



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:44 AM GMT

PDB ID : 2E67  
Title : Crystal structure of the hypothetical protein TTHB029 from *Thermus thermophilus* HB8  
Authors : Imagawa, T.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2006-12-26  
Resolution : 2.90 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

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

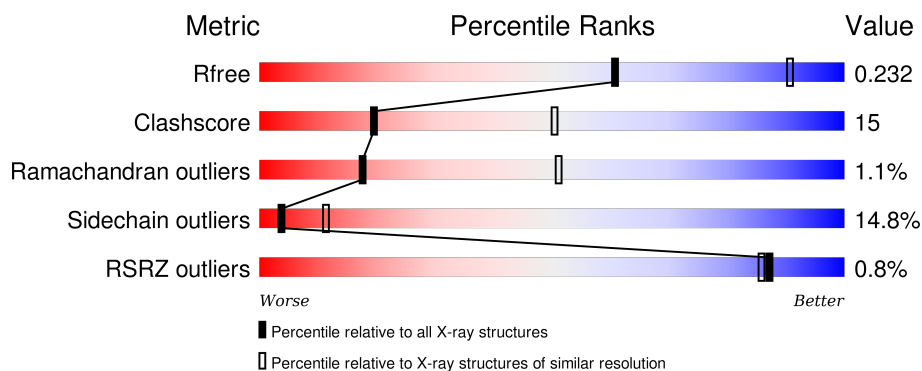
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	264	<div> <div>71%</div> <div>23%</div> <div>5%</div> </div>
1	B	264	<div> <div>61%</div> <div>31%</div> <div>6%</div> </div>
1	C	264	<div> <div>2%</div> <div>54%</div> <div>39%</div> <div>6%</div> </div>
1	D	264	<div> <div>67%</div> <div>27%</div> <div>5%</div> </div>
1	E	264	<div> <div>%</div> <div>72%</div> <div>22%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	264	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	D	304	-	-	-	X
2	MG	E	305	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12678 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 Hypothetical protein TTHB029.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			2090	1352	364	372	2			
1	B	263	Total	C	N	O	S	0	0	0
			2090	1352	364	372	2			
1	C	263	Total	C	N	O	S	0	0	0
			2090	1352	364	372	2			
1	D	263	Total	C	N	O	S	0	0	0
			2090	1352	364	372	2			
1	E	263	Total	C	N	O	S	0	0	0
			2090	1352	364	372	2			
1	F	263	Total	C	N	O	S	0	0	0
			2090	1352	364	372	2			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Mg	0	0
			1	1		
2	E	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	F	1	Total	Mg	0	0
			1	1		

- Molecule 3 is water.

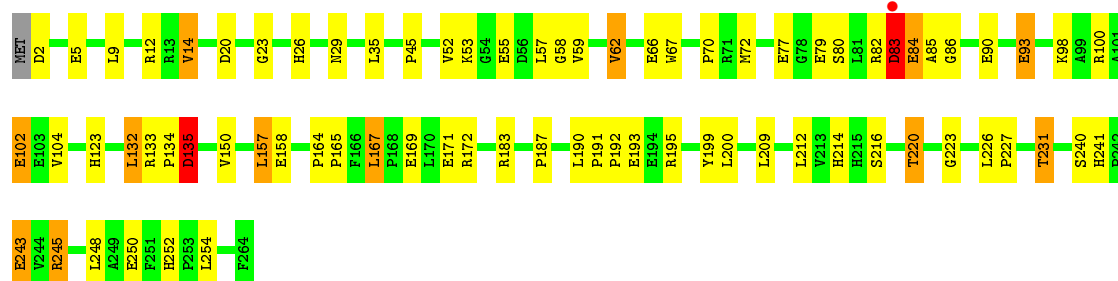
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	25	Total 25	O 25	0	0
3	B	29	Total 29	O 29	0	0
3	C	16	Total 16	O 16	0	0
3	D	26	Total 26	O 26	0	0
3	E	15	Total 15	O 15	0	0
3	F	21	Total 21	O 21	0	0

### 3 Residue-property plots

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

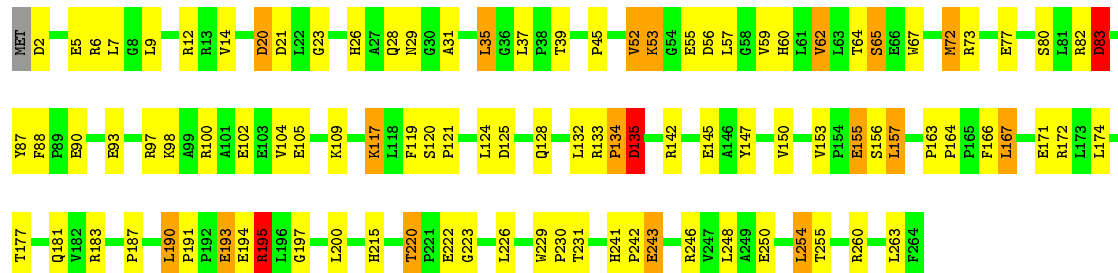
#### • Molecule 1: Hypothetical protein TTHB029

Chain A: 



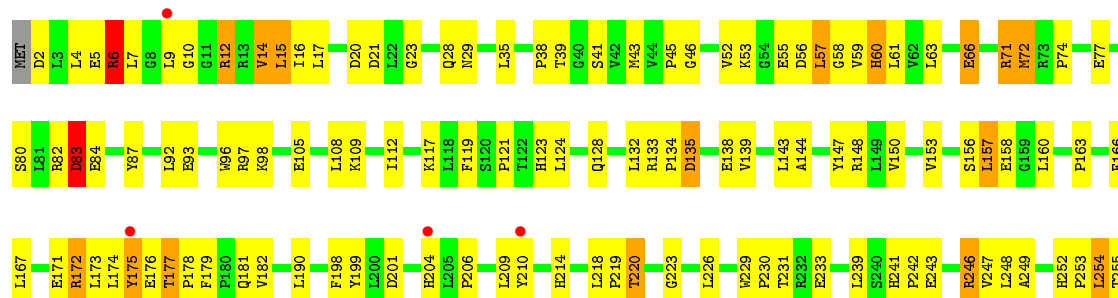
#### • Molecule 1: Hypothetical protein TTHB029

Chain B: 



