



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:17 AM UTC

PDB ID : 1ULS / pdb_00001uls
Title : Crystal structure of tt0140 from *Thermus thermophilus* HB8
Authors : Hisanaga, Y.; Ago, H.; Hamada, K.; Sugahara, M.; Nodake, Y.; Kuramitsu, S.;
Yokoyama, S.; Miyano, M.; RIKEN Structural Genomics/Proteomics Initiative
(RSGI)
Deposited on : 2003-09-16
Resolution : 2.40 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

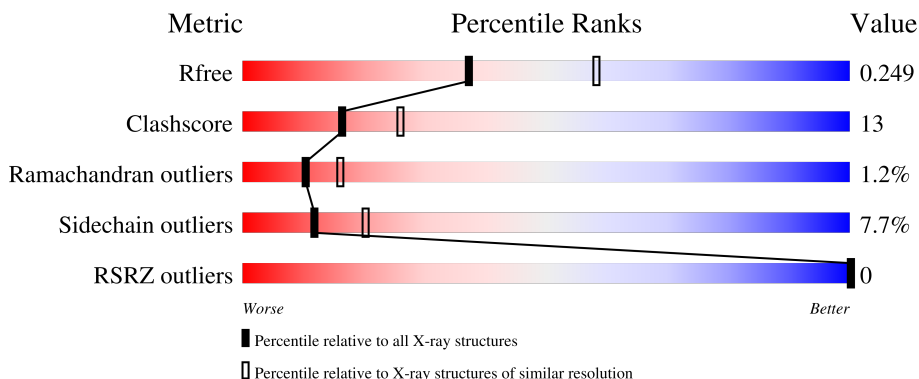
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	245	 70% 22% 7% .
1	B	245	 69% 26% .
1	C	245	 69% 24% . .
1	D	245	 71% 27% .
1	E	245	 67% 29% .

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Mol	Chain	Length	Quality of chain	
1	F	245	 71%	26% ..
1	G	245	 74%	24% .
1	H	245	 70%	24% 6%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 15244 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 putative 3-oxoacyl-acyl carrier protein reductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	242	Total 1810	C 1149	N 324	O 330	S 1	Se 6	0	0	0
1	B	245	Total 1828	C 1160	N 327	O 334	S 1	Se 6	0	0	0
1	C	239	Total 1781	C 1131	N 317	O 327	S 1	Se 5	0	0	0
1	D	245	Total 1828	C 1160	N 327	O 334	S 1	Se 6	0	0	0
1	E	245	Total 1828	C 1160	N 327	O 334	S 1	Se 6	0	0	0
1	F	242	Total 1810	C 1149	N 324	O 330	S 1	Se 6	0	0	0
1	G	245	Total 1828	C 1160	N 327	O 334	S 1	Se 6	0	0	0
1	H	245	Total 1828	C 1160	N 327	O 334	S 1	Se 6	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	89	Total 89	O 89	0	0
2	B	90	Total 90	O 90	0	0
2	C	84	Total 84	O 84	0	0
2	D	99	Total 99	O 99	0	0
2	E	89	Total 89	O 89	0	0
2	F	78	Total 78	O 78	0	0

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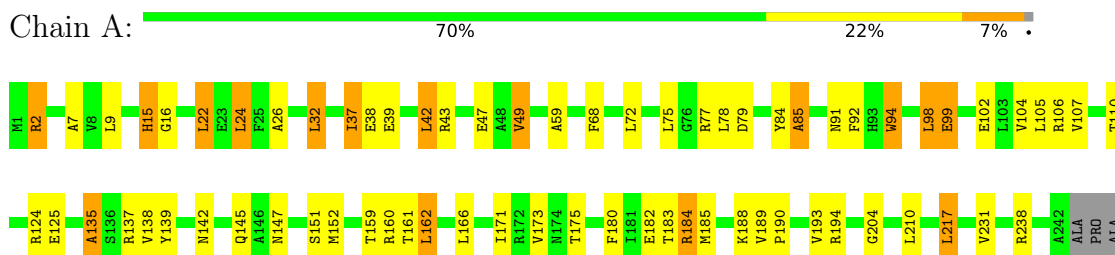
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	87	Total O 87 87	0	0
2	H	87	Total O 87 87	0	0

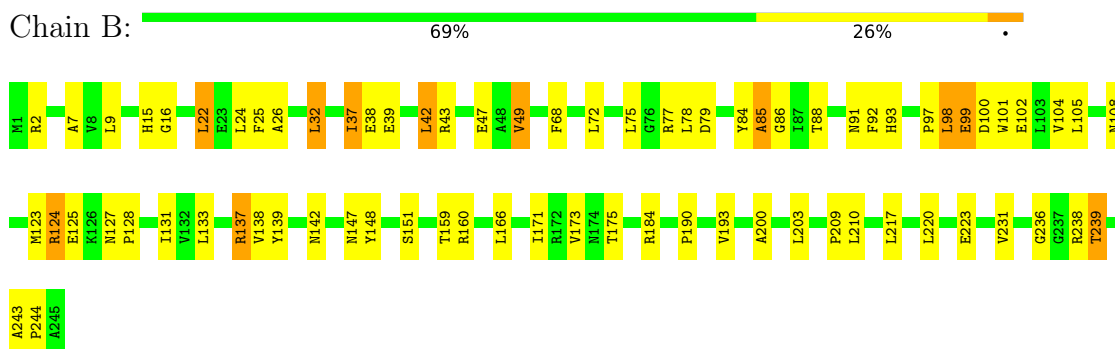
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

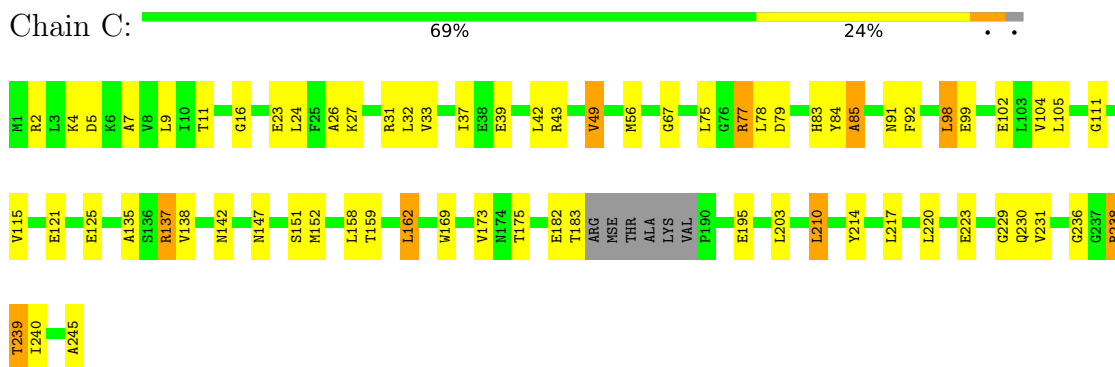
- Molecule 1: putative 3-oxoacyl-acyl carrier protein reductase



