



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 11:34 pm GMT

PDB ID : 2Q4F  
Title : Ensemble refinement of the crystal structure of putative histidine-containing phosphotransfer protein from rice, Ak104879  
Authors : Levin, E.J.; Kondrashov, D.A.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)  
Deposited on : 2007-05-31  
Resolution : 2.00 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

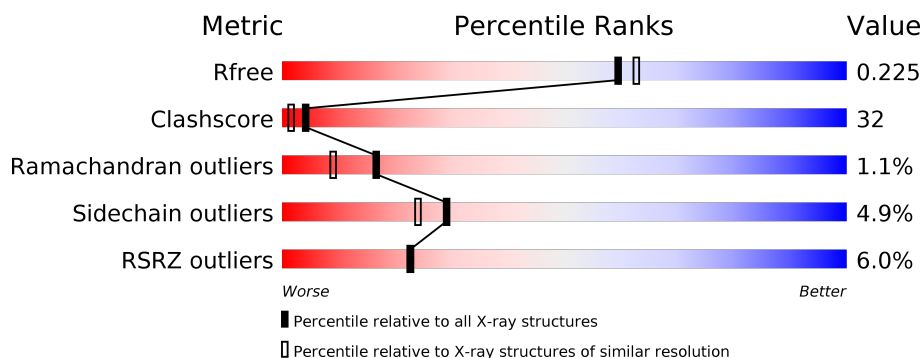
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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	1-A	149	
1	1-B	149	
1	2-A	149	
1	2-B	149	
1	3-A	149	
1	3-B	149	

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Mol	Chain	Length	Quality of chain
1	4-A	149	
1	4-B	149	
1	5-A	149	
1	5-B	149	
1	6-A	149	
1	6-B	149	
1	7-A	149	
1	7-B	149	
1	8-A	149	
1	8-B	149	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20000 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 Histidine-containing phosphotransfer protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	140	Total	C	N	O	S	0	0	0
			1102	692	188	213	9			
1	2-A	140	Total	C	N	O	S	0	0	0
			1102	692	188	213	9			
1	3-A	140	Total	C	N	O	S	0	0	0
			1102	692	188	213	9			
1	4-A	140	Total	C	N	O	S	0	0	0
			1102	692	188	213	9			
1	5-A	140	Total	C	N	O	S	0	0	0
			1102	692	188	213	9			
1	6-A	140	Total	C	N	O	S	0	0	0
			1102	692	188	213	9			
1	7-A	140	Total	C	N	O	S	0	0	0
			1102	692	188	213	9			
1	8-A	140	Total	C	N	O	S	0	0	0
			1102	692	188	213	9			
1	1-B	136	Total	C	N	O	S	0	0	0
			1079	679	184	207	9			
1	2-B	136	Total	C	N	O	S	0	0	0
			1079	679	184	207	9			
1	3-B	136	Total	C	N	O	S	0	0	0
			1079	679	184	207	9			
1	4-B	136	Total	C	N	O	S	0	0	0
			1079	679	184	207	9			
1	5-B	136	Total	C	N	O	S	0	0	0
			1079	679	184	207	9			
1	6-B	136	Total	C	N	O	S	0	0	0
			1079	679	184	207	9			
1	7-B	136	Total	C	N	O	S	0	0	0
			1079	679	184	207	9			
1	8-B	136	Total	C	N	O	S	0	0	0
			1079	679	184	207	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	EXPRESSION TAG	UNP Q6VAK4
B	1	SER	-	EXPRESSION TAG	UNP Q6VAK4

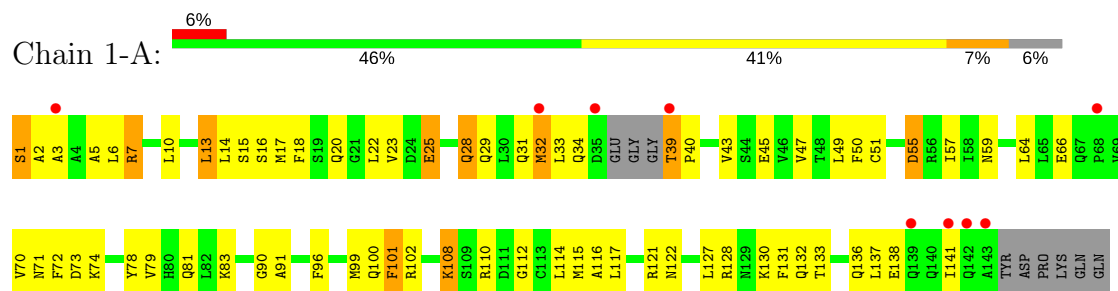
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	1-A	172	Total	O	0	0
			172	172		
2	2-A	169	Total	O	0	0
			169	169		
2	3-A	172	Total	O	0	0
			172	172		
2	4-A	172	Total	O	0	0
			172	172		
2	5-A	172	Total	O	0	0
			172	172		
2	6-A	171	Total	O	0	0
			171	171		
2	7-A	172	Total	O	0	0
			172	172		
2	8-A	173	Total	O	0	0
			173	173		
2	1-B	147	Total	O	0	0
			147	147		
2	2-B	150	Total	O	0	0
			150	150		
2	3-B	147	Total	O	0	0
			147	147		
2	4-B	147	Total	O	0	0
			147	147		
2	5-B	147	Total	O	0	0
			147	147		
2	6-B	148	Total	O	0	0
			148	148		
2	7-B	147	Total	O	0	0
			147	147		
2	8-B	146	Total	O	0	0
			146	146		

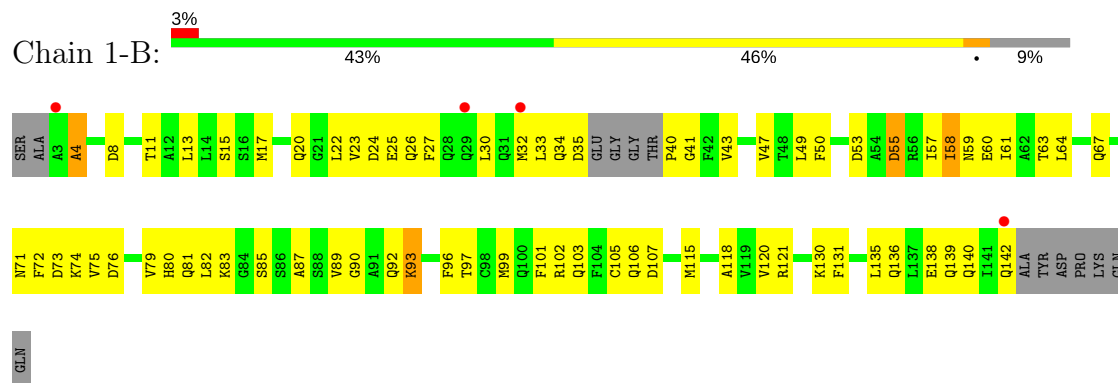
### 3 Residue-property plots [i](#)

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

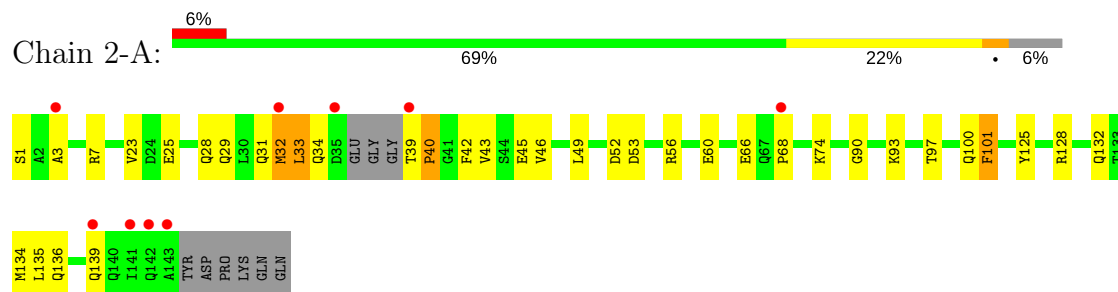
- Molecule 1: Histidine-containing phosphotransfer protein 1



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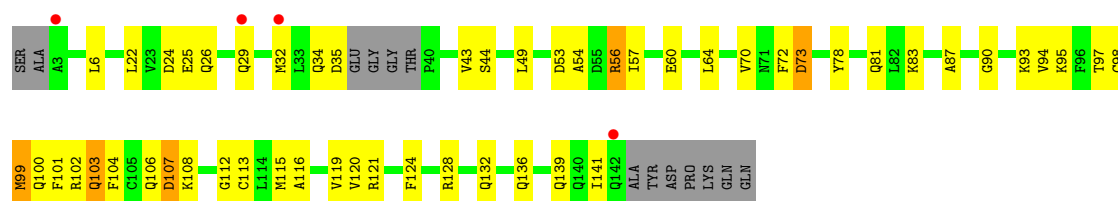


- Molecule 1: Histidine-containing phosphotransfer protein 1

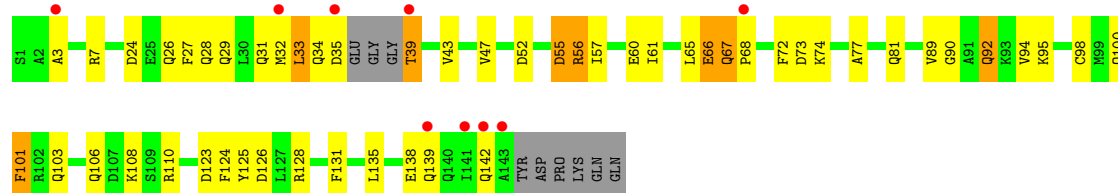


- Molecule 1: Histidine-containing phosphotransfer protein 1

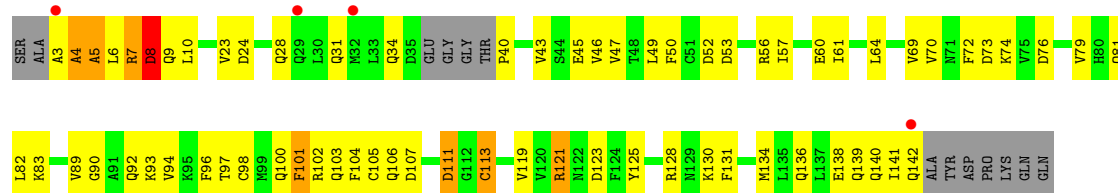




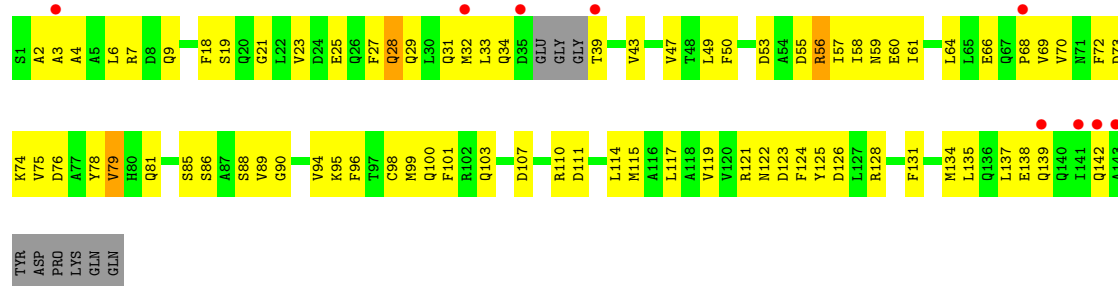
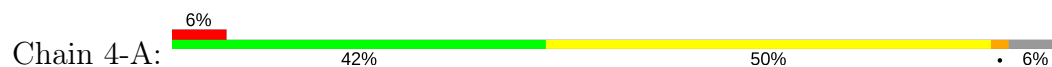
• Molecule 1: Histidine-containing phosphotransfer protein 1



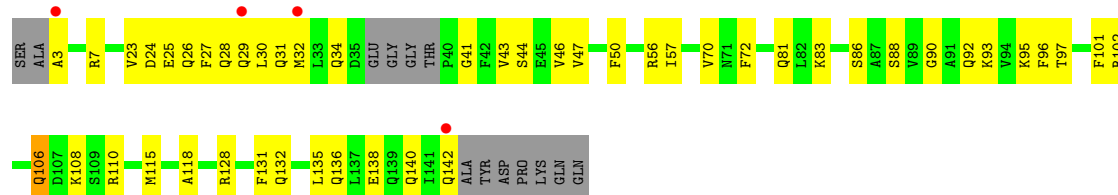
• Molecule 1: Histidine-containing phosphotransfer protein 1



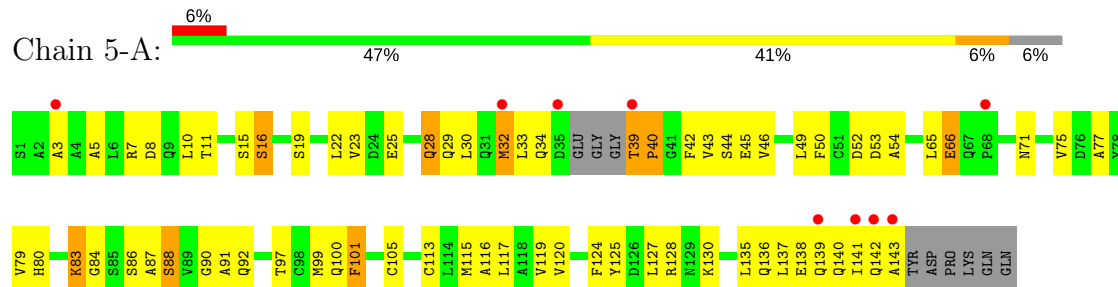
• Molecule 1: Histidine-containing phosphotransfer protein 1



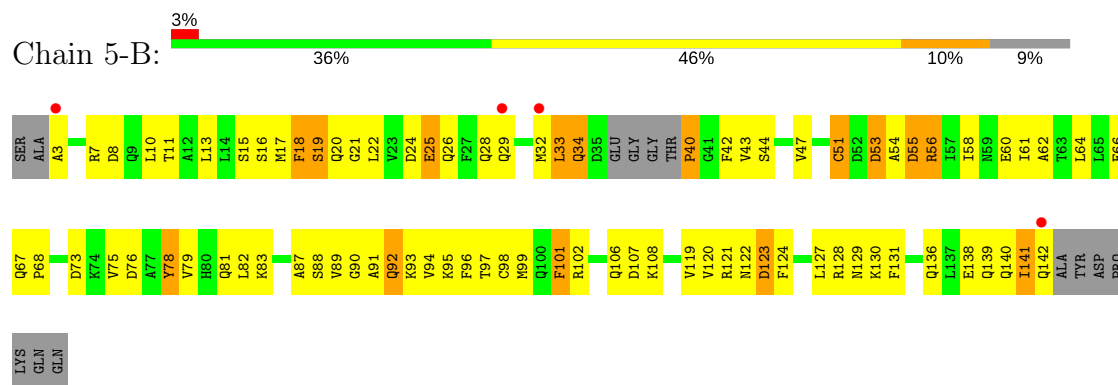
• Molecule 1: Histidine-containing phosphotransfer protein 1



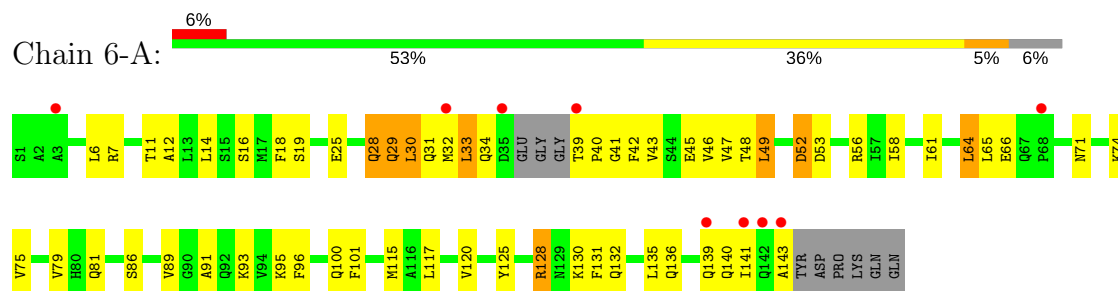
## • Molecule 1: Histidine-containing phosphotransfer protein 1



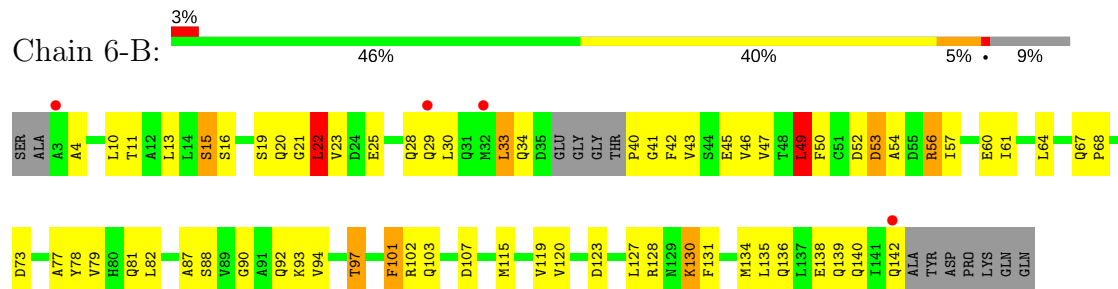
## • Molecule 1: Histidine-containing phosphotransfer protein 1