#### • Molecule 1: Hypothetical protein TTHB029

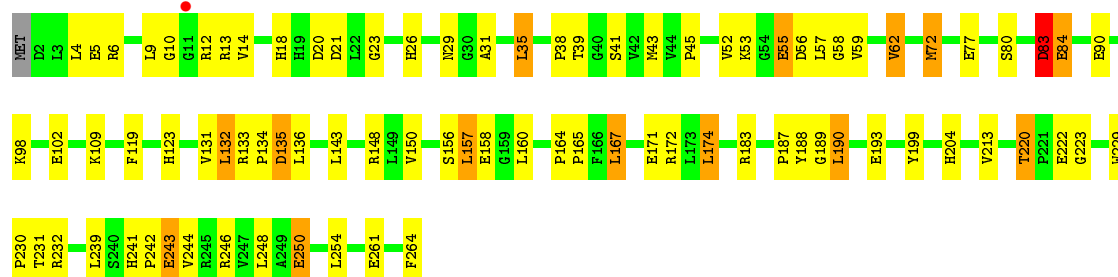
Chain C: 





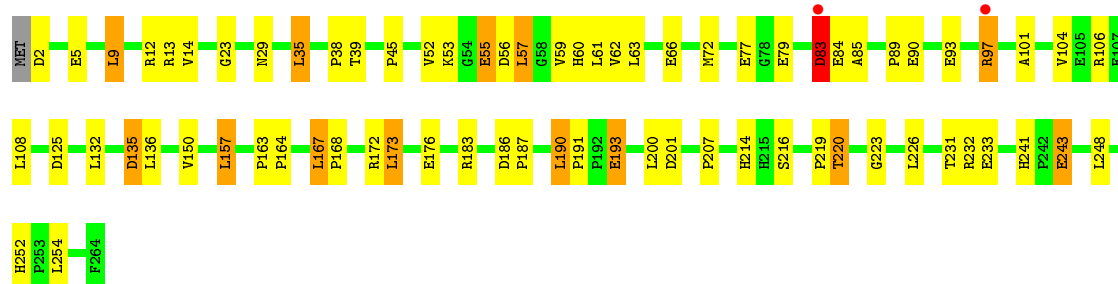
• Molecule 1: Hypothetical protein TTHB029

Chain D: 67% 27% 5%



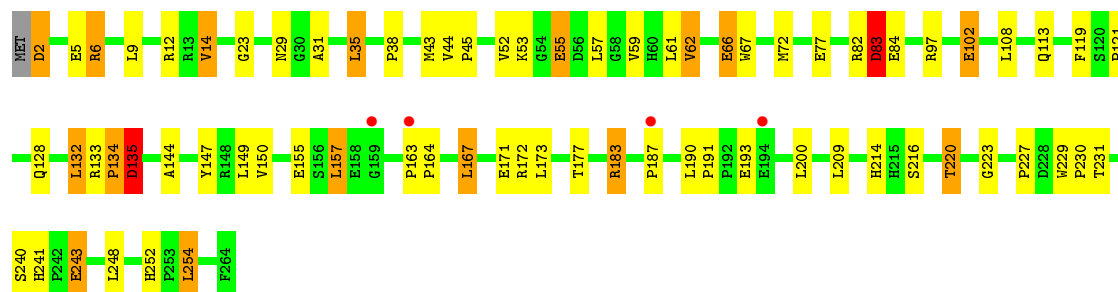
• Molecule 1: Hypothetical protein TTHB029

Chain E: 72% 22% 5%



• Molecule 1: Hypothetical protein TTHB029

Chain F: 72% 21% 6%



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	202.01Å 202.01Å 345.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.90 48.05 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.90) 100.0 (48.05-2.90)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.21 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.219 , 0.259 0.192 , 0.232	Depositor DCC
$R_{free}$ test set	3027 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.7	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 43.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 60144 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12678	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.92	1/2156 (0.0%)	0.93	3/2948 (0.1%)
1	B	0.87	0/2156	0.92	3/2948 (0.1%)
1	C	0.88	1/2156 (0.0%)	0.93	2/2948 (0.1%)
1	D	0.87	3/2156 (0.1%)	0.89	4/2948 (0.1%)
1	E	0.78	1/2156 (0.0%)	0.88	4/2948 (0.1%)
1	F	0.77	0/2156	0.84	2/2948 (0.1%)
All	All	0.85	6/12936 (0.0%)	0.90	18/17688 (0.1%)

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	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	1
1	F	0	2
All	All	0	11

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	83	ASP	CB-CG	6.87	1.66	1.51
1	D	83	ASP	CB-CG	6.64	1.65	1.51
1	D	55	GLU	CG-CD	5.67	1.60	1.51
1	C	138	GLU	CG-CD	5.60	1.60	1.51
1	E	55	GLU	CG-CD	5.33	1.59	1.51
1	D	261	GLU	CG-CD	5.00	1.59	1.51

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	263	LEU	CA-CB-CG	7.36	132.22	115.30
1	A	245	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	A	135	ASP	N-CA-CB	-5.80	100.16	110.60
1	E	57	LEU	CB-CG-CD1	5.73	120.73	111.00
1	C	71	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	E	35	LEU	CA-CB-CG	5.70	128.41	115.30
1	A	183	ARG	CG-CD-NE	5.63	123.61	111.80
1	B	135	ASP	N-CA-CB	-5.62	100.48	110.60
1	D	232	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	D	21	ASP	CB-CG-OD2	5.27	123.04	118.30
1	B	263	LEU	CA-CB-CG	5.26	127.41	115.30
1	E	232	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	D	174	LEU	CA-CB-CG	5.17	127.18	115.30
1	F	135	ASP	N-CA-CB	-5.14	101.36	110.60
1	F	254	LEU	CA-CB-CG	5.14	127.11	115.30
1	B	72	MET	CG-SD-CE	-5.07	92.09	100.20
1	E	9	LEU	CA-CB-CG	5.06	126.93	115.30
1	D	12	ARG	NE-CZ-NH2	5.01	122.80	120.30

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	134	PRO	Peptide
1	A	83	ASP	Peptide
1	B	134	PRO	Peptide
1	B	83	ASP	Peptide
1	C	134	PRO	Peptide
1	C	83	ASP	Peptide
1	D	134	PRO	Peptide
1	D	83	ASP	Peptide
1	E	83	ASP	Peptide
1	F	134	PRO	Peptide
1	F	83	ASP	Peptide

## 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	2090	0	2067	54	1
1	B	2090	0	2067	75	0
1	C	2090	0	2067	87	0
1	D	2090	0	2067	64	0
1	E	2090	0	2067	49	0
1	F	2090	0	2067	55	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	25	0	0	6	0
3	B	29	0	0	9	0
3	C	16	0	0	7	0
3	D	26	0	0	13	1
3	E	15	0	0	6	0
3	F	21	0	0	7	0
All	All	12678	0	12402	374	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 15.