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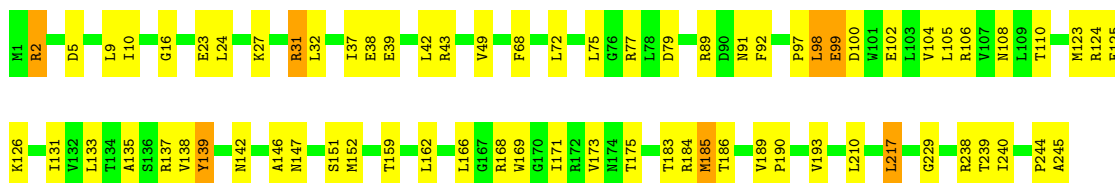


- Molecule 1: putative 3-oxoacyl-acyl carrier protein reductase



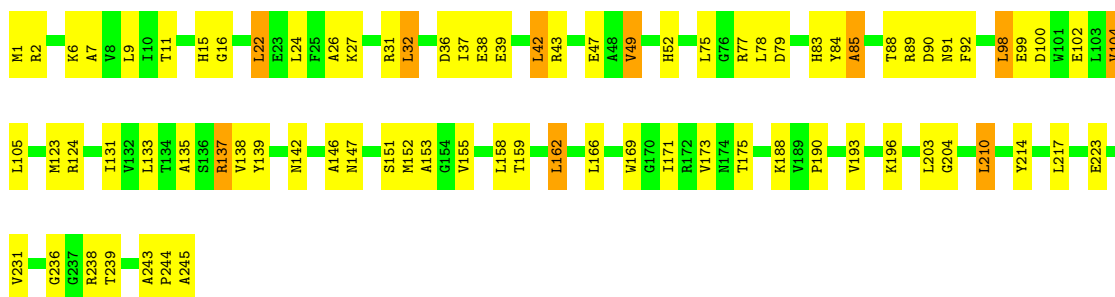
- Molecule 1: putative 3-oxoacyl-acyl carrier protein reductase

Chain D:  71% 27%



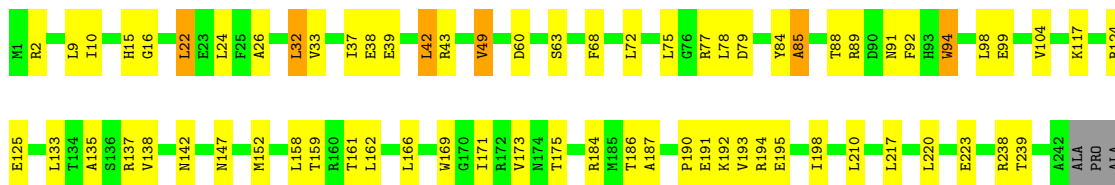
- Molecule 1: putative 3-oxoacyl-acyl carrier protein reductase

Chain E:  67% 29%



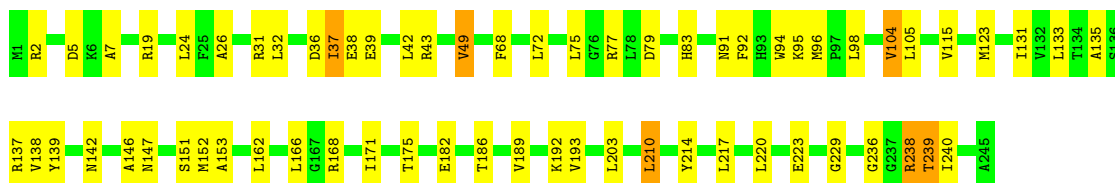
- Molecule 1: putative 3-oxoacyl-acyl carrier protein reductase

Chain F:  71% 26%



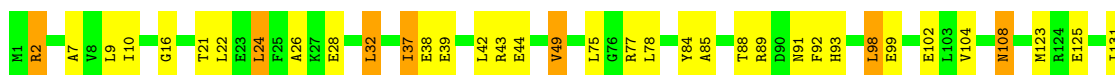
- Molecule 1: putative 3-oxoacyl-acyl carrier protein reductase

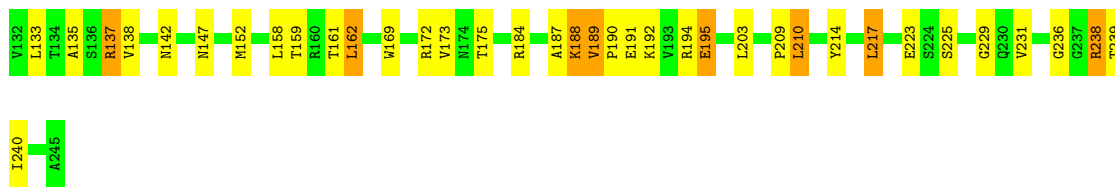
Chain G:  74% 24%



- Molecule 1: putative 3-oxoacyl-acyl carrier protein reductase

Chain H:  70% 24% 6%





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	77.26Å 77.33Å 78.67Å 90.12° 90.96° 95.12°	Depositor
Resolution (Å)	46.40 – 2.40 46.40 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.6 (46.40-2.40) 93.7 (46.40-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 2.39Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.196 , 0.252 0.194 , 0.249	Depositor DCC
R_{free} test set	7033 reflections (10.10%)	wwPDB-VP
Wilson B-factor (Å ²)	18.8	Xtrriage
Anisotropy	0.711	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 5.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.267 for -h,-k,l 0.010 for k,h,-l 0.010 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15244	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.41	0/1836	0.92	7/2479 (0.3%)
1	B	0.42	0/1855	0.92	4/2505 (0.2%)
1	C	0.42	0/1808	0.92	4/2442 (0.2%)
1	D	0.44	0/1855	0.94	5/2505 (0.2%)
1	E	0.44	0/1855	0.95	9/2505 (0.4%)
1	F	0.42	0/1836	0.92	4/2479 (0.2%)
1	G	0.44	0/1855	0.92	4/2505 (0.2%)
1	H	0.43	0/1855	0.91	5/2505 (0.2%)
All	All	0.43	0/14755	0.92	42/19925 (0.2%)

