



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:40 AM GMT

PDB ID : 2I3O  
Title : Crystal structure of gamma-glutamyl transferase related protein from Thermoplasma acidophilum  
Authors : Rao, K.N.; Eswaramoorthy, S.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2006-08-19  
Resolution : 2.03 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

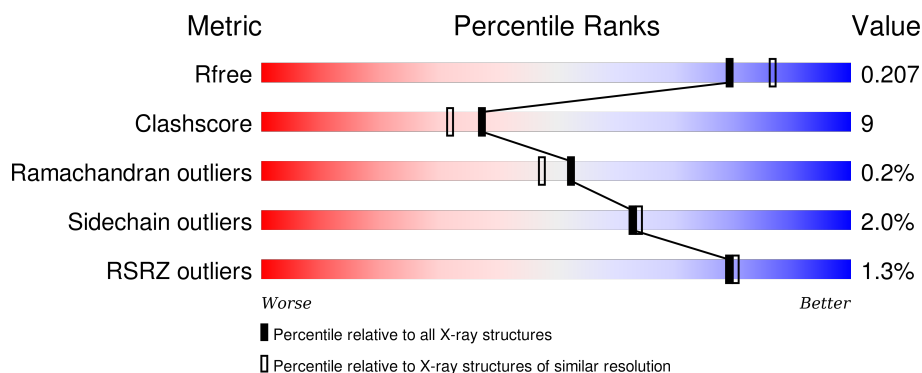
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.03 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	7858 (2.04-2.00)
Clashscore	102246	9060 (2.04-2.00)
Ramachandran outliers	100387	8952 (2.04-2.00)
Sidechain outliers	100360	8951 (2.04-2.00)
RSRZ outliers	91569	7873 (2.04-2.00)

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	516	<div> <div>2%</div> <div>80%</div> <div>16%</div> <div>••</div> </div>
1	B	516	<div> <div>2%</div> <div>82%</div> <div>14%</div> <div>••</div> </div>
1	C	516	<div> <div>2%</div> <div>81%</div> <div>16%</div> <div>••</div> </div>
1	D	516	<div> <div>2%</div> <div>80%</div> <div>18%</div> <div>•</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16382 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 Gamma-glutamyltransferase related protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	504	Total	C	N	O	S	Se	0	0	0
			3856	2423	653	760	3	17			
1	B	503	Total	C	N	O	S	Se	0	0	0
			3853	2421	654	759	3	16			
1	C	503	Total	C	N	O	S	Se	0	0	0
			3844	2415	652	758	3	16			
1	D	514	Total	C	N	O	S	Se	0	0	0
			3942	2473	674	775	3	17			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
A	46	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
A	73	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
A	93	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
A	126	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
A	171	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
A	195	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
A	267	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
A	277	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
A	289	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
A	305	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
A	352	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
A	385	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
A	398	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
A	412	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
A	422	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
A	426	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
B	46	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
B	73	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
B	93	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	126	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
B	171	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
B	195	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
B	267	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
B	277	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
B	289	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
B	305	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
B	352	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
B	385	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
B	398	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
B	412	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
B	422	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
B	426	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
C	1	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
C	46	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
C	73	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
C	93	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
C	126	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
C	171	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
C	195	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
C	267	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
C	277	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
C	289	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
C	305	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
C	352	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
C	385	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
C	398	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
C	412	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
C	422	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
C	426	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
D	1	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
D	46	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
D	73	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
D	93	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
D	126	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
D	171	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
D	195	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
D	267	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
D	277	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
D	289	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
D	305	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
D	352	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	385	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
D	398	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
D	412	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
D	422	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4
D	426	MSE	MET	MODIFIED RESIDUE	UNP Q9HJH4

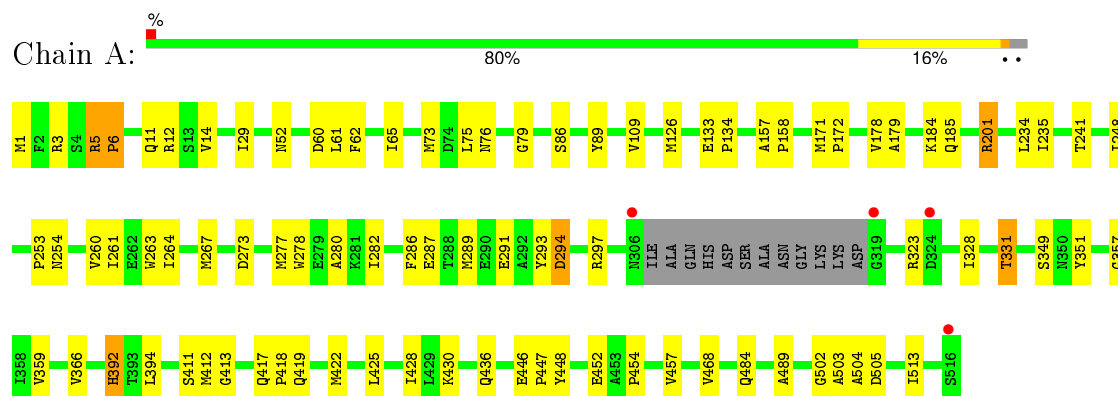
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	205	Total O 205 205	0	0
2	B	239	Total O 239 239	0	0
2	C	220	Total O 220 220	0	0
2	D	223	Total O 223 223	0	0

