



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:19 AM GMT

PDB ID : 2Q52
Title : Ensemble refinement of the crystal structure of a glycolipid transfer-like protein from *Galdieria sulphuraria*
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 : 1.38 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

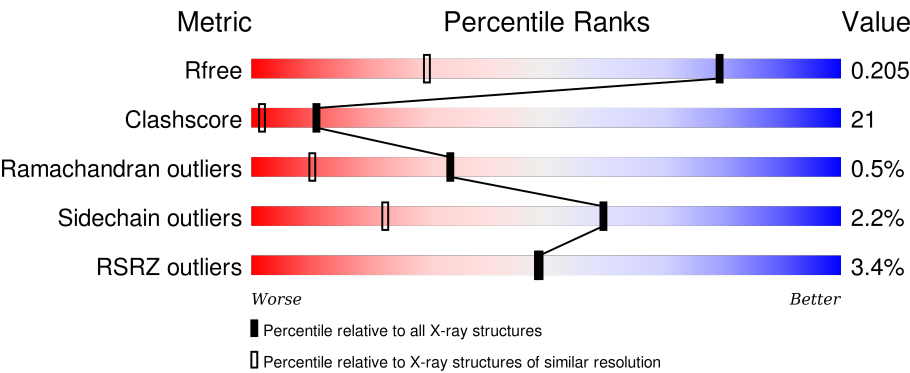
MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.38 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	1918 (1.40-1.36)
Clashscore	102246	2042 (1.40-1.36)
Ramachandran outliers	100387	1993 (1.40-1.36)
Sidechain outliers	100360	1992 (1.40-1.36)
RSRZ outliers	91569	1917 (1.40-1.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	224	<div><div>2%</div><div><div></div><div>53%</div><div>36%</div><div>•</div><div>8%</div></div></div>
1	1-B	224	<div><div>4%</div><div><div></div><div>61%</div><div>30%</div><div>•</div><div>8%</div></div></div>
1	2-A	224	<div><div>2%</div><div><div></div><div>54%</div><div>36%</div><div>•</div><div>8%</div></div></div>
1	2-B	224	<div><div>4%</div><div><div></div><div>59%</div><div>31%</div><div>•</div><div>8%</div></div></div>
1	3-A	224	<div><div>2%</div><div><div></div><div>63%</div><div>27%</div><div>•</div><div>8%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	3-B	224	
1	4-A	224	
1	4-B	224	
1	5-A	224	
1	5-B	224	
1	6-A	224	
1	6-B	224	
1	7-A	224	
1	7-B	224	
1	8-A	224	
1	8-B	224	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 29856 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 Glycolipid transfer-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	206	Total	C	N	O	S	0	0	0
			1674	1085	287	296	6			
1	2-A	206	Total	C	N	O	S	0	0	0
			1674	1085	287	296	6			
1	3-A	206	Total	C	N	O	S	0	0	0
			1674	1085	287	296	6			
1	4-A	206	Total	C	N	O	S	0	0	0
			1674	1085	287	296	6			
1	5-A	206	Total	C	N	O	S	0	0	0
			1674	1085	287	296	6			
1	6-A	206	Total	C	N	O	S	0	0	0
			1674	1085	287	296	6			
1	7-A	206	Total	C	N	O	S	0	0	0
			1674	1085	287	296	6			
1	8-A	206	Total	C	N	O	S	0	0	0
			1674	1085	287	296	6			
1	1-B	206	Total	C	N	O	S	0	0	0
			1674	1085	287	296	6			
1	2-B	206	Total	C	N	O	S	0	0	0
			1674	1085	287	296	6			
1	3-B	206	Total	C	N	O	S	0	0	0
			1674	1085	287	296	6			
1	4-B	206	Total	C	N	O	S	0	0	0
			1674	1085	287	296	6			
1	5-B	206	Total	C	N	O	S	0	0	0
			1674	1085	287	296	6			
1	6-B	206	Total	C	N	O	S	0	0	0
			1674	1085	287	296	6			
1	7-B	206	Total	C	N	O	S	0	0	0
			1674	1085	287	296	6			
1	8-B	206	Total	C	N	O	S	0	0	0
			1674	1085	287	296	6			