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	37	ILE	N-CA-C	9.13	119.94	110.72
1	B	32	LEU	N-CA-C	7.38	121.58	110.14
1	C	32	LEU	N-CA-C	7.35	122.01	110.17
1	A	32	LEU	N-CA-C	7.22	121.62	110.42
1	H	32	LEU	N-CA-C	7.21	121.79	110.17
1	F	37	ILE	N-CA-C	6.98	117.77	110.72
1	E	37	ILE	N-CA-C	6.89	117.68	110.72
1	G	32	LEU	N-CA-C	6.72	120.99	110.17
1	F	32	LEU	N-CA-C	6.69	120.94	110.17
1	D	92	PHE	N-CA-C	-6.61	101.18	110.50
1	D	32	LEU	N-CA-C	6.61	120.81	110.17
1	H	37	ILE	N-CA-C	6.49	118.07	111.00
1	A	37	ILE	N-CA-C	6.38	117.16	110.72
1	E	32	LEU	N-CA-C	6.24	119.87	109.95
1	E	92	PHE	N-CA-C	-6.17	101.81	110.50
1	C	92	PHE	N-CA-C	-6.03	102.00	110.50
1	E	204	GLY	N-CA-C	5.91	122.11	113.48
1	H	92	PHE	N-CA-C	-5.88	101.58	110.28
1	B	92	PHE	N-CA-C	-5.85	102.40	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	92	PHE	N-CA-C	-5.82	102.44	110.35
1	A	204	GLY	N-CA-C	5.79	121.93	113.48
1	F	92	PHE	N-CA-C	-5.76	102.38	110.50
1	E	52	HIS	CA-C-N	5.76	125.94	119.90
1	E	52	HIS	C-N-CA	5.76	125.94	119.90
1	D	108	ASN	N-CA-C	5.72	117.38	111.03
1	A	135	ALA	CA-C-O	5.69	121.24	117.94
1	F	184	ARG	N-CA-C	5.68	118.20	111.33
1	C	37	ILE	N-CA-C	5.66	117.17	111.00
1	A	92	PHE	N-CA-C	-5.58	102.63	110.50
1	B	37	ILE	N-CA-C	5.56	117.06	111.00
1	A	184	ARG	N-CA-C	-5.56	106.70	112.93
1	E	31	ARG	N-CA-C	-5.50	98.80	108.20
1	B	93	HIS	N-CA-C	5.38	117.84	111.33
1	C	31	ARG	N-CA-C	-5.30	99.14	108.20
1	G	153	ALA	N-CA-C	-5.29	105.59	111.36
1	E	90	ASP	N-CA-C	5.28	117.54	110.35
1	H	93	HIS	N-CA-C	5.24	117.67	111.33
1	D	31	ARG	N-CA-C	-5.22	100.00	108.41
1	H	108	ASN	N-CA-C	5.21	116.81	111.03
1	A	145	GLN	N-CA-C	5.21	117.54	110.88
1	D	185	MSE	N-CA-C	-5.20	106.96	113.15
1	E	153	ALA	N-CA-C	-5.20	105.79	111.82

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	1810	0	1856	47	0
1	B	1828	0	1873	51	0
1	C	1781	0	1817	50	0
1	D	1828	0	1873	54	0
1	E	1828	0	1873	55	0
1	F	1810	0	1856	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1828	0	1873	52	0
1	H	1828	0	1873	55	0
2	A	89	0	0	3	0
2	B	90	0	0	7	0
2	C	84	0	0	3	0
2	D	99	0	0	3	0
2	E	89	0	0	5	0
2	F	78	0	0	1	0
2	G	87	0	0	4	0
2	H	87	0	0	2	0
All	All	15244	0	14894	382	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 13.

