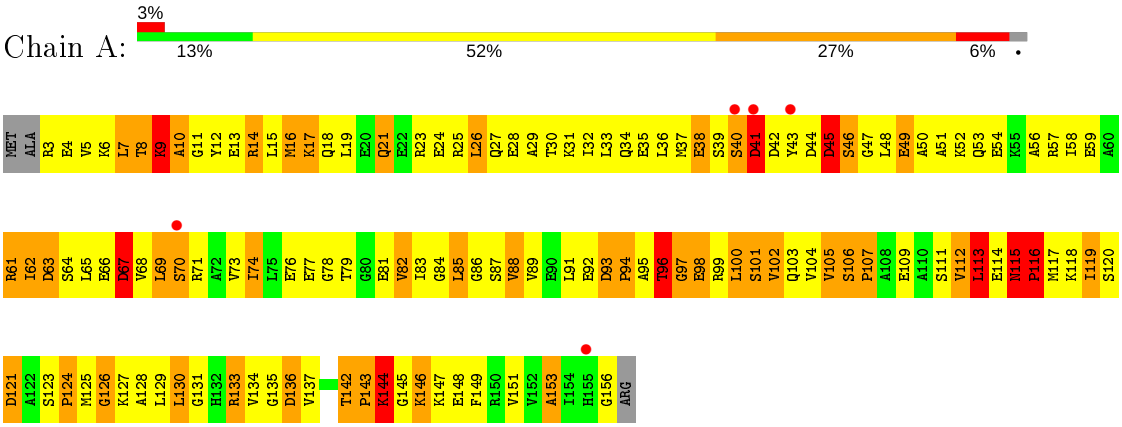
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	154	Total	C	N	O	S	0	0	0
			1180	728	206	242	4			
1	B	155	Total	C	N	O	S	0	0	0
			1185	731	207	243	4			
1	C	155	Total	C	N	O	S	0	0	0
			1185	731	207	243	4			

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 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.

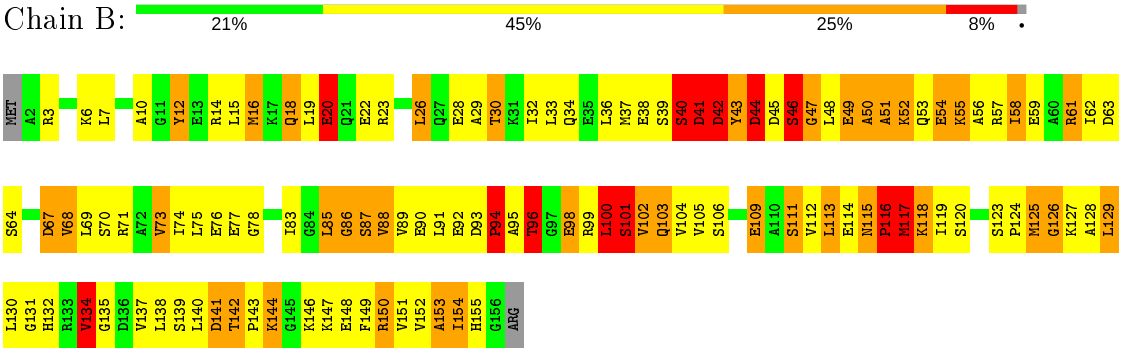
- Molecule 1: anti-cleavage anti-GreA transcription factor Gfh1

Chain A:



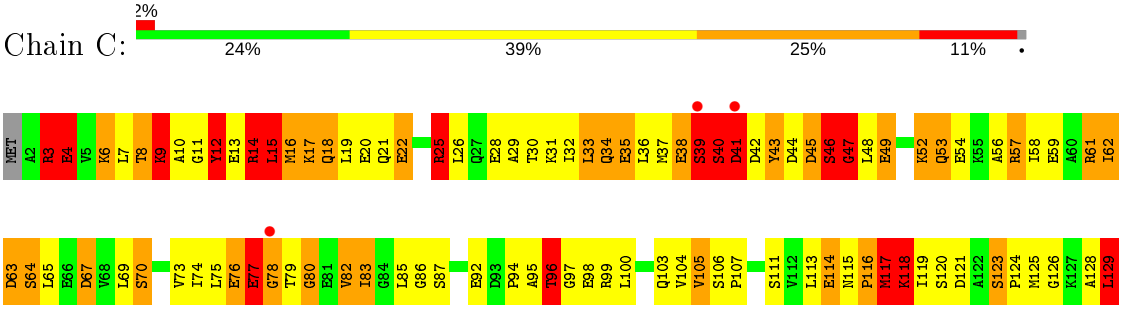
- Molecule 1: anti-cleavage anti-GreA transcription factor Gfh1

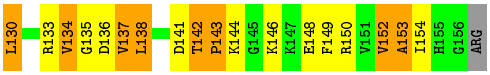
Chain B:



- Molecule 1: anti-cleavage anti-GreA transcription factor Gfh1

Chain C:




L130
R133
V134
G135
D136
V137
L138
D141
T142
P143
K144
G145
K146
K147
E148
F149
R150
V151
V152
A153
I154
H155
G156
ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	191.20Å 76.40Å 53.10Å 90.00° 101.90° 90.00°	Depositor
Resolution (Å)	30.00 – 3.30 29.59 – 3.20	Depositor EDS
% Data completeness (in resolution range)	92.5 (30.00-3.30) 91.6 (29.59-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.250 , 0.325 0.262 , 0.310	Depositor DCC
R_{free} test set	1113 reflections (9.10%)	wwPDB-VP
Wilson B-factor (Å^2)	80.5	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 61.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	3550	wwPDB-VP
Average B, all atoms (Å^2)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	1.31	3/1189 (0.3%)	1.49	10/1597 (0.6%)
1	B	1.45	10/1194 (0.8%)	1.67	18/1604 (1.1%)
1	C	1.75	13/1194 (1.1%)	1.66	31/1604 (1.9%)
All	All	1.51	26/3577 (0.7%)	1.61	59/4805 (1.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	3
1	C	0	5
All	All	0	8

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	47	GLY	N-CA	26.90	1.86	1.46
1	C	78	GLY	N-CA	15.47	1.69	1.46
1	C	40	SER	CB-OG	12.16	1.58	1.42
1	B	44	ASP	C-O	11.76	1.45	1.23
1	B	101	SER	N-CA	10.50	1.67	1.46
1	B	46	SER	CB-OG	8.07	1.52	1.42
1	C	43	TYR	CG-CD2	7.70	1.49	1.39
1	C	154	ILE	N-CA	7.57	1.61	1.46
1	B	41	ASP	C-O	-7.51	1.09	1.23
1	A	46	SER	N-CA	-7.48	1.31	1.46
1	C	118	LYS	N-CA	-7.21	1.31	1.46
1	B	16	MET	SD-CE	6.99	2.17	1.77
1	C	45	ASP	N-CA	6.60	1.59	1.46
1	C	22	GLU	CD-OE2	6.52	1.32	1.25
1	C	6	LYS	CD-CE	6.04	1.66	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	16	MET	SD-CE	5.99	2.11	1.77
1	B	73	VAL	CA-CB	-5.64	1.42	1.54
1	C	43	TYR	CE1-CZ	5.55	1.45	1.38
1	A	16	MET	SD-CE	5.50	2.08	1.77
1	B	20	GLU	CG-CD	5.47	1.60	1.51
1	A	97	GLY	N-CA	5.45	1.54	1.46
1	C	41	ASP	CB-CG	5.36	1.63	1.51
1	B	109	GLU	CD-OE1	5.35	1.31	1.25
1	B	12	TYR	CE1-CZ	5.29	1.45	1.38
1	C	44	ASP	N-CA	5.22	1.56	1.46
1	B	20	GLU	CD-OE2	5.09	1.31	1.25