## • Molecule 1: Histidine-containing phosphotransfer protein 1



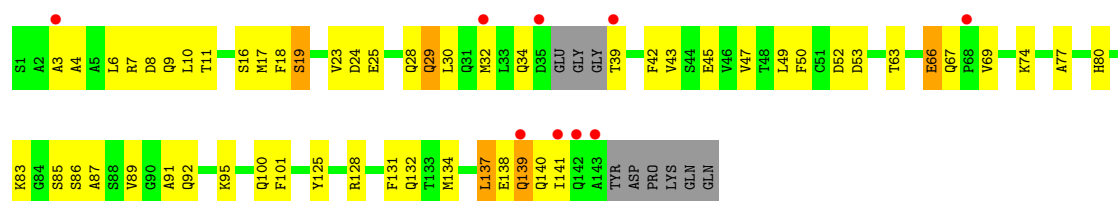
## • Molecule 1: Histidine-containing phosphotransfer protein 1



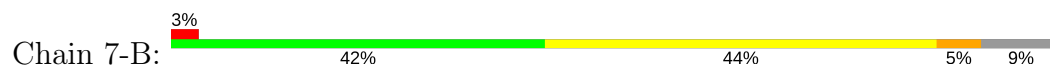
## • Molecule 1: Histidine-containing phosphotransfer protein 1







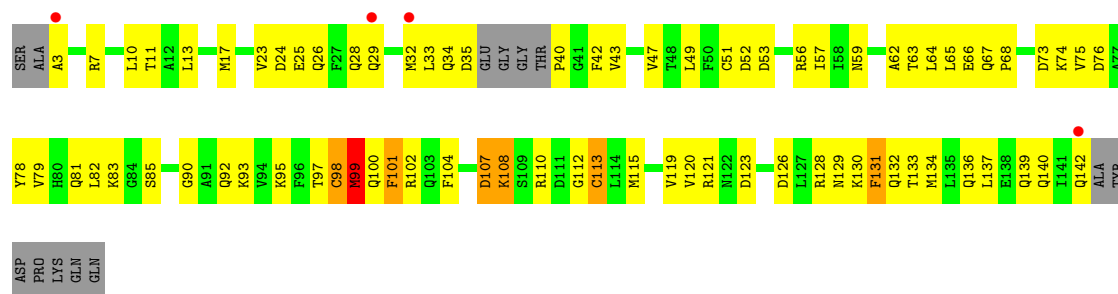
- Molecule 1: Histidine-containing phosphotransfer protein 1



- Molecule 1: Histidine-containing phosphotransfer protein 1



- Molecule 1: Histidine-containing phosphotransfer protein 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.56Å 100.56Å 69.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.77 – 2.00 37.77 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.0 (37.77-2.00) 99.0 (37.77-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.22 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.145 , 0.222 0.156 , 0.225	Depositor DCC
$R_{free}$ test set	1248 reflections (5.38%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.5	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 63.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	20000	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.08% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	1-A	1.03	0/1115	0.83	1/1501 (0.1%)
1	1-B	0.99	0/1092	0.89	3/1468 (0.2%)
1	2-A	1.01	2/1115 (0.2%)	0.77	0/1501
1	2-B	0.93	0/1092	0.86	2/1468 (0.1%)
1	3-A	1.04	3/1115 (0.3%)	0.83	1/1501 (0.1%)
1	3-B	1.03	1/1092 (0.1%)	0.92	2/1468 (0.1%)
1	4-A	1.02	0/1115	0.93	5/1501 (0.3%)
1	4-B	0.95	0/1092	0.86	0/1468
1	5-A	1.12	2/1115 (0.2%)	0.92	0/1501
1	5-B	1.11	2/1092 (0.2%)	1.01	4/1468 (0.3%)
1	6-A	1.13	3/1115 (0.3%)	0.90	3/1501 (0.2%)
1	6-B	1.06	0/1092	1.00	6/1468 (0.4%)
1	7-A	1.12	3/1115 (0.3%)	0.90	1/1501 (0.1%)
1	7-B	1.07	2/1092 (0.2%)	0.94	3/1468 (0.2%)
1	8-A	1.14	3/1115 (0.3%)	0.89	2/1501 (0.1%)
1	8-B	1.17	3/1092 (0.3%)	0.96	2/1468 (0.1%)
All	All	1.06	24/17656 (0.1%)	0.90	35/23752 (0.1%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	8-B	113	CYS	CB-SG	-8.95	1.67	1.82
1	8-B	98	CYS	CB-SG	-8.49	1.67	1.82
1	5-B	51	CYS	CB-SG	7.64	1.95	1.82
1	3-B	113	CYS	CB-SG	-7.42	1.69	1.82
1	7-A	125	TYR	CD2-CE2	7.00	1.49	1.39
1	8-A	125	TYR	CD2-CE2	6.87	1.49	1.39
1	6-A	125	TYR	CD2-CE2	6.86	1.49	1.39
1	5-A	125	TYR	CD2-CE2	6.82	1.49	1.39
1	3-A	125	TYR	CD2-CE2	6.40	1.49	1.39
1	2-A	125	TYR	CD2-CE2	6.36	1.48	1.39
1	3-A	66	GLU	CG-CD	6.30	1.61	1.51
1	8-B	99	MET	CG-SD	6.23	1.97	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2-A	45	GLU	CB-CG	6.12	1.63	1.52
1	8-A	105	CYS	CB-SG	-5.97	1.72	1.81
1	6-A	52	ASP	CB-CG	5.75	1.63	1.51
1	7-A	66	GLU	CG-CD	5.60	1.60	1.51
1	7-B	51	CYS	CB-SG	5.17	1.91	1.82
1	5-A	66	GLU	CG-CD	5.08	1.59	1.51
1	5-B	94	VAL	CB-CG2	5.08	1.63	1.52
1	3-A	66	GLU	CB-CG	5.07	1.61	1.52
1	7-B	119	VAL	CB-CG2	5.05	1.63	1.52
1	6-A	120	VAL	CB-CG1	5.04	1.63	1.52
1	7-A	4	ALA	CA-CB	5.03	1.63	1.52
1	8-A	120	VAL	CB-CG1	5.02	1.63	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4-A	121	ARG	NE-CZ-NH1	9.77	125.19	120.30
1	6-B	52	ASP	CB-CG-OD1	8.35	125.81	118.30
1	5-B	123	ASP	CB-CG-OD2	-7.91	111.18	118.30
1	7-A	137	LEU	CA-CB-CG	7.76	133.15	115.30
1	5-B	121	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	2-B	121	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	3-B	111	ASP	CB-CG-OD1	-7.60	111.46	118.30
1	1-B	121	ARG	NE-CZ-NH2	-7.35	116.62	120.30
1	3-B	121	ARG	NE-CZ-NH2	-7.29	116.65	120.30
1	4-A	56	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	4-A	121	ARG	NE-CZ-NH2	-7.11	116.74	120.30
1	4-A	56	ARG	NE-CZ-NH1	6.99	123.79	120.30
1	5-B	56	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	8-A	73	ASP	CB-CG-OD1	6.33	124.00	118.30
1	8-B	33	LEU	CA-CB-CG	6.21	129.57	115.30
1	6-B	49	LEU	CA-CB-CG	5.99	129.07	115.30
1	1-B	33	LEU	CA-CB-CG	5.88	128.82	115.30
1	6-A	128	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	4-A	107	ASP	CB-CA-C	-5.79	98.81	110.40
1	6-B	53	ASP	CB-CG-OD1	5.67	123.40	118.30
1	3-A	52	ASP	CB-CG-OD1	-5.62	113.25	118.30
1	8-B	121	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	7-B	56	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	7-B	56	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	6-B	56	ARG	NE-CZ-NH1	-5.51	117.54	120.30
1	6-A	128	ARG	NE-CZ-NH1	5.47	123.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-B	41	GLY	N-CA-C	-5.46	99.45	113.10
1	6-B	22	LEU	CA-CB-CG	-5.26	103.20	115.30
1	1-A	49	LEU	CA-CB-CG	5.25	127.38	115.30
1	5-B	123	ASP	CB-CG-OD1	5.18	122.97	118.30
1	7-B	73	ASP	CB-CG-OD2	5.10	122.89	118.30
1	6-A	49	LEU	CA-CB-CG	5.08	126.97	115.30
1	6-B	56	ARG	NE-CZ-NH2	5.07	122.83	120.30
1	8-A	128	ARG	NE-CZ-NH2	-5.00	117.80	120.30
1	2-B	101	PHE	N-CA-C	5.00	124.51	111.00

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	1-A	1102	0	1092	87	0
1	1-B	1079	0	1068	85	0
1	2-A	1102	0	1092	36	0
1	2-B	1079	0	1068	68	0
1	3-A	1102	0	1092	50	0
1	3-B	1079	0	1068	83	0
1	4-A	1102	0	1092	72	0
1	4-B	1079	0	1068	48	0
1	5-A	1102	0	1092	78	0
1	5-B	1079	0	1068	107	0
1	6-A	1102	0	1092	74	0
1	6-B	1079	0	1068	73	0
1	7-A	1102	0	1092	58	0
1	7-B	1079	0	1068	100	0
1	8-A	1102	0	1092	69	0
1	8-B	1079	0	1068	73	0
2	1-A	172	0	0	23	0
2	1-B	147	0	0	17	0
2	2-A	169	0	0	12	0
2	2-B	150	0	0	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	3-A	172	0	0	17	0
2	3-B	147	0	0	15	0
2	4-A	172	0	0	18	0
2	4-B	147	0	0	15	0
2	5-A	172	0	0	17	0
2	5-B	147	0	0	28	0
2	6-A	171	0	0	15	0
2	6-B	148	0	0	17	0
2	7-A	172	0	0	18	0
2	7-B	147	0	0	21	0
2	8-A	173	0	0	17	0
2	8-B	146	0	0	18	0
All	All	20000	0	17280	1128	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 32.