All (382) 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:135:ALA:HA	1:E:152:MSE:CE	1.79	1.12
1:E:135:ALA:CA	1:E:152:MSE:HE2	1.79	1.11
1:A:160:ARG:HH12	1:D:245:ALA:HB2	1.11	1.08
1:A:160:ARG:NH1	1:D:245:ALA:HB2	1.81	0.96
1:H:104:VAL:HG21	1:H:147:ASN:HB2	1.53	0.88
1:H:189:VAL:HB	1:H:190:PRO:HA	1.58	0.84
1:C:159:THR:HG23	1:C:173:VAL:HG12	1.61	0.83
1:A:39:GLU:O	1:A:43:ARG:HG3	1.79	0.81
1:H:189:VAL:HB	1:H:190:PRO:CA	2.11	0.81
1:C:104:VAL:HG21	1:C:147:ASN:HB2	1.63	0.80
1:F:39:GLU:O	1:F:43:ARG:HG3	1.82	0.80
1:C:39:GLU:O	1:C:43:ARG:HG3	1.83	0.79
1:E:99:GLU:HG3	2:E:271:HOH:O	1.82	0.78
1:D:104:VAL:HG21	1:D:147:ASN:HB2	1.65	0.77
1:E:152:MSE:HE3	1:E:152:MSE:HA	1.66	0.77
1:E:7:ALA:HB1	1:E:75:LEU:HD13	1.66	0.76
1:H:238:ARG:O	1:H:238:ARG:HD3	1.86	0.76
1:F:191:GLU:O	1:F:195:GLU:HG3	1.86	0.76
1:G:238:ARG:O	1:G:238:ARG:HD3	1.87	0.75
1:G:192:LYS:H	1:G:192:LYS:HD2	1.51	0.75
1:D:68:PHE:O	1:D:72:LEU:HD23	1.86	0.74
1:F:135:ALA:O	1:F:152:MSE:HE3	1.88	0.74
1:C:238:ARG:O	1:C:238:ARG:HD3	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:ARG:NH1	1:C:245:ALA:HB2	2.03	0.73
1:G:239:THR:HG22	2:G:289:HOH:O	1.89	0.72
1:G:68:PHE:O	1:G:72:LEU:HD23	1.90	0.72
1:E:135:ALA:HA	1:E:152:MSE:HE2	0.86	0.71
1:A:104:VAL:HG21	1:A:147:ASN:HB2	1.72	0.71
1:H:104:VAL:CG2	1:H:147:ASN:HB2	2.21	0.70
1:H:238:ARG:HG3	1:H:238:ARG:HH11	1.56	0.70
1:A:135:ALA:O	1:A:152:MSE:HE3	1.91	0.70
1:D:135:ALA:O	1:D:152:MSE:HE3	1.91	0.69
1:G:186:THR:O	1:G:189:VAL:HG23	1.92	0.69
1:C:104:VAL:CG2	1:C:147:ASN:HB2	2.22	0.69
1:B:22:LEU:HD23	1:B:32:LEU:HD13	1.74	0.69
1:D:104:VAL:CG2	1:D:147:ASN:HB2	2.23	0.68
1:G:37:ILE:HG23	1:G:38:GLU:HG3	1.75	0.68
2:C:305:HOH:O	1:D:239:THR:HG22	1.93	0.68
1:A:99:GLU:HG2	2:A:271:HOH:O	1.93	0.67
1:D:37:ILE:HG23	1:D:38:GLU:HG3	1.77	0.67
1:C:7:ALA:HB1	1:C:75:LEU:HD13	1.77	0.66
1:B:104:VAL:HG21	1:B:147:ASN:HB2	1.77	0.66
1:B:39:GLU:O	1:B:43:ARG:HG3	1.97	0.65
1:G:229:GLY:HA3	1:H:240:ILE:HD11	1.78	0.65
1:D:159:THR:HG23	1:D:173:VAL:HG12	1.78	0.64
1:G:39:GLU:O	1:G:43:ARG:HG3	1.97	0.64
1:D:184:ARG:HG2	1:D:184:ARG:HH11	1.63	0.64
1:F:104:VAL:HG21	1:F:147:ASN:HB2	1.80	0.64
1:H:7:ALA:HB1	1:H:75:LEU:HD13	1.79	0.64
1:H:37:ILE:HG23	1:H:38:GLU:HG3	1.80	0.64
1:H:39:GLU:O	1:H:43:ARG:HG3	1.98	0.64
1:C:239:THR:HG22	2:C:306:HOH:O	1.97	0.63
1:F:2:ARG:HD3	1:F:223:GLU:OE1	1.99	0.62
1:E:203:LEU:HD12	1:E:236:GLY:HA2	1.79	0.62
1:H:159:THR:HG23	1:H:173:VAL:HG12	1.81	0.62
1:C:39:GLU:HG2	1:C:43:ARG:HD2	1.81	0.61
1:D:39:GLU:O	1:D:43:ARG:HG3	2.00	0.61
1:G:5:ASP:OD2	1:G:31:ARG:HD2	2.00	0.61
1:A:104:VAL:CG2	1:A:147:ASN:HB2	2.29	0.61
1:G:135:ALA:O	1:G:152:MSE:HE3	2.00	0.61
1:G:192:LYS:H	1:G:192:LYS:CD	2.14	0.61
1:E:190:PRO:HG2	1:E:193:VAL:HB	1.81	0.61
1:G:210:LEU:HB2	2:G:255:HOH:O	2.01	0.61
1:B:239:THR:HG22	2:B:269:HOH:O	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:THR:HG21	1:D:146:ALA:HA	1.83	0.60
1:B:104:VAL:CG2	1:B:147:ASN:HB2	2.32	0.60
1:E:105:LEU:HD23	1:E:151:SER:HB3	1.84	0.60
1:B:160:ARG:HH12	1:C:245:ALA:HB2	1.67	0.60
1:F:238:ARG:HG2	2:F:280:HOH:O	2.00	0.60
1:B:2:ARG:HD3	1:B:223:GLU:OE1	2.02	0.59
1:B:7:ALA:HB1	1:B:75:LEU:HD13	1.85	0.59
1:H:189:VAL:HB	1:H:190:PRO:C	2.28	0.59
1:A:238:ARG:HG2	2:A:328:HOH:O	2.02	0.58
1:B:160:ARG:CZ	1:C:245:ALA:HB2	2.32	0.58
1:E:159:THR:HG23	1:E:173:VAL:HG12	1.85	0.58
1:C:135:ALA:O	1:C:152:MSE:HE3	2.02	0.58
1:A:22:LEU:HD23	1:A:32:LEU:HD13	1.86	0.58
1:A:166:LEU:HB3	1:A:171:ILE:HB	1.86	0.57
1:B:190:PRO:HG2	1:B:193:VAL:HB	1.85	0.57
1:H:190:PRO:C	1:H:192:LYS:H	2.12	0.57
1:F:104:VAL:CG2	1:F:147:ASN:HB2	2.35	0.57
1:A:159:THR:HG23	1:A:173:VAL:HG12	1.86	0.56
1:H:188:LYS:O	1:H:188:LYS:HG2	2.06	0.56
1:B:22:LEU:CD2	1:B:32:LEU:HD13	2.35	0.56
1:F:135:ALA:C	1:F:152:MSE:HE3	2.30	0.56
1:C:111:GLY:O	1:C:115:VAL:HG23	2.05	0.56
1:G:31:ARG:NH2	1:G:75:LEU:O	2.39	0.56
1:G:238:ARG:HD3	1:G:238:ARG:C	2.30	0.56
1:A:43:ARG:O	1:A:47:GLU:HG3	2.06	0.56
1:F:9:LEU:C	1:F:9:LEU:HD23	2.31	0.55
1:G:189:VAL:HG12	1:G:193:VAL:HB	1.87	0.55
1:C:2:ARG:HD3	1:C:223:GLU:OE1	2.06	0.55
1:C:26:ALA:HB2	1:C:49:VAL:HG13	1.88	0.55
1:C:158:LEU:HG	1:C:162:LEU:HD22	1.87	0.55
1:F:38:GLU:O	1:F:42:LEU:HB2	2.06	0.55
1:G:105:LEU:HD23	1:G:151:SER:HB3	1.89	0.55
1:H:133:LEU:O	1:H:175:THR:HA	2.06	0.55
1:H:238:ARG:HG3	1:H:238:ARG:NH1	2.21	0.55
1:A:37:ILE:HG23	1:A:38:GLU:HG3	1.89	0.55
1:B:133:LEU:O	1:B:175:THR:HA	2.06	0.55
1:C:125:GLU:HG2	1:C:169:TRP:CZ3	2.42	0.55
1:E:175:THR:CG2	1:E:231:VAL:HG22	2.37	0.55
1:E:1:MSE:HE2	1:E:27:LYS:O	2.07	0.54
1:A:98:LEU:HD22	1:A:102:GLU:HG3	1.89	0.54
1:D:138:VAL:HG13	1:D:142:ASN:CB	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:238:ARG:HH21	1:E:243:ALA:HB3	1.72	0.54
1:E:175:THR:HG23	1:E:231:VAL:HA	1.89	0.54
1:A:9:LEU:C	1:A:9:LEU:HD23	2.33	0.54
1:B:22:LEU:HD22	1:B:49:VAL:HG11	1.89	0.54
1:D:238:ARG:O	1:D:238:ARG:HD3	2.08	0.54
1:E:22:LEU:CD2	1:E:32:LEU:HD13	2.38	0.54
1:A:124:ARG:O	1:A:125:GLU:HB2	2.06	0.54
1:A:182:GLU:HA	1:A:182:GLU:OE1	2.07	0.54
1:B:124:ARG:O	1:B:125:GLU:HB2	2.07	0.53
1:H:10:ILE:HD13	1:H:21:THR:HG22	1.90	0.53
1:B:123:MSE:HE1	1:B:131:ILE:HG13	1.91	0.53
1:G:189:VAL:HG11	1:G:193:VAL:HG11	1.91	0.53
1:B:26:ALA:CB	1:B:49:VAL:HG22	2.38	0.53
1:B:98:LEU:HD22	1:B:102:GLU:HG3	1.90	0.53
1:H:158:LEU:HG	1:H:162:LEU:HD22	1.90	0.53
1:D:9:LEU:C	1:D:9:LEU:HD23	2.33	0.53
1:F:238:ARG:HD2	1:F:238:ARG:O	2.08	0.53
1:A:161:THR:HG21	1:D:146:ALA:CA	2.39	0.53
1:E:2:ARG:HD3	1:E:223:GLU:OE1	2.08	0.53
1:H:26:ALA:HB2	1:H:49:VAL:HG13	1.92	0.52
1:H:187:ALA:C	1:H:189:VAL:H	2.17	0.52