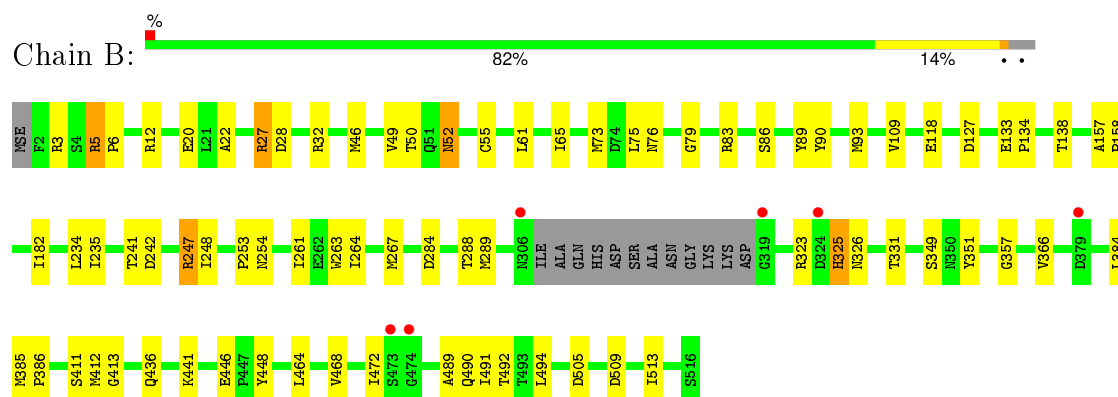
### 3 Residue-property plots

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.

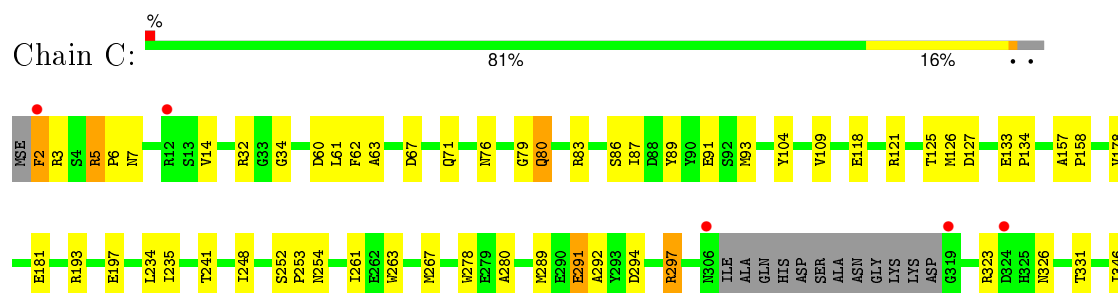
#### • Molecule 1: Gamma-glutamyltransferase related protein

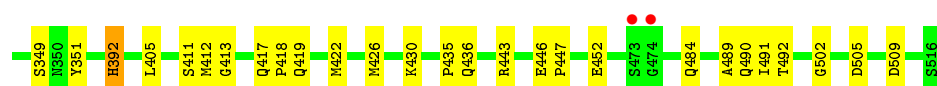


#### • Molecule 1: Gamma-glutamyltransferase related protein

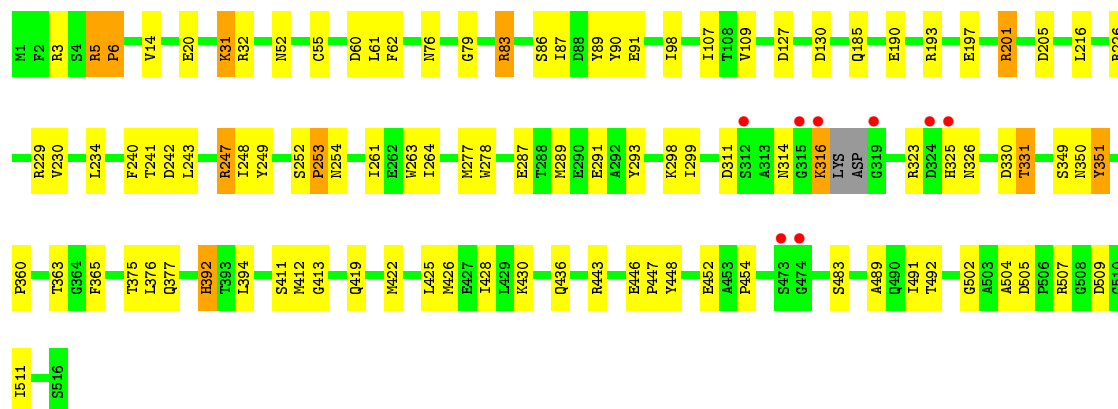
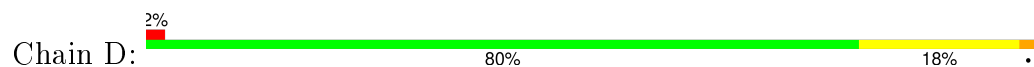