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	116	PRO	CA-N-CD	-12.61	93.85	111.50
1	B	117	MET	C-N-CA	12.60	153.20	121.70
1	A	46	SER	N-CA-C	-11.99	78.61	111.00
1	B	118	LYS	N-CA-CB	11.87	131.97	110.60
1	B	41	ASP	CA-C-N	-11.60	91.69	117.20
1	B	154	ILE	N-CA-CB	-9.84	88.17	110.80
1	C	47	GLY	N-CA-C	9.30	136.34	113.10
1	C	78	GLY	N-CA-C	9.21	136.14	113.10
1	B	73	VAL	CB-CA-C	-9.05	94.20	111.40
1	C	118	LYS	N-CA-CB	8.98	126.77	110.60
1	C	83	ILE	N-CA-CB	8.93	131.34	110.80
1	C	117	MET	C-N-CA	8.61	143.23	121.70
1	B	100	LEU	C-N-CA	-8.60	100.20	121.70
1	B	44	ASP	O-C-N	-8.35	109.34	122.70
1	A	46	SER	N-CA-CB	8.31	122.96	110.50
1	C	45	ASP	N-CA-C	-8.28	88.64	111.00
1	B	44	ASP	CA-C-N	7.68	134.09	117.20
1	A	41	ASP	N-CA-C	-7.23	91.47	111.00
1	C	4	GLU	C-N-CA	7.11	139.48	121.70
1	B	85	LEU	CA-CB-CG	-6.93	99.36	115.30
1	A	41	ASP	CA-C-N	-6.92	101.98	117.20
1	A	45	ASP	CB-CG-OD2	6.80	124.42	118.30
1	C	14	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	C	3	ARG	N-CA-C	-6.72	92.87	111.00
1	C	77	GLU	C-N-CA	-6.60	108.45	122.30
1	C	152	VAL	CB-CA-C	-6.44	99.17	111.40
1	C	45	ASP	N-CA-CB	6.28	121.91	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	154	ILE	N-CA-CB	6.28	125.24	110.80
1	A	41	ASP	CB-CA-C	6.26	122.92	110.40
1	C	41	ASP	CA-C-N	-6.21	103.53	117.20
1	C	40	SER	N-CA-C	6.21	127.76	111.00
1	B	42	ASP	C-N-CA	6.14	137.04	121.70
1	C	83	ILE	N-CA-C	-6.07	94.60	111.00
1	A	43	TYR	C-N-CA	5.94	136.54	121.70
1	C	12	TYR	CA-CB-CG	5.84	124.50	113.40
1	C	15	LEU	CA-CB-CG	-5.84	101.87	115.30
1	C	41	ASP	CB-CG-OD2	5.83	123.54	118.30
1	B	41	ASP	C-N-CA	5.82	136.26	121.70
1	C	61	ARG	CG-CD-NE	-5.75	99.73	111.80
1	C	25	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	C	129	LEU	CA-CB-CG	5.60	128.18	115.30
1	A	151	VAL	N-CA-C	-5.59	95.90	111.00
1	B	102	VAL	CB-CA-C	-5.58	100.79	111.40
1	B	42	ASP	CA-C-O	5.55	131.76	120.10
1	A	113	LEU	CA-CB-CG	-5.54	102.55	115.30
1	B	86	GLY	C-N-CA	-5.49	107.99	121.70
1	B	42	ASP	CA-C-N	-5.48	105.15	117.20
1	A	67	ASP	CB-CG-OD2	5.47	123.22	118.30
1	C	154	ILE	N-CA-C	-5.44	96.31	111.00
1	B	94	PRO	CA-N-CD	-5.41	103.93	111.50
1	C	137	VAL	CB-CA-C	-5.37	101.21	111.40
1	C	16	MET	CG-SD-CE	5.30	108.67	100.20
1	C	130	LEU	CA-CB-CG	-5.20	103.35	115.30
1	C	41	ASP	N-CA-C	5.20	125.03	111.00
1	C	104	VAL	C-N-CA	-5.17	108.78	121.70
1	C	41	ASP	C-N-CA	5.12	134.51	121.70
1	B	40	SER	CA-C-N	-5.04	106.12	117.20
1	C	45	ASP	CB-CG-OD1	5.02	122.81	118.30
1	C	40	SER	C-N-CA	5.01	134.22	121.70

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	40	SER	Peptide
1	B	41	ASP	Mainchain
1	B	44	ASP	Mainchain
1	C	153	ALA	Peptide
1	C	39	SER	Peptide

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Mol	Chain	Res	Type	Group
1	C	40	SER	Peptide
1	C	46	SER	Peptide
1	C	77	GLU	Peptide

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	1180	0	1201	166	0
1	B	1185	0	1205	189	1
1	C	1185	0	1206	151	0
All	All	3550	0	3612	492	1

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 69.