1:A:22:LEU:CD2	1:A:32:LEU:HD13	2.39	0.52
1:C:11:THR:OG1	1:C:83:HIS:HA	2.09	0.52
1:F:159:THR:HG23	1:F:173:VAL:HG12	1.90	0.52
1:B:160:ARG:HD3	2:B:312:HOH:O	2.09	0.52
1:H:104:VAL:HG21	1:H:147:ASN:CB	2.35	0.52
1:B:166:LEU:HB3	1:B:171:ILE:HB	1.91	0.52
1:E:22:LEU:HD23	1:E:32:LEU:HD13	1.91	0.52
1:B:159:THR:HG23	1:B:173:VAL:HG12	1.92	0.52
1:B:123:MSE:HE1	1:B:131:ILE:CG1	2.40	0.51
1:B:231:VAL:HG23	2:B:294:HOH:O	2.08	0.51
1:C:238:ARG:HD3	1:C:238:ARG:C	2.35	0.51
1:E:26:ALA:CB	1:E:49:VAL:HG22	2.40	0.51
1:D:31:ARG:NH2	1:D:75:LEU:O	2.44	0.51
1:D:166:LEU:HB3	1:D:171:ILE:HB	1.93	0.51
1:H:22:LEU:HD22	1:H:32:LEU:HD13	1.93	0.51
1:C:56:MSE:HE2	1:C:67:GLY:HA3	1.92	0.51
1:B:9:LEU:HD23	1:B:9:LEU:C	2.35	0.51
1:C:229:GLY:HA3	1:D:240:ILE:HD11	1.93	0.51
1:B:238:ARG:HE	1:B:243:ALA:HB2	1.76	0.51
1:A:77:ARG:NH1	1:A:79:ASP:OD1	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:TYR:O	1:B:85:ALA:C	2.54	0.50
1:B:97:PRO:HG2	1:B:100:ASP:CG	2.37	0.50
1:G:83:HIS:CE1	1:G:115:VAL:HG21	2.47	0.50
1:H:2:ARG:HG2	1:H:28:GLU:OE1	2.10	0.50
1:F:26:ALA:CB	1:F:49:VAL:HG22	2.41	0.50
1:A:94:TRP:CD1	1:A:94:TRP:H	2.29	0.50
1:D:183:THR:OG1	1:D:184:ARG:N	2.44	0.50
1:E:190:PRO:HG2	1:E:193:VAL:CG2	2.42	0.50
1:G:77:ARG:NH1	1:G:79:ASP:OD1	2.44	0.50
1:G:229:GLY:HA3	1:H:240:ILE:CD1	2.40	0.50
1:A:189:VAL:CG1	1:A:193:VAL:HB	2.41	0.50
1:E:36:ASP:HB3	2:E:288:HOH:O	2.10	0.50
1:C:84:TYR:O	1:C:85:ALA:C	2.54	0.50
1:D:138:VAL:HG13	1:D:142:ASN:HB3	1.93	0.50
1:D:189:VAL:HG22	1:D:190:PRO:HD2	1.94	0.50
1:E:6:LYS:HG2	2:E:304:HOH:O	2.11	0.50
1:F:186:THR:HG22	1:F:187:ALA:O	2.11	0.50
1:G:104:VAL:CG2	1:G:147:ASN:HB2	2.42	0.50
1:H:203:LEU:HD12	1:H:236:GLY:HA2	1.94	0.50
1:A:68:PHE:O	1:A:72:LEU:HD23	2.11	0.49
1:C:195:GLU:HA	1:C:195:GLU:OE1	2.12	0.49
1:A:190:PRO:HG2	1:A:193:VAL:HG23	1.93	0.49
1:B:190:PRO:HG2	1:B:193:VAL:CG2	2.41	0.49
1:C:203:LEU:HD12	1:C:236:GLY:HA2	1.94	0.49
1:E:123:MSE:HE1	1:E:131:ILE:HG13	1.94	0.49
1:G:19:ARG:NH1	1:G:19:ARG:HG2	2.27	0.49
1:G:19:ARG:HG2	1:G:19:ARG:HH11	1.75	0.49
1:C:138:VAL:HG12	1:C:138:VAL:O	2.12	0.49
1:E:100:ASP:O	1:E:104:VAL:HG13	2.12	0.49
1:F:9:LEU:HD23	1:F:10:ILE:N	2.26	0.49
1:F:94:TRP:CD1	1:F:94:TRP:H	2.28	0.49
1:F:220:LEU:HD23	1:F:220:LEU:O	2.12	0.49
1:D:123:MSE:CE	1:D:131:ILE:HD11	2.43	0.49
1:H:2:ARG:HD2	1:H:223:GLU:OE1	2.12	0.49
1:H:135:ALA:O	1:H:152:MSE:HE3	2.12	0.49
1:E:9:LEU:C	1:E:9:LEU:HD23	2.36	0.49
1:E:43:ARG:O	1:E:47:GLU:HG3	2.12	0.49
1:B:175:THR:CG2	1:B:231:VAL:HG22	2.42	0.49
1:E:39:GLU:O	1:E:43:ARG:HG3	2.13	0.49
1:G:123:MSE:HE3	1:G:171:ILE:HD13	1.94	0.49
1:H:88:THR:O	1:H:89:ARG:CD	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:77:ARG:NH1	1:E:79:ASP:OD1	2.46	0.48
1:F:166:LEU:HB3	1:F:171:ILE:HB	1.95	0.48
1:H:125:GLU:HG2	1:H:169:TRP:CZ3	2.49	0.48
1:A:184:ARG:HG2	2:A:286:HOH:O	2.12	0.48
1:B:203:LEU:HD12	1:B:236:GLY:HA2	1.95	0.48
1:B:37:ILE:HG22	2:B:296:HOH:O	2.13	0.48
1:C:98:LEU:HD22	1:C:102:GLU:HG3	1.95	0.48
1:G:192:LYS:HD2	1:G:192:LYS:N	2.23	0.48
1:H:88:THR:O	1:H:89:ARG:HD3	2.13	0.48
1:C:245:ALA:C	1:D:244:PRO:HG3	2.38	0.48
1:D:9:LEU:HD23	1:D:10:ILE:N	2.29	0.48
1:D:23:GLU:O	1:D:27:LYS:HG3	2.14	0.48
1:A:162:LEU:HB3	1:A:173:VAL:HG21	1.95	0.48
1:B:138:VAL:HG12	1:B:138:VAL:O	2.13	0.48
1:B:160:ARG:NH2	1:C:245:ALA:HB2	2.29	0.48
1:B:77:ARG:NH1	1:B:79:ASP:OD1	2.47	0.48
1:G:238:ARG:HG3	1:G:238:ARG:HH11	1.78	0.48
1:B:43:ARG:O	1:B:47:GLU:HG3	2.14	0.47
1:D:138:VAL:O	1:D:138:VAL:HG12	2.14	0.47
1:E:133:LEU:O	1:E:175:THR:HA	2.13	0.47
1:F:125:GLU:HG2	1:F:169:TRP:CZ3	2.49	0.47
1:B:105:LEU:HD23	1:B:151:SER:HB3	1.96	0.47
1:G:133:LEU:O	1:G:175:THR:HA	2.13	0.47
1:G:135:ALA:C	1:G:152:MSE:HE3	2.39	0.47
1:C:121:GLU:HG2	2:C:275:HOH:O	2.13	0.47
1:D:123:MSE:HE1	1:D:131:ILE:HD11	1.95	0.47
1:C:245:ALA:O	1:D:244:PRO:HG3	2.14	0.47
1:A:175:THR:CG2	1:A:231:VAL:HG22	2.44	0.47
1:F:22:LEU:HD23	1:F:32:LEU:HD13	1.95	0.47
1:A:238:ARG:HD2	1:A:238:ARG:O	2.15	0.47
1:H:98:LEU:HD22	1:H:102:GLU:HG3	1.95	0.47
1:A:104:VAL:HG21	1:A:147:ASN:CB	2.44	0.47
1:B:184:ARG:NH1	2:B:327:HOH:O	2.48	0.47
1:B:209:PRO:HG2	2:B:284:HOH:O	2.13	0.47
1:D:184:ARG:C	1:D:186:THR:H	2.22	0.47
1:G:7:ALA:HB1	1:G:75:LEU:HD13	1.97	0.47
1:G:138:VAL:HG12	1:G:138:VAL:O	2.14	0.47
1:B:68:PHE:O	1:B:72:LEU:HD23	2.15	0.47
1:A:84:TYR:O	1:A:85:ALA:C	2.57	0.47
1:F:68:PHE:O	1:F:72:LEU:HD23	2.15	0.47
1:G:168:ARG:HG2	2:G:299:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:LEU:HD23	1:C:220:LEU:O	2.14	0.47
1:C:229:GLY:HA3	1:D:240:ILE:CD1	2.45	0.47
1:C:137:ARG:NH1	1:C:138:VAL:HG22	2.30	0.46
1:E:38:GLU:O	1:E:42:LEU:HB2	2.15	0.46
1:F:133:LEU:O	1:F:175:THR:HA	2.15	0.46
1:H:123:MSE:HE1	1:H:131:ILE:HG13	1.96	0.46
1:D:97:PRO:HB2	1:D:99:GLU:HG3	1.97	0.46
1:E:104:VAL:HG21	1:E:147:ASN:HB2	1.96	0.46
1:H:189:VAL:CB	1:H:190:PRO:HA	2.38	0.46
1:A:138:VAL:HG13	1:A:142:ASN:HB3	1.98	0.46
1:E:190:PRO:HG2	1:E:193:VAL:CB	2.46	0.46
1:H:24:LEU:HD11	1:H:217:LEU:HD12	1.97	0.46
1:E:104:VAL:CG2	1:E:147:ASN:HB2	2.45	0.46
1:A:180:PHE:HZ	1:A:194:ARG:HH21	1.62	0.46
1:C:238:ARG:HG3	1:C:238:ARG:HH11	1.80	0.46
1:F:117:LYS:NZ	1:G:96:MSE:O	2.49	0.46
1:H:184:ARG:HA	1:H:184:ARG:NE	2.30	0.46
1:E:152:MSE:HE1	1:E:155:VAL:HG21	1.97	0.46
1:A:138:VAL:HG13	1:A:142:ASN:CB	2.46	0.46
1:D:89:ARG:HG2	1:D:100:ASP:CG	2.40	0.46
1:E:137:ARG:NH2	1:E:142:ASN:OD1	2.49	0.45
1:G:123:MSE:HE1	1:G:131:ILE:HG13	1.99	0.45
1:E:146:ALA:CA	1:H:161:THR:HG21	2.46	0.45
1:H:209:PRO:HG2	2:H:253:HOH:O	2.15	0.45
1:A:138:VAL:HG12	1:A:138:VAL:O	2.16	0.45
1:C:4:LYS:O	1:C:5:ASP:HB2	2.16	0.45