All (374) 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:84:GLU:HA	3:A:325:HOH:O	1.11	1.26
1:C:84:GLU:HA	3:C:318:HOH:O	1.34	1.25
3:B:330:HOH:O	1:C:178:PRO:HD3	1.32	1.23
1:F:84:GLU:HA	3:F:327:HOH:O	1.45	1.16
1:B:220:THR:HG22	1:B:223:GLY:H	1.02	1.14
1:D:188:TYR:HA	3:D:328:HOH:O	1.48	1.10
1:A:220:THR:HG22	1:A:223:GLY:H	1.03	1.07
1:C:220:THR:HG22	1:C:223:GLY:H	1.13	1.06
1:D:220:THR:HG21	3:D:314:HOH:O	1.56	1.04
1:E:220:THR:HG22	1:E:223:GLY:H	1.24	1.02
1:F:23:GLY:H	1:F:29:ASN:HD21	1.00	1.00
1:F:220:THR:HG22	1:F:223:GLY:H	1.25	0.99
1:E:157:LEU:H	1:E:157:LEU:HD23	1.20	0.98
1:B:117:LYS:HD2	1:C:175:TYR:O	1.66	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:84:GLU:HA	3:D:326:HOH:O	1.66	0.95
1:A:93:GLU:HB2	3:A:314:HOH:O	1.68	0.94
1:B:97:ARG:HD3	3:B:314:HOH:O	1.66	0.94
1:C:10:GLY:HA2	3:C:319:HOH:O	1.66	0.93
1:E:23:GLY:H	1:E:29:ASN:HD21	1.16	0.93
1:B:220:THR:HG22	1:B:223:GLY:N	1.85	0.91
1:B:67:TRP:HH2	3:B:331:HOH:O	1.54	0.89
1:E:157:LEU:H	1:E:157:LEU:CD2	1.86	0.88
1:E:220:THR:HG21	3:E:309:HOH:O	1.73	0.88
1:A:220:THR:HG22	1:A:223:GLY:N	1.88	0.87
1:D:220:THR:HG22	1:D:223:GLY:H	1.36	0.87
1:C:43:MET:HB3	1:C:72:MET:HE1	1.57	0.86
1:C:220:THR:HG21	3:C:304:HOH:O	1.75	0.86
1:B:83:ASP:O	3:B:329:HOH:O	1.93	0.86
1:F:119:PHE:O	1:F:121:PRO:HD3	1.77	0.85
1:A:23:GLY:H	1:A:29:ASN:HD21	1.21	0.84
1:D:84:GLU:CA	3:D:326:HOH:O	2.23	0.84
1:F:23:GLY:H	1:F:29:ASN:ND2	1.76	0.84
1:A:157:LEU:CD2	1:A:157:LEU:H	1.91	0.83
1:C:23:GLY:H	1:C:29:ASN:HD21	1.24	0.83
1:E:191:PRO:HB2	1:E:193:GLU:OE1	1.77	0.82
1:C:241:HIS:HD2	1:C:242:PRO:HD2	1.45	0.82
1:A:220:THR:CG2	1:A:223:GLY:H	1.91	0.81
1:C:220:THR:HG22	1:C:223:GLY:N	1.93	0.81
1:F:23:GLY:N	1:F:29:ASN:HD21	1.81	0.79
1:B:23:GLY:H	1:B:29:ASN:HD21	1.30	0.78
1:B:83:ASP:OD2	3:B:304:HOH:O	2.02	0.77
1:A:200:LEU:HD21	1:A:243:GLU:HB3	1.65	0.77
1:B:157:LEU:H	1:B:157:LEU:HD23	1.50	0.76
1:E:157:LEU:CD2	1:E:157:LEU:N	2.48	0.76
1:D:83:ASP:O	3:D:321:HOH:O	2.03	0.75
1:A:220:THR:HG21	3:A:302:HOH:O	1.87	0.74
1:E:62:VAL:HG11	1:E:72:MET:HE1	1.69	0.74
1:D:23:GLY:H	1:D:29:ASN:HD21	1.32	0.74
1:C:4:LEU:HD22	1:C:14:VAL:HG11	1.70	0.73
1:B:77:GLU:HA	1:B:82:ARG:NH2	2.03	0.73
1:C:43:MET:HB3	1:C:72:MET:CE	2.18	0.73
1:A:157:LEU:H	1:A:157:LEU:HD23	1.54	0.73
1:A:26:HIS:ND1	3:A:311:HOH:O	2.22	0.72
1:B:193:GLU:H	1:B:193:GLU:CD	1.92	0.72
1:F:241:HIS:HD2	1:F:243:GLU:H	1.36	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:45:PRO:HB2	1:F:72:MET:HE2	1.72	0.72
1:C:241:HIS:CD2	1:C:242:PRO:HD2	2.26	0.71
1:E:241:HIS:HD2	1:E:243:GLU:HB2	1.56	0.70
1:F:220:THR:HG21	3:F:308:HOH:O	1.90	0.70
1:F:220:THR:HG22	1:F:223:GLY:N	2.04	0.70
1:C:220:THR:CG2	1:C:223:GLY:H	1.97	0.69
1:A:157:LEU:CD2	1:A:157:LEU:N	2.55	0.69
1:C:153:VAL:HG12	1:C:181:GLN:HG2	1.75	0.69
1:D:5:GLU:HA	1:D:5:GLU:OE2	1.93	0.69
1:A:67:TRP:CD1	1:A:227:PRO:HD2	2.28	0.68
1:E:23:GLY:N	1:E:29:ASN:HD21	1.91	0.68
1:F:84:GLU:CA	3:F:327:HOH:O	2.16	0.68
1:D:220:THR:HG22	1:D:223:GLY:N	2.09	0.68
1:A:133:ARG:NH1	1:A:135:ASP:OD1	2.26	0.68
1:A:12:ARG:NH1	1:A:252:HIS:HB2	2.09	0.68
1:B:60:HIS:HA	1:B:125:ASP:OD2	1.93	0.67
1:F:66:GLU:HG2	1:F:128:GLN:HE22	1.58	0.67
1:E:241:HIS:CD2	1:E:243:GLU:HB2	2.30	0.66
1:A:187:PRO:HA	1:A:190:LEU:HD23	1.78	0.66
1:A:23:GLY:H	1:A:29:ASN:ND2	1.94	0.65
1:C:109:LYS:HG2	1:C:147:TYR:OH	1.95	0.65
1:C:219:PRO:HA	1:C:233:GLU:OE1	1.97	0.64
1:B:142:ARG:O	1:B:145:GLU:HB3	1.98	0.64
1:D:62:VAL:HG11	1:D:72:MET:HE1	1.78	0.63
1:A:70:PRO:HD2	1:A:226:LEU:HD11	1.79	0.63
1:B:174:LEU:HD21	1:B:181:GLN:OE1	1.99	0.63
1:C:5:GLU:OE2	1:C:5:GLU:HA	1.98	0.63
1:B:191:PRO:HB2	1:B:193:GLU:OE1	1.99	0.62
1:D:241:HIS:HD2	1:D:242:PRO:HD2	1.64	0.62
1:F:55:GLU:CD	1:F:55:GLU:H	2.00	0.62
1:E:23:GLY:H	1:E:29:ASN:ND2	1.93	0.62
1:F:157:LEU:N	1:F:157:LEU:HD23	2.15	0.62
1:F:193:GLU:CD	1:F:193:GLU:H	2.02	0.62
1:F:157:LEU:H	1:F:157:LEU:HD23	1.64	0.62
1:D:43:MET:HB3	1:D:72:MET:CE	2.29	0.62
1:F:77:GLU:HA	1:F:82:ARG:NH2	2.15	0.62
1:A:102:GLU:CD	1:A:102:GLU:H	2.03	0.61
1:D:45:PRO:HB2	1:D:72:MET:HG2	1.82	0.61