All (492) 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:A:74:ILE:CD1	1:A:74:ILE:CG1	1.80	1.59
1:C:78:GLY:N	1:C:78:GLY:CA	1.69	1.56
1:A:16:MET:SD	1:A:16:MET:CE	2.08	1.42
1:C:16:MET:SD	1:C:16:MET:CE	2.11	1.36
1:C:47:GLY:N	1:C:47:GLY:CA	1.86	1.36
1:B:16:MET:CE	1:B:16:MET:SD	2.17	1.33
1:B:129:LEU:H	1:B:129:LEU:CD1	1.24	1.28
1:B:129:LEU:N	1:B:129:LEU:HD12	1.16	1.27
1:B:96:THR:HG21	1:B:98:GLU:HG3	1.19	1.18
1:B:112:VAL:CA	1:B:117:MET:HE2	1.74	1.17
1:A:85:LEU:N	1:A:85:LEU:HD12	1.42	1.17
1:A:28:GLU:HB2	1:C:25:ARG:HG2	1.20	1.16
1:B:112:VAL:CB	1:B:117:MET:HE2	1.77	1.15
1:B:129:LEU:N	1:B:129:LEU:CD1	1.84	1.12
1:A:85:LEU:CD1	1:A:85:LEU:H	1.62	1.11
1:C:8:THR:HG22	1:C:135:GLY:O	1.47	1.11
1:A:61:ARG:HG2	1:A:61:ARG:HH11	1.09	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:ILE:HG12	1:B:154:ILE:CD1	1.82	1.10
1:C:96:THR:HG23	1:C:96:THR:O	1.49	1.10
1:A:113:LEU:HD23	1:A:113:LEU:N	1.52	1.10
1:C:80:GLY:HA2	1:C:133:ARG:HG2	1.22	1.10
1:B:129:LEU:H	1:B:129:LEU:HD13	1.09	1.07
1:B:54:GLU:OE1	1:B:54:GLU:CA	2.00	1.07
1:A:115:ASN:HB3	1:A:116:PRO:HD2	1.33	1.06
1:A:85:LEU:HD12	1:A:85:LEU:H	0.96	1.05
1:A:95:ALA:O	1:A:96:THR:HB	1.51	1.05
1:B:112:VAL:HA	1:B:117:MET:HE2	1.40	1.03
1:A:85:LEU:N	1:A:85:LEU:CD1	2.17	1.03
1:B:96:THR:CG2	1:B:98:GLU:HG3	1.89	1.03
1:C:80:GLY:CA	1:C:133:ARG:HG2	1.89	1.02
1:B:51:ALA:O	1:B:54:GLU:HB2	1.59	1.02
1:C:96:THR:CG2	1:C:96:THR:O	2.04	1.01
1:A:115:ASN:HB3	1:A:116:PRO:CD	1.91	1.01
1:B:112:VAL:HB	1:B:117:MET:CE	1.92	1.00
1:A:115:ASN:O	1:A:116:PRO:C	1.99	0.99
1:C:115:ASN:HB3	1:C:116:PRO:CD	1.94	0.98
1:A:88:VAL:HG13	1:A:103:GLN:HB2	1.42	0.97
1:B:114:GLU:OE1	1:B:118:LYS:HE3	1.64	0.97
1:C:134:VAL:CG1	1:C:153:ALA:H	1.76	0.97
1:C:107:PRO:HD3	1:C:121:ASP:OD1	1.62	0.97
1:B:3:ARG:HG3	1:B:71:ARG:HH12	1.31	0.96
1:A:82:VAL:HG12	1:A:83:ILE:H	1.30	0.94
1:B:44:ASP:O	1:B:45:ASP:HB2	1.67	0.94
1:B:112:VAL:CB	1:B:117:MET:CE	2.44	0.93
1:B:16:MET:HG2	1:B:69:LEU:HD21	1.50	0.93
1:C:3:ARG:O	1:C:4:GLU:CB	2.15	0.93
1:A:145:GLY:C	1:A:146:LYS:HD3	1.88	0.93
1:B:54:GLU:HA	1:B:54:GLU:OE1	1.12	0.93
1:C:105:VAL:HG21	1:C:118:LYS:HB3	1.48	0.92
1:C:38:GLU:O	1:C:40:SER:HB3	1.70	0.91
1:C:125:MET:O	1:C:129:LEU:HD12	1.70	0.90
1:B:125:MET:O	1:B:129:LEU:HD13	1.71	0.90
1:C:3:ARG:O	1:C:4:GLU:HB2	1.69	0.90
1:C:134:VAL:HG13	1:C:153:ALA:H	1.36	0.89
1:C:105:VAL:CG2	1:C:118:LYS:HB3	2.01	0.89
1:A:61:ARG:CG	1:A:61:ARG:HH11	1.84	0.89
1:B:40:SER:C	1:B:42:ASP:H	1.76	0.89
1:B:42:ASP:N	1:B:42:ASP:OD2	2.04	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:TYR:O	1:B:16:MET:HG3	1.73	0.89
1:A:100:LEU:HD12	1:A:101:SER:N	1.88	0.88
1:A:113:LEU:CD2	1:A:113:LEU:N	2.31	0.86
1:A:87:SER:HA	1:A:156:GLY:O	1.75	0.86
1:B:6:LYS:HD3	1:B:75:LEU:HD11	1.57	0.85
1:B:3:ARG:HG3	1:B:71:ARG:NH1	1.92	0.85
1:A:121:ASP:OD1	1:A:121:ASP:C	2.16	0.83
1:C:115:ASN:HB3	1:C:116:PRO:HD2	1.60	0.83
1:C:77:GLU:C	1:C:78:GLY:CA	2.46	0.83
1:C:64:SER:O	1:C:67:ASP:HB3	1.77	0.83
1:C:15:LEU:HD12	1:C:137:VAL:HG11	1.62	0.82
1:B:83:ILE:HG12	1:B:154:ILE:HD12	1.58	0.82
1:A:24:GLU:HG3	1:C:25:ARG:HD2	1.62	0.82
1:C:53:GLN:HA	1:C:53:GLN:OE1	1.79	0.81
1:C:62:ILE:HG22	1:C:63:ASP:N	1.91	0.81
1:A:5:VAL:HB	1:A:71:ARG:HB3	1.62	0.81
1:B:34:GLN:NE2	1:B:55:LYS:NZ	2.29	0.81
1:A:61:ARG:HG2	1:A:61:ARG:NH1	1.91	0.81
1:B:96:THR:CG2	1:B:98:GLU:CG	2.59	0.80
1:C:7:LEU:O	1:C:75:LEU:HG	1.81	0.80
1:B:143:PRO:HG3	1:C:114:GLU:HG3	1.63	0.80
1:C:38:GLU:O	1:C:40:SER:CB	2.29	0.80
1:A:112:VAL:C	1:A:113:LEU:HD23	2.01	0.79
1:B:92:GLU:O	1:B:94:PRO:CD	2.30	0.79
1:C:10:ALA:O	1:C:14:ARG:HB2	1.82	0.79
1:C:8:THR:CG2	1:C:135:GLY:O	2.31	0.79
1:B:112:VAL:HA	1:B:117:MET:HG2	1.67	0.77
1:B:96:THR:HG21	1:B:98:GLU:CG	2.07	0.77
1:A:88:VAL:HG13	1:A:103:GLN:CB	2.14	0.76
1:A:19:LEU:HD21	1:A:66:GLU:HG2	1.66	0.76
1:C:45:ASP:O	1:C:47:GLY:N	2.18	0.76
1:B:92:GLU:O	1:B:94:PRO:HD3	1.87	0.74
1:C:83:ILE:HG22	1:C:130:LEU:HD12	1.69	0.74
1:B:74:ILE:CG2	1:B:75:LEU:N	2.50	0.74
1:B:16:MET:C	1:B:18:GLN:H	1.89	0.73
1:B:22:GLU:OE2	1:B:61:ARG:HD3	1.88	0.73
1:A:100:LEU:HD12	1:A:101:SER:H	1.54	0.72
1:C:26:LEU:O	1:C:26:LEU:HD12	1.88	0.72
1:C:33:LEU:O	1:C:36:LEU:N	2.22	0.72