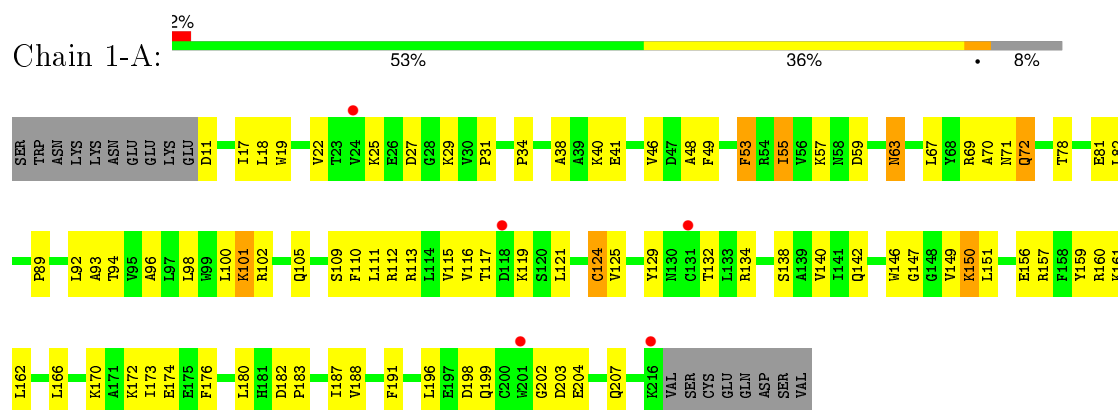
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	1-A	201	Total O 201 201	0	0
2	2-A	206	Total O 206 206	0	0
2	3-A	212	Total O 212 212	0	0
2	4-A	202	Total O 202 202	0	0
2	5-A	201	Total O 201 201	0	0
2	6-A	202	Total O 202 202	0	0
2	7-A	204	Total O 204 204	0	0
2	8-A	206	Total O 206 206	0	0
2	1-B	183	Total O 183 183	0	0
2	2-B	178	Total O 178 178	0	0
2	3-B	172	Total O 172 172	0	0
2	4-B	182	Total O 182 182	0	0
2	5-B	183	Total O 183 183	0	0
2	6-B	182	Total O 182 182	0	0
2	7-B	180	Total O 180 180	0	0
2	8-B	178	Total O 178 178	0	0

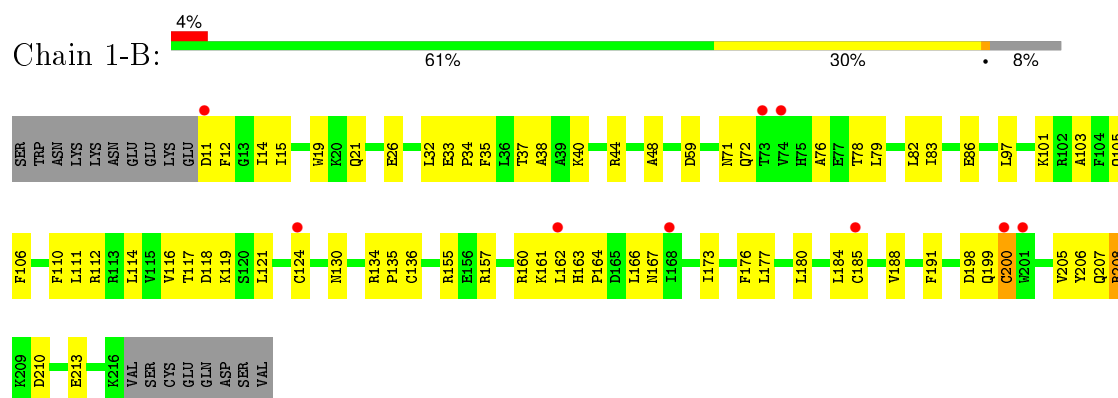
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

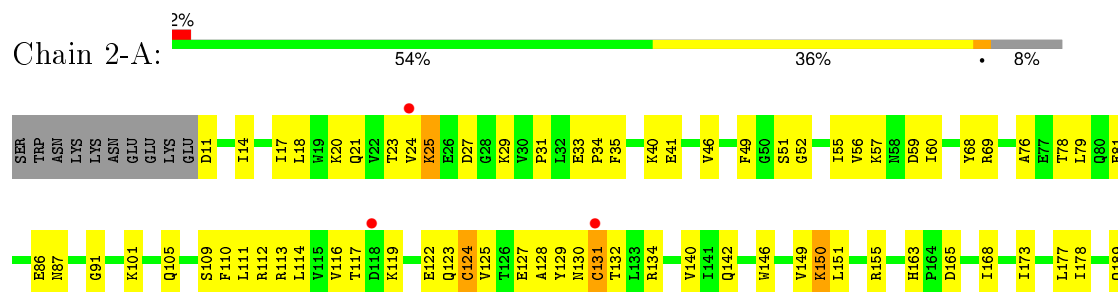
• Molecule 1: Glycolipid transfer-like protein



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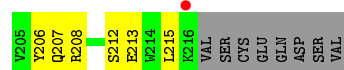




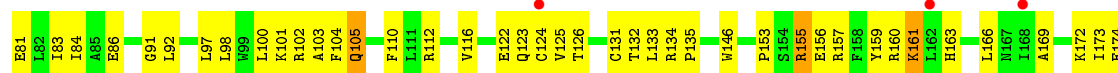
- Molecule 1: Glycolipid transfer-like protein