1:B:62:VAL:HG11	1:B:72:MET:HE1	1.82	0.61
1:D:189:GLY:N	3:D:328:HOH:O	2.31	0.61
1:B:157:LEU:H	1:B:157:LEU:CD2	2.13	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:MET:HB3	1:D:72:MET:HE1	1.82	0.61
1:D:55:GLU:HG3	3:D:320:HOH:O	1.99	0.61
1:A:241:HIS:HD2	1:A:243:GLU:H	1.49	0.60
1:F:43:MET:HB3	1:F:72:MET:HE1	1.81	0.60
1:E:193:GLU:CD	1:E:193:GLU:H	2.05	0.60
1:E:200:LEU:HD21	1:E:243:GLU:HB3	1.84	0.60
1:F:157:LEU:CD2	1:F:157:LEU:N	2.65	0.60
1:F:62:VAL:HG11	1:F:72:MET:HE1	1.84	0.59
1:A:62:VAL:HG11	1:A:72:MET:HE1	1.83	0.59
1:B:2:ASP:O	1:B:5:GLU:HB2	2.03	0.59
1:D:220:THR:CG2	1:D:223:GLY:H	2.14	0.59
1:C:46:GLY:N	1:C:72:MET:HE2	2.16	0.59
1:A:45:PRO:HB2	1:A:72:MET:CE	2.33	0.58
1:C:23:GLY:H	1:C:29:ASN:ND2	2.00	0.58
1:B:98:LYS:HD3	3:B:304:HOH:O	2.02	0.58
1:D:10:GLY:N	3:D:322:HOH:O	2.36	0.58
1:F:220:THR:CG2	1:F:223:GLY:H	2.09	0.58
1:C:241:HIS:HD2	1:C:242:PRO:CD	2.16	0.58
1:A:26:HIS:CE1	3:A:311:HOH:O	2.56	0.58
1:C:61:LEU:HD22	1:C:108:LEU:HD22	1.86	0.58
1:E:61:LEU:HD13	1:E:108:LEU:HD13	1.86	0.58
1:B:157:LEU:CD2	1:B:157:LEU:N	2.67	0.58
1:B:93:GLU:HG2	1:B:97:ARG:HH11	1.68	0.58
1:B:191:PRO:HG2	1:B:194:GLU:OE1	2.04	0.58
1:C:12:ARG:NH2	1:C:12:ARG:HB3	2.19	0.58
1:E:191:PRO:CB	1:E:193:GLU:OE1	2.50	0.57
1:F:200:LEU:HD21	1:F:243:GLU:HB3	1.86	0.57
1:B:97:ARG:CD	3:B:314:HOH:O	2.37	0.57
1:E:214:HIS:HD2	1:E:216:SER:OG	1.88	0.57
1:B:195:ARG:HH21	1:B:195:ARG:HB2	1.70	0.57
1:D:43:MET:HE1	1:D:72:MET:SD	2.45	0.56
1:D:133:ARG:NH1	1:D:135:ASP:OD1	2.38	0.56
1:C:66:GLU:HG2	1:C:128:GLN:NE2	2.20	0.56
1:C:41:SER:HB2	1:C:60:HIS:N	2.20	0.56
1:F:187:PRO:HA	1:F:190:LEU:HD23	1.88	0.56
1:C:43:MET:HE1	1:C:72:MET:SD	2.46	0.56
1:C:2:ASP:O	1:C:5:GLU:HB2	2.05	0.56
1:C:71:ARG:HB2	1:C:87:TYR:CE1	2.41	0.56
1:C:15:LEU:HD12	1:C:16:ILE:N	2.20	0.56
1:D:187:PRO:HA	1:D:190:LEU:HD23	1.86	0.56
1:B:133:ARG:NH1	1:B:135:ASP:OD2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:ASP:C	3:D:326:HOH:O	2.45	0.55
1:F:102:GLU:H	1:F:102:GLU:CD	2.10	0.55
1:D:83:ASP:N	3:D:326:HOH:O	2.38	0.55
1:C:43:MET:CB	1:C:72:MET:CE	2.83	0.55
1:B:23:GLY:H	1:B:29:ASN:ND2	2.01	0.55
1:F:214:HIS:HD2	1:F:216:SER:OG	1.90	0.55
1:C:229:TRP:N	1:C:230:PRO:CD	2.70	0.55
1:F:66:GLU:HG2	1:F:128:GLN:NE2	2.21	0.55
1:A:191:PRO:HB2	1:A:193:GLU:OE1	2.06	0.55
1:C:5:GLU:C	1:C:7:LEU:H	2.10	0.55
1:A:45:PRO:HB2	1:A:72:MET:HE2	1.89	0.55
1:C:119:PHE:O	1:C:121:PRO:HD3	2.07	0.55
1:D:58:GLY:HA3	1:D:123:HIS:CE1	2.42	0.55
1:B:241:HIS:CD2	1:B:242:PRO:HD2	2.41	0.54
1:A:23:GLY:N	1:A:29:ASN:HD21	1.97	0.54
1:C:45:PRO:HB2	1:C:72:MET:HG2	1.90	0.54
1:B:102:GLU:H	1:B:102:GLU:CD	2.11	0.54
1:D:80:SER:HB2	1:D:98:LYS:O	2.07	0.54
1:C:157:LEU:H	1:C:157:LEU:CD2	2.21	0.54
1:C:77:GLU:HG2	1:E:77:GLU:CG	2.38	0.54
1:B:220:THR:HG21	3:B:306:HOH:O	2.08	0.53
1:C:108:LEU:O	1:C:112:ILE:HG13	2.08	0.53
1:F:2:ASP:O	1:F:5:GLU:HB2	2.08	0.53
1:D:119:PHE:HB2	3:D:323:HOH:O	2.08	0.53
1:F:191:PRO:HB2	1:F:193:GLU:OE1	2.08	0.53
1:D:83:ASP:CA	3:D:326:HOH:O	2.55	0.53
1:A:2:ASP:O	1:A:5:GLU:HB2	2.07	0.53
1:D:43:MET:CB	1:D:72:MET:HE3	2.38	0.53
1:F:113:GLN:NE2	1:F:147:TYR:OH	2.42	0.53
1:A:214:HIS:HD2	1:A:216:SER:OG	1.92	0.53
1:C:84:GLU:CA	3:C:318:HOH:O	2.14	0.53
1:E:220:THR:HG22	1:E:223:GLY:N	2.08	0.53
1:A:157:LEU:H	1:A:157:LEU:HD22	1.70	0.52
1:A:157:LEU:N	1:A:157:LEU:HD22	2.23	0.52
1:E:101:ALA:HB2	1:E:135:ASP:OD2	2.10	0.52
1:D:31:ALA:O	1:D:35:LEU:HB2	2.09	0.52
1:A:80:SER:HA	1:A:98:LYS:HE2	1.90	0.52
1:B:254:LEU:HD22	1:B:255:THR:O	2.08	0.52
1:F:214:HIS:HE1	3:F:320:HOH:O	1.92	0.52
1:F:83:ASP:CA	3:F:327:HOH:O	2.56	0.52
1:D:157:LEU:HD13	1:D:174:LEU:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:164:PRO:HA	1:E:167:LEU:HD23	1.91	0.52
1:D:13:ARG:NH1	1:D:250:GLU:O	2.43	0.52
1:C:61:LEU:HD11	1:C:124:LEU:HG	1.90	0.52
1:E:83:ASP:O	1:E:85:ALA:N	2.43	0.51
1:B:23:GLY:N	1:B:29:ASN:HD21	2.05	0.51
1:A:193:GLU:CD	1:A:193:GLU:H	2.13	0.51
1:D:220:THR:HG23	3:F:307:HOH:O	2.10	0.51
1:F:241:HIS:CD2	1:F:243:GLU:HB2	2.45	0.51
1:A:55:GLU:N	1:A:55:GLU:OE2	2.30	0.51