1:C:240:ILE:HD11	1:D:229:GLY:HA3	1.98	0.45
1:E:166:LEU:HB3	1:E:171:ILE:HB	1.99	0.45
1:G:26:ALA:CB	1:G:49:VAL:HG22	2.47	0.45
1:A:175:THR:HG23	1:A:231:VAL:HG22	1.97	0.45
1:E:146:ALA:HA	1:H:161:THR:HG21	1.97	0.45
1:G:138:VAL:HG13	1:G:142:ASN:HB3	1.98	0.45
1:G:240:ILE:HD11	1:H:229:GLY:HA3	1.98	0.45
1:H:138:VAL:O	1:H:138:VAL:HG12	2.16	0.45
1:A:38:GLU:O	1:A:42:LEU:HB2	2.16	0.45
1:E:11:THR:OG1	1:E:83:HIS:HA	2.16	0.45
1:F:84:TYR:O	1:F:85:ALA:C	2.59	0.45
1:F:138:VAL:HG13	1:F:142:ASN:CB	2.46	0.45
1:G:2:ARG:HD3	1:G:223:GLU:OE1	2.16	0.45
1:G:189:VAL:HG11	1:G:193:VAL:CG1	2.46	0.45
1:H:138:VAL:HG13	1:H:142:ASN:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2:ARG:H	1:D:2:ARG:HG2	1.64	0.45
1:F:161:THR:HG21	1:G:146:ALA:CA	2.47	0.45
1:F:192:LYS:HD2	1:F:192:LYS:HA	1.86	0.45
1:B:88:THR:HG22	1:B:148:TYR:CD1	2.51	0.45
1:D:168:ARG:HG2	2:D:310:HOH:O	2.16	0.45
1:G:166:LEU:HB3	1:G:171:ILE:HB	1.98	0.45
1:H:9:LEU:C	1:H:9:LEU:HD23	2.42	0.45
1:H:189:VAL:CB	1:H:190:PRO:CA	2.87	0.45
1:E:2:ARG:HD3	1:E:223:GLU:CD	2.42	0.45
1:E:84:TYR:O	1:E:85:ALA:C	2.60	0.44
1:G:210:LEU:HD22	1:G:214:TYR:CD1	2.52	0.44
1:F:77:ARG:NH1	1:F:79:ASP:OD1	2.51	0.44
1:G:36:ASP:HB3	2:G:286:HOH:O	2.17	0.44
1:C:33:VAL:HG23	1:C:75:LEU:HD11	1.99	0.44
1:D:5:ASP:OD1	1:D:31:ARG:HD2	2.18	0.44
1:D:190:PRO:HG2	1:D:193:VAL:CG2	2.47	0.44
1:H:189:VAL:HB	1:H:191:GLU:N	2.31	0.44
1:B:137:ARG:NH2	1:B:238:ARG:NH2	2.66	0.44
1:E:188:LYS:N	1:E:188:LYS:HD3	2.32	0.44
1:F:39:GLU:CG	1:F:43:ARG:HD2	2.48	0.44
1:F:88:THR:O	1:F:89:ARG:HD2	2.17	0.44
1:G:203:LEU:HD12	1:G:236:GLY:HA2	2.00	0.44
1:C:137:ARG:NH2	1:C:238:ARG:CZ	2.81	0.44
1:H:210:LEU:HD22	1:H:214:TYR:CD1	2.52	0.44
1:C:9:LEU:C	1:C:9:LEU:HD23	2.43	0.43
1:E:196:LYS:NZ	1:E:245:ALA:HB1	2.33	0.43
1:E:158:LEU:HG	1:E:162:LEU:HD22	2.00	0.43
1:A:7:ALA:HB1	1:A:75:LEU:HD13	2.00	0.43
1:A:26:ALA:CB	1:A:49:VAL:HG22	2.49	0.43
1:C:138:VAL:HG13	1:C:142:ASN:HB3	2.00	0.43
1:E:239:THR:HG22	2:E:303:HOH:O	2.19	0.43
1:F:124:ARG:HH11	1:F:124:ARG:HB3	1.83	0.43
1:H:188:LYS:C	1:H:189:VAL:HG22	2.44	0.43
1:A:106:ARG:O	1:A:110:THR:HB	2.18	0.43
1:B:97:PRO:HB2	1:B:99:GLU:HG3	2.01	0.43
1:C:23:GLU:O	1:C:27:LYS:HG3	2.18	0.43
1:D:125:GLU:HG2	1:D:169:TRP:CZ3	2.53	0.43
1:C:77:ARG:NH1	1:C:79:ASP:OD1	2.52	0.43
1:C:175:THR:CG2	1:C:231:VAL:HG22	2.48	0.43
1:A:15:HIS:ND1	1:A:15:HIS:N	2.66	0.43
1:G:104:VAL:HG21	1:G:147:ASN:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:190:PRO:C	1:H:192:LYS:N	2.72	0.43
1:F:138:VAL:HG13	1:F:142:ASN:HB3	2.00	0.43
1:D:138:VAL:HG13	1:D:142:ASN:HB2	2.00	0.43
1:C:182:GLU:O	1:C:183:THR:C	2.61	0.43
1:H:84:TYR:O	1:H:85:ALA:C	2.61	0.43
1:A:59:ALA:HB2	1:A:107:VAL:HG22	2.01	0.42
1:D:123:MSE:HE1	1:D:131:ILE:CD1	2.49	0.42
1:D:133:LEU:O	1:D:175:THR:HA	2.19	0.42
1:E:138:VAL:O	1:E:138:VAL:HG12	2.17	0.42
1:H:172:ARG:HD3	1:H:225:SER:O	2.19	0.42
1:A:24:LEU:HD11	1:A:217:LEU:HD12	1.99	0.42
1:B:101:TRP:CZ3	1:B:147:ASN:HA	2.54	0.42
1:B:190:PRO:HG2	1:B:193:VAL:CB	2.49	0.42
1:C:104:VAL:HG21	1:C:147:ASN:CB	2.43	0.42
1:D:184:ARG:HG2	1:D:184:ARG:NH1	2.31	0.42
1:E:210:LEU:HD22	1:E:214:TYR:CD1	2.54	0.42
1:F:138:VAL:O	1:F:138:VAL:HG12	2.19	0.42
1:G:240:ILE:CD1	1:H:229:GLY:HA3	2.48	0.42
1:D:2:ARG:NH1	1:D:217:LEU:HD13	2.34	0.42
1:F:33:VAL:HG23	1:F:75:LEU:HD11	2.01	0.42
1:A:2:ARG:NH1	1:A:2:ARG:HG3	2.34	0.42
1:E:98:LEU:HD22	1:E:102:GLU:HG3	2.01	0.42
1:G:138:VAL:HG13	1:G:142:ASN:CB	2.50	0.42
1:C:230:GLN:HG3	2:D:257:HOH:O	2.19	0.42
1:G:49:VAL:O	1:G:49:VAL:HG13	2.19	0.42
1:B:127:ASN:HB2	1:B:128:PRO:HD2	2.01	0.42
1:D:98:LEU:O	1:D:102:GLU:HG3	2.19	0.42
1:H:195:GLU:HA	1:H:195:GLU:OE1	2.20	0.42
1:E:152:MSE:CE	1:E:152:MSE:HA	2.42	0.42
1:H:104:VAL:O	1:H:108:ASN:HB2	2.19	0.42
1:H:194:ARG:HH11	1:H:194:ARG:HG2	1.85	0.42
1:A:183:THR:C	1:A:185:MSE:H	2.28	0.42
1:B:86:GLY:HA2	1:B:108:ASN:OD1	2.20	0.41
1:F:161:THR:HG21	1:G:146:ALA:HA	2.02	0.41
1:F:194:ARG:NH1	1:F:198:ILE:CD1	2.83	0.41
1:G:123:MSE:HE2	1:G:131:ILE:HD11	2.02	0.41
1:A:105:LEU:HD23	1:A:151:SER:HB3	2.02	0.41
1:C:182:GLU:HA	1:C:182:GLU:OE1	2.20	0.41
1:F:158:LEU:HD12	1:F:162:LEU:HD13	2.02	0.41
1:F:190:PRO:HG2	1:F:193:VAL:CG2	2.49	0.41
1:E:88:THR:O	1:E:89:ARG:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:ARG:O	1:A:188:LYS:NZ	2.49	0.41
1:D:124:ARG:O	1:D:125:GLU:HB2	2.20	0.41
1:D:139:TYR:CE1	1:D:245:ALA:HB3	2.55	0.41
1:D:184:ARG:HG3	2:D:276:HOH:O	2.19	0.41
1:B:25:PHE:HE2	1:B:220:LEU:HD13	1.85	0.41
1:D:105:LEU:HD23	1:D:151:SER:HB3	2.03	0.41
1:H:175:THR:HG23	1:H:231:VAL:HA	2.03	0.41
1:C:105:LEU:HD23	1:C:151:SER:HB3	2.02	0.41
1:D:106:ARG:O	1:D:110:THR:HB	2.20	0.41
1:E:166:LEU:HD13	1:E:171:ILE:HG21	2.03	0.41
1:B:200:ALA:HB1	2:B:287:HOH:O	2.21	0.41
1:D:123:MSE:HE1	1:D:131:ILE:HG13	2.02	0.41
1:E:238:ARG:HE	1:E:243:ALA:HB2	1.85	0.41
1:F:162:LEU:HB3	1:F:173:VAL:HG21	2.02	0.41
1:G:94:TRP:CD1	1:G:95:LYS:HG3	2.56	0.41
1:G:138:VAL:O	1:G:138:VAL:CG1	2.68	0.41
1:B:38:GLU:O	1:B:42:LEU:HB2	2.21	0.41
1:D:238:ARG:HD3	1:D:238:ARG:C	2.46	0.41
1:E:135:ALA:CB	1:E:152:MSE:HE2	2.46	0.41
1:H:137:ARG:NH1	2:H:287:HOH:O	2.53	0.41
1:E:238:ARG:NH1	2:E:259:HOH:O	2.53	0.40
1:D:77:ARG:NH1	1:D:79:ASP:OD1	2.54	0.40
1:C:138:VAL:HG13	1:C:142:ASN:CB	2.52	0.40
1:D:98:LEU:HD22	1:D:102:GLU:HG3	2.03	0.40
1:E:166:LEU:HA	1:E:169:TRP:HD1	1.86	0.40
1:G:220:LEU:O	1:G:220:LEU:HD23	2.21	0.40
1:B:138:VAL:HG13	1:B:142:ASN:HB3	2.03	0.40
1:B:220:LEU:O	1:B:220:LEU:HD23	2.21	0.40
1:C:210:LEU:HD22	1:C:214:TYR:CD1	2.56	0.40
1:E:196:LYS:HZ2	1:E:245:ALA:HB1	1.86	0.40
1:F:60:ASP:HB3	1:F:63:SER:HB3	2.03	0.40