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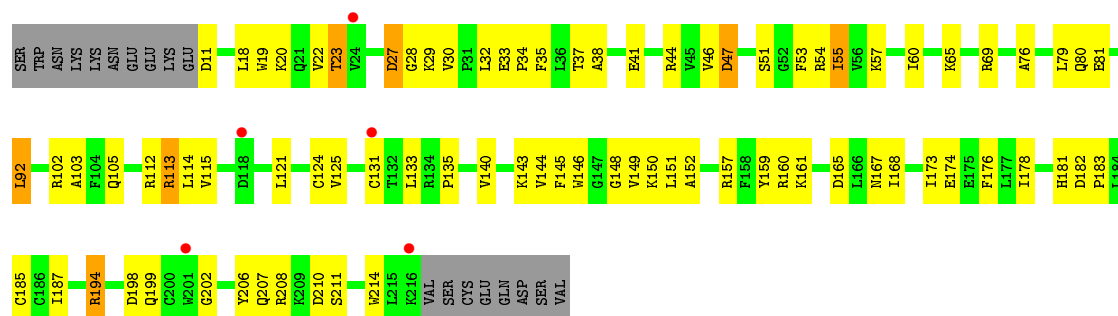


- Molecule 1: Glycolipid transfer-like protein

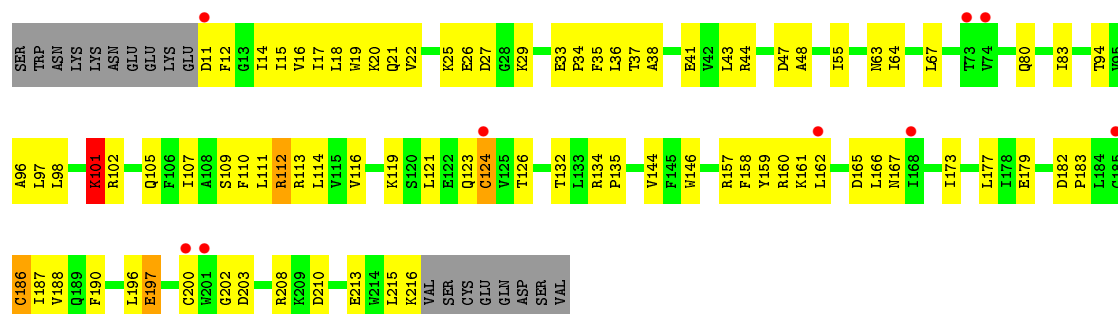


- Molecule 1: Glycolipid transfer-like protein

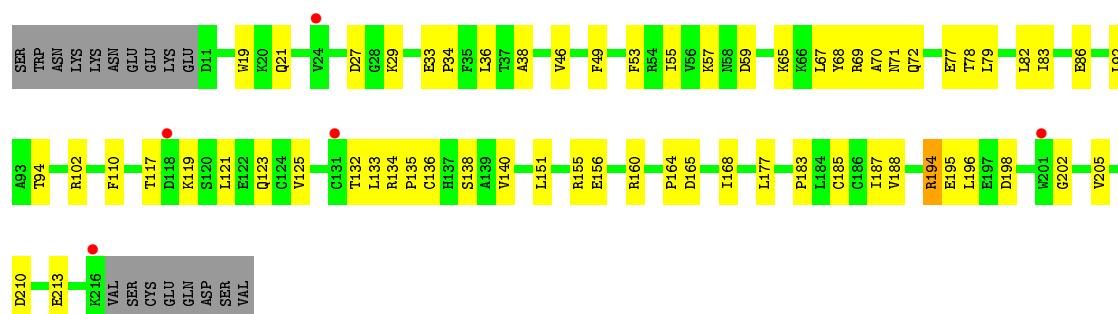




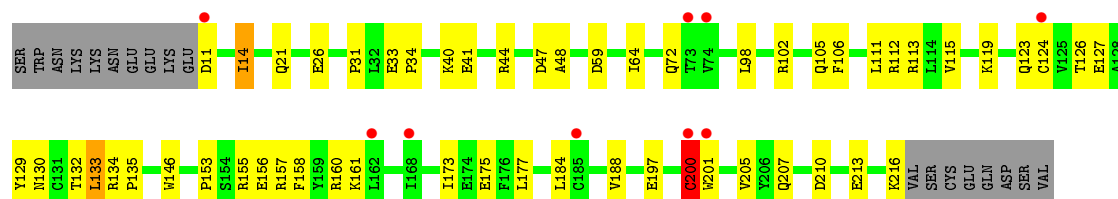
- Molecule 1: Glycolipid transfer-like protein