#### • Molecule 1: Gamma-glutamyltransferase related protein





- Molecule 1: Gamma-glutamyltransferase related protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.08 Å   95.47 Å   119.04 Å 90.00°   109.79°   90.00°	Depositor
Resolution (Å)	30.47 – 2.03 30.47 – 2.03	Depositor EDS
% Data completeness (in resolution range)	96.3 (30.47-2.03) 96.4 (30.47-2.03)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.81 (at 2.03 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.183 , 0.207 0.183 , 0.207	Depositor DCC
$R_{free}$ test set	3836 reflections (2.53%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.0	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 48.2	EDS
Estimated twinning fraction	0.025 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 156636 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	16382	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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 ⓘ

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	0.35	3/3917 (0.1%)	0.60	1/5282 (0.0%)
1	B	0.35	3/3915 (0.1%)	0.62	2/5280 (0.0%)
1	C	0.36	4/3905 (0.1%)	0.63	3/5268 (0.1%)
1	D	0.37	5/4005 (0.1%)	0.60	2/5398 (0.0%)
All	All	0.36	15/15742 (0.1%)	0.61	8/21228 (0.0%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	252	SER	C-N	7.80	1.49	1.34
1	D	254	ASN	C-N	-7.13	1.17	1.34
1	C	252	SER	C-N	5.76	1.45	1.34
1	D	254	ASN	C-O	5.44	1.33	1.23
1	B	254	ASN	C-O	5.42	1.33	1.23
1	A	254	ASN	C-O	5.41	1.33	1.23
1	C	254	ASN	C-O	5.40	1.33	1.23
1	C	253	PRO	N-CD	5.29	1.55	1.47
1	B	253	PRO	N-CD	5.29	1.55	1.47
1	A	253	PRO	N-CD	5.28	1.55	1.47
1	D	253	PRO	N-CD	5.24	1.55	1.47
1	B	253	PRO	C-N	-5.05	1.22	1.34
1	C	253	PRO	C-N	-5.05	1.22	1.34
1	D	253	PRO	C-N	-5.04	1.22	1.34
1	A	253	PRO	C-N	-5.04	1.22	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	252	SER	O-C-N	-9.37	103.29	121.10
1	A	253	PRO	C-N-CA	7.15	139.59	121.70
1	C	253	PRO	C-N-CA	7.14	139.56	121.70
1	B	253	PRO	C-N-CA	7.14	139.56	121.70
1	D	253	PRO	C-N-CA	7.12	139.50	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	252	SER	CA-C-N	6.43	135.11	117.10
1	B	254	ASN	CA-C-N	6.05	130.51	117.20
1	D	252	SER	O-C-N	-5.54	110.57	121.10

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3856	0	3734	80	0
1	B	3853	0	3728	59	0
1	C	3844	0	3714	68	0
1	D	3942	0	3826	81	0
2	A	205	0	0	7	0
2	B	239	0	0	2	0
2	C	220	0	0	8	0
2	D	223	0	0	6	0
All	All	16382	0	15002	283	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 9.