There are no symmetry-related clashes.

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	240/245 (98%)	229 (95%)	8 (3%)	3 (1%)	9	14
1	B	243/245 (99%)	233 (96%)	6 (2%)	4 (2%)	7	11
1	C	235/245 (96%)	223 (95%)	9 (4%)	3 (1%)	9	14
1	D	243/245 (99%)	230 (95%)	11 (4%)	2 (1%)	16	25
1	E	243/245 (99%)	230 (95%)	9 (4%)	4 (2%)	7	11
1	F	240/245 (98%)	225 (94%)	12 (5%)	3 (1%)	9	14
1	G	243/245 (99%)	231 (95%)	11 (4%)	1 (0%)	30	43
1	H	243/245 (99%)	226 (93%)	13 (5%)	4 (2%)	7	11
All	All	1930/1960 (98%)	1827 (95%)	79 (4%)	24 (1%)	10	16

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	GLY
1	A	85	ALA
1	A	91	ASN
1	B	244	PRO
1	C	16	GLY
1	C	91	ASN
1	E	16	GLY
1	E	85	ALA
1	F	16	GLY
1	F	85	ALA
1	G	91	ASN
1	H	16	GLY
1	H	91	ASN
1	H	189	VAL
1	B	85	ALA
1	C	85	ALA
1	D	91	ASN
1	F	91	ASN
1	B	16	GLY
1	E	91	ASN
1	H	188	LYS
1	B	91	ASN
1	D	16	GLY
1	E	244	PRO