1:B:43:TYR:HA	1:B:48:LEU:HD12	1.72	0.72
1:C:82:VAL:HG12	1:C:83:ILE:N	2.03	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:GLU:HB2	1:C:25:ARG:CG	2.10	0.72
1:B:34:GLN:NE2	1:B:55:LYS:HZ1	1.85	0.72
1:B:85:LEU:O	1:B:87:SER:N	2.22	0.72
1:A:16:MET:O	1:A:18:GLN:N	2.22	0.72
1:B:128:ALA:C	1:B:129:LEU:HD12	2.04	0.72
1:A:115:ASN:CB	1:A:116:PRO:CD	2.64	0.71
1:A:24:GLU:HG2	1:C:21:GLN:HG2	1.72	0.71
1:A:119:ILE:CD1	1:A:125:MET:HG2	2.21	0.71
1:A:49:GLU:HG3	1:A:53:GLN:NE2	2.05	0.71
1:C:57:ARG:O	1:C:61:ARG:HB2	1.91	0.71
1:B:92:GLU:C	1:B:94:PRO:HD3	2.10	0.71
1:A:4:GLU:OE2	1:A:6:LYS:HE3	1.90	0.71
1:B:40:SER:C	1:B:42:ASP:N	2.43	0.71
1:C:82:VAL:CG1	1:C:83:ILE:H	2.04	0.70
1:B:83:ILE:HB	1:B:131:GLY:H	1.56	0.70
1:B:112:VAL:CG1	1:B:117:MET:HE2	2.21	0.70
1:B:112:VAL:HG12	1:B:117:MET:CE	2.21	0.70
1:B:50:ALA:O	1:B:51:ALA:C	2.31	0.70
1:B:92:GLU:O	1:B:94:PRO:HD2	1.92	0.69
1:B:83:ILE:HG12	1:B:154:ILE:HD11	1.71	0.69
1:C:82:VAL:HG12	1:C:83:ILE:H	1.56	0.69
1:A:147:LYS:HB3	1:A:149:PHE:CE1	2.27	0.69
1:A:82:VAL:HG12	1:A:83:ILE:N	2.07	0.69
1:B:51:ALA:O	1:B:54:GLU:N	2.26	0.69
1:C:134:VAL:HG13	1:C:153:ALA:N	2.06	0.69
1:A:49:GLU:OE1	1:A:49:GLU:HA	1.92	0.68
1:C:34:GLN:O	1:C:38:GLU:HB2	1.94	0.68
1:A:124:PRO:O	1:A:128:ALA:N	2.24	0.68
1:B:83:ILE:CG1	1:B:154:ILE:CD1	2.69	0.68
1:B:112:VAL:CG1	1:B:117:MET:CE	2.72	0.68
1:B:125:MET:O	1:B:126:GLY:C	2.28	0.68
1:A:38:GLU:C	1:A:40:SER:H	1.96	0.67
1:B:74:ILE:HG23	1:B:75:LEU:N	2.09	0.67
1:B:114:GLU:HG2	1:C:143:PRO:HG3	1.74	0.67
1:C:115:ASN:O	1:C:116:PRO:C	2.32	0.67
1:B:141:ASP:HB3	1:B:146:LYS:HG2	1.76	0.67
1:C:95:ALA:O	1:C:96:THR:HB	1.95	0.67
1:B:88:VAL:O	1:B:154:ILE:HA	1.95	0.67
1:C:48:LEU:HD11	1:C:52:LYS:HB2	1.77	0.66
1:A:87:SER:CA	1:A:156:GLY:O	2.43	0.66
1:B:125:MET:HA	1:B:128:ALA:HB3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:VAL:HG11	1:B:130:LEU:HD13	1.78	0.66
1:B:74:ILE:HG23	1:B:75:LEU:H	1.61	0.66
1:B:88:VAL:HG23	1:B:155:HIS:O	1.96	0.66
1:C:48:LEU:HD12	1:C:48:LEU:O	1.94	0.66
1:C:56:ALA:HA	1:C:59:GLU:HB2	1.76	0.66
1:A:49:GLU:O	1:A:50:ALA:C	2.34	0.66
1:A:93:ASP:O	1:A:97:GLY:N	2.20	0.66
1:B:16:MET:C	1:B:18:GLN:N	2.46	0.66
1:B:95:ALA:O	1:B:96:THR:HB	1.95	0.66
1:A:96:THR:HG21	1:A:98:GLU:OE1	1.96	0.66
1:A:17:LYS:O	1:A:21:GLN:HB2	1.97	0.65
1:C:4:GLU:OE1	1:C:4:GLU:HA	1.95	0.65
1:A:15:LEU:HD13	1:A:137:VAL:HG21	1.78	0.65
1:B:132:HIS:CG	1:B:138:LEU:HD11	2.31	0.65
1:C:95:ALA:O	1:C:96:THR:CB	2.43	0.65
1:B:114:GLU:CG	1:C:143:PRO:HG3	2.27	0.65
1:A:115:ASN:O	1:A:116:PRO:O	2.14	0.65
1:A:67:ASP:C	1:A:67:ASP:OD1	2.35	0.65
1:C:82:VAL:CG1	1:C:83:ILE:N	2.59	0.65
1:A:133:ARG:O	1:A:136:ASP:HB2	1.96	0.65
1:B:26:LEU:HG	1:B:26:LEU:O	1.97	0.65
1:B:20:GLU:OE1	1:B:20:GLU:HA	1.96	0.64
1:C:37:MET:O	1:C:40:SER:HB3	1.97	0.64
1:A:35:GLU:HA	1:A:38:GLU:OE1	1.97	0.64
1:C:48:LEU:CD1	1:C:52:LYS:HB2	2.29	0.63
1:A:12:TYR:CD1	1:A:69:LEU:HD23	2.34	0.63
1:A:142:THR:HG22	1:A:145:GLY:N	2.13	0.63
1:A:15:LEU:HD11	1:A:94:PRO:HG2	1.80	0.63
1:C:17:LYS:O	1:C:21:GLN:HB2	1.99	0.63
1:C:115:ASN:CB	1:C:116:PRO:CD	2.72	0.62
1:C:69:LEU:H	1:C:69:LEU:HD12	1.64	0.62
1:C:96:THR:O	1:C:98:GLU:N	2.31	0.62
1:B:55:LYS:O	1:B:59:GLU:HB3	2.00	0.62
1:A:145:GLY:CA	1:A:146:LYS:HD3	2.28	0.62
1:A:12:TYR:CE1	1:A:69:LEU:HD23	2.35	0.61
1:A:61:ARG:CG	1:A:61:ARG:NH1	2.50	0.61
1:B:33:LEU:O	1:B:37:MET:HB2	1.99	0.61
1:B:89:VAL:CG1	1:B:91:LEU:HD21	2.30	0.61
1:C:64:SER:OG	1:C:65:LEU:N	2.32	0.61
1:B:64:SER:O	1:B:67:ASP:HB3	2.01	0.61
1:A:24:GLU:O	1:C:25:ARG:HG3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:GLN:NE2	1:B:55:LYS:HZ2	1.98	0.61
1:B:96:THR:CG2	1:B:98:GLU:CB	2.79	0.61
1:A:76:GLU:OE1	1:A:76:GLU:HA	2.00	0.60
1:B:125:MET:O	1:B:126:GLY:O	2.19	0.60
1:A:7:LEU:HD22	1:A:135:GLY:O	2.01	0.60
1:A:8:THR:HG22	1:A:135:GLY:O	2.02	0.60
1:B:134:VAL:HG13	1:B:153:ALA:H	1.66	0.60
1:A:56:ALA:O	1:A:57:ARG:C	2.36	0.60
1:A:28:GLU:CB	1:C:25:ARG:HG2	2.14	0.59
1:C:8:THR:O	1:C:9:LYS:C	2.37	0.59
1:B:54:GLU:O	1:B:56:ALA:N	2.35	0.59
1:C:62:ILE:HG22	1:C:63:ASP:H	1.66	0.59
1:A:121:ASP:OD1	1:A:121:ASP:O	2.20	0.59
1:B:114:GLU:OE1	1:B:118:LYS:CE	2.45	0.59
1:C:22:GLU:CD	1:C:61:ARG:NH1	2.56	0.59