All (1128) 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:B:97:THR:HG23	2:B:185:HOH:O	1.34	1.23
1:B:57:ILE:HG21	1:B:82:LEU:HB2	1.34	1.10
1:B:97:THR:HG23	2:B:186:HOH:O	1.52	1.10
1:A:57:ILE:HD13	1:A:82:LEU:HD13	1.33	1.08
1:A:43:VAL:O	1:A:47:VAL:HG23	1.53	1.08
1:B:97:THR:HG21	1:B:120:VAL:HA	1.32	1.08
1:B:72:PHE:O	1:B:76:ASP:HB2	1.56	1.06
1:B:26:GLN:HA	1:B:29:GLN:HG3	1.33	1.06
1:B:79:VAL:HB	2:B:295:HOH:O	1.53	1.05
1:A:5:ALA:HA	1:A:8:ASP:OD2	1.60	1.02
1:B:99:MET:O	2:B:174:HOH:O	1.79	1.01
1:A:10:LEU:HD21	1:A:138:GLU:HG2	1.41	1.01
1:A:130:LYS:NZ	2:A:165:HOH:O	1.83	1.00
1:A:39:THR:HG22	1:A:42:PHE:HB2	1.44	0.99
1:B:79:VAL:HB	2:B:296:HOH:O	1.61	0.98
1:B:28:GLN:HA	1:B:31:GLN:OE1	1.63	0.98
1:A:71:ASN:ND2	1:A:74:LYS:HG3	1.80	0.97
1:B:6:LEU:HA	1:B:9:GLN:OE1	1.64	0.96
1:B:103:GLN:HG3	2:B:155:HOH:O	1.66	0.96
2:A:260:HOH:O	1:B:40:PRO:HD3	1.64	0.95
1:A:24:ASP:HB3	1:A:92:GLN:OE1	1.65	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:VAL:HG12	1:B:98:CYS:SG	2.06	0.95
1:B:66:GLU:OE1	2:B:214:HOH:O	1.85	0.95
1:A:29:GLN:HA	1:A:32:MET:HG3	1.50	0.94
1:A:25:GLU:OE2	2:A:318:HOH:O	1.84	0.94
1:B:136:GLN:NE2	1:B:140:GLN:HG2	1.82	0.94
1:A:29:GLN:HA	1:A:32:MET:HG3	1.50	0.93
1:B:81:GLN:O	1:B:85:SER:HB2	1.68	0.93
1:A:81:GLN:OE1	1:B:49:LEU:HB3	1.69	0.92
1:B:56:ARG:NH1	2:B:191:HOH:O	1.74	0.92
1:A:39:THR:HG23	1:A:42:PHE:HB2	1.51	0.92
1:A:66:GLU:OE1	2:A:296:HOH:O	1.89	0.91
1:A:128:ARG:NH1	2:A:176:HOH:O	1.95	0.90
1:B:67:GLN:HB2	1:B:70:VAL:HA	1.54	0.90
1:B:65:LEU:HD21	1:B:113:CYS:SG	2.12	0.90
1:A:55:ASP:OD1	2:A:282:HOH:O	1.89	0.90
1:A:39:THR:HG21	1:B:76:ASP:OD2	1.72	0.90
1:B:83:LYS:HD2	1:B:99:MET:HG3	1.53	0.89
1:A:58:ILE:HG23	1:A:117:LEU:HD11	1.54	0.89
1:B:29:GLN:HA	1:B:32:MET:HG3	1.52	0.88
1:B:29:GLN:HA	1:B:32:MET:HG3	1.55	0.88
1:A:100:GLN:HG3	2:A:202:HOH:O	1.74	0.88
1:B:26:GLN:NE2	1:B:29:GLN:HG3	1.88	0.88
1:B:136:GLN:HE22	1:B:140:GLN:HE21	1.23	0.87
1:B:87:ALA:HB2	1:B:95:LYS:HD2	1.53	0.87
1:B:136:GLN:NE2	1:B:140:GLN:HG3	1.88	0.87
1:B:87:ALA:CB	1:B:95:LYS:HD2	2.04	0.86
1:B:56:ARG:NH2	2:B:179:HOH:O	2.07	0.86
1:A:68:PRO:HD2	2:A:189:HOH:O	1.74	0.86
1:B:26:GLN:HB2	1:B:90:GLY:HA2	1.55	0.86
1:B:129:ASN:ND2	2:B:214:HOH:O	2.10	0.85
1:A:66:GLU:HG3	2:A:248:HOH:O	1.75	0.85
1:B:60:GLU:OE2	2:B:235:HOH:O	1.94	0.85
1:B:26:GLN:HA	1:B:29:GLN:CG	2.07	0.85
1:B:25:GLU:O	1:B:28:GLN:HB3	1.77	0.84
1:A:86:SER:HB2	1:A:91:ALA:HB3	1.60	0.84
1:B:20:GLN:O	1:B:20:GLN:HG2	1.73	0.84
1:A:68:PRO:HD2	2:A:188:HOH:O	1.78	0.84
1:A:57:ILE:CD1	1:A:82:LEU:HD13	2.06	0.84
1:B:88:SER:HB2	2:B:271:HOH:O	1.78	0.84
1:B:49:LEU:HD21	2:B:280:HOH:O	1.77	0.83
1:A:68:PRO:HD2	2:A:187:HOH:O	1.77	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:LEU:HA	1:A:9:GLN:HE21	1.43	0.83
1:A:55:ASP:OD1	2:A:181:HOH:O	1.95	0.83
1:B:139:GLN:HG3	1:B:142:GLN:NE2	1.93	0.83
1:B:44:SER:HB2	2:B:170:HOH:O	1.78	0.83
1:B:18:PHE:O	1:B:20:GLN:N	2.11	0.83
1:B:93:LYS:HE2	2:B:177:HOH:O	1.77	0.83
1:B:60:GLU:OE2	2:B:286:HOH:O	1.96	0.83
1:B:60:GLU:O	1:B:64:LEU:HG	1.79	0.82
1:B:50:PHE:CD2	1:B:89:VAL:HG11	2.15	0.82
1:B:126:ASP:OD2	2:B:275:HOH:O	1.96	0.82
1:A:6:LEU:HA	1:A:9:GLN:NE2	1.95	0.81
1:B:34:GLN:NE2	1:B:43:VAL:H	1.77	0.81
1:B:129:ASN:HB3	2:B:215:HOH:O	1.81	0.81
1:A:39:THR:HG22	1:A:42:PHE:HB2	1.61	0.81
1:A:30:LEU:HD22	1:A:43:VAL:HG22	1.62	0.81
1:A:21:GLY:HA2	2:A:178:HOH:O	1.80	0.81
1:B:136:GLN:HE21	1:B:140:GLN:HG2	1.45	0.81
1:B:61:ILE:HD11	1:B:78:TYR:HB3	1.63	0.81
1:B:7:ARG:O	1:B:10:LEU:N	2.12	0.81
1:B:3:ALA:N	1:B:7:ARG:HH21	1.78	0.80
1:A:34:GLN:HE21	1:A:43:VAL:H	1.26	0.80
1:B:102:ARG:HG2	2:B:295:HOH:O	1.81	0.80
1:A:74:LYS:NZ	2:A:269:HOH:O	2.13	0.80
1:B:136:GLN:HE22	1:B:140:GLN:HG3	1.47	0.80
1:B:24:ASP:OD1	1:B:26:GLN:N	2.15	0.80
1:B:97:THR:HG21	1:B:120:VAL:CA	2.12	0.79
1:B:56:ARG:NH1	2:B:193:HOH:O	1.89	0.79
1:B:50:PHE:CE2	1:B:89:VAL:HG11	2.18	0.79
1:A:69:VAL:HA	2:A:208:HOH:O	1.84	0.78
1:B:97:THR:HG23	2:B:185:HOH:O	1.83	0.77
1:B:24:ASP:N	1:B:90:GLY:O	2.13	0.77
1:A:57:ILE:HG21	1:A:82:LEU:HD22	1.65	0.77
1:A:39:THR:HG23	1:B:73:ASP:HA	1.64	0.77
1:A:13:LEU:HD13	1:A:13:LEU:C	2.04	0.77
1:B:131:PHE:O	1:B:134:MET:HB3	1.85	0.76
1:B:97:THR:CG2	2:B:185:HOH:O	2.33	0.76
1:A:34:GLN:HB2	1:A:43:VAL:HG23	1.67	0.76
1:B:97:THR:HG22	2:B:185:HOH:O	1.85	0.76
1:A:57:ILE:HD11	1:A:81:GLN:NE2	2.01	0.76
1:A:55:ASP:O	1:A:59:ASN:ND2	2.19	0.76
1:B:34:GLN:HE21	1:B:43:VAL:H	1.31	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:GLN:HB2	1:B:90:GLY:HA2	1.68	0.76
1:B:97:THR:HG22	1:B:120:VAL:HG22	1.68	0.76
1:A:66:GLU:HG2	2:A:248:HOH:O	1.86	0.76
1:B:56:ARG:NH2	2:B:180:HOH:O	2.16	0.75
1:A:72:PHE:O	1:A:76:ASP:HB2	1.86	0.75
1:B:128:ARG:NE	2:B:161:HOH:O	2.09	0.75
1:B:3:ALA:HA	1:B:7:ARG:NH1	2.01	0.75
1:A:22:LEU:HB3	1:A:127:LEU:HD13	1.67	0.75
1:B:142:GLN:HB2	2:B:225:HOH:O	1.87	0.75
1:B:111:ASP:OD2	2:B:210:HOH:O	2.04	0.75
1:A:57:ILE:CG2	1:A:82:LEU:HD22	2.16	0.75
1:B:20:GLN:O	2:B:274:HOH:O	2.05	0.75
1:A:45:GLU:O	1:A:49:LEU:HB2	1.87	0.75
1:B:92:GLN:NE2	2:B:250:HOH:O	2.19	0.74
1:B:56:ARG:HD3	2:B:192:HOH:O	1.87	0.74
1:A:137:LEU:HA	1:A:140:GLN:HE21	1.51	0.74
1:B:103:GLN:HE22	1:B:106:GLN:NE2	1.86	0.74
1:B:96:PHE:O	1:B:99:MET:HB2	1.87	0.74
1:B:15:SER:OG	2:B:276:HOH:O	2.05	0.74
1:B:25:GLU:CD	1:B:25:GLU:H	1.91	0.74
1:A:9:GLN:OE1	2:A:294:HOH:O	2.06	0.74
1:A:16:SER:HA	1:A:19:SER:OG	1.88	0.73
1:A:41:GLY:O	1:A:45:GLU:HG2	1.87	0.73
1:B:24:ASP:HB3	1:B:92:GLN:NE2	2.03	0.73
1:A:81:GLN:NE2	1:B:49:LEU:HD11	2.02	0.73
1:B:33:LEU:O	1:B:33:LEU:HG	1.86	0.73
1:B:28:GLN:HG2	1:B:32:MET:HE2	1.70	0.73
1:B:52:ASP:OD2	2:B:251:HOH:O	2.05	0.73
1:A:117:LEU:HD12	1:A:117:LEU:O	1.89	0.73
1:A:64:LEU:O	1:A:66:GLU:N	2.21	0.73
1:A:50:PHE:HE1	1:A:85:SER:HG	1.37	0.73
1:B:64:LEU:O	1:B:67:GLN:HG2	1.89	0.73
1:B:125:TYR:HB3	2:B:176:HOH:O	1.89	0.72
1:B:110:ARG:O	1:B:113:CYS:HB3	1.89	0.72
1:A:134:MET:O	1:A:138:GLU:HG3	1.90	0.72
1:A:34:GLN:HE21	1:A:43:VAL:H	1.37	0.72
1:A:66:GLU:OE1	2:A:300:HOH:O	2.05	0.72
1:B:3:ALA:N	2:B:222:HOH:O	2.23	0.72
1:B:60:GLU:HG3	2:B:285:HOH:O	1.88	0.72
1:A:23:VAL:HA	1:A:90:GLY:O	1.89	0.72
1:A:52:ASP:OD1	2:A:200:HOH:O	2.08	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:GLN:OE1	2:A:312:HOH:O	2.08	0.71
1:B:20:GLN:O	1:B:20:GLN:HG2	1.89	0.71
1:B:53:ASP:O	1:B:56:ARG:N	2.22	0.71
1:B:91:ALA:HB1	1:B:127:LEU:CD2	2.20	0.71
1:A:29:GLN:O	1:A:33:LEU:HB2	1.89	0.71
1:B:106:GLN:OE1	2:B:201:HOH:O	2.08	0.71
1:A:34:GLN:HG3	1:A:40:PRO:O	1.90	0.71
1:A:66:GLU:HG3	2:A:247:HOH:O	1.90	0.71
1:B:55:ASP:OD2	2:B:293:HOH:O	2.08	0.71
1:A:6:LEU:HD23	1:A:9:GLN:NE2	2.06	0.71
1:B:129:ASN:OD1	2:B:216:HOH:O	2.07	0.71
1:B:32:MET:O	1:B:35:ASP:N	2.22	0.71
1:B:73:ASP:OD2	2:B:177:HOH:O	2.09	0.70
1:B:57:ILE:O	1:B:60:GLU:N	2.22	0.70
1:B:128:ARG:NH1	2:B:181:HOH:O	1.93	0.70
1:A:74:LYS:HE3	2:A:266:HOH:O	1.90	0.70
1:B:64:LEU:HD21	1:B:74:LYS:HE2	1.72	0.70
1:A:53:ASP:OD2	1:B:81:GLN:NE2	2.25	0.70
1:A:102:ARG:HB3	1:A:102:ARG:NH1	2.05	0.70
1:B:113:CYS:O	1:B:116:ALA:HB3	1.91	0.70
1:A:56:ARG:NH2	2:A:310:HOH:O	2.20	0.70
1:A:138:GLU:O	1:A:142:GLN:HG3	1.92	0.70
1:A:44:SER:OG	2:A:175:HOH:O	2.09	0.70
1:A:39:THR:HG21	1:B:73:ASP:HA	1.72	0.70
1:B:28:GLN:HA	1:B:31:GLN:OE1	1.91	0.70
1:B:53:ASP:OD1	2:B:190:HOH:O	2.09	0.69
1:A:123:ASP:OD1	2:A:157:HOH:O	2.09	0.69
1:A:66:GLU:OE1	2:A:300:HOH:O	2.09	0.69
1:A:112:GLY:O	1:A:116:ALA:HB2	1.91	0.69
1:A:20:GLN:OE1	2:A:287:HOH:O	2.08	0.69
1:B:30:LEU:HD23	1:B:43:VAL:HG13	1.74	0.69
1:B:72:PHE:O	1:B:76:ASP:CB	2.39	0.69
1:B:136:GLN:HE21	1:B:140:GLN:CD	1.95	0.69
1:A:34:GLN:NE2	1:A:43:VAL:H	1.91	0.69
1:B:25:GLU:O	1:B:29:GLN:HG2	1.92	0.69
1:A:39:THR:HB	1:B:76:ASP:OD2	1.92	0.69
1:A:2:ALA:O	2:A:193:HOH:O	2.11	0.69
1:A:39:THR:HG23	1:A:39:THR:O	1.91	0.69
1:A:30:LEU:CD2	1:A:43:VAL:HG22	2.23	0.69
1:B:75:VAL:O	1:B:79:VAL:HG23	1.92	0.69
1:B:108:LYS:NZ	2:B:287:HOH:O	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:GLN:HE21	1:B:29:GLN:HG3	1.57	0.69
1:A:34:GLN:HE21	1:A:43:VAL:H	1.40	0.69
1:B:101:PHE:CZ	1:B:113:CYS:HB2	2.27	0.69
1:B:53:ASP:O	1:B:57:ILE:HG13	1.93	0.69
1:B:140:GLN:C	1:B:142:GLN:H	1.96	0.68
1:B:20:GLN:O	2:B:275:HOH:O	2.10	0.68
1:A:103:GLN:OE1	2:A:312:HOH:O	2.11	0.68
1:B:28:GLN:HG2	1:B:32:MET:CE	2.23	0.68
1:B:24:ASP:HB3	1:B:92:GLN:HB2	1.75	0.68
1:A:122:ASN:OD1	2:A:150:HOH:O	2.11	0.68
1:A:134:MET:HG2	1:A:134:MET:O	1.92	0.68
1:B:15:SER:OG	2:B:278:HOH:O	2.11	0.68
1:B:94:VAL:HG13	1:B:120:VAL:HG13	1.75	0.68
1:A:3:ALA:O	1:A:7:ARG:HG3	1.93	0.68
1:B:81:GLN:O	1:B:85:SER:CB	2.42	0.68
1:A:73:ASP:OD2	1:B:41:GLY:N	2.24	0.68
1:B:128:ARG:O	1:B:132:GLN:HG3	1.94	0.68
1:B:53:ASP:HB3	2:B:181:HOH:O	1.94	0.68
1:A:66:GLU:HG2	2:A:269:HOH:O	1.92	0.68
1:B:138:GLU:OE1	2:B:263:HOH:O	2.12	0.68
1:B:135:LEU:HD23	1:B:138:GLU:OE1	1.94	0.68
1:B:56:ARG:HD2	2:B:287:HOH:O	1.94	0.67
1:B:56:ARG:HH12	1:B:57:ILE:CG1	2.07	0.67
1:B:107:ASP:CG	2:B:291:HOH:O	2.33	0.67
1:A:74:LYS:NZ	2:A:270:HOH:O	2.02	0.67
1:B:30:LEU:HD11	1:B:46:VAL:HG11	1.76	0.67
1:B:128:ARG:O	1:B:132:GLN:HG3	1.95	0.67
1:B:32:MET:O	1:B:35:ASP:N	2.24	0.67
1:A:120:VAL:O	1:A:120:VAL:HG12	1.95	0.67
1:A:39:THR:HG23	1:A:39:THR:O	1.93	0.67
1:A:52:ASP:OD2	2:A:296:HOH:O	2.12	0.67
1:A:49:LEU:HD13	2:B:192:HOH:O	1.94	0.67
1:A:32:MET:HA	1:A:35:ASP:OD2	1.95	0.66
1:B:3:ALA:HA	1:B:7:ARG:CZ	2.26	0.66
1:A:23:VAL:HA	1:A:90:GLY:O	1.96	0.66
1:B:75:VAL:O	1:B:79:VAL:HG23	1.95	0.66
1:B:56:ARG:HH12	1:B:57:ILE:HG13	1.61	0.66
1:A:34:GLN:HE21	1:A:43:VAL:H	1.43	0.66
1:B:17:MET:HG2	1:B:130:LYS:HG2	1.78	0.66
1:A:68:PRO:HD2	2:A:188:HOH:O	1.95	0.66
1:A:39:THR:HG23	1:A:39:THR:O	1.93	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ASN:OD1	2:B:295:HOH:O	2.13	0.66
1:A:8:ASP:O	1:A:11:THR:N	2.28	0.66
1:A:45:GLU:OE1	2:A:155:HOH:O	2.12	0.66
1:A:61:ILE:HG21	1:A:117:LEU:HD13	1.78	0.65
1:B:72:PHE:HE1	1:B:113:CYS:SG	2.19	0.65
1:B:28:GLN:O	1:B:32:MET:HG3	1.97	0.65
1:B:93:LYS:CE	2:B:274:HOH:O	2.43	0.65
1:B:104:PHE:HA	1:B:107:ASP:OD2	1.96	0.65
1:B:56:ARG:O	1:B:56:ARG:HG2	1.96	0.65
1:A:18:PHE:O	2:A:178:HOH:O	2.15	0.65
1:B:94:VAL:O	1:B:98:CYS:SG	2.54	0.65
1:B:8:ASP:OD2	2:B:229:HOH:O	2.15	0.65
1:B:16:SER:O	1:B:20:GLN:HB2	1.97	0.65
1:B:103:GLN:O	1:B:107:ASP:N	2.29	0.65
1:A:29:GLN:HA	1:A:32:MET:HG2	1.78	0.65
1:A:81:GLN:OE1	1:B:49:LEU:CB	2.43	0.65
1:A:6:LEU:HD23	1:A:9:GLN:HE22	1.62	0.65
1:A:53:ASP:OD2	2:A:298:HOH:O	2.14	0.64
1:A:125:TYR:HA	1:A:128:ARG:HB3	1.79	0.64
1:A:42:PHE:O	1:A:45:GLU:HB2	1.96	0.64
1:A:138:GLU:O	1:A:142:GLN:HG3	1.97	0.64
1:A:27:PHE:HB2	1:A:89:VAL:O	1.97	0.64
1:B:97:THR:CG2	1:B:120:VAL:HG22	2.26	0.64
1:A:88:SER:OG	2:A:214:HOH:O	2.15	0.64
1:A:10:LEU:HA	1:A:137:LEU:HD13	1.80	0.64
1:B:104:PHE:HB3	1:B:113:CYS:HB3	1.80	0.64
1:A:77:ALA:O	1:A:80:HIS:HB3	1.98	0.64
1:B:26:GLN:HB2	1:B:90:GLY:CA	2.26	0.64
1:B:128:ARG:NH2	2:B:161:HOH:O	2.26	0.64
1:A:128:ARG:NH2	2:A:262:HOH:O	2.30	0.64
1:B:34:GLN:NE2	1:B:43:VAL:HG23	2.13	0.63
1:B:103:GLN:NE2	1:B:107:ASP:OD1	2.28	0.63
1:B:72:PHE:CE1	1:B:113:CYS:SG	2.91	0.63
1:A:10:LEU:HD22	1:A:141:ILE:HD12	1.79	0.63
1:A:8:ASP:O	1:A:11:THR:HB	1.99	0.63
1:B:140:GLN:C	1:B:142:GLN:H	1.99	0.63
1:A:43:VAL:C	1:A:47:VAL:HG23	2.19	0.63
1:A:71:ASN:O	1:A:75:VAL:HG23	1.99	0.63
1:B:104:PHE:CE2	1:B:112:GLY:O	2.52	0.63
1:B:94:VAL:CG1	1:B:98:CYS:SG	2.85	0.63
1:B:71:ASN:OD1	1:B:73:ASP:HB2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:GLN:NE2	1:A:43:VAL:H	1.97	0.62
2:A:246:HOH:O	1:B:40:PRO:HG3	1.98	0.62
1:A:50:PHE:HE1	1:A:85:SER:OG	1.81	0.62
1:B:11:THR:HG22	2:B:270:HOH:O	1.98	0.62
1:B:139:GLN:O	1:B:142:GLN:HB3	2.00	0.62
1:B:57:ILE:HD11	1:B:81:GLN:NE2	2.14	0.62
1:B:70:VAL:HB	1:B:72:PHE:CE2	2.34	0.62
1:A:29:GLN:NE2	2:A:309:HOH:O	2.28	0.62
1:A:34:GLN:NE2	1:A:43:VAL:H	1.98	0.62
1:A:61:ILE:O	1:A:65:LEU:HG	2.00	0.62
1:B:121:ARG:HD3	1:B:125:TYR:HE2	1.64	0.62
1:A:57:ILE:HG21	1:A:82:LEU:HB2	1.82	0.62
1:A:6:LEU:HB3	1:A:141:ILE:CG1	2.30	0.62
1:A:79:VAL:HG11	1:A:101:PHE:HB3	1.80	0.62
1:A:70:VAL:HB	1:A:72:PHE:CE2	2.33	0.62
1:B:53:ASP:O	1:B:57:ILE:HD12	2.00	0.62
1:A:134:MET:HE3	2:A:167:HOH:O	1.98	0.62
1:B:136:GLN:HE22	1:B:139:GLN:HE22	1.48	0.62
1:A:34:GLN:NE2	1:A:43:VAL:H	1.97	0.61
1:B:93:LYS:HD3	1:B:123:ASP:OD1	2.00	0.61
1:B:53:ASP:HB3	2:B:180:HOH:O	1.99	0.61
1:A:57:ILE:HD11	1:A:81:GLN:NE2	2.14	0.61
1:B:83:LYS:NZ	2:B:203:HOH:O	2.33	0.61
1:B:49:LEU:HD23	1:B:49:LEU:O	2.00	0.61
1:B:136:GLN:NE2	1:B:139:GLN:HE22	1.98	0.61
1:B:11:THR:O	1:B:15:SER:HB3	1.99	0.61
1:A:136:GLN:HA	1:A:139:GLN:NE2	2.15	0.61
1:A:72:PHE:CD2	1:A:108:LYS:HG2	2.35	0.61
1:A:66:GLU:CG	2:A:247:HOH:O	2.47	0.61
1:B:81:GLN:NE2	2:B:180:HOH:O	2.33	0.61
1:B:23:VAL:HA	1:B:90:GLY:O	2.00	0.61
1:A:34:GLN:HE21	1:A:43:VAL:H	1.48	0.61
1:A:115:MET:O	1:A:119:VAL:HG23	2.01	0.61
1:A:4:ALA:HA	1:A:7:ARG:HH21	1.65	0.61
1:B:21:GLY:HA2	1:B:92:GLN:OE1	2.01	0.61
1:A:55:ASP:HB3	2:A:213:HOH:O	2.01	0.61
1:A:13:LEU:CD1	1:A:13:LEU:C	2.68	0.61
1:A:66:GLU:CB	2:A:300:HOH:O	2.48	0.61
1:A:107:ASP:O	1:A:108:LYS:HB2	2.01	0.61
1:B:34:GLN:HG2	1:B:34:GLN:O	2.00	0.61
1:B:18:PHE:O	1:B:21:GLY:N	2.26	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:GLN:O	2:B:284:HOH:O	2.16	0.61
1:A:98:CYS:O	1:A:101:PHE:HB3	2.01	0.60
1:A:30:LEU:HD21	1:A:43:VAL:HA	1.82	0.60
1:B:24:ASP:OD1	1:B:26:GLN:HG2	2.02	0.60
1:B:83:LYS:HD2	1:B:99:MET:CG	2.27	0.60
1:B:93:LYS:HE3	2:B:274:HOH:O	2.01	0.60
1:B:93:LYS:HD3	1:B:123:ASP:CG	2.21	0.60
1:A:3:ALA:O	1:A:7:ARG:HG3	2.02	0.60
1:B:20:GLN:HB3	2:B:275:HOH:O	2.00	0.60
1:A:30:LEU:HD21	1:A:46:VAL:HG21	1.83	0.60
1:B:134:MET:O	1:B:138:GLU:HG3	2.01	0.60
1:B:104:PHE:CE1	1:B:112:GLY:HA3	2.37	0.60
1:B:101:PHE:HE1	1:B:105:CYS:SG	2.24	0.60
1:B:97:THR:HG21	1:B:120:VAL:N	2.16	0.60
1:B:24:ASP:OD1	1:B:25:GLU:N	2.34	0.60
1:A:86:SER:CB	1:A:91:ALA:HB3	2.30	0.60
1:B:56:ARG:O	1:B:60:GLU:HG3	2.02	0.60
1:B:97:THR:O	1:B:101:PHE:N	2.35	0.60
1:B:142:GLN:OE1	1:B:142:GLN:HA	2.02	0.60
1:B:50:PHE:O	1:B:54:ALA:N	2.34	0.60
1:B:6:LEU:O	1:B:9:GLN:HB2	2.01	0.59
1:A:47:VAL:HB	1:A:135:LEU:HD21	1.83	0.59
1:A:80:HIS:HB3	2:A:170:HOH:O	2.00	0.59
1:B:141:ILE:HG22	1:B:141:ILE:O	2.02	0.59
1:A:85:SER:OG	1:A:86:SER:N	2.32	0.59
1:B:97:THR:HB	2:B:187:HOH:O	2.02	0.59
1:A:39:THR:HA	1:B:73:ASP:OD1	2.02	0.59
1:A:29:GLN:O	1:A:32:MET:N	2.33	0.59
1:B:3:ALA:HA	1:B:7:ARG:HD2	1.84	0.59
1:B:3:ALA:N	1:B:7:ARG:NH2	2.47	0.59
1:A:2:ALA:O	1:A:5:ALA:HB3	2.03	0.59
1:A:95:LYS:HE3	1:A:96:PHE:CE1	2.38	0.59
1:B:44:SER:OG	1:B:135:LEU:HD22	2.03	0.59
1:A:33:LEU:HB3	1:B:102:ARG:HH12	1.68	0.59
1:B:63:THR:O	1:B:67:GLN:NE2	2.36	0.59
1:B:4:ALA:O	1:B:5:ALA:C	2.41	0.59
1:A:23:VAL:C	1:A:92:GLN:HE21	2.05	0.59
1:A:66:GLU:CG	2:A:248:HOH:O	2.40	0.59
1:A:5:ALA:O	1:A:8:ASP:HB2	2.02	0.59
1:B:134:MET:O	1:B:138:GLU:HG3	2.02	0.58
1:A:130:LYS:NZ	2:A:165:HOH:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:PHE:HA	1:B:134:MET:HE2	1.84	0.58
1:B:97:THR:CG2	2:B:186:HOH:O	2.29	0.58
1:A:50:PHE:CE1	1:A:86:SER:HA	2.38	0.58
1:A:101:PHE:O	1:A:101:PHE:HD1	1.86	0.58
1:A:28:GLN:HA	1:A:31:GLN:OE1	2.03	0.58
1:B:139:GLN:O	1:B:142:GLN:HB3	2.03	0.58
1:B:66:GLU:HA	1:B:110:ARG:HH11	1.68	0.58
1:A:10:LEU:O	1:A:14:LEU:HG	2.03	0.58
1:B:82:LEU:HA	1:B:85:SER:HB3	1.85	0.58
1:A:25:GLU:OE1	1:A:29:GLN:OE1	2.20	0.58
1:B:93:LYS:HE2	2:B:178:HOH:O	2.03	0.58
1:A:97:THR:CG2	1:A:119:VAL:HG12	2.34	0.58
1:B:126:ASP:O	1:B:130:LYS:HD3	2.03	0.58
1:B:96:PHE:O	1:B:97:THR:C	2.41	0.58
1:B:97:THR:C	1:B:99:MET:H	2.06	0.58
1:B:104:PHE:CB	1:B:113:CYS:HB3	2.33	0.58
1:B:107:ASP:O	2:B:170:HOH:O	2.17	0.58
1:B:18:PHE:C	1:B:20:GLN:N	2.54	0.58
1:B:53:ASP:HB3	2:B:179:HOH:O	2.03	0.58
1:A:17:MET:HB3	1:A:23:VAL:HG22	1.86	0.58
1:B:87:ALA:HA	2:B:191:HOH:O	2.04	0.58
1:B:20:GLN:NE2	2:B:282:HOH:O	2.27	0.58
1:B:56:ARG:NH1	2:B:192:HOH:O	2.24	0.58
1:B:97:THR:HG21	1:B:120:VAL:CA	2.33	0.58
1:A:39:THR:OG1	1:B:73:ASP:HA	2.03	0.58
1:B:103:GLN:HA	1:B:103:GLN:OE1	2.04	0.58
1:A:80:HIS:HB2	2:A:185:HOH:O	2.03	0.58
1:B:98:CYS:C	1:B:100:GLN:H	2.07	0.58
1:A:73:ASP:OD1	2:A:173:HOH:O	2.17	0.58
1:A:3:ALA:O	1:A:6:LEU:N	2.37	0.58
1:B:102:ARG:HG2	2:B:296:HOH:O	2.02	0.57
1:A:17:MET:O	1:A:23:VAL:HG22	2.04	0.57
1:A:29:GLN:HB3	2:A:309:HOH:O	2.03	0.57