1:C:12:ARG:HB3	1:C:12:ARG:HH21	1.74	0.51
1:C:39:THR:HA	1:C:56:ASP:O	2.10	0.51
1:B:55:GLU:N	1:B:55:GLU:OE2	2.33	0.51
1:B:155:GLU:OE1	1:B:183:ARG:HG3	2.10	0.51
1:C:117:LYS:HG2	1:E:85:ALA:HA	1.93	0.51
1:C:38:PRO:HB3	1:C:55:GLU:HG2	1.92	0.50
1:B:67:TRP:CH2	3:B:331:HOH:O	2.41	0.50
1:D:241:HIS:CD2	1:D:242:PRO:HD2	2.45	0.50
1:E:63:LEU:O	1:E:89:PRO:HD2	2.12	0.50
1:C:14:VAL:HG22	1:C:209:LEU:CD1	2.42	0.50
1:D:23:GLY:H	1:D:29:ASN:ND2	2.06	0.50
1:D:193:GLU:CD	1:D:193:GLU:H	2.15	0.50
1:C:214:HIS:HE1	3:C:315:HOH:O	1.94	0.50
1:C:58:GLY:HA3	1:C:123:HIS:CD2	2.47	0.50
1:D:220:THR:CG2	3:D:314:HOH:O	2.31	0.50
1:F:144:ALA:HB1	1:F:149:LEU:O	2.12	0.49
1:B:7:LEU:HB3	1:B:9:LEU:HD23	1.93	0.49
1:E:93:GLU:HG2	1:E:97:ARG:HH11	1.77	0.49
1:B:187:PRO:HA	1:B:190:LEU:HD23	1.94	0.49
1:B:187:PRO:HB2	1:B:195:ARG:HE	1.77	0.49
1:A:14:VAL:HG22	1:A:209:LEU:HD13	1.94	0.49
1:B:220:THR:CG2	1:B:223:GLY:H	1.96	0.49
1:A:58:GLY:HA3	1:A:123:HIS:CE1	2.47	0.49
1:B:164:PRO:HA	1:B:167:LEU:HD23	1.94	0.49
1:D:43:MET:HB2	1:D:72:MET:HE3	1.93	0.49
1:B:200:LEU:HD21	1:B:243:GLU:HB3	1.94	0.49
1:B:117:LYS:CD	1:C:175:TYR:O	2.50	0.49
1:D:23:GLY:N	1:D:29:ASN:HD21	2.06	0.49
1:D:109:LYS:HG3	1:D:143:LEU:HD21	1.95	0.48
1:C:105:GLU:HG3	1:C:139:VAL:HG13	1.95	0.48
1:D:55:GLU:H	1:D:55:GLU:CD	2.17	0.48
1:A:199:TYR:CE2	1:A:212:LEU:HD21	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:164:PRO:N	1:D:165:PRO:HD2	2.29	0.48
1:C:4:LEU:HB2	3:C:319:HOH:O	2.13	0.48
1:F:44:VAL:N	1:F:45:PRO:CD	2.76	0.48
1:C:74:PRO:HD2	1:C:82:ARG:HH12	1.78	0.48
1:C:43:MET:CB	1:C:72:MET:HE3	2.44	0.48
1:D:80:SER:HA	1:D:98:LYS:HE2	1.96	0.48
1:E:226:LEU:HD12	1:E:226:LEU:N	2.28	0.47
1:A:77:GLU:OE2	1:B:77:GLU:HG2	2.14	0.47
1:D:164:PRO:HA	1:D:167:LEU:HD23	1.96	0.47
1:F:164:PRO:HA	1:F:167:LEU:HD22	1.95	0.47
1:C:66:GLU:HG2	1:C:128:GLN:HE22	1.77	0.47
1:D:148:ARG:HA	1:D:264:PHE:CE1	2.50	0.47
1:B:124:LEU:HA	1:B:124:LEU:HD12	1.56	0.47
1:F:67:TRP:CD1	1:F:227:PRO:HD2	2.50	0.47
1:E:214:HIS:HE1	3:E:312:HOH:O	1.97	0.47
1:B:241:HIS:HD2	1:B:243:GLU:H	1.60	0.47
1:F:2:ASP:O	1:F:6:ARG:HG2	2.15	0.47
1:B:64:THR:OG1	1:B:128:GLN:NE2	2.48	0.47
1:B:100:ARG:O	1:B:104:VAL:HG23	2.15	0.47
1:C:220:THR:HG23	3:E:306:HOH:O	2.14	0.47
1:D:84:GLU:H	1:D:84:GLU:CD	2.17	0.47
1:C:4:LEU:HD21	1:C:209:LEU:HB2	1.97	0.47
1:F:133:ARG:NH1	1:F:135:ASP:OD1	2.47	0.47
1:E:60:HIS:ND1	1:E:125:ASP:OD2	2.38	0.47
1:B:157:LEU:HD23	1:B:157:LEU:N	2.24	0.46
1:D:241:HIS:HD2	1:D:242:PRO:CD	2.28	0.46
1:E:187:PRO:HA	1:E:190:LEU:HD23	1.96	0.46
1:C:83:ASP:N	3:C:318:HOH:O	2.49	0.46
1:A:167:LEU:HA	1:A:167:LEU:HD13	1.73	0.46
1:B:105:GLU:CD	1:B:142:ARG:HH22	2.19	0.46
1:C:148:ARG:HG2	1:C:264:PHE:CD1	2.51	0.46
1:C:198:PHE:CD2	1:C:198:PHE:C	2.88	0.46
1:B:80:SER:HA	1:B:98:LYS:HE2	1.98	0.46
1:E:219:PRO:HB3	1:E:233:GLU:CD	2.36	0.46
1:C:80:SER:HA	1:C:98:LYS:HE2	1.96	0.46
1:E:106:ARG:NE	3:E:316:HOH:O	2.31	0.45
1:D:77:GLU:HG2	1:F:77:GLU:OE2	2.16	0.45
1:A:85:ALA:HB1	3:A:326:HOH:O	2.15	0.45
1:E:173:LEU:HA	1:E:176:GLU:HB2	1.98	0.45
1:F:83:ASP:C	3:F:327:HOH:O	2.55	0.45
1:D:38:PRO:HB3	1:D:55:GLU:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:GLU:HG2	1:E:77:GLU:HG2	1.98	0.45
1:C:254:LEU:HD22	1:C:255:THR:O	2.16	0.45
1:A:164:PRO:HA	1:A:167:LEU:HD23	1.99	0.45
1:F:61:LEU:HD13	1:F:108:LEU:HD13	1.99	0.45
1:D:102:GLU:H	1:D:102:GLU:CD	2.20	0.45
1:C:29:ASN:HD22	1:C:29:ASN:N	2.13	0.45
1:F:14:VAL:HG22	1:F:209:LEU:HD12	1.99	0.45
1:C:43:MET:HB2	1:C:72:MET:HE3	1.99	0.45
1:B:153:VAL:O	1:B:181:GLN:HA	2.16	0.45
1:D:199:TYR:CE2	1:D:239:LEU:HD21	2.51	0.45
1:E:12:ARG:NH1	1:E:252:HIS:HB2	2.32	0.45
1:B:45:PRO:HD2	1:B:72:MET:CE	2.47	0.45
1:E:2:ASP:HA	1:E:5:GLU:HB2	1.99	0.45
1:D:4:LEU:HB3	1:D:10:GLY:HA2	1.99	0.45
1:D:157:LEU:H	1:D:157:LEU:HD22	1.82	0.45
1:A:132:LEU:HD12	1:A:132:LEU:HA	1.84	0.45
1:B:119:PHE:O	1:B:121:PRO:HD3	2.16	0.45
1:C:92:LEU:HD22	1:C:96:TRP:CZ2	2.52	0.44
1:B:39:THR:HA	1:B:56:ASP:O	2.16	0.44
1:A:169:GLU:N	1:A:169:GLU:OE2	2.47	0.44
1:C:77:GLU:OE2	1:E:77:GLU:HG3	2.16	0.44