1:B:112:VAL:HG12	1:B:117:MET:HE1	1.84	0.59
1:B:26:LEU:HB2	1:B:58:ILE:HG21	1.84	0.59
1:A:14:ARG:NH1	1:A:137:VAL:O	2.36	0.58
1:B:61:ARG:HH11	1:B:61:ARG:HG2	1.68	0.58
1:C:142:THR:HG23	1:C:143:PRO:HD2	1.84	0.58
1:B:83:ILE:CG1	1:B:154:ILE:HD11	2.31	0.58
1:B:96:THR:CG2	1:B:98:GLU:HB2	2.34	0.58
1:C:7:LEU:HD21	1:C:150:ARG:HD2	1.86	0.58
1:B:115:ASN:HB2	1:B:116:PRO:HD2	1.86	0.58
1:A:142:THR:HG22	1:A:145:GLY:C	2.23	0.57
1:A:91:LEU:O	1:A:99:ARG:HA	2.03	0.57
1:B:12:TYR:CB	1:B:74:ILE:HD11	2.33	0.57
1:C:37:MET:O	1:C:40:SER:CB	2.51	0.57
1:A:74:ILE:CB	1:A:74:ILE:CD1	2.78	0.57
1:B:32:ILE:O	1:B:36:LEU:N	2.30	0.57
1:C:33:LEU:O	1:C:35:GLU:N	2.36	0.57
1:B:62:ILE:O	1:B:64:SER:N	2.38	0.57
1:B:125:MET:O	1:B:129:LEU:CD1	2.50	0.57
1:C:62:ILE:CG2	1:C:63:ASP:N	2.60	0.57
1:C:115:ASN:HB3	1:C:116:PRO:HD3	1.84	0.57
1:C:18:GLN:NE2	1:C:148:GLU:HG3	2.20	0.57
1:A:44:ASP:N	1:A:44:ASP:OD1	2.35	0.57
1:B:51:ALA:O	1:B:54:GLU:CB	2.45	0.57
1:A:142:THR:HG23	1:A:144:LYS:N	2.20	0.56
1:A:16:MET:HG3	1:A:69:LEU:CD2	2.35	0.56
1:A:125:MET:HA	1:A:128:ALA:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:LEU:HD12	1:B:100:LEU:HD23	1.86	0.56
1:B:112:VAL:CA	1:B:117:MET:CE	2.67	0.56
1:A:16:MET:C	1:A:18:GLN:H	2.09	0.56
1:A:25:ARG:HG2	1:C:28:GLU:OE1	2.06	0.56
1:B:137:VAL:O	1:B:138:LEU:HD23	2.06	0.56
1:C:92:GLU:O	1:C:94:PRO:HD3	2.06	0.56
1:B:128:ALA:HB3	1:B:129:LEU:CD1	2.36	0.56
1:A:9:LYS:O	1:A:10:ALA:C	2.44	0.55
1:C:28:GLU:O	1:C:32:ILE:HG13	2.06	0.55
1:C:105:VAL:O	1:C:121:ASP:N	2.38	0.55
1:B:115:ASN:CB	1:B:116:PRO:HD2	2.37	0.55
1:B:96:THR:HG23	1:B:98:GLU:CG	2.36	0.55
1:B:150:ARG:O	1:B:152:VAL:HG23	2.07	0.55
1:B:16:MET:O	1:B:18:GLN:N	2.40	0.55
1:B:105:VAL:HG11	1:B:118:LYS:HD3	1.89	0.55
1:B:116:PRO:O	1:B:117:MET:C	2.44	0.54
1:C:35:GLU:HA	1:C:39:SER:HB2	1.88	0.54
1:B:83:ILE:HD12	1:B:129:LEU:O	2.07	0.54
1:B:12:TYR:HB3	1:B:74:ILE:HD11	1.88	0.54
1:B:112:VAL:HB	1:B:117:MET:HE3	1.87	0.54
1:B:139:SER:HB3	1:B:148:GLU:HG2	1.88	0.54
1:C:3:ARG:O	1:C:4:GLU:HB3	2.06	0.54
1:B:89:VAL:HG11	1:B:91:LEU:HD21	1.88	0.54
1:A:13:GLU:O	1:A:17:LYS:HG2	2.08	0.54
1:A:120:SER:O	1:A:123:SER:OG	2.26	0.53
1:B:44:ASP:OD1	1:B:46:SER:CB	2.56	0.53
1:C:19:LEU:O	1:C:20:GLU:C	2.45	0.53
1:A:6:LYS:HG3	1:A:73:VAL:HB	1.90	0.53
1:B:114:GLU:OE1	1:B:118:LYS:HG3	2.08	0.53
1:B:67:ASP:O	1:B:68:VAL:C	2.46	0.53
1:A:68:VAL:O	1:A:70:SER:N	2.40	0.53
1:B:44:ASP:OD1	1:B:46:SER:OG	2.19	0.53
1:C:12:TYR:O	1:C:16:MET:HG3	2.08	0.53
1:C:92:GLU:O	1:C:149:PHE:HA	2.09	0.53
1:C:53:GLN:CA	1:C:53:GLN:OE1	2.56	0.53
1:A:143:PRO:C	1:A:145:GLY:H	2.12	0.53
1:A:9:LYS:O	1:A:11:GLY:N	2.42	0.53
1:C:16:MET:O	1:C:17:LYS:C	2.46	0.53
1:A:124:PRO:O	1:A:128:ALA:CB	2.57	0.52
1:A:8:THR:OG1	1:A:9:LYS:N	2.40	0.52
1:A:83:ILE:HB	1:A:131:GLY:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:VAL:HG12	1:B:117:MET:HE2	1.86	0.52
1:C:11:GLY:O	1:C:15:LEU:N	2.43	0.52
1:C:142:THR:CG2	1:C:143:PRO:N	2.72	0.52
1:A:100:LEU:HD12	1:A:100:LEU:C	2.21	0.52
1:A:96:THR:CG2	1:A:98:GLU:OE1	2.58	0.52
1:B:120:SER:HB3	1:B:123:SER:HB3	1.91	0.52
1:B:28:GLU:O	1:B:32:ILE:HG12	2.09	0.52
1:A:100:LEU:CD1	1:A:100:LEU:C	2.76	0.52
1:B:134:VAL:HA	1:B:151:VAL:HG12	1.90	0.52
1:C:96:THR:HG22	1:C:98:GLU:H	1.73	0.52
1:A:87:SER:N	1:A:156:GLY:O	2.43	0.52
1:A:28:GLU:O	1:A:28:GLU:HG3	2.10	0.52
1:A:5:VAL:HG12	1:A:5:VAL:O	2.10	0.52
1:B:138:LEU:O	1:B:149:PHE:N	2.35	0.52
1:B:41:ASP:HA	1:B:42:ASP:OD2	2.09	0.52
1:A:56:ALA:O	1:A:59:GLU:N	2.43	0.52
1:B:152:VAL:HG12	1:B:152:VAL:O	2.10	0.52
1:B:62:ILE:O	1:B:63:ASP:C	2.45	0.52
1:A:130:LEU:HD12	1:A:131:GLY:N	2.25	0.52
1:C:80:GLY:HA3	1:C:133:ARG:HG2	1.86	0.51
1:A:5:VAL:HB	1:A:71:ARG:CB	2.38	0.51
1:A:93:ASP:C	1:A:93:ASP:OD2	2.49	0.51
1:B:54:GLU:O	1:B:57:ARG:N	2.44	0.51
1:B:50:ALA:O	1:B:52:LYS:N	2.43	0.51
1:B:112:VAL:CG1	1:B:117:MET:HE1	2.41	0.51
1:A:49:GLU:CG	1:A:53:GLN:NE2	2.72	0.51
1:C:16:MET:O	1:C:19:LEU:N	2.42	0.50
1:B:26:LEU:HB2	1:B:58:ILE:CG2	2.41	0.50
1:B:95:ALA:O	1:B:96:THR:CB	2.60	0.50
1:A:16:MET:O	1:A:19:LEU:N	2.43	0.50
1:B:92:GLU:OE2	1:B:150:ARG:NH1	2.45	0.50
1:A:103:GLN:CG	1:A:104:VAL:N	2.73	0.50