All (283) 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:6:PRO:HD3	2:B:536:HOH:O	1.58	1.02
2:A:517:HOH:O	1:B:6:PRO:HD3	1.59	1.00
1:A:52:ASN:HD21	1:A:185:GLN:HE22	1.10	0.99
2:C:527:HOH:O	1:D:6:PRO:HD3	1.61	0.98
1:A:73:MSE:HE3	1:A:75:LEU:HB2	1.46	0.97
1:A:294:ASP:HA	1:A:297:ARG:NH1	1.82	0.94
1:C:6:PRO:HD3	2:D:518:HOH:O	1.66	0.94
1:A:65:ILE:HD12	1:A:73:MSE:HE2	1.48	0.91
1:D:98:ILE:HG13	1:D:376:LEU:HD21	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:376:LEU:HG	2:D:560:HOH:O	1.69	0.91
1:B:331:THR:HG23	1:B:349:SER:HB2	1.49	0.91
1:D:52:ASN:HD21	1:D:185:GLN:HE22	1.14	0.90
1:C:7:ASN:HD21	1:C:436:GLN:H	1.17	0.86
1:D:316:LYS:HD3	1:D:316:LYS:H	1.44	0.82
1:B:46:MSE:HE1	1:B:138:THR:HB	1.60	0.82
1:A:263:TRP:HB3	1:A:422:MSE:HE3	1.61	0.82
1:B:73:MSE:HE3	1:B:75:LEU:HB2	1.60	0.82
1:B:248:ILE:HD13	1:B:264:ILE:HD13	1.63	0.81
1:A:29:ILE:HD12	1:A:126:MSE:HE1	1.62	0.80
1:B:267:MSE:HA	1:B:267:MSE:HE2	1.61	0.80
1:A:331:THR:HB	1:A:349:SER:HB2	1.62	0.79
1:C:412:MSE:HE1	1:C:484:GLN:HB2	1.63	0.79
1:C:80:GLN:NE2	1:C:80:GLN:H	1.81	0.79
1:D:20:GLU:HB2	1:D:511:ILE:HD12	1.66	0.77
1:A:1:MSE:HE1	1:A:3:ARG:NH2	2.00	0.77
1:A:328:ILE:HG13	2:A:553:HOH:O	1.85	0.77
1:B:65:ILE:HD12	1:B:73:MSE:HE2	1.67	0.76
1:C:331:THR:HG23	1:C:349:SER:HB2	1.67	0.76
1:A:294:ASP:HA	1:A:297:ARG:HH11	1.49	0.75
1:C:80:GLN:HE21	1:C:80:GLN:H	1.35	0.73
1:D:83:ARG:HH11	1:D:83:ARG:HB3	1.54	0.73
1:A:1:MSE:HE1	1:A:3:ARG:HH22	1.51	0.73
1:A:323:ARG:HH22	1:A:328:ILE:HG12	1.55	0.72
1:C:3:ARG:HH11	1:C:3:ARG:HG2	1.55	0.71
1:D:52:ASN:ND2	1:D:185:GLN:HE22	1.88	0.70
1:B:241:THR:HB	1:B:261:ILE:HG23	1.74	0.70
1:B:65:ILE:HD12	1:B:73:MSE:CE	2.23	0.68
1:A:289:MSE:HE1	1:A:446:GLU:OE1	1.95	0.67
1:A:457:VAL:HG21	1:A:468:VAL:HG11	1.77	0.67
1:A:411:SER:HB2	1:A:489:ALA:HB2	1.77	0.67
1:A:52:ASN:ND2	1:A:185:GLN:HE22	1.89	0.66
1:A:65:ILE:HD12	1:A:73:MSE:CE	2.22	0.66
1:B:267:MSE:HE3	1:B:288:THR:CG2	2.25	0.66
1:C:289:MSE:HE1	1:C:446:GLU:OE1	1.95	0.66
1:D:253:PRO:HB3	1:D:299:ILE:HG23	1.78	0.65
1:C:125:THR:HB	2:C:554:HOH:O	1.96	0.65
1:A:331:THR:HG23	1:A:412:MSE:HG3	1.78	0.65
1:C:419:GLN:HE22	1:C:446:GLU:H	1.45	0.65
1:C:7:ASN:ND2	1:C:436:GLN:H	1.93	0.65
1:B:46:MSE:HE1	1:B:138:THR:CB	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:316:LYS:CD	1:D:316:LYS:H	2.09	0.64
1:D:242:ASP:OD2	1:D:247:ARG:HD3	1.98	0.64
1:A:412:MSE:HG2	1:A:413:GLY:N	2.13	0.64
1:C:331:THR:H	1:C:412:MSE:HG3	1.63	0.64
1:D:331:THR:HG23	1:D:412:MSE:HG3	1.78	0.64
1:B:127:ASP:HB3	2:B:594:HOH:O	1.98	0.64
1:C:241:THR:HB	1:C:261:ILE:HG23	1.80	0.64
1:D:287:GLU:O	1:D:291:GLU:HG3	1.99	0.63
1:B:411:SER:HB2	1:B:489:ALA:HB2	1.79	0.63
1:D:331:THR:HG23	1:D:412:MSE:HA	1.82	0.62
1:C:412:MSE:HG2	1:C:413:GLY:N	2.14	0.62
1:C:291:GLU:HG2	1:C:292:ALA:N	2.14	0.61
1:D:32:ARG:HH21	1:D:130:ASP:HB3	1.65	0.61
1:D:52:ASN:HD21	1:D:185:GLN:NE2	1.94	0.61
1:B:289:MSE:HE1	1:B:446:GLU:OE1	2.00	0.61
1:D:316:LYS:HD3	1:D:316:LYS:N	2.16	0.60
1:B:267:MSE:HE3	1:B:288:THR:HG21	1.84	0.60
1:C:76:ASN:HB3	1:C:234:LEU:HB2	1.84	0.60
1:C:60:ASP:OD2	1:C:392:HIS:HE1	1.84	0.59
1:B:22:ALA:HA	1:B:46:MSE:HG2	1.84	0.59
1:D:443:ARG:HD3	2:D:520:HOH:O	2.01	0.59