1:B:26:GLN:HB2	1:B:90:GLY:CA	2.32	0.57
1:B:67:GLN:HB2	1:B:70:VAL:CA	2.32	0.57
1:B:18:PHE:O	1:B:19:SER:C	2.42	0.57
1:B:10:LEU:O	1:B:13:LEU:N	2.37	0.57
1:B:53:ASP:HB3	2:B:180:HOH:O	2.04	0.57
1:A:78:TYR:CZ	1:B:49:LEU:HD21	2.39	0.57
1:A:7:ARG:HG3	2:A:241:HOH:O	2.03	0.57
1:A:34:GLN:NE2	1:A:43:VAL:H	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:LEU:HB3	1:B:127:LEU:HD13	1.86	0.57
1:B:136:GLN:NE2	1:B:139:GLN:NE2	2.52	0.57
1:B:87:ALA:HA	2:B:193:HOH:O	2.04	0.57
1:A:56:ARG:O	1:A:60:GLU:HG2	2.05	0.57
1:A:39:THR:HG23	1:A:39:THR:O	2.03	0.57
1:B:34:GLN:NE2	1:B:43:VAL:HG23	2.20	0.57
1:B:22:LEU:H	1:B:22:LEU:HD12	1.70	0.57
1:B:24:ASP:HB2	1:B:25:GLU:OE2	2.05	0.57
1:B:49:LEU:C	1:B:49:LEU:HD23	2.25	0.57
1:B:103:GLN:O	1:B:107:ASP:N	2.33	0.57
1:B:82:LEU:O	1:B:85:SER:HB3	2.04	0.57
1:B:87:ALA:HA	1:B:95:LYS:CD	2.35	0.56
1:A:6:LEU:HB3	1:A:141:ILE:HG12	1.87	0.56
1:B:136:GLN:NE2	1:B:140:GLN:CG	2.64	0.56
1:B:88:SER:CB	2:B:271:HOH:O	2.43	0.56
1:B:87:ALA:CA	1:B:95:LYS:HD2	2.34	0.56
1:B:83:LYS:HD3	1:B:98:CYS:O	2.05	0.56
1:B:56:ARG:O	1:B:60:GLU:HG3	2.04	0.56
1:B:34:GLN:HE21	1:B:43:VAL:H	1.53	0.56
1:A:115:MET:O	1:A:119:VAL:HG23	2.05	0.56
1:A:10:LEU:HD21	1:A:138:GLU:CG	2.25	0.56
1:A:139:GLN:NE2	1:A:139:GLN:C	2.58	0.56
1:A:110:ARG:O	1:A:110:ARG:HG2	2.05	0.56
1:A:31:GLN:HA	1:A:43:VAL:HG21	1.86	0.56
1:B:102:ARG:HG2	2:B:297:HOH:O	2.05	0.56
1:B:32:MET:O	1:B:35:ASP:HB2	2.04	0.56
1:A:18:PHE:O	1:A:21:GLY:N	2.36	0.56
2:A:258:HOH:O	1:B:40:PRO:HD3	2.05	0.56
1:B:6:LEU:HD23	1:B:6:LEU:N	2.21	0.56
1:A:91:ALA:HA	1:A:127:LEU:HD21	1.86	0.56
1:B:80:HIS:CD2	1:B:83:LYS:HE3	2.41	0.56
1:B:106:GLN:C	1:B:106:GLN:HE21	2.09	0.56
1:A:66:GLU:HG2	2:A:268:HOH:O	2.04	0.56
1:B:72:PHE:CE1	1:B:108:LYS:HA	2.41	0.56
1:A:138:GLU:O	1:A:142:GLN:HG3	2.06	0.56
1:A:137:LEU:HA	1:A:140:GLN:NE2	2.18	0.56
1:A:64:LEU:O	1:A:70:VAL:HG22	2.04	0.56
1:A:58:ILE:HG23	1:A:117:LEU:CD1	2.33	0.56
1:B:83:LYS:NZ	2:B:207:HOH:O	2.34	0.56
1:B:34:GLN:HE21	1:B:42:PHE:HB3	1.70	0.56
1:B:131:PHE:HD1	1:B:134:MET:HE2	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:GLN:HA	1:A:31:GLN:OE1	2.06	0.55
1:A:81:GLN:C	1:A:81:GLN:OE1	2.45	0.55
1:B:108:LYS:HE2	2:B:250:HOH:O	2.06	0.55
1:A:28:GLN:O	1:A:32:MET:HG2	2.06	0.55
1:A:28:GLN:O	1:A:32:MET:HE2	2.06	0.55
1:B:61:ILE:HA	1:B:64:LEU:HD12	1.87	0.55
1:B:97:THR:HG21	1:B:119:VAL:CG1	2.36	0.55
1:B:140:GLN:O	1:B:142:GLN:N	2.39	0.55
1:B:26:GLN:NE2	1:B:29:GLN:CG	2.67	0.55
1:A:29:GLN:NE2	2:A:309:HOH:O	2.33	0.55
1:B:74:LYS:HE2	2:B:231:HOH:O	2.06	0.55
1:A:66:GLU:HG2	2:A:247:HOH:O	2.07	0.55
1:B:11:THR:O	2:B:198:HOH:O	2.18	0.55
1:B:101:PHE:CE1	1:B:113:CYS:HB2	2.40	0.55
1:A:100:GLN:OE1	2:A:224:HOH:O	2.18	0.55
1:B:41:GLY:O	1:B:44:SER:HB3	2.07	0.55
1:A:29:GLN:O	1:A:32:MET:HB2	2.06	0.55
1:A:100:GLN:HG3	2:A:203:HOH:O	2.06	0.55
1:A:96:PHE:HD1	1:A:99:MET:SD	2.30	0.55
1:B:41:GLY:O	1:B:45:GLU:HG2	2.06	0.55
1:A:131:PHE:O	1:A:135:LEU:HG	2.07	0.55
1:B:138:GLU:OE1	2:B:265:HOH:O	2.18	0.55
1:B:26:GLN:HG3	2:B:193:HOH:O	2.06	0.55
1:A:45:GLU:HG3	1:B:73:ASP:CB	2.37	0.54
1:A:124:PHE:CZ	1:A:128:ARG:HD2	2.42	0.54
1:A:137:LEU:HG	2:A:183:HOH:O	2.07	0.54
1:A:23:VAL:HA	1:A:90:GLY:O	2.07	0.54
1:B:93:LYS:NZ	2:B:274:HOH:O	2.39	0.54
1:A:112:GLY:O	1:A:116:ALA:CB	2.56	0.54
1:B:4:ALA:CB	2:B:221:HOH:O	2.55	0.54
1:B:56:ARG:NH1	1:B:57:ILE:HG13	2.22	0.54
1:A:94:VAL:HG22	1:A:123:ASP:HB3	1.90	0.54
1:A:97:THR:O	1:A:101:PHE:HB2	2.08	0.54
1:A:93:LYS:HB2	2:A:151:HOH:O	2.06	0.54
1:A:51:CYS:HB3	2:A:209:HOH:O	2.06	0.54
1:B:3:ALA:HB1	1:B:7:ARG:NH1	2.22	0.54
1:B:93:LYS:HD3	1:B:123:ASP:CG	2.28	0.54
1:B:141:ILE:HG22	1:B:141:ILE:O	2.08	0.54
1:B:26:GLN:HE21	1:B:26:GLN:HA	1.72	0.54
1:B:101:PHE:HD1	1:B:101:PHE:O	1.91	0.54
1:A:28:GLN:O	1:A:32:MET:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:PHE:CE2	1:A:28:GLN:HB2	2.43	0.54
1:B:136:GLN:HE22	1:B:140:GLN:NE2	2.00	0.54
1:A:93:LYS:HB2	2:A:151:HOH:O	2.06	0.54
1:B:23:VAL:HA	1:B:90:GLY:O	2.08	0.54
1:A:22:LEU:HD12	1:A:130:LYS:HG3	1.90	0.54
1:B:51:CYS:SG	1:B:128:ARG:HG3	2.48	0.54
1:B:91:ALA:O	1:B:92:GLN:C	2.46	0.53
1:B:26:GLN:NE2	1:B:26:GLN:HA	2.23	0.53
1:A:102:ARG:HB3	1:A:102:ARG:HH11	1.72	0.53
1:A:17:MET:HE1	1:A:23:VAL:HG11	1.89	0.53
1:A:53:ASP:OD2	1:B:81:GLN:NE2	2.41	0.53
1:B:104:PHE:CD1	1:B:112:GLY:HA3	2.44	0.53
1:B:92:GLN:HG2	1:B:96:PHE:CE2	2.43	0.53
1:B:97:THR:C	1:B:99:MET:N	2.62	0.53
1:B:10:LEU:O	1:B:13:LEU:HB3	2.09	0.53
1:A:123:ASP:O	1:A:126:ASP:HB2	2.09	0.53
1:A:83:LYS:HD2	1:A:99:MET:HG2	1.90	0.53
1:B:97:THR:HG21	1:B:119:VAL:HG12	1.90	0.53
1:A:57:ILE:HD13	1:A:82:LEU:CD1	2.23	0.53
1:B:98:CYS:O	1:B:100:GLN:N	2.41	0.53
1:B:47:VAL:HG13	1:B:131:PHE:CD2	2.44	0.53
1:B:61:ILE:HD13	1:B:79:VAL:HG22	1.89	0.53
1:A:34:GLN:HE21	1:A:43:VAL:H	1.56	0.53
1:A:9:GLN:OE1	2:A:255:HOH:O	2.19	0.53
1:B:3:ALA:HB3	2:B:222:HOH:O	2.08	0.53
1:A:135:LEU:O	1:A:139:GLN:HG3	2.09	0.53
1:A:103:GLN:NE2	1:A:107:ASP:OD1	2.42	0.53
1:B:104:PHE:CE1	1:B:112:GLY:HA3	2.44	0.53
1:B:4:ALA:HB3	2:B:221:HOH:O	2.07	0.53
1:A:138:GLU:OE1	1:A:142:GLN:HG3	2.07	0.53
1:B:11:THR:HG22	2:B:267:HOH:O	2.08	0.53
1:A:3:ALA:HB3	2:A:273:HOH:O	2.09	0.53
1:A:25:GLU:OE1	2:A:315:HOH:O	2.18	0.53
1:A:18:PHE:CE1	1:A:23:VAL:HG23	2.43	0.53
1:B:102:ARG:HG2	2:B:296:HOH:O	2.08	0.53
1:A:24:ASP:OD2	1:A:92:GLN:HB3	2.09	0.53
1:B:56:ARG:HD3	2:B:191:HOH:O	2.09	0.53
1:B:107:ASP:O	1:B:108:LYS:HB2	2.08	0.52
1:B:24:ASP:HB3	1:B:92:GLN:NE2	2.23	0.52
1:A:137:LEU:HD23	1:A:140:GLN:HE22	1.73	0.52
1:B:13:LEU:O	1:B:17:MET:HG3	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:GLN:NE2	1:B:43:VAL:H	2.05	0.52
1:A:101:PHE:HD1	1:A:101:PHE:O	1.92	0.52
1:A:45:GLU:HB3	1:B:77:ALA:HB2	1.92	0.52
1:B:34:GLN:NE2	1:B:43:VAL:H	2.06	0.52
1:B:43:VAL:O	1:B:47:VAL:HG23	2.09	0.52
1:B:57:ILE:HG21	1:B:82:LEU:CB	2.21	0.52
1:A:135:LEU:O	1:A:139:GLN:HG3	2.09	0.52
1:B:29:GLN:HA	1:B:32:MET:HE3	1.92	0.52
1:A:2:ALA:C	2:A:193:HOH:O	2.48	0.52
1:B:32:MET:O	1:B:35:ASP:HB2	2.09	0.52
1:B:34:GLN:NE2	1:B:43:VAL:HG23	2.25	0.52
1:A:100:GLN:HG2	2:A:202:HOH:O	2.10	0.52
1:B:56:ARG:NH1	1:B:56:ARG:HG2	2.25	0.52
1:A:97:THR:HG21	1:A:119:VAL:HG12	1.91	0.52
1:B:34:GLN:NE2	1:B:43:VAL:H	2.07	0.52
1:B:15:SER:HB2	2:B:198:HOH:O	2.09	0.52
1:B:32:MET:C	1:B:34:GLN:N	2.64	0.52
1:B:56:ARG:HG2	1:B:56:ARG:HH11	1.75	0.52
1:B:30:LEU:HD21	1:B:46:VAL:HG11	1.91	0.52
1:A:75:VAL:CG1	1:A:105:CYS:SG	2.98	0.52
1:A:39:THR:O	1:A:39:THR:HG23	2.10	0.52
1:B:98:CYS:C	1:B:100:GLN:N	2.61	0.52
1:A:132:GLN:O	1:A:136:GLN:HG3	2.10	0.52
1:A:110:ARG:O	1:A:114:LEU:HG	2.10	0.52
1:A:94:VAL:CG2	1:A:123:ASP:HB3	2.39	0.52
1:B:56:ARG:NH2	2:B:181:HOH:O	2.40	0.51
1:B:79:VAL:HG11	1:B:101:PHE:HB3	1.91	0.51
1:A:18:PHE:CD1	1:A:23:VAL:HG23	2.46	0.51
1:B:94:VAL:O	1:B:98:CYS:SG	2.61	0.51
1:B:58:ILE:HG13	1:B:82:LEU:HD21	1.92	0.51
1:A:17:MET:CE	1:A:23:VAL:HG11	2.39	0.51
1:B:102:ARG:O	1:B:106:GLN:HB3	2.11	0.51
1:A:94:VAL:O	1:A:98:CYS:N	2.39	0.51
1:A:103:GLN:O	1:A:106:GLN:N	2.44	0.51
1:B:92:GLN:HG2	1:B:96:PHE:CZ	2.46	0.51
1:B:79:VAL:HG11	1:B:101:PHE:HB3	1.93	0.51
1:A:50:PHE:CE1	1:A:85:SER:OG	2.53	0.51
1:B:131:PHE:CD1	1:B:134:MET:HE2	2.45	0.51
1:A:2:ALA:N	2:A:304:HOH:O	2.42	0.51
1:A:33:LEU:HD12	1:A:33:LEU:N	2.26	0.51
1:A:80:HIS:CE1	2:A:291:HOH:O	2.63	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:LEU:HA	1:B:33:LEU:HD13	1.93	0.51
1:B:67:GLN:HG2	2:B:151:HOH:O	2.11	0.51
1:B:87:ALA:HB2	1:B:95:LYS:HD2	1.93	0.51
1:B:32:MET:C	1:B:34:GLN:N	2.64	0.51
1:B:25:GLU:HA	1:B:28:GLN:HB3	1.93	0.51
1:A:49:LEU:HD21	1:B:81:GLN:OE1	2.11	0.51
1:B:76:ASP:OD1	1:B:102:ARG:HG2	2.11	0.51
1:B:24:ASP:HB2	1:B:25:GLU:OE2	2.11	0.51
1:A:137:LEU:HD23	1:A:140:GLN:NE2	2.25	0.51
1:A:28:GLN:O	1:A:32:MET:HG2	2.11	0.51
1:A:71:ASN:OD1	1:A:73:ASP:HB2	2.11	0.51
1:A:131:PHE:O	1:A:134:MET:HB3	2.11	0.51
1:A:100:GLN:HG2	2:A:202:HOH:O	2.11	0.50
1:A:40:PRO:O	2:A:235:HOH:O	2.19	0.50
1:A:25:GLU:O	1:A:29:GLN:HG3	2.12	0.50
1:B:130:LYS:HD2	2:B:294:HOH:O	2.11	0.50
1:B:24:ASP:HB3	1:B:92:GLN:NE2	2.26	0.50
1:A:13:LEU:O	1:A:13:LEU:HD13	2.10	0.50
1:B:34:GLN:HE21	1:B:43:VAL:H	1.58	0.50
1:A:24:ASP:CB	1:A:92:GLN:OE1	2.49	0.50
1:A:45:GLU:O	1:A:49:LEU:HB2	2.10	0.50
1:A:100:GLN:HG3	2:A:203:HOH:O	2.10	0.50
1:A:16:SER:HA	1:A:19:SER:OG	2.10	0.50
1:A:60:GLU:OE1	1:A:60:GLU:HA	2.11	0.50
1:A:139:GLN:O	1:A:143:ALA:O	2.28	0.50
1:B:22:LEU:N	1:B:22:LEU:HD12	2.26	0.50
1:A:138:GLU:OE1	1:A:141:ILE:HD11	2.11	0.50
1:B:71:ASN:O	1:B:75:VAL:HG23	2.12	0.50
1:A:66:GLU:CD	2:A:300:HOH:O	2.47	0.50
1:A:10:LEU:HD21	1:A:138:GLU:OE2	2.11	0.50
1:B:131:PHE:CD1	1:B:134:MET:CE	2.95	0.50
1:B:115:MET:O	1:B:119:VAL:HG23	2.11	0.50
1:A:80:HIS:CD2	1:B:42:PHE:HZ	2.30	0.50
1:B:56:ARG:HD3	2:B:193:HOH:O	2.12	0.50
1:A:46:VAL:O	1:A:47:VAL:C	2.49	0.50
1:A:29:GLN:HB3	2:A:310:HOH:O	2.11	0.50
1:B:34:GLN:HE21	1:B:43:VAL:H	1.59	0.50
1:B:57:ILE:CD1	1:B:81:GLN:OE1	2.59	0.50
1:B:83:LYS:NZ	2:B:209:HOH:O	2.29	0.50
1:B:102:ARG:HG2	2:B:296:HOH:O	2.11	0.50
1:A:67:GLN:HG3	2:A:217:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:ASP:OD2	1:B:40:PRO:N	2.44	0.50
1:B:67:GLN:O	1:B:68:PRO:C	2.50	0.50
1:B:34:GLN:CD	1:B:40:PRO:N	2.65	0.50
1:A:11:THR:O	1:A:15:SER:HB2	2.12	0.50
1:B:3:ALA:HB1	1:B:7:ARG:NH2	2.27	0.50
1:A:86:SER:CA	1:A:91:ALA:HB3	2.41	0.50
1:B:17:MET:SD	1:B:130:LYS:HB3	2.52	0.50
1:B:106:GLN:HB2	2:B:201:HOH:O	2.11	0.50
1:A:29:GLN:HB3	2:A:306:HOH:O	2.11	0.50
1:B:70:VAL:HB	1:B:72:PHE:CE2	2.46	0.50
1:B:31:GLN:HA	1:B:43:VAL:HG21	1.94	0.50
1:A:7:ARG:HG3	1:A:7:ARG:NH1	2.26	0.50
1:A:61:ILE:HD11	1:A:78:TYR:HB3	1.93	0.50
1:B:87:ALA:HA	1:B:95:LYS:HD3	1.93	0.49
1:A:30:LEU:CD2	1:A:43:VAL:HA	2.41	0.49
1:A:45:GLU:HG3	1:B:73:ASP:HB3	1.93	0.49
1:B:57:ILE:CG2	1:B:82:LEU:HD22	2.42	0.49
1:A:49:LEU:HD13	2:B:192:HOH:O	2.12	0.49
1:B:34:GLN:NE2	1:B:43:VAL:H	2.10	0.49
1:B:26:GLN:HG3	2:B:193:HOH:O	2.11	0.49
1:A:34:GLN:NE2	1:A:43:VAL:HB	2.27	0.49
1:A:33:LEU:HB3	1:B:102:ARG:HH12	1.77	0.49
1:B:64:LEU:CD2	1:B:74:LYS:HE2	2.41	0.49
1:A:33:LEU:HD13	2:A:311:HOH:O	2.12	0.49
1:A:79:VAL:HG11	1:A:101:PHE:HB2	1.94	0.49
1:B:57:ILE:HD11	1:B:81:GLN:NE2	2.27	0.49
1:A:53:ASP:CG	1:A:56:ARG:HH21	2.15	0.49
1:A:61:ILE:HD13	1:A:79:VAL:CG2	2.42	0.49
1:A:29:GLN:HB3	2:A:310:HOH:O	2.11	0.49
1:A:103:GLN:HE21	1:A:107:ASP:CG	2.16	0.49
1:B:25:GLU:H	1:B:25:GLU:CD	2.15	0.49
1:B:102:ARG:O	1:B:106:GLN:CB	2.60	0.49
1:B:34:GLN:NE2	1:B:43:VAL:H	2.09	0.49
1:B:4:ALA:O	1:B:5:ALA:O	2.30	0.49
1:A:71:ASN:ND2	2:A:238:HOH:O	1.96	0.49
1:B:47:VAL:HG11	1:B:131:PHE:HB3	1.94	0.49
1:A:30:LEU:HD11	1:A:89:VAL:HA	1.93	0.49
1:B:103:GLN:O	1:B:106:GLN:HB3	2.12	0.49
1:A:33:LEU:N	1:A:33:LEU:CD1	2.76	0.49
1:B:21:GLY:O	1:B:92:GLN:HB3	2.12	0.49
1:B:97:THR:HG21	1:B:120:VAL:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:GLN:O	1:B:33:LEU:HD13	2.13	0.49
1:B:24:ASP:OD1	1:B:26:GLN:CG	2.61	0.49
1:B:101:PHE:CE1	1:B:105:CYS:SG	3.04	0.49
1:B:133:THR:O	1:B:137:LEU:HG	2.13	0.49
1:B:25:GLU:O	1:B:29:GLN:N	2.37	0.49
1:B:60:GLU:O	1:B:64:LEU:HG	2.13	0.49
1:B:57:ILE:O	1:B:59:ASN:N	2.45	0.49
1:B:97:THR:CG2	1:B:120:VAL:HG23	2.42	0.49
1:A:134:MET:O	1:A:135:LEU:C	2.51	0.49
1:A:83:LYS:O	1:A:87:ALA:HB2	2.12	0.49
1:A:100:GLN:HG3	2:A:201:HOH:O	2.12	0.49
1:A:66:GLU:HG2	2:A:270:HOH:O	2.11	0.49
1:B:136:GLN:O	1:B:139:GLN:HB3	2.12	0.49
1:A:100:GLN:CG	2:A:202:HOH:O	2.60	0.49
1:B:99:MET:HE2	2:B:290:HOH:O	2.13	0.49
1:A:80:HIS:O	1:A:83:LYS:HB3	2.13	0.49
1:A:128:ARG:HD3	2:A:176:HOH:O	2.11	0.49
1:A:66:GLU:CG	2:A:247:HOH:O	2.60	0.49
1:B:33:LEU:HD12	2:B:222:HOH:O	2.13	0.49
1:B:24:ASP:OD1	1:B:90:GLY:HA2	2.13	0.49
1:A:94:VAL:HG22	1:A:123:ASP:CB	2.42	0.49
1:A:141:ILE:O	1:A:143:ALA:N	2.42	0.49
1:B:34:GLN:NE2	1:B:43:VAL:H	2.10	0.49
1:A:115:MET:HG2	2:A:282:HOH:O	2.12	0.49
1:B:10:LEU:O	1:B:13:LEU:N	2.46	0.48
1:B:101:PHE:CD1	1:B:101:PHE:O	2.66	0.48
1:B:34:GLN:HG3	1:B:42:PHE:HB3	1.94	0.48
1:A:100:GLN:HG3	2:A:203:HOH:O	2.12	0.48
1:A:53:ASP:O	1:A:57:ILE:HG13	2.12	0.48
1:B:29:GLN:O	1:B:33:LEU:N	2.46	0.48
1:B:108:LYS:HE2	2:B:246:HOH:O	2.12	0.48
1:B:18:PHE:C	1:B:20:GLN:H	2.15	0.48
1:B:72:PHE:CD1	1:B:105:CYS:HA	2.48	0.48
1:B:82:LEU:CA	1:B:85:SER:HB3	2.43	0.48
1:A:6:LEU:CA	1:A:9:GLN:HE21	2.18	0.48
1:B:61:ILE:HD13	1:B:79:VAL:HG22	1.94	0.48
1:B:141:ILE:CG2	1:B:141:ILE:O	2.61	0.48
1:B:140:GLN:C	1:B:142:GLN:N	2.65	0.48
1:A:10:LEU:CA	1:A:137:LEU:HD13	2.42	0.48
1:A:25:GLU:O	1:A:29:GLN:HG3	2.12	0.48
1:A:56:ARG:O	1:A:60:GLU:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:GLN:HG3	2:B:250:HOH:O	2.14	0.48
1:A:116:ALA:O	1:A:120:VAL:N	2.38	0.48
1:A:84:GLY:HA2	1:A:87:ALA:HB3	1.94	0.48
2:A:173:HOH:O	1:B:40:PRO:CB	2.61	0.48
1:A:93:LYS:HB2	2:A:151:HOH:O	2.13	0.48
1:A:138:GLU:O	1:A:141:ILE:HB	2.13	0.48
1:A:13:LEU:HD23	1:A:133:THR:HG21	1.95	0.48
1:A:20:GLN:CD	2:A:287:HOH:O	2.51	0.48
1:A:17:MET:HB3	1:A:23:VAL:CG2	2.43	0.48
1:A:40:PRO:O	2:A:236:HOH:O	2.20	0.48
1:A:7:ARG:HH11	1:A:7:ARG:HG3	1.78	0.48
1:A:122:ASN:O	1:A:126:ASP:HB2	2.13	0.48
1:B:97:THR:CG2	1:B:119:VAL:HG12	2.43	0.48
1:A:57:ILE:HG21	1:A:82:LEU:CD2	2.40	0.48
1:B:23:VAL:O	1:B:23:VAL:HG23	2.13	0.48
1:A:58:ILE:HA	1:A:61:ILE:HG13	1.94	0.48
1:B:60:GLU:CD	1:B:78:TYR:HE2	2.17	0.48
1:A:81:GLN:OE1	1:A:82:LEU:N	2.47	0.48
1:A:9:GLN:HB3	2:A:294:HOH:O	2.11	0.48
1:B:99:MET:O	2:B:173:HOH:O	2.20	0.48
1:B:63:THR:HG22	1:B:67:GLN:NE2	2.28	0.48
1:B:93:LYS:NZ	2:B:178:HOH:O	2.46	0.48
1:A:29:GLN:HB3	2:A:309:HOH:O	2.14	0.48
1:A:128:ARG:O	1:A:132:GLN:HG2	2.14	0.48
1:A:11:THR:HG22	2:A:267:HOH:O	2.13	0.48
1:A:50:PHE:CE1	1:A:86:SER:HA	2.48	0.48
1:A:139:GLN:O	1:A:140:GLN:C	2.52	0.48
1:A:57:ILE:HG23	1:A:78:TYR:CD1	2.48	0.48
1:B:103:GLN:NE2	1:B:107:ASP:OD1	2.46	0.47
1:A:136:GLN:O	1:A:139:GLN:HB2	2.14	0.47
1:A:113:CYS:O	1:A:117:LEU:N	2.45	0.47
1:B:10:LEU:HD22	1:B:138:GLU:HG2	1.96	0.47
1:B:57:ILE:O	1:B:58:ILE:C	2.52	0.47
1:B:87:ALA:HB2	1:B:95:LYS:HD2	1.96	0.47
1:B:3:ALA:HA	1:B:7:ARG:CD	2.43	0.47
1:A:120:VAL:O	1:A:120:VAL:CG1	2.62	0.47
1:A:14:LEU:HD12	2:A:305:HOH:O	2.13	0.47
1:B:23:VAL:HA	1:B:90:GLY:O	2.14	0.47
1:B:97:THR:CG2	2:B:185:HOH:O	2.17	0.47
1:B:53:ASP:CG	2:B:180:HOH:O	2.52	0.47
1:B:23:VAL:HA	1:B:90:GLY:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ASN:ND2	2:A:190:HOH:O	2.42	0.47
1:A:66:GLU:HG2	2:A:247:HOH:O	2.14	0.47
1:B:82:LEU:HD12	1:B:82:LEU:O	2.13	0.47
1:A:28:GLN:HG2	1:A:32:MET:HE2	1.97	0.47
2:A:173:HOH:O	1:B:40:PRO:HB2	2.13	0.47
1:B:26:GLN:NE2	1:B:29:GLN:HB2	2.29	0.47
1:B:136:GLN:NE2	1:B:140:GLN:HE21	2.02	0.47
1:B:87:ALA:HA	1:B:95:LYS:HD2	1.95	0.47
1:A:14:LEU:O	1:A:18:PHE:HD1	1.97	0.47
1:A:22:LEU:C	1:A:92:GLN:HG2	2.35	0.47
1:A:41:GLY:HA2	1:A:142:GLN:HE22	1.79	0.47
1:A:63:THR:O	1:A:67:GLN:HG2	2.14	0.47
1:A:64:LEU:HD11	1:A:74:LYS:HG2	1.95	0.47
1:B:57:ILE:HA	1:B:60:GLU:OE1	2.15	0.47
1:B:57:ILE:HD11	1:B:81:GLN:CD	2.35	0.47
1:A:96:PHE:O	1:A:99:MET:HB2	2.13	0.47
1:B:142:GLN:CB	2:B:225:HOH:O	2.55	0.47
1:A:115:MET:HG3	2:A:169:HOH:O	2.13	0.47
1:B:131:PHE:O	1:B:135:LEU:HG	2.14	0.47
1:B:30:LEU:HD21	1:B:46:VAL:CG1	2.45	0.47
1:A:26:GLN:HB2	1:A:90:GLY:CA	2.44	0.47
1:B:139:GLN:C	1:B:141:ILE:N	2.68	0.47
1:B:5:ALA:O	1:B:8:ASP:HB2	2.14	0.47
1:B:122:ASN:HB3	2:B:172:HOH:O	2.15	0.47
1:B:140:GLN:O	1:B:142:GLN:N	2.46	0.47
1:A:72:PHE:HA	1:A:75:VAL:HB	1.97	0.47
1:A:66:GLU:CG	2:A:247:HOH:O	2.60	0.47
1:B:139:GLN:O	1:B:142:GLN:HB3	2.14	0.47
1:B:56:ARG:HH12	1:B:57:ILE:HG12	1.80	0.47
1:A:128:ARG:O	1:A:132:GLN:HG2	2.14	0.47
1:A:66:GLU:HB3	2:A:300:HOH:O	2.15	0.47
1:B:96:PHE:O	1:B:100:GLN:HG3	2.15	0.47
1:A:75:VAL:HG12	1:A:105:CYS:SG	2.55	0.47
1:B:91:ALA:CB	1:B:127:LEU:CD2	2.92	0.47
1:B:24:ASP:OD1	1:B:90:GLY:HA2	2.15	0.47
1:B:80:HIS:HD2	1:B:83:LYS:HE3	1.80	0.47
1:B:83:LYS:HB3	1:B:83:LYS:HE3	1.63	0.47
1:A:29:GLN:HA	1:A:32:MET:CG	2.32	0.47
1:A:4:ALA:CA	1:A:7:ARG:HH21	2.27	0.47
1:A:12:ALA:O	1:A:16:SER:N	2.43	0.46
1:A:135:LEU:O	1:A:139:GLN:HG3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:GLN:HG3	2:B:228:HOH:O	2.15	0.46
1:B:47:VAL:HG13	1:B:131:PHE:CD2	2.51	0.46
1:A:71:ASN:CG	1:A:74:LYS:HG3	2.35	0.46
1:B:13:LEU:O	1:B:17:MET:HG3	2.15	0.46
1:B:57:ILE:HD11	1:B:81:GLN:NE2	2.29	0.46
1:A:95:LYS:HE3	1:A:96:PHE:CE1	2.50	0.46