1:A:58:ILE:O	1:A:59:GLU:C	2.46	0.50
1:A:82:VAL:HG22	1:A:133:ARG:NH1	2.27	0.50
1:B:87:SER:O	1:B:103:GLN:HB2	2.12	0.50
1:B:89:VAL:HG12	1:B:91:LEU:CD2	2.41	0.50
1:C:22:GLU:OE1	1:C:61:ARG:NH1	2.44	0.50
1:A:26:LEU:O	1:A:29:ALA:HB3	2.11	0.50
1:A:84:GLY:C	1:A:85:LEU:HD12	2.23	0.50
1:C:49:GLU:OE1	1:C:49:GLU:HA	2.11	0.50
1:A:130:LEU:HD12	1:A:130:LEU:C	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:ILE:HA	1:C:61:ARG:HB2	1.93	0.50
1:B:19:LEU:CD1	1:B:62:ILE:HG23	2.42	0.49
1:A:25:ARG:O	1:C:28:GLU:HG2	2.12	0.49
1:A:14:ARG:HD3	1:A:148:GLU:OE2	2.12	0.49
1:B:57:ARG:O	1:B:61:ARG:HB2	2.12	0.49
1:A:105:VAL:CG2	1:A:119:ILE:O	2.61	0.49
1:B:92:GLU:C	1:B:94:PRO:CD	2.78	0.49
1:B:132:HIS:CD2	1:B:138:LEU:HD11	2.47	0.49
1:B:54:GLU:C	1:B:56:ALA:N	2.66	0.49
1:B:89:VAL:HG12	1:B:91:LEU:HD21	1.93	0.49
1:C:19:LEU:C	1:C:21:GLN:N	2.62	0.49
1:C:6:LYS:HB3	1:C:75:LEU:HD21	1.94	0.49
1:B:105:VAL:HG23	1:B:106:SER:O	2.13	0.49
1:B:44:ASP:O	1:B:45:ASP:CB	2.47	0.49
1:B:44:ASP:OD1	1:B:46:SER:HB3	2.13	0.49
1:C:33:LEU:O	1:C:34:GLN:C	2.51	0.49
1:C:45:ASP:C	1:C:47:GLY:N	2.65	0.49
1:C:92:GLU:O	1:C:94:PRO:CD	2.61	0.49
1:A:88:VAL:CG1	1:A:103:GLN:HB2	2.29	0.49
1:B:125:MET:O	1:B:128:ALA:HB3	2.13	0.49
1:B:47:GLY:HA2	1:B:50:ALA:CB	2.42	0.49
1:C:105:VAL:HG22	1:C:118:LYS:HB3	1.90	0.48
1:A:18:GLN:O	1:A:21:GLN:HB3	2.13	0.48
1:A:19:LEU:HD11	1:A:62:ILE:HG23	1.94	0.48
1:A:119:ILE:HD11	1:A:125:MET:HG2	1.95	0.48
1:A:4:GLU:CD	1:A:6:LYS:HE3	2.32	0.48
1:B:83:ILE:HD13	1:B:89:VAL:HG21	1.94	0.48
1:A:29:ALA:O	1:A:32:ILE:HB	2.14	0.48
1:A:44:ASP:HB3	1:A:48:LEU:HG	1.95	0.48
1:A:77:GLU:C	1:A:79:THR:H	2.17	0.48
1:B:28:GLU:OE1	1:B:28:GLU:HA	2.13	0.48
1:C:92:GLU:O	1:C:150:ARG:N	2.42	0.48
1:A:49:GLU:CD	1:A:53:GLN:NE2	2.66	0.48
1:C:67:ASP:O	1:C:70:SER:HB3	2.14	0.48
1:C:18:GLN:O	1:C:22:GLU:HG2	2.13	0.48
1:C:61:ARG:O	1:C:62:ILE:C	2.51	0.48
1:A:49:GLU:HG3	1:A:53:GLN:HE22	1.77	0.48
1:C:16:MET:C	1:C:18:GLN:N	2.64	0.48
1:C:15:LEU:CD1	1:C:137:VAL:HG11	2.39	0.47
1:B:85:LEU:O	1:B:104:VAL:O	2.32	0.47
1:B:142:THR:CG2	1:B:143:PRO:N	2.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:VAL:HB	1:B:119:ILE:HD13	1.97	0.47
1:C:138:LEU:O	1:C:149:PHE:N	2.34	0.47
1:C:62:ILE:O	1:C:64:SER:N	2.48	0.47
1:C:67:ASP:C	1:C:67:ASP:OD1	2.52	0.47
1:B:34:GLN:O	1:B:37:MET:HB3	2.14	0.47
1:B:67:ASP:O	1:B:70:SER:OG	2.25	0.47
1:C:39:SER:O	1:C:40:SER:OG	2.29	0.47
1:A:105:VAL:HG21	1:A:118:LYS:HB3	1.96	0.47
1:B:59:GLU:O	1:B:63:ASP:N	2.28	0.47
1:B:105:VAL:HG21	1:B:109:GLU:O	2.15	0.47
1:C:119:ILE:HD13	1:C:125:MET:HG2	1.96	0.47
1:B:126:GLY:O	1:B:127:LYS:C	2.54	0.46
1:B:49:GLU:HA	1:B:49:GLU:OE1	2.15	0.46
1:A:38:GLU:C	1:A:40:SER:N	2.67	0.46
1:B:134:VAL:HG13	1:B:153:ALA:N	2.30	0.46
1:C:47:GLY:O	1:C:49:GLU:N	2.48	0.46
1:C:114:GLU:OE1	1:C:118:LYS:HD2	2.15	0.46
1:B:89:VAL:O	1:B:101:SER:HA	2.16	0.46
1:B:138:LEU:HA	1:B:138:LEU:HD23	1.43	0.46
1:C:120:SER:HB3	1:C:123:SER:HB3	1.97	0.46
1:C:142:THR:HG23	1:C:143:PRO:CD	2.45	0.46
1:B:47:GLY:O	1:B:50:ALA:N	2.49	0.46
1:C:111:SER:H	1:C:118:LYS:HB2	1.81	0.46
1:A:103:GLN:HG2	1:A:105:VAL:HG13	1.98	0.46
1:B:14:ARG:C	1:B:16:MET:H	2.19	0.46
1:A:100:LEU:O	1:A:100:LEU:HG	2.12	0.46
1:B:6:LYS:O	1:B:135:GLY:HA2	2.16	0.46
1:A:119:ILE:HD12	1:A:125:MET:HG2	1.94	0.46
1:B:61:ARG:NH1	1:B:61:ARG:HG2	2.29	0.45
1:A:124:PRO:O	1:A:128:ALA:HB2	2.17	0.45
1:A:65:LEU:O	1:A:66:GLU:C	2.52	0.45
1:A:6:LYS:O	1:A:135:GLY:CA	2.63	0.45
1:B:44:ASP:C	1:B:46:SER:H	2.19	0.45
1:C:130:LEU:HD12	1:C:130:LEU:HA	1.29	0.45
1:C:13:GLU:C	1:C:15:LEU:N	2.68	0.45
1:C:16:MET:O	1:C:18:GLN:N	2.50	0.45
1:C:54:GLU:OE2	1:C:58:ILE:HD11	2.17	0.45
1:C:80:GLY:CA	1:C:133:ARG:CG	2.79	0.45
1:A:61:ARG:HG3	1:A:95:ALA:HB1	1.99	0.45
1:A:6:LYS:O	1:A:135:GLY:HA3	2.17	0.45
1:C:114:GLU:OE1	1:C:118:LYS:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:GLU:O	1:C:39:SER:C	2.55	0.45
1:A:74:ILE:H	1:A:74:ILE:HG13	1.60	0.45
1:B:16:MET:O	1:B:19:LEU:N	2.50	0.45
1:A:48:LEU:O	1:A:52:LYS:HB2	2.17	0.45
1:C:61:ARG:NH1	1:C:61:ARG:HG2	2.32	0.45
1:A:105:VAL:HG22	1:A:119:ILE:O	2.17	0.44
1:A:19:LEU:HA	1:A:19:LEU:HD12	1.77	0.44
1:C:83:ILE:CG2	1:C:130:LEU:HD12	2.44	0.44