1:C:177:THR:HG23	1:C:179:PHE:H	1.82	0.44
1:C:77:GLU:HG2	1:E:77:GLU:OE2	2.17	0.44
1:C:5:GLU:O	1:C:7:LEU:N	2.51	0.44
1:E:187:PRO:HA	1:E:190:LEU:CD2	2.48	0.44
1:D:135:ASP:HB3	1:D:136:LEU:H	1.66	0.44
1:C:77:GLU:HA	1:C:82:ARG:NH2	2.33	0.44
1:E:186:ASP:HA	1:E:187:PRO:HD2	1.83	0.44
1:E:55:GLU:N	1:E:55:GLU:OE2	2.45	0.44
1:B:194:GLU:O	1:B:197:GLY:N	2.50	0.44
1:A:45:PRO:HB2	1:A:72:MET:HE3	2.00	0.44
1:D:39:THR:HA	1:D:56:ASP:O	2.18	0.44
1:C:17:LEU:O	1:C:39:THR:HB	2.18	0.44
1:D:26:HIS:HB3	1:D:222:GLU:OE2	2.18	0.44
1:E:104:VAL:HG11	1:E:136:LEU:HD22	2.00	0.44
1:D:132:LEU:HD12	1:D:132:LEU:HA	1.86	0.43
1:B:164:PRO:HA	1:B:167:LEU:CD2	2.48	0.43
1:D:243:GLU:O	1:D:246:ARG:HB3	2.18	0.43
1:B:65:SER:HB2	1:B:88:PHE:HB2	2.00	0.43
1:B:133:ARG:NE	1:B:135:ASP:OD2	2.51	0.43
1:F:229:TRP:CG	1:F:230:PRO:HD3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:63:LEU:HD21	1:E:108:LEU:HD21	2.00	0.43
1:B:195:ARG:CG	1:B:195:ARG:HH21	2.31	0.43
1:E:38:PRO:HD2	3:E:307:HOH:O	2.17	0.43
1:B:31:ALA:O	1:B:35:LEU:HB2	2.18	0.43
1:C:6:ARG:H	1:C:6:ARG:HG2	1.62	0.43
1:A:200:LEU:CD2	1:A:243:GLU:HB3	2.42	0.43
1:B:45:PRO:HB2	1:B:72:MET:HE3	2.00	0.43
1:B:195:ARG:HA	1:B:195:ARG:HD3	1.63	0.43
1:F:6:ARG:HG2	1:F:6:ARG:H	1.55	0.43
1:C:199:TYR:CE2	1:C:239:LEU:HD21	2.53	0.43
1:F:38:PRO:HB3	1:F:55:GLU:CG	2.49	0.43
1:D:77:GLU:HG2	1:F:77:GLU:HG2	2.01	0.43
1:C:133:ARG:NH1	1:C:135:ASP:OD1	2.52	0.43
1:B:35:LEU:O	1:B:37:LEU:HG	2.19	0.42
1:B:62:VAL:HG21	1:B:72:MET:HE2	2.01	0.42
1:E:214:HIS:CE1	3:E:312:HOH:O	2.70	0.42
1:D:157:LEU:H	1:D:157:LEU:CD2	2.32	0.42
1:B:52:VAL:O	1:B:53:LYS:HG3	2.18	0.42
1:E:163:PRO:HA	1:E:164:PRO:HD2	1.71	0.42
1:A:29:ASN:N	1:A:29:ASN:HD22	2.16	0.42
1:B:187:PRO:HB2	1:B:195:ARG:NE	2.34	0.42
1:A:195:ARG:NH1	1:A:231:THR:HB	2.33	0.42
1:B:21:ASP:OD1	1:B:215:HIS:HD2	2.03	0.42
1:A:12:ARG:CZ	1:A:252:HIS:HB2	2.49	0.42
1:A:191:PRO:HA	1:A:192:PRO:HD3	1.94	0.42
1:A:58:GLY:N	1:A:123:HIS:CE1	2.88	0.42
1:D:229:TRP:CG	1:D:230:PRO:HD3	2.54	0.42
1:F:132:LEU:HD12	1:F:132:LEU:HA	1.94	0.42
1:B:82:ARG:HA	1:B:87:TYR:O	2.20	0.42
1:C:246:ARG:O	1:C:249:ALA:N	2.44	0.42
1:F:133:ARG:HA	1:F:134:PRO:HD3	1.81	0.42
1:C:38:PRO:CB	1:C:55:GLU:HG2	2.50	0.42
1:C:177:THR:HG23	1:C:179:PHE:N	2.35	0.42
1:C:93:GLU:CG	1:C:97:ARG:NH1	2.83	0.42
1:D:58:GLY:N	1:D:123:HIS:CE1	2.88	0.41
1:F:163:PRO:HA	1:F:164:PRO:HD2	1.79	0.41
1:A:82:ARG:HB2	1:A:86:GLY:HA2	2.01	0.41
1:B:73:ARG:NH1	1:B:87:TYR:CZ	2.88	0.41
1:F:229:TRP:N	1:F:230:PRO:CD	2.83	0.41
1:F:183:ARG:HH11	1:F:209:LEU:H	1.67	0.41
1:C:163:PRO:HG2	1:C:166:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:LEU:O	1:C:144:ALA:C	2.59	0.41
1:C:157:LEU:N	1:C:157:LEU:CD2	2.83	0.41
1:D:244:VAL:C	1:D:246:ARG:H	2.24	0.41
1:B:163:PRO:HG2	1:B:166:PHE:CE1	2.55	0.41
1:C:252:HIS:HA	1:C:253:PRO:HD2	1.95	0.41
1:A:100:ARG:O	1:A:104:VAL:HG23	2.20	0.41
1:F:12:ARG:NH1	1:F:252:HIS:HB2	2.35	0.41
1:A:164:PRO:HA	1:A:167:LEU:CD2	2.50	0.41
1:C:93:GLU:HG2	1:C:97:ARG:HH12	1.85	0.41
1:E:13:ARG:HG3	1:E:207:PRO:HA	2.02	0.41
1:B:26:HIS:HB3	1:B:222:GLU:OE2	2.20	0.41
1:D:58:GLY:CA	1:D:123:HIS:CE1	3.03	0.41
1:C:206:PRO:HG2	1:C:210:TYR:OH	2.20	0.41
1:B:193:GLU:CD	1:B:193:GLU:N	2.69	0.41
1:C:218:LEU:HA	1:C:219:PRO:HD3	1.97	0.41
1:F:164:PRO:HA	1:F:167:LEU:CD2	2.51	0.41
1:C:21:ASP:HB2	1:C:28:GLN:NE2	2.36	0.41
1:B:62:VAL:HG21	1:B:72:MET:CE	2.51	0.41
1:C:246:ARG:O	1:C:247:VAL:C	2.57	0.41
1:F:121:PRO:HB2	1:F:149:LEU:HD21	2.03	0.40
1:E:45:PRO:HD2	1:E:72:MET:CE	2.49	0.40
1:C:58:GLY:N	1:C:123:HIS:CE1	2.89	0.40
1:A:164:PRO:N	1:A:165:PRO:HD2	2.36	0.40
1:A:195:ARG:HA	1:A:195:ARG:HD3	1.86	0.40
1:D:18:HIS:HE1	1:D:41:SER:OG	2.04	0.40
1:F:31:ALA:O	1:F:35:LEU:HB2	2.22	0.40
1:E:39:THR:HA	1:E:56:ASP:O	2.22	0.40
1:C:57:LEU:HB3	1:C:119:PHE:CE1	2.57	0.40
1:B:20:ASP:O	1:B:28:GLN:NE2	2.54	0.40
1:B:109:LYS:HG2	1:B:147:TYR:OH	2.22	0.40
1:E:226:LEU:CD1	1:E:226:LEU:N	2.85	0.40
1:B:229:TRP:CG	1:B:230:PRO:HD3	2.57	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:A:250:GLU:CG	3:D:330:HOH:O[10_455]	2.11	0.09