5.3.2 Protein sidechains

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	180/175 (103%)	165 (92%)	15 (8%)	10	17
1	B	181/175 (103%)	167 (92%)	14 (8%)	12	20
1	C	176/175 (101%)	163 (93%)	13 (7%)	13	22
1	D	181/175 (103%)	168 (93%)	13 (7%)	13	23
1	E	181/175 (103%)	167 (92%)	14 (8%)	12	20
1	F	180/175 (103%)	167 (93%)	13 (7%)	13	23
1	G	181/175 (103%)	168 (93%)	13 (7%)	13	23
1	H	181/175 (103%)	165 (91%)	16 (9%)	9	15
All	All	1441/1400 (103%)	1330 (92%)	111 (8%)	12	20

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	15	HIS
1	A	22	LEU
1	A	24	LEU
1	A	42	LEU
1	A	49	VAL
1	A	78	LEU
1	A	94	TRP
1	A	98	LEU
1	A	99	GLU
1	A	137	ARG
1	A	139	TYR
1	A	162	LEU
1	A	210	LEU
1	A	217	LEU
1	B	15	HIS
1	B	22	LEU
1	B	24	LEU
1	B	42	LEU

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Mol	Chain	Res	Type
1	B	49	VAL
1	B	78	LEU
1	B	98	LEU
1	B	99	GLU
1	B	124	ARG
1	B	137	ARG
1	B	139	TYR
1	B	210	LEU
1	B	217	LEU
1	B	239	THR
1	C	24	LEU
1	C	42	LEU
1	C	49	VAL
1	C	77	ARG
1	C	78	LEU
1	C	98	LEU
1	C	99	GLU
1	C	137	ARG
1	C	162	LEU
1	C	210	LEU
1	C	217	LEU
1	C	238	ARG
1	C	239	THR
1	D	2	ARG
1	D	24	LEU
1	D	42	LEU
1	D	49	VAL
1	D	98	LEU
1	D	99	GLU
1	D	126	LYS
1	D	137	ARG
1	D	139	TYR
1	D	162	LEU
1	D	185	MSE
1	D	210	LEU
1	D	217	LEU
1	E	15	HIS
1	E	22	LEU
1	E	24	LEU
1	E	42	LEU
1	E	49	VAL
1	E	78	LEU

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Mol	Chain	Res	Type
1	E	98	LEU
1	E	104	VAL
1	E	124	ARG
1	E	137	ARG
1	E	139	TYR
1	E	162	LEU
1	E	210	LEU
1	E	217	LEU
1	F	15	HIS
1	F	22	LEU
1	F	24	LEU
1	F	42	LEU
1	F	49	VAL
1	F	78	LEU
1	F	94	TRP
1	F	98	LEU
1	F	99	GLU
1	F	137	ARG
1	F	210	LEU
1	F	217	LEU
1	F	239	THR
1	G	24	LEU
1	G	42	LEU
1	G	49	VAL
1	G	98	LEU
1	G	104	VAL
1	G	137	ARG
1	G	139	TYR
1	G	162	LEU
1	G	182	GLU
1	G	210	LEU
1	G	217	LEU
1	G	238	ARG
1	G	239	THR
1	H	2	ARG
1	H	24	LEU
1	H	42	LEU
1	H	44	GLU
1	H	49	VAL
1	H	77	ARG
1	H	78	LEU
1	H	98	LEU

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Mol	Chain	Res	Type
1	H	99	GLU
1	H	137	ARG
1	H	162	LEU
1	H	195	GLU
1	H	210	LEU
1	H	217	LEU
1	H	238	ARG
1	H	239	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	HIS
1	A	74	HIS
1	B	52	HIS
1	C	52	HIS
1	C	74	HIS
1	D	52	HIS
1	D	91	ASN
1	D	230	GLN
1	E	52	HIS
1	E	74	HIS
1	F	52	HIS
1	F	74	HIS
1	G	74	HIS
1	G	230	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	236/245 (96%)	-1.66	0 100 100	10, 20, 45, 74	0
1	B	239/245 (97%)	-1.67	0 100 100	11, 20, 40, 71	0
1	C	234/245 (95%)	-1.66	0 100 100	10, 19, 39, 94	0
1	D	239/245 (97%)	-1.70	0 100 100	9, 19, 35, 53	0
1	E	239/245 (97%)	-1.68	0 100 100	10, 20, 43, 56	0
1	F	236/245 (96%)	-1.67	0 100 100	8, 21, 40, 52	0
1	G	239/245 (97%)	-1.69	0 100 100	5, 19, 35, 48	0
1	H	239/245 (97%)	-1.66	0 100 100	8, 20, 58, 88	0
All	All	1901/1960 (96%)	-1.67	0 100 100	5, 20, 40, 94	0

There are no RSRZ outliers to report.

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 oligosaccharides 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.