1:C:85:LEU:HD12	1:C:85:LEU:N	2.32	0.44
1:C:96:THR:CG2	1:C:98:GLU:H	2.29	0.44
1:A:119:ILE:HD12	1:A:125:MET:CG	2.47	0.44
1:B:96:THR:HG22	1:B:98:GLU:HB2	2.00	0.44
1:A:24:GLU:CG	1:C:21:GLN:HG2	2.46	0.44
1:A:16:MET:HG3	1:A:69:LEU:HD22	1.98	0.44
1:A:82:VAL:CG1	1:A:83:ILE:H	2.16	0.44
1:B:10:ALA:O	1:B:14:ARG:HB2	2.17	0.44
1:B:85:LEU:C	1:B:87:SER:N	2.71	0.44
1:A:6:LYS:CG	1:A:73:VAL:HB	2.47	0.44
1:B:44:ASP:H	1:B:48:LEU:HD12	1.82	0.44
1:C:32:ILE:O	1:C:35:GLU:HB3	2.18	0.44
1:A:113:LEU:O	1:A:114:GLU:C	2.53	0.44
1:B:61:ARG:HG2	1:B:95:ALA:HB1	1.99	0.44
1:B:77:GLU:HG3	1:B:78:GLY:H	1.83	0.44
1:C:119:ILE:CD1	1:C:125:MET:HG2	2.48	0.44
1:A:29:ALA:O	1:A:30:THR:C	2.55	0.44
1:A:28:GLU:OE2	1:C:54:GLU:OE2	2.35	0.43
1:C:142:THR:HG22	1:C:144:LYS:N	2.32	0.43
1:B:29:ALA:O	1:B:30:THR:C	2.57	0.43
1:C:76:GLU:O	1:C:76:GLU:HG3	2.19	0.43
1:B:147:LYS:HB2	1:B:149:PHE:HE1	1.83	0.43
1:B:85:LEU:HA	1:B:85:LEU:HD12	1.25	0.43
1:A:66:GLU:O	1:A:69:LEU:N	2.51	0.43
1:B:125:MET:CA	1:B:128:ALA:HB3	2.45	0.43
1:B:37:MET:O	1:B:40:SER:CB	2.66	0.43
1:B:54:GLU:HB3	1:B:55:LYS:H	1.51	0.43
1:C:39:SER:C	1:C:40:SER:HG	2.22	0.43
1:B:102:VAL:CB	1:B:119:ILE:HD13	2.48	0.43
1:B:129:LEU:HD11	1:B:140:LEU:HD21	2.01	0.43
1:A:106:SER:HA	1:A:107:PRO:HD3	1.83	0.43
1:A:45:ASP:O	1:A:49:GLU:CB	2.66	0.43
1:B:67:ASP:C	1:B:67:ASP:OD1	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:GLU:HG3	1:C:143:PRO:HD3	2.00	0.43
1:C:69:LEU:N	1:C:69:LEU:HD12	2.32	0.43
1:A:126:GLY:O	1:A:127:LYS:C	2.57	0.43
1:A:47:GLY:O	1:A:51:ALA:HB3	2.19	0.43
1:C:114:GLU:O	1:C:117:MET:HG3	2.18	0.43
1:C:96:THR:HG22	1:C:96:THR:O	2.08	0.43
1:B:67:ASP:O	1:B:70:SER:N	2.51	0.42
1:A:98:GLU:HG2	1:A:98:GLU:O	2.19	0.42
1:C:115:ASN:O	1:C:117:MET:N	2.51	0.42
1:C:47:GLY:C	1:C:49:GLU:N	2.71	0.42
1:A:49:GLU:O	1:A:51:ALA:N	2.52	0.42
1:B:102:VAL:HG21	1:B:119:ILE:CD1	2.48	0.42
1:B:138:LEU:O	1:B:148:GLU:HA	2.20	0.42
1:A:101:SER:C	1:A:102:VAL:HG12	2.39	0.42
1:A:15:LEU:HD11	1:A:94:PRO:CG	2.46	0.42
1:A:83:ILE:O	1:A:130:LEU:CD1	2.67	0.42
1:C:19:LEU:O	1:C:21:GLN:N	2.53	0.42
1:B:100:LEU:HD12	1:B:101:SER:N	2.35	0.42
1:B:102:VAL:HG21	1:B:119:ILE:HD13	2.01	0.42
1:A:115:ASN:O	1:A:117:MET:N	2.50	0.42
1:B:93:ASP:O	1:B:96:THR:HG22	2.19	0.42
1:A:14:ARG:HA	1:A:17:LYS:HG3	2.02	0.42
1:B:61:ARG:O	1:B:62:ILE:C	2.57	0.42
1:B:87:SER:O	1:B:103:GLN:CB	2.68	0.42
1:A:114:GLU:OE1	1:A:118:LYS:HD2	2.20	0.42
1:A:67:ASP:O	1:A:67:ASP:OD1	2.38	0.42
1:C:11:GLY:HA2	1:C:137:VAL:HG23	2.02	0.42
1:B:115:ASN:CB	1:B:116:PRO:CD	2.97	0.41
1:A:134:VAL:HG13	1:A:153:ALA:H	1.85	0.41
1:A:66:GLU:O	1:A:67:ASP:C	2.58	0.41
1:B:142:THR:HG22	1:B:144:LYS:N	2.34	0.41
1:C:125:MET:O	1:C:129:LEU:CD1	2.54	0.41
1:A:96:THR:HG21	1:A:98:GLU:CD	2.40	0.41
1:A:62:ILE:HG22	1:A:63:ASP:N	2.34	0.41
1:B:7:LEU:HA	1:B:135:GLY:O	2.20	0.41
1:C:126:GLY:C	1:C:128:ALA:N	2.71	0.41
1:C:38:GLU:O	1:C:40:SER:OG	2.38	0.41
1:B:33:LEU:HD23	1:B:34:GLN:HG2	2.02	0.41
1:A:109:GLU:H	1:A:109:GLU:HG2	1.65	0.41
1:A:6:LYS:O	1:A:7:LEU:HD23	2.21	0.41
1:B:152:VAL:O	1:B:153:ALA:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:ASP:C	1:B:47:GLY:N	2.72	0.41
1:C:29:ALA:O	1:C:30:THR:C	2.59	0.41
1:A:102:VAL:HG23	1:A:103:GLN:N	2.34	0.41
1:A:37:MET:O	1:A:40:SER:HB2	2.21	0.41
1:B:37:MET:O	1:B:40:SER:OG	2.38	0.41
1:B:41:ASP:CA	1:B:42:ASP:OD2	2.68	0.41
1:C:36:LEU:O	1:C:40:SER:HA	2.21	0.41
1:B:111:SER:OG	1:B:113:LEU:HB2	2.21	0.41
1:A:45:ASP:O	1:A:49:GLU:HB2	2.21	0.41
1:C:78:GLY:HA2	1:C:133:ARG:HH12	1.85	0.40
1:C:45:ASP:O	1:C:47:GLY:CA	2.68	0.40
1:A:40:SER:O	1:A:41:ASP:HB3	2.21	0.40
1:C:15:LEU:HD23	1:C:69:LEU:HD11	2.02	0.40
1:A:36:LEU:C	1:A:38:GLU:N	2.75	0.40
1:A:85:LEU:O	1:A:86:GLY:C	2.60	0.40
1:C:33:LEU:C	1:C:35:GLU:N	2.75	0.40
1:A:27:GLN:O	1:A:28:GLU:C	2.53	0.40
1:A:16:MET:CG	1:A:69:LEU:HD22	2.51	0.40
1:B:15:LEU:HD23	1:B:15:LEU:HA	1.88	0.40
1:B:83:ILE:HD13	1:B:83:ILE:HG21	1.60	0.40
1:C:129:LEU:H	1:C:129:LEU:HD12	1.86	0.40
1:C:38:GLU:C	1:C:40:SER:HB3	2.39	0.40
1:A:142:THR:CG2	1:A:144:LYS:C	2.90	0.40
1:A:23:ARG:C	1:A:25:ARG:H	2.25	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ASP:OD2	1:B:44:ASP:OD2[2_556]	1.87	0.33