1:B:7:ARG:O	1:B:8:ASP:C	2.52	0.46
1:A:3:ALA:O	1:A:7:ARG:HG3	2.16	0.46
1:A:92:GLN:HB2	1:A:95:LYS:HZ1	1.81	0.46
1:B:83:LYS:HE3	1:B:87:ALA:HB2	1.96	0.46
1:B:28:GLN:HA	1:B:31:GLN:OE1	2.15	0.46
1:B:6:LEU:HD23	1:B:6:LEU:H	1.81	0.46
1:B:13:LEU:HD11	1:B:130:LYS:HG3	1.98	0.46
1:B:28:GLN:O	1:B:32:MET:HE2	2.15	0.46
1:A:16:SER:O	1:A:19:SER:N	2.48	0.46
1:B:115:MET:O	1:B:118:ALA:HB3	2.15	0.46
1:A:92:GLN:CB	1:A:95:LYS:NZ	2.79	0.46
1:B:10:LEU:CD2	1:B:138:GLU:HG2	2.46	0.46
1:B:57:ILE:HD11	1:B:81:GLN:NE2	2.31	0.46
1:A:30:LEU:HD11	1:A:46:VAL:HG11	1.96	0.46
1:A:49:LEU:O	1:A:52:ASP:HB2	2.16	0.46
1:A:39:THR:O	1:A:39:THR:CG2	2.64	0.46
1:A:66:GLU:HG2	2:A:269:HOH:O	2.16	0.46
1:A:45:GLU:OE1	1:A:45:GLU:HA	2.16	0.46
1:B:61:ILE:O	1:B:62:ALA:C	2.54	0.46
1:A:34:GLN:NE2	1:A:43:VAL:H	2.13	0.46
1:A:66:GLU:HG2	2:A:268:HOH:O	2.16	0.46
1:B:60:GLU:OE2	2:B:234:HOH:O	2.20	0.46
1:A:16:SER:O	1:A:17:MET:C	2.54	0.46
1:A:28:GLN:HA	1:A:31:GLN:OE1	2.15	0.46
1:B:8:ASP:O	1:B:11:THR:HB	2.15	0.46
1:B:131:PHE:O	1:B:135:LEU:HG	2.16	0.46
1:B:81:GLN:OE1	1:B:82:LEU:N	2.49	0.45
1:A:138:GLU:OE1	1:A:142:GLN:CG	2.63	0.45
1:A:104:PHE:CD2	1:A:116:ALA:HB2	2.51	0.45
1:A:69:VAL:CG1	2:A:207:HOH:O	2.64	0.45
1:B:136:GLN:NE2	1:B:140:GLN:CD	2.67	0.45
1:B:29:GLN:O	1:B:32:MET:HB2	2.16	0.45
1:A:39:THR:HA	1:B:73:ASP:OD1	2.17	0.45
1:A:101:PHE:O	1:A:102:ARG:C	2.55	0.45
1:B:13:LEU:O	1:B:17:MET:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:ARG:NH1	2:B:181:HOH:O	2.42	0.45
1:B:64:LEU:HD11	1:B:74:LYS:HG2	1.97	0.45
1:B:136:GLN:O	1:B:140:GLN:HG3	2.15	0.45
1:B:25:GLU:O	1:B:29:GLN:HG2	2.16	0.45
1:B:83:LYS:HE3	1:B:83:LYS:O	2.16	0.45
1:B:23:VAL:HA	1:B:90:GLY:O	2.16	0.45
1:B:136:GLN:O	1:B:139:GLN:HB3	2.16	0.45
1:A:32:MET:HE2	1:A:32:MET:N	2.31	0.45
1:B:47:VAL:HG13	1:B:131:PHE:CD2	2.51	0.45
1:A:49:LEU:HA	1:A:49:LEU:HD12	1.54	0.45
1:A:18:PHE:CZ	1:A:28:GLN:HB2	2.52	0.45
1:A:50:PHE:CD2	1:A:131:PHE:HE2	2.35	0.45
1:B:82:LEU:HA	1:B:85:SER:CB	2.46	0.45
1:A:86:SER:HB3	1:A:91:ALA:HB3	1.99	0.45
1:B:97:THR:HB	1:B:120:VAL:HG22	1.98	0.45
1:A:67:GLN:NE2	2:A:284:HOH:O	2.49	0.45
1:B:97:THR:CG2	2:B:186:HOH:O	2.64	0.45
1:A:22:LEU:HD12	1:A:130:LYS:HG3	1.99	0.45
1:A:83:LYS:HD2	1:A:99:MET:CG	2.46	0.45
1:B:94:VAL:O	1:B:97:THR:HB	2.15	0.45
1:B:136:GLN:OE1	1:B:139:GLN:OE1	2.34	0.45
1:A:57:ILE:HD11	1:A:81:GLN:HE22	1.80	0.45
1:B:139:GLN:HG3	1:B:142:GLN:HE21	1.78	0.45
1:A:80:HIS:HD2	1:B:42:PHE:HZ	1.63	0.45
1:A:60:GLU:O	1:A:64:LEU:HG	2.17	0.45
1:B:136:GLN:O	1:B:140:GLN:HG3	2.17	0.45
1:B:47:VAL:CG1	1:B:135:LEU:HD11	2.47	0.45
1:B:29:GLN:O	1:B:33:LEU:CD1	2.65	0.45
1:B:27:PHE:HB2	1:B:90:GLY:HA3	1.98	0.45
1:A:85:SER:O	1:A:88:SER:N	2.40	0.45
1:B:28:GLN:HG3	2:B:227:HOH:O	2.16	0.45
1:A:29:GLN:HB3	1:A:29:GLN:HE21	1.43	0.45
1:B:101:PHE:CD1	1:B:101:PHE:C	2.89	0.45
1:B:83:LYS:HD2	1:B:99:MET:HG2	1.99	0.45
1:A:111:ASP:HA	1:A:114:LEU:HD12	1.99	0.45
1:B:128:ARG:O	1:B:132:GLN:HG3	2.17	0.45
1:B:56:ARG:CG	1:B:56:ARG:HH11	2.30	0.45
1:A:90:GLY:O	1:A:92:GLN:N	2.50	0.45
1:A:139:GLN:NE2	2:A:231:HOH:O	2.50	0.45
1:A:27:PHE:CZ	1:A:31:GLN:NE2	2.85	0.45
1:B:23:VAL:HA	1:B:90:GLY:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:LEU:HG	2:B:158:HOH:O	2.16	0.45
1:A:139:GLN:NE2	2:A:232:HOH:O	2.50	0.45
1:B:93:LYS:NZ	2:B:273:HOH:O	2.30	0.45
1:B:90:GLY:O	1:B:92:GLN:N	2.50	0.45
1:A:53:ASP:CG	1:A:56:ARG:HH21	2.18	0.45
1:B:100:GLN:HA	2:B:218:HOH:O	2.17	0.45
1:B:29:GLN:HB3	2:B:223:HOH:O	2.17	0.45
1:A:27:PHE:HB2	1:A:89:VAL:O	2.17	0.45
1:A:83:LYS:HE2	2:A:232:HOH:O	2.16	0.45
1:A:22:LEU:CD1	1:A:130:LYS:HG3	2.47	0.45
1:B:130:LYS:NZ	2:B:296:HOH:O	2.47	0.44
1:B:69:VAL:HA	2:B:185:HOH:O	2.16	0.44
1:A:29:GLN:HB3	2:A:311:HOH:O	2.17	0.44
1:A:66:GLU:HG3	2:A:164:HOH:O	2.17	0.44
1:A:42:PHE:O	1:A:46:VAL:HG23	2.17	0.44
1:B:58:ILE:HG13	1:B:82:LEU:CD2	2.47	0.44
1:B:82:LEU:HA	1:B:85:SER:HB2	2.00	0.44
1:A:91:ALA:HB2	1:A:127:LEU:CD2	2.47	0.44
1:A:30:LEU:HD21	1:A:46:VAL:CG2	2.46	0.44
1:B:34:GLN:HE21	1:B:43:VAL:H	1.65	0.44
1:B:139:GLN:C	1:B:141:ILE:H	2.21	0.44
1:A:1:SER:HB2	1:A:2:ALA:H	1.56	0.44
1:B:24:ASP:CG	1:B:26:GLN:HG2	2.38	0.44
1:A:77:ALA:HB2	1:B:45:GLU:HB2	1.99	0.44
1:B:132:GLN:NE2	2:B:259:HOH:O	2.50	0.44
1:B:79:VAL:HG11	1:B:101:PHE:CB	2.47	0.44
1:A:83:LYS:NZ	2:A:277:HOH:O	2.51	0.44
1:A:123:ASP:OD1	2:A:277:HOH:O	2.21	0.44
1:A:55:ASP:CG	2:A:282:HOH:O	2.45	0.44
1:B:64:LEU:HD23	2:B:232:HOH:O	2.17	0.44
1:B:101:PHE:HZ	1:B:117:LEU:HB2	1.83	0.44
1:A:135:LEU:O	1:A:139:GLN:HG3	2.16	0.44
1:A:79:VAL:HG22	2:A:200:HOH:O	2.18	0.44
1:A:30:LEU:HD11	1:A:46:VAL:CG1	2.46	0.44
1:A:47:VAL:CG1	1:A:135:LEU:HD21	2.47	0.44
1:A:68:PRO:O	1:A:110:ARG:NH2	2.47	0.44
1:B:98:CYS:O	1:B:101:PHE:HB3	2.17	0.44
1:B:32:MET:C	1:B:34:GLN:N	2.70	0.44
1:A:3:ALA:O	1:A:7:ARG:HG3	2.18	0.44
1:B:7:ARG:O	1:B:9:GLN:N	2.51	0.44
1:A:30:LEU:HB3	1:A:43:VAL:HG22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:LEU:HA	2:B:225:HOH:O	2.18	0.44
1:B:15:SER:CB	2:B:276:HOH:O	2.63	0.44
1:A:13:LEU:O	1:A:16:SER:CB	2.66	0.44
1:A:139:GLN:NE2	2:A:232:HOH:O	2.51	0.44
1:B:93:LYS:O	1:B:97:THR:OG1	2.27	0.44
1:A:138:GLU:O	1:A:139:GLN:C	2.56	0.44
1:B:79:VAL:HG11	1:B:101:PHE:HB3	1.99	0.44
1:B:110:ARG:O	1:B:113:CYS:CB	2.64	0.44
1:A:66:GLU:HG2	2:A:268:HOH:O	2.17	0.44
1:A:28:GLN:HE22	1:A:32:MET:CE	2.30	0.44
1:B:29:GLN:O	1:B:33:LEU:HB2	2.17	0.44
1:A:24:ASP:OD1	1:A:90:GLY:HA3	2.18	0.44
1:B:34:GLN:HE21	1:B:43:VAL:H	1.64	0.44
1:B:22:LEU:N	1:B:22:LEU:HD12	2.33	0.43
1:B:50:PHE:CD1	1:B:89:VAL:HG11	2.52	0.43
1:A:29:GLN:HA	1:A:32:MET:CG	2.36	0.43
1:A:34:GLN:HE21	1:A:42:PHE:HB3	1.82	0.43
1:A:74:LYS:HE2	1:A:78:TYR:HE2	1.82	0.43
1:B:22:LEU:N	1:B:22:LEU:HD12	2.33	0.43
1:A:55:ASP:CG	1:A:59:ASN:ND2	2.71	0.43
1:A:39:THR:OG1	1:B:73:ASP:HA	2.18	0.43
1:A:128:ARG:O	1:A:132:GLN:N	2.45	0.43
2:A:266:HOH:O	1:B:49:LEU:HD23	2.18	0.43
1:A:136:GLN:HA	1:A:139:GLN:CD	2.38	0.43
1:A:64:LEU:C	1:A:66:GLU:H	2.20	0.43
1:B:97:THR:HG22	2:B:186:HOH:O	2.18	0.43
1:A:83:LYS:C	1:A:83:LYS:HD3	2.38	0.43
1:B:93:LYS:NZ	2:B:274:HOH:O	2.51	0.43
1:B:54:ALA:HB3	1:B:124:PHE:CZ	2.53	0.43
1:A:6:LEU:HB3	1:A:141:ILE:HG13	2.00	0.43
1:B:128:ARG:CZ	2:B:161:HOH:O	2.49	0.43
1:B:123:ASP:O	1:B:124:PHE:C	2.55	0.43
1:B:56:ARG:O	1:B:60:GLU:N	2.44	0.43
1:B:43:VAL:O	1:B:47:VAL:N	2.36	0.43
1:B:22:LEU:N	1:B:22:LEU:HD12	2.33	0.43
1:B:70:VAL:HG23	1:B:110:ARG:CZ	2.47	0.43
1:B:73:ASP:OD2	2:B:250:HOH:O	2.21	0.43
1:A:97:THR:HG23	1:A:119:VAL:HG12	1.98	0.43
1:B:54:ALA:CB	1:B:82:LEU:HD11	2.49	0.43
1:B:20:GLN:O	1:B:20:GLN:CG	2.52	0.43
1:B:25:GLU:HG2	1:B:26:GLN:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:GLN:HE22	1:A:43:VAL:HB	1.83	0.43
1:B:101:PHE:CZ	1:B:117:LEU:HB2	2.54	0.43
1:B:29:GLN:HG2	1:B:29:GLN:H	1.59	0.43
1:A:136:GLN:HG2	1:A:140:GLN:HE21	1.83	0.43
1:A:33:LEU:HA	1:A:33:LEU:HD12	1.77	0.43
1:A:119:VAL:HG11	2:A:224:HOH:O	2.18	0.43
1:B:97:THR:HG22	2:B:185:HOH:O	2.10	0.43
1:A:74:LYS:HE2	2:A:189:HOH:O	2.19	0.43
1:B:22:LEU:H	1:B:22:LEU:CD1	2.32	0.43
1:B:141:ILE:O	1:B:141:ILE:CG2	2.66	0.43
1:B:26:GLN:CA	1:B:26:GLN:NE2	2.80	0.43
1:A:79:VAL:HG11	1:A:101:PHE:CB	2.48	0.43
1:B:104:PHE:CD1	1:B:112:GLY:HA3	2.54	0.43
1:A:131:PHE:O	1:A:135:LEU:HG	2.18	0.43
1:A:91:ALA:HA	1:A:127:LEU:CD2	2.48	0.43
1:B:32:MET:C	1:B:34:GLN:H	2.21	0.43
1:A:6:LEU:HD21	1:A:140:GLN:OE1	2.19	0.43
1:A:13:LEU:O	1:A:16:SER:N	2.51	0.43
1:A:33:LEU:HB3	1:B:102:ARG:NH1	2.33	0.43
1:B:67:GLN:O	1:B:68:PRO:C	2.56	0.43
1:B:67:GLN:CG	2:B:151:HOH:O	2.67	0.43
1:B:32:MET:C	1:B:34:GLN:H	2.21	0.43
1:B:82:LEU:C	1:B:85:SER:HB3	2.38	0.43
1:B:115:MET:O	1:B:118:ALA:HB3	2.19	0.43
1:A:83:LYS:HE3	1:A:99:MET:CG	2.48	0.42
1:B:55:ASP:OD1	1:B:128:ARG:NH1	2.52	0.42
1:B:66:GLU:HB2	2:B:214:HOH:O	2.18	0.42
1:B:97:THR:OG1	1:B:120:VAL:HG22	2.19	0.42
1:B:67:GLN:OE1	1:B:67:GLN:HA	2.17	0.42
1:B:64:LEU:HD11	1:B:74:LYS:HG2	2.00	0.42
1:A:134:MET:O	1:A:137:LEU:N	2.52	0.42
1:A:95:LYS:O	1:A:99:MET:HG3	2.19	0.42
1:B:93:LYS:CE	2:B:274:HOH:O	2.63	0.42
1:B:106:GLN:CG	1:B:106:GLN:O	2.67	0.42
1:A:78:TYR:CD2	1:B:49:LEU:HD12	2.55	0.42
1:B:49:LEU:CD2	2:B:242:HOH:O	2.67	0.42
1:B:60:GLU:OE1	1:B:78:TYR:HE2	2.02	0.42
1:B:119:VAL:O	1:B:120:VAL:C	2.57	0.42
1:B:59:ASN:O	1:B:62:ALA:HB3	2.19	0.42
1:B:79:VAL:HG21	1:B:101:PHE:CG	2.54	0.42
1:A:39:THR:CG2	1:A:39:THR:O	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ASP:O	1:A:59:ASN:ND2	2.52	0.42
1:B:72:PHE:HB3	1:B:105:CYS:HB3	2.02	0.42
1:A:55:ASP:OD1	2:A:182:HOH:O	2.22	0.42
1:B:3:ALA:HB1	1:B:7:ARG:HH11	1.83	0.42
1:A:57:ILE:HD11	1:A:81:GLN:HE21	1.84	0.42
1:B:3:ALA:HA	1:B:7:ARG:HH11	1.82	0.42
1:A:73:ASP:HB3	1:B:45:GLU:HG3	2.02	0.42
1:B:140:GLN:C	1:B:142:GLN:N	2.68	0.42
1:B:25:GLU:O	1:B:29:GLN:HG2	2.19	0.42
1:B:51:CYS:SG	1:B:128:ARG:HG3	2.60	0.42
1:B:79:VAL:CG1	1:B:98:CYS:HA	2.50	0.42
1:B:34:GLN:HB2	1:B:43:VAL:HG23	2.00	0.42
1:A:34:GLN:HG3	1:A:39:THR:O	2.19	0.42
1:A:49:LEU:HD21	1:B:81:GLN:OE1	2.20	0.42
1:A:42:PHE:O	1:A:46:VAL:HG23	2.19	0.42
1:A:136:GLN:HB2	1:A:136:GLN:HE21	1.66	0.42
1:B:119:VAL:O	1:B:120:VAL:C	2.56	0.42
1:A:40:PRO:O	2:A:236:HOH:O	2.21	0.42
1:A:53:ASP:CG	1:A:56:ARG:NH2	2.73	0.42
2:A:170:HOH:O	1:B:46:VAL:HG13	2.20	0.42
1:B:73:ASP:O	1:B:76:ASP:HB3	2.19	0.42
1:B:97:THR:CG2	1:B:120:VAL:CG2	2.97	0.42
1:B:136:GLN:NE2	1:B:139:GLN:OE1	2.53	0.42
1:A:69:VAL:HB	2:A:189:HOH:O	2.19	0.42
1:B:75:VAL:CG1	1:B:105:CYS:SG	3.08	0.42
1:B:61:ILE:CD1	1:B:79:VAL:HG22	2.49	0.42
1:A:47:VAL:HG13	1:A:131:PHE:CD2	2.54	0.42
1:A:3:ALA:O	1:A:7:ARG:HG3	2.20	0.42
1:B:136:GLN:NE2	1:B:140:GLN:CG	2.68	0.42
1:B:50:PHE:CE1	1:B:86:SER:HA	2.54	0.42
1:A:30:LEU:HD11	1:A:46:VAL:HB	2.02	0.42
1:A:47:VAL:HG13	1:A:131:PHE:CD2	2.55	0.42
1:A:127:LEU:HD22	2:A:151:HOH:O	2.19	0.42
1:A:66:GLU:HG3	2:A:164:HOH:O	2.18	0.42
1:B:13:LEU:O	1:B:16:SER:HB3	2.19	0.42
1:B:71:ASN:OD1	1:B:73:ASP:CB	2.67	0.42
1:A:18:PHE:CE1	1:A:23:VAL:CG2	3.02	0.42
1:A:79:VAL:HG23	1:A:98:CYS:HB3	2.02	0.42
1:B:103:GLN:OE1	1:B:106:GLN:HG2	2.20	0.42
1:B:6:LEU:O	1:B:141:ILE:HD11	2.20	0.42
1:B:49:LEU:HD23	2:B:242:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ILE:HD13	1:A:79:VAL:HG23	2.01	0.42
1:B:15:SER:CB	2:B:198:HOH:O	2.66	0.42
1:B:139:GLN:O	1:B:141:ILE:N	2.53	0.42
1:B:93:LYS:NZ	2:B:274:HOH:O	2.53	0.42
1:A:57:ILE:O	1:A:58:ILE:C	2.58	0.42
1:B:30:LEU:C	1:B:32:MET:H	2.23	0.42
1:A:137:LEU:HD23	1:A:137:LEU:HA	1.91	0.41
1:A:28:GLN:OE1	1:A:29:GLN:N	2.53	0.41
1:B:97:THR:HG21	1:B:120:VAL:HG23	2.02	0.41
1:B:13:LEU:HA	2:B:224:HOH:O	2.20	0.41
1:B:115:MET:O	1:B:119:VAL:HG23	2.20	0.41
1:B:130:LYS:HA	1:B:130:LYS:HD2	1.81	0.41
1:A:116:ALA:O	1:A:120:VAL:HG23	2.20	0.41
1:A:92:GLN:O	1:A:95:LYS:HB3	2.20	0.41
1:B:92:GLN:O	1:B:95:LYS:HB3	2.20	0.41
1:A:52:ASP:CG	2:A:210:HOH:O	2.58	0.41
1:A:47:VAL:O	1:A:51:CYS:HB2	2.20	0.41
1:B:139:GLN:O	1:B:142:GLN:CB	2.68	0.41
1:B:29:GLN:HA	1:B:32:MET:HE2	2.02	0.41
1:A:116:ALA:HA	1:A:119:VAL:HB	2.02	0.41
1:B:24:ASP:OD1	1:B:90:GLY:CA	2.68	0.41
1:A:136:GLN:HG2	1:A:140:GLN:HE21	1.85	0.41
1:A:137:LEU:HD23	2:A:183:HOH:O	2.20	0.41
1:A:139:GLN:NE2	1:A:139:GLN:O	2.52	0.41
1:A:114:LEU:HD11	2:A:321:HOH:O	2.19	0.41
1:A:128:ARG:NH1	1:A:132:GLN:HG3	2.36	0.41
1:A:39:THR:CG2	1:A:39:THR:O	2.63	0.41
1:B:127:LEU:HD11	1:B:131:PHE:CZ	2.55	0.41
1:B:107:ASP:O	2:B:170:HOH:O	2.21	0.41
1:B:83:LYS:NZ	1:B:99:MET:CE	2.84	0.41
1:B:26:GLN:HB2	1:B:90:GLY:CA	2.50	0.41
1:B:104:PHE:CD2	1:B:112:GLY:C	2.93	0.41
1:B:67:GLN:O	1:B:68:PRO:C	2.58	0.41
1:B:30:LEU:HD11	1:B:46:VAL:HG11	2.03	0.41
1:A:49:LEU:HD21	1:B:81:GLN:OE1	2.21	0.41
1:A:140:GLN:HA	1:A:143:ALA:O	2.19	0.41
1:B:130:LYS:HD2	2:B:295:HOH:O	2.20	0.41
1:A:57:ILE:HG22	1:A:58:ILE:N	2.35	0.41
1:B:10:LEU:O	1:B:11:THR:C	2.58	0.41
1:B:47:VAL:HG11	1:B:131:PHE:HB3	2.02	0.41
2:A:259:HOH:O	1:B:40:PRO:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LEU:HD12	1:A:33:LEU:HA	1.83	0.41
1:A:75:VAL:O	1:A:79:VAL:HG12	2.21	0.41
1:B:23:VAL:HB	1:B:27:PHE:CB	2.51	0.41
1:A:23:VAL:HA	1:A:90:GLY:O	2.20	0.41
1:B:115:MET:O	1:B:119:VAL:HG23	2.20	0.41
1:A:47:VAL:HG13	1:A:131:PHE:CD2	2.56	0.41
1:B:92:GLN:HG2	1:B:96:PHE:CE2	2.54	0.41
1:B:93:LYS:NZ	2:B:235:HOH:O	2.53	0.41
1:A:25:GLU:O	1:A:29:GLN:HG3	2.20	0.41
1:A:74:LYS:HE2	2:A:189:HOH:O	2.20	0.41
1:B:83:LYS:HG3	1:B:95:LYS:HG3	2.02	0.41
1:B:32:MET:O	1:B:35:ASP:N	2.52	0.41
1:B:22:LEU:CD2	1:B:130:LYS:HG2	2.51	0.41
1:B:61:ILE:HD13	1:B:79:VAL:CG2	2.51	0.41
1:A:65:LEU:HD11	1:A:113:CYS:HB3	2.02	0.41
1:B:32:MET:C	1:B:34:GLN:H	2.24	0.41
1:B:97:THR:HG22	1:B:120:VAL:HG23	2.03	0.41
1:A:33:LEU:HA	1:A:33:LEU:HD12	1.80	0.41
1:B:100:GLN:HG3	2:B:186:HOH:O	2.20	0.41
1:A:46:VAL:CG1	1:A:89:VAL:HG12	2.51	0.41
1:B:56:ARG:NE	2:B:287:HOH:O	2.53	0.41
1:B:60:GLU:OE2	1:B:78:TYR:HE2	2.04	0.41
1:A:30:LEU:O	1:A:30:LEU:HD23	2.20	0.41
1:A:31:GLN:HB2	1:A:32:MET:CE	2.51	0.41
1:A:124:PHE:O	1:A:128:ARG:N	2.47	0.41
1:B:58:ILE:CD1	1:B:120:VAL:HG12	2.51	0.41
1:B:91:ALA:HB1	1:B:127:LEU:HD22	2.00	0.41
1:B:62:ALA:O	1:B:66:GLU:HG3	2.20	0.41
1:A:32:MET:C	1:A:34:GLN:H	2.23	0.41
1:A:32:MET:C	1:A:34:GLN:N	2.74	0.41
1:A:49:LEU:CD1	2:B:192:HOH:O	2.69	0.41
1:B:57:ILE:HG21	1:B:82:LEU:HB2	2.03	0.41
1:A:77:ALA:O	1:A:80:HIS:HB3	2.20	0.41
1:A:87:ALA:HB2	1:A:95:LYS:HD3	2.03	0.41
1:B:25:GLU:O	1:B:28:GLN:HB3	2.20	0.41
1:A:50:PHE:HD2	1:A:131:PHE:HE2	1.68	0.41
1:A:39:THR:N	1:B:106:GLN:HE22	2.18	0.41
1:A:39:THR:CG2	1:A:42:PHE:HB2	2.37	0.41
1:A:61:ILE:HG23	1:A:75:VAL:HG13	2.03	0.41
1:A:81:GLN:HE21	1:B:49:LEU:HD11	1.83	0.41
1:A:128:ARG:HG2	1:A:132:GLN:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:LYS:HZ3	1:A:108:LYS:CB	2.34	0.41
1:A:117:LEU:O	1:A:121:ARG:HG3	2.21	0.41
1:A:39:THR:N	1:B:106:GLN:NE2	2.68	0.41
1:B:25:GLU:C	1:B:28:GLN:HB3	2.39	0.40
1:B:56:ARG:CD	2:B:287:HOH:O	2.62	0.40
1:A:101:PHE:O	1:A:101:PHE:CD1	2.72	0.40
1:A:55:ASP:O	1:A:56:ARG:O	2.39	0.40
1:B:136:GLN:O	1:B:140:GLN:HG3	2.21	0.40
1:B:64:LEU:HD23	2:B:233:HOH:O	2.19	0.40
1:A:103:GLN:O	1:A:104:PHE:C	2.57	0.40
1:A:25:GLU:O	1:A:28:GLN:HB3	2.21	0.40
1:A:96:PHE:HD1	1:A:99:MET:SD	2.44	0.40
1:A:3:ALA:O	1:A:7:ARG:NE	2.50	0.40
1:B:3:ALA:CB	1:B:7:ARG:NH1	2.83	0.40
1:B:47:VAL:HG13	1:B:131:PHE:CD2	2.56	0.40
1:A:39:THR:HA	1:A:40:PRO:HD2	1.90	0.40
1:B:83:LYS:HB2	1:B:98:CYS:HB3	2.03	0.40
1:A:53:ASP:O	1:A:54:ALA:C	2.60	0.40
1:B:93:LYS:HD2	2:B:273:HOH:O	2.20	0.40
1:A:65:LEU:HD23	1:A:65:LEU:HA	1.92	0.40
1:B:95:LYS:HA	1:B:98:CYS:SG	2.61	0.40
1:B:92:GLN:HG2	1:B:96:PHE:CZ	2.57	0.40
1:A:136:GLN:HG2	1:A:140:GLN:NE2	2.37	0.40
1:A:61:ILE:HD13	1:A:79:VAL:HG22	2.03	0.40
1:B:97:THR:CG2	1:B:120:VAL:HG23	2.51	0.40
1:B:24:ASP:O	1:B:27:PHE:HB3	2.22	0.40
1:A:66:GLU:HG2	2:A:246:HOH:O	2.21	0.40
1:A:66:GLU:HG3	2:A:247:HOH:O	2.20	0.40
1:B:25:GLU:HA	1:B:28:GLN:HB3	2.03	0.40
1:B:67:GLN:HA	1:B:68:PRO:HD3	1.97	0.40
1:A:100:GLN:CG	2:A:202:HOH:O	2.67	0.40
1:A:102:ARG:HB3	1:A:102:ARG:CZ	2.51	0.40
1:A:59:ASN:ND2	2:A:319:HOH:O	2.47	0.40
1:A:1:SER:HB2	2:A:301:HOH:O	2.22	0.40
1:A:95:LYS:NZ	2:A:256:HOH:O	2.51	0.40
1:A:74:LYS:HE2	2:A:189:HOH:O	2.21	0.40
1:B:81:GLN:HG3	2:B:184:HOH:O	2.21	0.40
1:A:56:ARG:O	1:A:59:ASN:HB2	2.21	0.40
1:A:68:PRO:CD	2:A:187:HOH:O	2.51	0.40
1:B:101:PHE:O	1:B:102:ARG:C	2.60	0.40
1:B:15:SER:HB2	2:B:198:HOH:O	2.21	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	1-A	136/149 (91%)	129 (95%)	7 (5%)	0	100	100
1	1-B	132/149 (89%)	123 (93%)	7 (5%)	2 (2%)	12	5
1	2-A	136/149 (91%)	133 (98%)	2 (2%)	1 (1%)	25	18
1	2-B	132/149 (89%)	125 (95%)	7 (5%)	0	100	100
1	3-A	136/149 (91%)	128 (94%)	5 (4%)	3 (2%)	8	3
1	3-B	132/149 (89%)	120 (91%)	8 (6%)	4 (3%)	5	1
1	4-A	136/149 (91%)	133 (98%)	2 (2%)	1 (1%)	25	18
1	4-B	132/149 (89%)	126 (96%)	6 (4%)	0	100	100
1	5-A	136/149 (91%)	122 (90%)	13 (10%)	1 (1%)	25	18
1	5-B	132/149 (89%)	117 (89%)	10 (8%)	5 (4%)	4	1
1	6-A	136/149 (91%)	128 (94%)	6 (4%)	2 (2%)	12	5
1	6-B	132/149 (89%)	124 (94%)	7 (5%)	1 (1%)	22	15
1	7-A	136/149 (91%)	132 (97%)	4 (3%)	0	100	100
1	7-B	132/149 (89%)	126 (96%)	5 (4%)	1 (1%)	22	15
1	8-A	136/149 (91%)	125 (92%)	10 (7%)	1 (1%)	25	18
1	8-B	132/149 (89%)	127 (96%)	4 (3%)	1 (1%)	22	15
All	All	2144/2384 (90%)	2018 (94%)	103 (5%)	23 (1%)	17	9