1:A:235:ILE:N	1:A:235:ILE:HD12	2.18	0.59
1:C:411:SER:HB2	1:C:489:ALA:HB2	1.84	0.59
1:D:31:LYS:HB3	1:D:31:LYS:NZ	2.18	0.59
1:A:436:GLN:HE22	1:A:504:ALA:H	1.51	0.59
1:D:79:GLY:HA3	1:D:109:VAL:O	2.01	0.59
1:C:67:ASP:OD2	1:C:71:GLN:HB2	2.02	0.59
1:C:331:THR:N	1:C:412:MSE:HG3	2.18	0.59
1:C:79:GLY:HA3	1:C:109:VAL:O	2.02	0.59
1:A:287:GLU:O	1:A:291:GLU:HG3	2.03	0.58
1:C:32:ARG:HH11	1:C:32:ARG:HB3	1.68	0.58
1:B:331:THR:H	1:B:412:MSE:HG3	1.68	0.58
1:D:436:GLN:HE22	1:D:504:ALA:H	1.49	0.58
1:A:133:GLU:HB3	1:A:134:PRO:HD3	1.85	0.58
1:D:411:SER:HB2	1:D:489:ALA:HB2	1.85	0.58
1:A:79:GLY:HA3	1:A:109:VAL:O	2.03	0.58
1:A:294:ASP:HA	1:A:297:ARG:HH12	1.67	0.57
1:B:412:MSE:HG2	1:B:413:GLY:N	2.18	0.57
1:C:32:ARG:HB3	1:C:32:ARG:NH1	2.20	0.57
1:C:323:ARG:HD3	1:C:452:GLU:OE1	2.05	0.57
1:D:331:THR:HB	1:D:349:SER:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:MSE:HE3	1:B:49:VAL:HB	1.86	0.56
1:B:267:MSE:HE3	1:B:288:THR:OG1	2.04	0.56
1:B:46:MSE:HE2	1:B:50:THR:HG23	1.86	0.56
1:A:331:THR:HG23	1:A:412:MSE:CG	2.36	0.56
1:D:412:MSE:HG2	1:D:413:GLY:N	2.20	0.55
1:A:331:THR:H	1:A:412:MSE:HG3	1.70	0.55
1:A:52:ASN:HD21	1:A:185:GLN:NE2	1.93	0.55
1:C:489:ALA:O	1:C:505:ASP:HB2	2.06	0.55
1:B:76:ASN:HB3	1:B:234:LEU:HB2	1.88	0.55
1:D:376:LEU:N	1:D:376:LEU:HD22	2.22	0.55
1:C:3:ARG:HG2	2:D:593:HOH:O	2.06	0.55
1:B:384:LEU:O	1:B:385:MSE:HE2	2.07	0.55
1:A:241:THR:HB	1:A:261:ILE:HG23	1.88	0.55
1:A:263:TRP:HB3	1:A:422:MSE:CE	2.34	0.55
1:C:331:THR:HG23	1:C:349:SER:CB	2.37	0.55
1:A:297:ARG:CZ	2:A:541:HOH:O	2.55	0.54
1:C:93:MSE:HE1	1:C:104:TYR:CZ	2.42	0.54
1:C:509:ASP:O	1:D:6:PRO:HG3	2.07	0.54
1:A:323:ARG:HD3	1:A:452:GLU:OE1	2.07	0.54
1:C:157:ALA:HB3	1:C:158:PRO:HD3	1.88	0.54
1:A:263:TRP:CZ2	1:A:289:MSE:HB2	2.42	0.54
1:D:425:LEU:HA	1:D:428:ILE:HG22	1.89	0.54
1:D:3:ARG:HG2	1:D:5:ARG:O	2.08	0.54
1:C:443:ARG:NH1	2:C:529:HOH:O	2.40	0.53
1:C:126:MSE:HG3	2:C:554:HOH:O	2.07	0.53
1:C:294:ASP:O	1:C:297:ARG:HD3	2.07	0.53
1:A:14:VAL:HG11	1:A:502:GLY:HA3	1.89	0.53
1:D:76:ASN:HB3	1:D:234:LEU:HB2	1.90	0.53
1:D:298:LYS:HB2	1:D:298:LYS:NZ	2.24	0.53
1:A:60:ASP:OD2	1:A:392:HIS:HE1	1.92	0.53
1:A:331:THR:HG23	1:A:412:MSE:HA	1.91	0.52
1:B:52:ASN:HD22	1:B:52:ASN:N	2.05	0.52
1:A:263:TRP:CB	1:A:422:MSE:HE3	2.34	0.52
1:D:448:TYR:CZ	1:D:454:PRO:HG3	2.44	0.52
1:D:375:THR:OG1	1:D:377:GLN:HG3	2.09	0.52
1:C:278:TRP:CG	1:C:430:LYS:HD2	2.44	0.52
1:D:248:ILE:CD1	1:D:264:ILE:HD13	2.40	0.52
1:B:331:THR:N	1:B:412:MSE:HG3	2.23	0.52
1:A:448:TYR:CZ	1:A:454:PRO:HG3	2.45	0.52
1:C:2:PHE:O	1:C:3:ARG:HB3	2.10	0.52
1:D:226:ARG:HG2	1:D:226:ARG:HH11	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:TYR:HA	1:B:93:MSE:HE3	1.91	0.52
1:B:323:ARG:HG2	1:B:325:HIS:HD2	1.74	0.52
1:D:127:ASP:HB3	2:D:625:HOH:O	2.10	0.51
1:B:331:THR:HG23	1:B:349:SER:CB	2.31	0.51
1:D:323:ARG:HD3	1:D:452:GLU:OE1	2.11	0.51
1:A:264:ILE:HG13	1:A:422:MSE:HE1	1.93	0.51
1:C:80:GLN:N	1:C:80:GLN:HE21	2.07	0.51
1:C:263:TRP:CG	1:C:422:MSE:HE2	2.46	0.51
1:D:278:TRP:CD2	1:D:430:LYS:HE2	2.46	0.51
1:B:157:ALA:HB3	1:B:158:PRO:HD3	1.93	0.51
1:D:263:TRP:CZ2	1:D:289:MSE:HB2	2.45	0.51