## 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	261/264 (99%)	253 (97%)	7 (3%)	1 (0%)	39	74
1	B	261/264 (99%)	244 (94%)	13 (5%)	4 (2%)	13	42
1	C	261/264 (99%)	225 (86%)	31 (12%)	5 (2%)	10	35
1	D	261/264 (99%)	239 (92%)	18 (7%)	4 (2%)	13	42
1	E	261/264 (99%)	239 (92%)	19 (7%)	3 (1%)	17	51
1	F	261/264 (99%)	248 (95%)	12 (5%)	1 (0%)	39	74
All	All	1566/1584 (99%)	1448 (92%)	100 (6%)	18 (1%)	17	51

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	135	ASP
1	B	135	ASP
1	B	195	ARG
1	C	135	ASP
1	C	201	ASP
1	D	135	ASP
1	E	84	GLU
1	F	135	ASP
1	C	6	ARG
1	D	204	HIS
1	C	172	ARG
1	D	250	GLU
1	E	168	PRO
1	E	201	ASP
1	B	250	GLU
1	C	176	GLU
1	B	134	PRO
1	D	131	VAL

### 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	216/217 (100%)	186 (86%)	30 (14%)	4	12
1	B	216/217 (100%)	181 (84%)	35 (16%)	3	9
1	C	216/217 (100%)	177 (82%)	39 (18%)	2	6
1	D	216/217 (100%)	186 (86%)	30 (14%)	4	12
1	E	216/217 (100%)	189 (88%)	27 (12%)	6	17
1	F	216/217 (100%)	185 (86%)	31 (14%)	4	12
All	All	1296/1302 (100%)	1104 (85%)	192 (15%)	4	11