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	3-B	4	ALA
1	3-B	5	ALA
1	5-B	19	SER

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Mol	Chain	Res	Type
1	6-A	65	LEU
1	1-B	4	ALA
1	3-B	8	ASP
1	5-A	40	PRO
1	5-B	18	PHE
1	5-B	92	GLN
1	5-B	141	ILE
1	6-B	4	ALA
1	7-B	141	ILE
1	8-A	47	VAL
1	8-B	99	MET
1	1-B	58	ILE
1	3-A	56	ARG
1	3-B	7	ARG
1	4-A	124	PHE
1	6-A	64	LEU
1	3-A	67	GLN
1	3-A	92	GLN
1	5-B	53	ASP
1	2-A	40	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	1-A	122/129 (95%)	110 (90%)	12 (10%)	9	5
1	1-B	120/129 (93%)	117 (98%)	3 (2%)	53	54
1	2-A	122/129 (95%)	119 (98%)	3 (2%)	53	54
1	2-B	120/129 (93%)	114 (95%)	6 (5%)	28	23
1	3-A	122/129 (95%)	117 (96%)	5 (4%)	35	31
1	3-B	120/129 (93%)	116 (97%)	4 (3%)	43	41
1	4-A	122/129 (95%)	117 (96%)	5 (4%)	35	31
1	4-B	120/129 (93%)	118 (98%)	2 (2%)	66	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	5-A	122/129 (95%)	114 (93%)	8 (7%)	19	14
1	5-B	120/129 (93%)	110 (92%)	10 (8%)	13	8
1	6-A	122/129 (95%)	115 (94%)	7 (6%)	24	18
1	6-B	120/129 (93%)	110 (92%)	10 (8%)	13	8
1	7-A	122/129 (95%)	118 (97%)	4 (3%)	43	41
1	7-B	120/129 (93%)	114 (95%)	6 (5%)	28	23
1	8-A	122/129 (95%)	119 (98%)	3 (2%)	53	54
1	8-B	120/129 (93%)	114 (95%)	6 (5%)	28	23
All	All	1936/2064 (94%)	1842 (95%)	94 (5%)	29	24