1:C:263:TRP:CZ2	1:C:289:MSE:HB2	2.47	0.50
1:B:263:TRP:CZ2	1:B:289:MSE:HB2	2.46	0.50
1:B:267:MSE:HE1	1:B:284:ASP:HB3	1.94	0.50
1:C:93:MSE:HE1	1:C:104:TYR:CE2	2.46	0.50
1:A:76:ASN:HB3	1:A:234:LEU:HB2	1.94	0.50
1:A:263:TRP:CG	1:A:422:MSE:HE3	2.46	0.50
1:D:323:ARG:HG2	1:D:447:PRO:O	2.11	0.50
1:D:193:ARG:NH1	1:D:197:GLU:CD	2.65	0.50
1:D:241:THR:HB	1:D:261:ILE:HG23	1.94	0.50
1:C:248:ILE:HD12	1:C:248:ILE:N	2.27	0.49
1:A:157:ALA:HB3	1:A:158:PRO:HD3	1.95	0.49
1:C:3:ARG:HG2	1:C:3:ARG:NH1	2.27	0.49
1:D:331:THR:H	1:D:412:MSE:HG3	1.77	0.49
1:B:267:MSE:HA	1:B:267:MSE:CE	2.37	0.49
1:B:79:GLY:HA3	1:B:109:VAL:O	2.12	0.49
1:B:323:ARG:HD2	1:B:448:TYR:HA	1.95	0.48
1:A:61:LEU:HD23	1:A:61:LEU:C	2.32	0.48
1:C:34:GLY:HA2	2:C:554:HOH:O	2.13	0.48
1:D:248:ILE:HD13	1:D:264:ILE:HD13	1.95	0.48
1:B:52:ASN:ND2	1:B:52:ASN:H	2.11	0.48
1:A:412:MSE:HE1	1:A:484:GLN:HB2	1.96	0.48
1:A:331:THR:N	1:A:412:MSE:HG3	2.29	0.48
1:D:61:LEU:HD23	1:D:61:LEU:C	2.34	0.48
1:C:118:GLU:OE2	1:C:121:ARG:NH2	2.47	0.48
1:A:323:ARG:HG2	1:A:447:PRO:O	2.15	0.47
1:B:472:ILE:N	1:B:472:ILE:HD12	2.29	0.47
1:B:133:GLU:HB3	1:B:134:PRO:HD3	1.96	0.47
1:A:278:TRP:CG	1:A:430:LYS:HD2	2.49	0.47
1:A:73:MSE:CE	1:A:75:LEU:HD22	2.44	0.47
1:D:489:ALA:O	1:D:505:ASP:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:ARG:HG2	1:C:447:PRO:O	2.14	0.47
1:B:27:ARG:HG3	1:B:513:ILE:HG22	1.97	0.47
1:D:289:MSE:HE1	1:D:446:GLU:OE2	2.14	0.47
1:A:267:MSE:HE1	1:A:280:ALA:CB	2.44	0.47
1:B:61:LEU:HD23	1:B:61:LEU:C	2.35	0.47
1:D:83:ARG:CB	1:D:83:ARG:HH11	2.27	0.47
1:A:248:ILE:HD12	1:A:248:ILE:N	2.30	0.47
1:D:331:THR:HG23	1:D:412:MSE:CG	2.44	0.47
1:D:491:ILE:HG12	1:D:492:THR:N	2.30	0.47
1:C:32:ARG:HH11	1:C:32:ARG:CB	2.28	0.47
1:D:226:ARG:NH1	1:D:230:VAL:HG11	2.30	0.47
1:B:118:GLU:HG3	1:B:235:ILE:HD11	1.97	0.47
1:A:513:ILE:HD13	1:B:20:GLU:OE2	2.15	0.46
1:A:436:GLN:NE2	1:A:503:ALA:HB1	2.30	0.46
1:B:52:ASN:ND2	1:B:52:ASN:N	2.64	0.46
1:C:419:GLN:NE2	1:C:446:GLU:H	2.09	0.46
1:B:52:ASN:HA	1:B:55:CYS:O	2.15	0.46
1:D:61:LEU:HD23	1:D:62:PHE:N	2.31	0.46
1:D:392:HIS:CD2	1:D:394:LEU:HB2	2.50	0.46
1:A:297:ARG:NE	2:A:541:HOH:O	2.49	0.46
1:C:263:TRP:CD1	1:C:422:MSE:HE2	2.51	0.46
1:D:87:ILE:O	1:D:91:GLU:HG3	2.16	0.45
1:A:282:ILE:HD11	1:A:286:PHE:HE1	1.80	0.45
1:A:293:TYR:OH	1:A:419:GLN:HG3	2.17	0.45
1:B:464:LEU:O	1:B:468:VAL:HG23	2.16	0.45
1:A:413:GLY:O	1:A:417:GLN:HG3	2.16	0.45
1:D:330:ASP:O	1:D:349:SER:HB2	2.16	0.45
1:D:293:TYR:OH	1:D:419:GLN:HG3	2.15	0.45
1:A:260:VAL:HG13	1:A:422:MSE:HE2	1.97	0.45
1:A:1:MSE:SE	1:A:1:MSE:O	2.85	0.45
1:D:247:ARG:HG3	1:D:249:TYR:CE2	2.52	0.45
1:B:489:ALA:O	1:B:505:ASP:HB2	2.17	0.45
1:D:483:SER:O	1:D:507:ARG:HD3	2.17	0.45
1:A:297:ARG:NH2	2:A:541:HOH:O	2.49	0.45
1:B:248:ILE:HD13	1:B:264:ILE:CD1	2.41	0.45
1:A:282:ILE:HD11	1:A:286:PHE:CE1	2.53	0.44
1:C:127:ASP:HB3	2:C:579:HOH:O	2.16	0.44
1:B:242:ASP:OD1	1:B:247:ARG:HG2	2.17	0.44
2:C:629:HOH:O	1:D:511:ILE:HD11	2.15	0.44
1:A:86:SER:O	1:A:89:TYR:HB3	2.18	0.44
1:D:205:ASP:HB2	1:D:229:ARG:HH12	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:GLU:HB3	1:C:134:PRO:HD3	1.99	0.44
1:C:7:ASN:ND2	1:C:435:PRO:HG2	2.32	0.44