5.3 Torsion angles

5.3.1 Protein backbone

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	152/157 (97%)	110 (72%)	26 (17%)	16 (10%)	0 3
1	B	153/157 (98%)	102 (67%)	32 (21%)	19 (12%)	0 1
1	C	153/157 (98%)	104 (68%)	27 (18%)	22 (14%)	0 1
All	All	458/471 (97%)	316 (69%)	85 (19%)	57 (12%)	0 1

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	17	LYS
1	A	41	ASP
1	A	45	ASP
1	A	116	PRO
1	B	40	SER
1	B	42	ASP
1	B	43	TYR
1	B	50	ALA
1	B	55	LYS
1	B	96	THR
1	C	4	GLU
1	C	33	LEU
1	C	43	TYR
1	C	46	SER
1	C	62	ILE
1	C	63	ASP
1	C	82	VAL
1	C	96	THR
1	C	97	GLY
1	C	116	PRO
1	A	49	GLU
1	A	96	THR
1	A	144	LYS
1	B	68	VAL
1	B	117	MET
1	C	9	LYS
1	C	34	GLN
1	C	40	SER
1	C	47	GLY
1	C	117	MET
1	A	69	LEU

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Mol	Chain	Res	Type
1	A	115	ASN
1	B	41	ASP
1	B	51	ALA
1	B	67	ASP
1	B	100	LEU
1	C	3	ARG
1	C	80	GLY
1	A	153	ALA
1	C	38	GLU
1	C	41	ASP
1	C	118	LYS
1	A	10	ALA
1	A	143	PRO
1	B	30	THR
1	B	153	ALA
1	A	126	GLY
1	B	115	ASN
1	B	134	VAL
1	A	82	VAL
1	B	126	GLY
1	A	78	GLY
1	B	86	GLY
1	C	86	GLY
1	B	47	GLY
1	C	143	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	129/131 (98%)	76 (59%)	53 (41%)	0 0
1	B	129/131 (98%)	91 (70%)	38 (30%)	0 1
1	C	129/131 (98%)	84 (65%)	45 (35%)	0 1
All	All	387/393 (98%)	251 (65%)	136 (35%)	0 1

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	7	LEU
1	A	8	THR
1	A	9	LYS
1	A	14	ARG
1	A	21	GLN
1	A	26	LEU
1	A	31	LYS
1	A	33	LEU
1	A	34	GLN
1	A	38	GLU
1	A	39	SER
1	A	40	SER
1	A	42	ASP
1	A	46	SER
1	A	54	GLU
1	A	61	ARG
1	A	62	ILE
1	A	63	ASP
1	A	64	SER
1	A	67	ASP
1	A	70	SER
1	A	74	ILE
1	A	81	GLU
1	A	85	LEU
1	A	88	VAL
1	A	89	VAL
1	A	92	GLU
1	A	93	ASP
1	A	94	PRO
1	A	96	THR
1	A	98	GLU
1	A	100	LEU
1	A	101	SER
1	A	102	VAL
1	A	105	VAL
1	A	106	SER
1	A	107	PRO
1	A	111	SER
1	A	112	VAL
1	A	113	LEU
1	A	115	ASN

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Mol	Chain	Res	Type
1	A	116	PRO
1	A	119	ILE
1	A	121	ASP
1	A	124	PRO
1	A	129	LEU
1	A	130	LEU
1	A	133	ARG
1	A	136	ASP
1	A	142	THR
1	A	144	LYS
1	A	146	LYS
1	B	18	GLN
1	B	20	GLU
1	B	23	ARG
1	B	26	LEU
1	B	38	GLU
1	B	39	SER
1	B	41	ASP
1	B	42	ASP
1	B	44	ASP
1	B	46	SER
1	B	49	GLU
1	B	52	LYS
1	B	53	GLN
1	B	54	GLU
1	B	58	ILE
1	B	61	ARG
1	B	73	VAL
1	B	76	GLU
1	B	87	SER
1	B	88	VAL
1	B	90	GLU
1	B	94	PRO
1	B	96	THR
1	B	98	GLU
1	B	99	ARG
1	B	101	SER
1	B	103	GLN
1	B	111	SER
1	B	113	LEU
1	B	116	PRO
1	B	124	PRO

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Mol	Chain	Res	Type
1	B	125	MET
1	B	129	LEU
1	B	134	VAL
1	B	141	ASP
1	B	142	THR
1	B	144	LYS
1	B	150	ARG
1	C	3	ARG
1	C	8	THR
1	C	9	LYS
1	C	12	TYR
1	C	14	ARG
1	C	15	LEU
1	C	17	LYS
1	C	18	GLN
1	C	25	ARG
1	C	31	LYS
1	C	35	GLU
1	C	39	SER
1	C	41	ASP
1	C	42	ASP
1	C	46	SER
1	C	49	GLU
1	C	52	LYS
1	C	53	GLN
1	C	57	ARG
1	C	64	SER
1	C	67	ASP
1	C	70	SER
1	C	73	VAL
1	C	74	ILE
1	C	76	GLU
1	C	79	THR
1	C	87	SER
1	C	96	THR
1	C	99	ARG
1	C	100	LEU
1	C	103	GLN
1	C	105	VAL
1	C	106	SER
1	C	113	LEU
1	C	114	GLU

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Mol	Chain	Res	Type
1	C	123	SER
1	C	124	PRO
1	C	129	LEU
1	C	134	VAL
1	C	136	ASP
1	C	138	LEU
1	C	141	ASP
1	C	142	THR
1	C	146	LYS
1	C	152	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	21	GLN
1	A	34	GLN
1	A	53	GLN
1	A	155	HIS
1	B	34	GLN
1	B	132	HIS
1	C	132	HIS

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	154/157 (98%)	-0.22	5 (3%) 47 46	51, 95, 194, 253	0
1	B	155/157 (98%)	-0.30	0 100 100	41, 79, 215, 265	0
1	C	155/157 (98%)	-0.17	3 (1%) 66 65	57, 92, 183, 226	0
All	All	464/471 (98%)	-0.23	8 (1%) 70 68	41, 90, 198, 265	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	39	SER	4.9
1	A	41	ASP	3.6
1	A	40	SER	3.6
1	A	43	TYR	3.6
1	C	41	ASP	3.3
1	C	78	GLY	3.1
1	A	70	SER	3.0
1	A	155	HIS	2.5

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.