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	1	SER
1	1-A	7	ARG
1	1-A	13	LEU
1	1-A	15	SER
1	1-A	25	GLU
1	1-A	28	GLN
1	1-A	32	MET
1	1-A	33	LEU
1	1-A	39	THR
1	1-A	55	ASP
1	1-A	101	PHE
1	1-A	108	LYS
1	1-B	55	ASP
1	1-B	93	LYS
1	1-B	101	PHE
1	2-A	32	MET
1	2-A	33	LEU
1	2-A	101	PHE
1	2-B	44	SER
1	2-B	56	ARG
1	2-B	73	ASP
1	2-B	99	MET
1	2-B	103	GLN
1	2-B	107	ASP
1	3-A	33	LEU
1	3-A	39	THR

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Mol	Chain	Res	Type
1	3-A	55	ASP
1	3-A	101	PHE
1	3-A	106	GLN
1	3-B	8	ASP
1	3-B	52	ASP
1	3-B	101	PHE
1	3-B	130	LYS
1	4-A	19	SER
1	4-A	28	GLN
1	4-A	31	GLN
1	4-A	79	VAL
1	4-A	101	PHE
1	4-B	101	PHE
1	4-B	106	GLN
1	5-A	16	SER
1	5-A	28	GLN
1	5-A	32	MET
1	5-A	39	THR
1	5-A	52	ASP
1	5-A	83	LYS
1	5-A	88	SER
1	5-A	101	PHE
1	5-B	25	GLU
1	5-B	33	LEU
1	5-B	34	GLN
1	5-B	40	PRO
1	5-B	44	SER
1	5-B	55	ASP
1	5-B	78	TYR
1	5-B	88	SER
1	5-B	89	VAL
1	5-B	101	PHE
1	6-A	25	GLU
1	6-A	28	GLN
1	6-A	29	GLN
1	6-A	30	LEU
1	6-A	33	LEU
1	6-A	48	THR
1	6-A	101	PHE
1	6-B	15	SER
1	6-B	16	SER
1	6-B	19	SER