1:A:489:ALA:O	1:A:505:ASP:HB2	2.18	0.44
1:B:86:SER:O	1:B:89:TYR:HB3	2.17	0.44
1:C:118:GLU:HG3	1:C:235:ILE:HD11	2.00	0.44
1:A:201:ARG:HB2	2:A:580:HOH:O	2.17	0.44
1:B:3:ARG:HG2	1:B:5:ARG:O	2.17	0.44
1:C:193:ARG:O	1:C:197:GLU:HG3	2.18	0.44
1:A:11:GLN:HG3	2:A:573:HOH:O	2.18	0.44
1:B:83:ARG:HD3	1:B:386:PRO:HB2	2.00	0.44
1:C:178:VAL:HG22	1:C:181:GLU:OE2	2.18	0.43
1:A:457:VAL:HG23	1:A:457:VAL:O	2.18	0.43
1:D:205:ASP:HB2	1:D:229:ARG:NH1	2.33	0.43
1:D:201:ARG:HB2	2:D:610:HOH:O	2.18	0.43
1:C:86:SER:O	1:C:89:TYR:HB3	2.17	0.43
1:D:331:THR:HG23	1:D:412:MSE:CA	2.48	0.43
1:D:243:LEU:HD21	1:D:277:MSE:HE2	1.99	0.43
1:D:205:ASP:CB	1:D:229:ARG:NH1	2.81	0.43
1:C:422:MSE:O	1:C:426:MSE:HG3	2.18	0.43
1:C:14:VAL:HG11	1:C:502:GLY:HA3	2.00	0.43
1:D:350:ASN:O	1:D:351:TYR:HB3	2.18	0.43
1:A:61:LEU:HD23	1:A:62:PHE:N	2.33	0.43
1:D:60:ASP:OD2	1:D:392:HIS:HE1	2.02	0.42
1:D:86:SER:O	1:D:89:TYR:HB3	2.18	0.42
1:A:392:HIS:CD2	1:A:394:LEU:HG	2.54	0.42
1:D:425:LEU:O	1:D:428:ILE:HG22	2.18	0.42
1:A:11:GLN:HG2	1:B:182:ILE:CD1	2.49	0.42
1:D:20:GLU:CD	1:D:511:ILE:HD12	2.40	0.42
1:A:425:LEU:O	1:A:428:ILE:HG22	2.20	0.42
1:D:316:LYS:N	1:D:316:LYS:CD	2.81	0.42
1:A:417:GLN:HB2	1:A:418:PRO:HD3	2.02	0.42
1:C:61:LEU:HD23	1:C:61:LEU:C	2.39	0.42
1:D:311:ASP:HB3	1:D:314:ASN:ND2	2.34	0.42
1:C:6:PRO:HG3	1:D:509:ASP:O	2.19	0.41
1:A:273:ASP:O	1:A:277:MSE:HG3	2.19	0.41
1:D:240:PHE:CD1	1:D:247:ARG:NE	2.88	0.41
1:D:363:THR:HB	1:D:365:PHE:CE2	2.54	0.41
1:A:6:PRO:HG3	1:B:509:ASP:O	2.21	0.41
1:C:278:TRP:CD2	1:C:430:LYS:HD2	2.55	0.41
1:A:357:GLY:H	1:A:366:VAL:CG1	2.34	0.41
1:D:14:VAL:HG11	1:D:502:GLY:HA3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:491:ILE:CG1	1:C:492:THR:N	2.83	0.41
1:A:171:MSE:N	1:A:172:PRO:CD	2.83	0.41
1:C:490:GLN:HE21	1:C:505:ASP:H	1.69	0.41
1:D:325:HIS:CG	1:D:326:ASN:N	2.88	0.41
1:C:63:ALA:CB	1:C:346:ILE:HG12	2.51	0.41
1:D:491:ILE:CG1	1:D:492:THR:N	2.83	0.41
1:C:61:LEU:HD23	1:C:62:PHE:N	2.35	0.41
1:B:491:ILE:HG22	1:B:492:THR:N	2.36	0.41
1:B:490:GLN:NE2	1:B:505:ASP:H	2.19	0.41
1:A:359:VAL:HG22	1:A:366:VAL:HG22	2.02	0.41
1:D:90:TYR:OH	1:D:107:ILE:HG21	2.21	0.41
1:C:5:ARG:O	1:C:436:GLN:HG2	2.20	0.41
1:B:28:ASP:O	1:B:32:ARG:HG3	2.21	0.41
1:D:422:MSE:O	1:D:426:MSE:HG3	2.21	0.41
1:D:216:LEU:HD21	1:D:360:PRO:HG3	2.02	0.41
1:C:83:ARG:HD3	2:C:634:HOH:O	2.21	0.41
1:C:87:ILE:O	1:C:91:GLU:HG3	2.21	0.41
1:B:357:GLY:H	1:B:366:VAL:CG1	2.34	0.40
1:C:267:MSE:HE1	1:C:280:ALA:CB	2.51	0.40
1:A:184:LYS:HB2	1:A:184:LYS:NZ	2.37	0.40
1:B:5:ARG:O	1:B:436:GLN:HG2	2.21	0.40
1:A:3:ARG:HG2	1:A:5:ARG:O	2.22	0.40
1:A:178:VAL:CG1	1:A:179:ALA:N	2.85	0.40
1:D:55:CYS:HA	1:D:349:SER:HA	2.04	0.40
1:A:235:ILE:CD1	1:A:235:ILE:N	2.84	0.40
1:B:325:HIS:N	1:B:325:HIS:CD2	2.88	0.40
1:B:441:LYS:HB3	1:B:441:LYS:NZ	2.36	0.40
1:C:417:GLN:HB2	1:C:418:PRO:HD3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	500/516 (97%)	486 (97%)	13 (3%)	1 (0%)	52	47
1	B	499/516 (97%)	486 (97%)	12 (2%)	1 (0%)	52	47
1	C	499/516 (97%)	487 (98%)	11 (2%)	1 (0%)	52	47
1	D	510/516 (99%)	495 (97%)	14 (3%)	1 (0%)	52	47
All	All	2008/2064 (97%)	1954 (97%)	50 (2%)	4 (0%)	52	47