All (192) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	14	VAL
1	A	20	ASP
1	A	35	LEU
1	A	52	VAL
1	A	53	LYS
1	A	57	LEU
1	A	59	VAL
1	A	62	VAL
1	A	66	GLU
1	A	79	GLU
1	A	83	ASP
1	A	84	GLU
1	A	90	GLU
1	A	93	GLU
1	A	102	GLU
1	A	132	LEU
1	A	150	VAL
1	A	157	LEU
1	A	158	GLU
1	A	167	LEU
1	A	171	GLU

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Mol	Chain	Res	Type
1	A	172	ARG
1	A	220	THR
1	A	231	THR
1	A	240	SER
1	A	243	GLU
1	A	245	ARG
1	A	248	LEU
1	A	254	LEU
1	B	6	ARG
1	B	12	ARG
1	B	14	VAL
1	B	20	ASP
1	B	35	LEU
1	B	52	VAL
1	B	53	LYS
1	B	57	LEU
1	B	59	VAL
1	B	62	VAL
1	B	65	SER
1	B	83	ASP
1	B	90	GLU
1	B	117	LYS
1	B	120	SER
1	B	132	LEU
1	B	150	VAL
1	B	155	GLU
1	B	156	SER
1	B	157	LEU
1	B	167	LEU
1	B	171	GLU
1	B	172	ARG
1	B	177	THR
1	B	190	LEU
1	B	193	GLU
1	B	195	ARG
1	B	220	THR
1	B	226	LEU
1	B	231	THR
1	B	243	GLU
1	B	246	ARG
1	B	248	LEU
1	B	254	LEU

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Mol	Chain	Res	Type
1	B	260	ARG
1	C	6	ARG
1	C	9	LEU
1	C	12	ARG
1	C	14	VAL
1	C	15	LEU
1	C	20	ASP
1	C	35	LEU
1	C	52	VAL
1	C	53	LYS
1	C	57	LEU
1	C	59	VAL
1	C	60	HIS
1	C	63	LEU
1	C	66	GLU
1	C	72	MET
1	C	83	ASP
1	C	132	LEU
1	C	150	VAL
1	C	156	SER
1	C	157	LEU
1	C	158	GLU
1	C	160	LEU
1	C	167	LEU
1	C	171	GLU
1	C	172	ARG
1	C	173	LEU
1	C	174	LEU
1	C	175	TYR
1	C	177	THR
1	C	182	VAL
1	C	190	LEU
1	C	204	HIS
1	C	220	THR
1	C	226	LEU
1	C	231	THR
1	C	243	GLU
1	C	246	ARG
1	C	248	LEU
1	C	254	LEU
1	D	6	ARG
1	D	9	LEU

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Mol	Chain	Res	Type
1	D	14	VAL
1	D	20	ASP
1	D	35	LEU
1	D	52	VAL
1	D	53	LYS
1	D	57	LEU
1	D	59	VAL
1	D	62	VAL
1	D	72	MET
1	D	84	GLU
1	D	90	GLU
1	D	132	LEU
1	D	150	VAL
1	D	156	SER
1	D	157	LEU
1	D	158	GLU
1	D	160	LEU
1	D	167	LEU
1	D	171	GLU
1	D	172	ARG
1	D	183	ARG
1	D	190	LEU
1	D	213	VAL
1	D	220	THR
1	D	231	THR
1	D	243	GLU
1	D	248	LEU
1	D	254	LEU
1	E	9	LEU
1	E	14	VAL
1	E	35	LEU
1	E	52	VAL
1	E	53	LYS
1	E	57	LEU
1	E	59	VAL
1	E	66	GLU
1	E	79	GLU
1	E	83	ASP
1	E	90	GLU
1	E	97	ARG
1	E	132	LEU
1	E	135	ASP

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Mol	Chain	Res	Type
1	E	150	VAL
1	E	157	LEU
1	E	167	LEU
1	E	172	ARG
1	E	173	LEU
1	E	183	ARG
1	E	190	LEU
1	E	193	GLU
1	E	220	THR
1	E	231	THR
1	E	243	GLU
1	E	248	LEU
1	E	254	LEU
1	F	2	ASP
1	F	6	ARG
1	F	9	LEU
1	F	14	VAL
1	F	35	LEU
1	F	52	VAL
1	F	53	LYS
1	F	55	GLU
1	F	57	LEU
1	F	59	VAL
1	F	62	VAL
1	F	66	GLU
1	F	83	ASP
1	F	97	ARG
1	F	102	GLU
1	F	132	LEU
1	F	150	VAL
1	F	155	GLU
1	F	157	LEU
1	F	167	LEU
1	F	171	GLU
1	F	172	ARG
1	F	173	LEU
1	F	177	THR
1	F	183	ARG
1	F	220	THR
1	F	231	THR
1	F	240	SER
1	F	243	GLU

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Mol	Chain	Res	Type
1	F	248	LEU
1	F	254	LEU

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

Mol	Chain	Res	Type
1	A	29	ASN
1	A	214	HIS
1	A	241	HIS
1	B	29	ASN
1	B	128	GLN
1	B	214	HIS
1	B	215	HIS
1	B	241	HIS
1	C	29	ASN
1	C	113	GLN
1	C	128	GLN
1	C	214	HIS
1	C	241	HIS
1	D	29	ASN
1	D	214	HIS
1	D	241	HIS
1	E	29	ASN
1	E	113	GLN
1	E	128	GLN
1	E	214	HIS
1	E	241	HIS
1	F	29	ASN
1	F	113	GLN
1	F	214	HIS
1	F	241	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	263/264 (99%)	-0.34	1 (0%) 93 92	7, 20, 41, 57	0
1	B	263/264 (99%)	-0.26	0 100 100	7, 26, 49, 61	0
1	C	263/264 (99%)	-0.02	4 (1%) 76 74	8, 32, 62, 79	0
1	D	263/264 (99%)	-0.12	1 (0%) 93 92	7, 26, 49, 60	0
1	E	263/264 (99%)	-0.14	2 (0%) 87 86	11, 35, 70, 82	0
1	F	263/264 (99%)	0.02	4 (1%) 76 74	10, 36, 62, 70	0
All	All	1578/1584 (99%)	-0.14	12 (0%) 87 86	7, 29, 59, 82	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	175	TYR	4.3
1	F	187	PRO	3.4
1	E	83	ASP	3.2
1	A	83	ASP	3.1
1	F	163	PRO	2.9
1	C	9	LEU	2.3
1	E	97	ARG	2.2
1	F	159	GLY	2.2
1	C	204	HIS	2.1
1	C	210	TYR	2.1
1	F	194	GLU	2.1
1	D	11	GLY	2.0

### 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 [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	D	304	1/1	0.90	0.23	5.92	13,13,13,13	0
2	MG	E	305	1/1	0.91	0.18	2.49	14,14,14,14	0
2	MG	C	303	1/1	0.88	0.23	1.98	20,20,20,20	0
2	MG	B	302	1/1	0.94	0.19	1.90	17,17,17,17	0
2	MG	A	301	1/1	0.97	0.15	0.29	10,10,10,10	0
2	MG	F	306	1/1	0.96	0.14	-0.15	18,18,18,18	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.