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Mol	Chain	Res	Type
1	6-B	22	LEU
1	6-B	33	LEU
1	6-B	49	LEU
1	6-B	88	SER
1	6-B	97	THR
1	6-B	101	PHE
1	6-B	130	LYS
1	7-A	19	SER
1	7-A	29	GLN
1	7-A	101	PHE
1	7-A	139	GLN
1	7-B	16	SER
1	7-B	29	GLN
1	7-B	83	LYS
1	7-B	89	VAL
1	7-B	101	PHE
1	7-B	139	GLN
1	8-A	28	GLN
1	8-A	35	ASP
1	8-A	101	PHE
1	8-B	63	THR
1	8-B	78	TYR
1	8-B	101	PHE
1	8-B	107	ASP
1	8-B	108	LYS
1	8-B	131	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	29	GLN
1	1-A	34	GLN
1	1-A	59	ASN
1	1-A	81	GLN
1	1-B	34	GLN
1	1-B	67	GLN
1	1-B	80	HIS
1	1-B	140	GLN
1	2-A	26	GLN
1	2-A	29	GLN
1	2-A	34	GLN
1	2-A	81	GLN

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Mol	Chain	Res	Type
1	2-A	139	GLN
1	2-B	34	GLN
1	2-B	92	GLN
1	2-B	142	GLN
1	3-A	26	GLN
1	3-A	29	GLN
1	3-A	34	GLN
1	3-A	139	GLN
1	3-B	34	GLN
1	3-B	92	GLN
1	3-B	106	GLN
1	3-B	132	GLN
1	3-B	142	GLN
1	4-A	9	GLN
1	4-A	28	GLN
1	4-A	29	GLN
1	4-A	34	GLN
1	4-A	59	ASN
1	4-A	81	GLN
1	4-A	142	GLN
1	4-B	92	GLN
1	4-B	106	GLN
1	4-B	136	GLN
1	4-B	142	GLN
1	5-A	20	GLN
1	5-A	26	GLN
1	5-A	29	GLN
1	5-A	34	GLN
1	5-A	80	HIS
1	5-A	81	GLN
1	5-A	92	GLN
1	5-A	136	GLN
1	5-A	139	GLN
1	5-B	34	GLN
1	5-B	81	GLN
1	5-B	92	GLN
1	5-B	136	GLN
1	5-B	142	GLN
1	6-A	29	GLN
1	6-A	34	GLN
1	6-A	81	GLN
1	6-A	140	GLN

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Mol	Chain	Res	Type
1	6-B	34	GLN
1	6-B	136	GLN
1	7-A	29	GLN
1	7-A	34	GLN
1	7-A	81	GLN
1	7-A	139	GLN
1	7-A	140	GLN
1	7-B	26	GLN
1	7-B	34	GLN
1	7-B	92	GLN
1	7-B	136	GLN
1	7-B	142	GLN
1	8-A	26	GLN
1	8-A	29	GLN
1	8-A	31	GLN
1	8-A	34	GLN
1	8-A	103	GLN
1	8-A	140	GLN
1	8-A	142	GLN
1	8-B	34	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 [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	1-A	140/149 (93%)	-0.15	9 (6%)	20	20	7, 14, 37, 55	140 (100%)
1	1-B	136/149 (91%)	-0.18	4 (2%)	52	52	5, 15, 38, 51	136 (100%)
1	2-A	140/149 (93%)	-0.15	9 (6%)	20	20	7, 14, 37, 55	140 (100%)
1	2-B	136/149 (91%)	-0.18	4 (2%)	52	52	5, 15, 38, 51	136 (100%)
1	3-A	140/149 (93%)	-0.15	9 (6%)	20	20	7, 14, 37, 55	140 (100%)
1	3-B	136/149 (91%)	-0.18	4 (2%)	52	52	5, 15, 38, 51	136 (100%)
1	4-A	140/149 (93%)	-0.15	9 (6%)	20	20	7, 14, 37, 55	140 (100%)
1	4-B	136/149 (91%)	-0.18	4 (2%)	52	52	5, 15, 38, 51	136 (100%)
1	5-A	140/149 (93%)	-0.15	9 (6%)	20	20	7, 14, 37, 55	140 (100%)
1	5-B	136/149 (91%)	-0.18	4 (2%)	52	52	5, 15, 38, 51	136 (100%)
1	6-A	140/149 (93%)	-0.15	9 (6%)	20	20	7, 14, 37, 55	140 (100%)
1	6-B	136/149 (91%)	-0.18	4 (2%)	52	52	5, 15, 38, 51	136 (100%)
1	7-A	140/149 (93%)	-0.15	9 (6%)	20	20	7, 14, 37, 55	140 (100%)
1	7-B	136/149 (91%)	-0.18	4 (2%)	52	52	5, 15, 38, 51	136 (100%)
1	8-A	140/149 (93%)	-0.15	9 (6%)	20	20	7, 14, 37, 55	140 (100%)
1	8-B	136/149 (91%)	-0.18	4 (2%)	52	52	5, 15, 38, 51	136 (100%)
All	All	2208/2384 (92%)	-0.17	104 (4%)	23	32	5, 15, 39, 55	2208 (100%)

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	35	ASP	4.4
1	2-A	35	ASP	4.4
1	3-A	35	ASP	4.4
1	4-A	35	ASP	4.4
1	5-A	35	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
1	6-A	35	ASP	4.4
1	7-A	35	ASP	4.4
1	8-A	35	ASP	4.4
1	1-A	142	GLN	4.3
1	2-A	142	GLN	4.3
1	3-A	142	GLN	4.3
1	4-A	142	GLN	4.3
1	5-A	142	GLN	4.3
1	6-A	142	GLN	4.3
1	7-A	142	GLN	4.3
1	8-A	142	GLN	4.3
1	1-B	3	ALA	4.2
1	2-B	3	ALA	4.2
1	3-B	3	ALA	4.2
1	4-B	3	ALA	4.2
1	5-B	3	ALA	4.2
1	6-B	3	ALA	4.2
1	7-B	3	ALA	4.2
1	8-B	3	ALA	4.2
1	1-A	141	ILE	3.7
1	2-A	141	ILE	3.7
1	3-A	141	ILE	3.7
1	4-A	141	ILE	3.7
1	5-A	141	ILE	3.7
1	6-A	141	ILE	3.7
1	7-A	141	ILE	3.7
1	8-A	141	ILE	3.7
1	1-A	68	PRO	3.1
1	2-A	68	PRO	3.1
1	3-A	68	PRO	3.1
1	4-A	68	PRO	3.1
1	5-A	68	PRO	3.1
1	6-A	68	PRO	3.1
1	7-A	68	PRO	3.1
1	8-A	68	PRO	3.1
1	1-A	32	MET	2.9
1	2-A	32	MET	2.9
1	3-A	32	MET	2.9
1	4-A	32	MET	2.9
1	5-A	32	MET	2.9
1	6-A	32	MET	2.9
1	7-A	32	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	8-A	32	MET	2.9
1	1-A	143	ALA	2.8
1	2-A	143	ALA	2.8
1	3-A	143	ALA	2.8
1	4-A	143	ALA	2.8
1	5-A	143	ALA	2.8
1	6-A	143	ALA	2.8
1	7-A	143	ALA	2.8
1	8-A	143	ALA	2.8
1	1-A	3	ALA	2.8
1	2-A	3	ALA	2.8
1	3-A	3	ALA	2.8
1	4-A	3	ALA	2.8
1	5-A	3	ALA	2.8
1	6-A	3	ALA	2.8
1	7-A	3	ALA	2.8
1	8-A	3	ALA	2.8
1	1-B	142	GLN	2.8
1	2-B	142	GLN	2.8
1	3-B	142	GLN	2.8
1	4-B	142	GLN	2.8
1	5-B	142	GLN	2.8
1	6-B	142	GLN	2.8
1	7-B	142	GLN	2.8
1	8-B	142	GLN	2.8
1	1-B	32	MET	2.6
1	2-B	32	MET	2.6
1	3-B	32	MET	2.6
1	4-B	32	MET	2.6
1	5-B	32	MET	2.6
1	6-B	32	MET	2.6
1	7-B	32	MET	2.6
1	8-B	32	MET	2.6
1	1-B	29	GLN	2.6
1	2-B	29	GLN	2.6
1	3-B	29	GLN	2.6
1	4-B	29	GLN	2.6
1	5-B	29	GLN	2.6
1	6-B	29	GLN	2.6
1	7-B	29	GLN	2.6
1	8-B	29	GLN	2.6
1	1-A	39	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	2-A	39	THR	2.5
1	3-A	39	THR	2.5
1	4-A	39	THR	2.5
1	5-A	39	THR	2.5
1	6-A	39	THR	2.5
1	7-A	39	THR	2.5
1	8-A	39	THR	2.5
1	1-A	139	GLN	2.1
1	2-A	139	GLN	2.1
1	3-A	139	GLN	2.1
1	4-A	139	GLN	2.1
1	5-A	139	GLN	2.1
1	6-A	139	GLN	2.1
1	7-A	139	GLN	2.1
1	8-A	139	GLN	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.