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	351	TYR
1	B	351	TYR
1	C	351	TYR
1	D	351	TYR

### 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	410/411 (100%)	403 (98%)	7 (2%)	68	70
1	B	410/411 (100%)	402 (98%)	8 (2%)	63	64
1	C	408/411 (99%)	400 (98%)	8 (2%)	63	64
1	D	420/411 (102%)	410 (98%)	10 (2%)	57	56
All	All	1648/1644 (100%)	1615 (98%)	33 (2%)	63	64

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	6	PRO
1	A	12	ARG
1	A	201	ARG
1	A	294	ASP
1	A	331	THR
1	A	392	HIS

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Mol	Chain	Res	Type
1	B	5	ARG
1	B	12	ARG
1	B	27	ARG
1	B	52	ASN
1	B	247	ARG
1	B	325	HIS
1	B	326	ASN
1	B	494	LEU
1	C	2	PHE
1	C	5	ARG
1	C	80	GLN
1	C	291	GLU
1	C	297	ARG
1	C	326	ASN
1	C	392	HIS
1	C	405	LEU
1	D	5	ARG
1	D	6	PRO
1	D	31	LYS
1	D	83	ARG
1	D	190	GLU
1	D	201	ARG
1	D	247	ARG
1	D	316	LYS
1	D	331	THR
1	D	392	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
1	A	148	ASN
1	A	185	GLN
1	A	350	ASN
1	A	392	HIS
1	A	436	GLN
1	A	490	GLN
1	B	52	ASN
1	B	69	ASN
1	B	148	ASN
1	B	173	ASN
1	B	185	GLN

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Mol	Chain	Res	Type
1	B	325	HIS
1	B	326	ASN
1	B	350	ASN
1	B	467	ASN
1	B	471	GLN
1	B	490	GLN
1	C	7	ASN
1	C	80	GLN
1	C	148	ASN
1	C	326	ASN
1	C	392	HIS
1	C	419	GLN
1	C	467	ASN
1	C	490	GLN
1	D	51	GLN
1	D	69	ASN
1	D	148	ASN
1	D	173	ASN
1	D	185	GLN
1	D	314	ASN
1	D	326	ASN
1	D	377	GLN
1	D	392	HIS
1	D	436	GLN
1	D	467	ASN
1	D	484	GLN
1	D	490	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	487/516 (94%)	-0.22	4 (0%) 87 88	11, 17, 34, 46	0
1	B	487/516 (94%)	-0.29	6 (1%) 81 82	8, 15, 33, 44	0
1	C	487/516 (94%)	-0.28	7 (1%) 78 79	8, 16, 33, 47	0
1	D	497/516 (96%)	-0.23	8 (1%) 74 76	10, 17, 32, 48	0
All	All	1958/2064 (94%)	-0.26	25 (1%) 79 80	8, 17, 33, 48	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	306	ASN	5.7
1	D	316	LYS	4.1
1	C	306	ASN	3.8
1	C	319	GLY	3.8
1	D	474	GLY	3.8
1	B	324	ASP	3.7
1	A	319	GLY	3.6
1	A	306	ASN	3.5
1	A	324	ASP	3.4
1	B	473	SER	3.4
1	D	324	ASP	3.4
1	B	319	GLY	3.3
1	D	319	GLY	3.2
1	A	516	SER	3.0
1	C	2	PHE	2.9
1	D	325	HIS	2.9
1	C	474	GLY	2.9
1	D	473	SER	2.8
1	D	312	SER	2.6
1	B	379	ASP	2.4
1	D	315	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	473	SER	2.3
1	C	324	ASP	2.2
1	B	474	GLY	2.1
1	C	12	ARG	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.