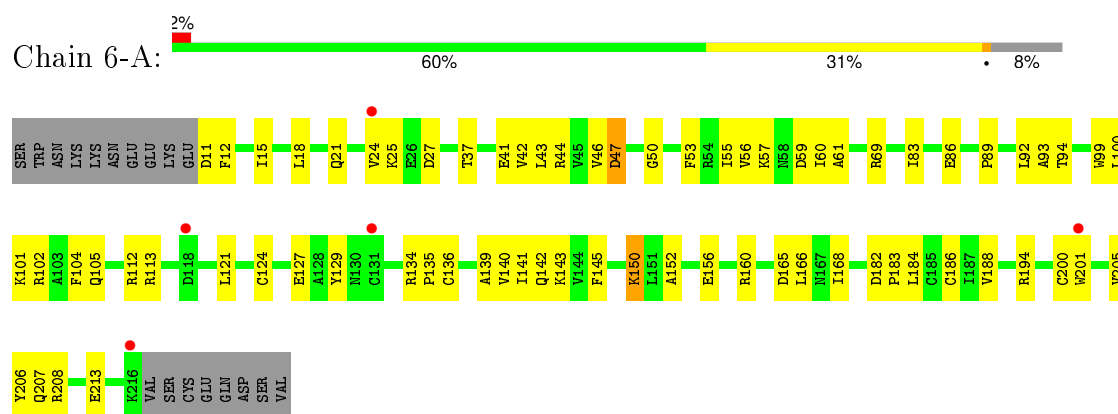
- Molecule 1: Glycolipid transfer-like protein



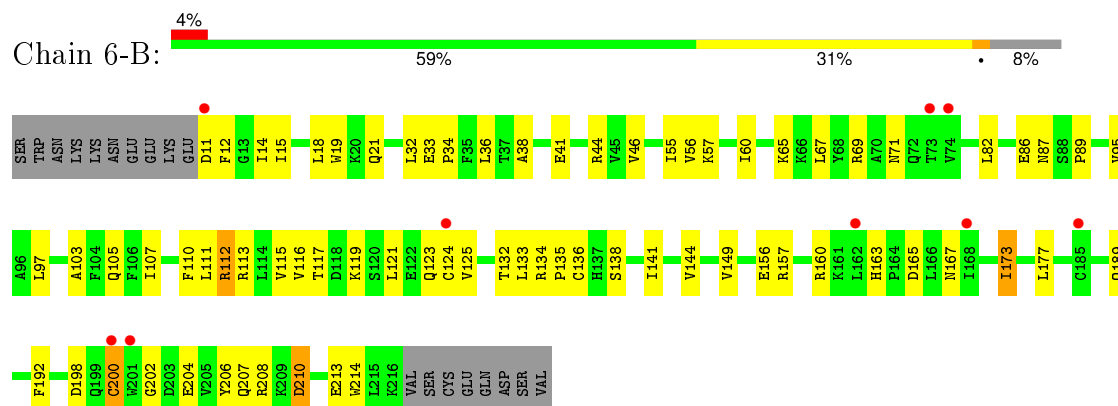
- Molecule 1: Glycolipid transfer-like protein



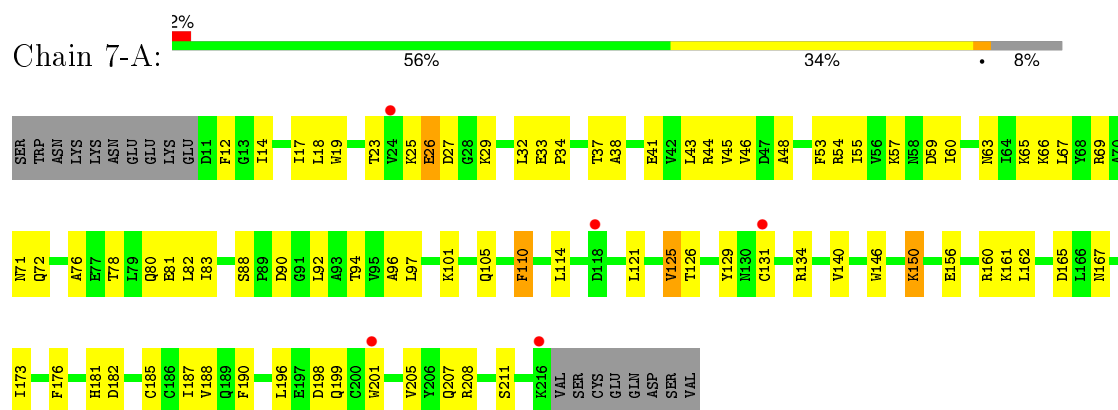
- Molecule 1: Glycolipid transfer-like protein



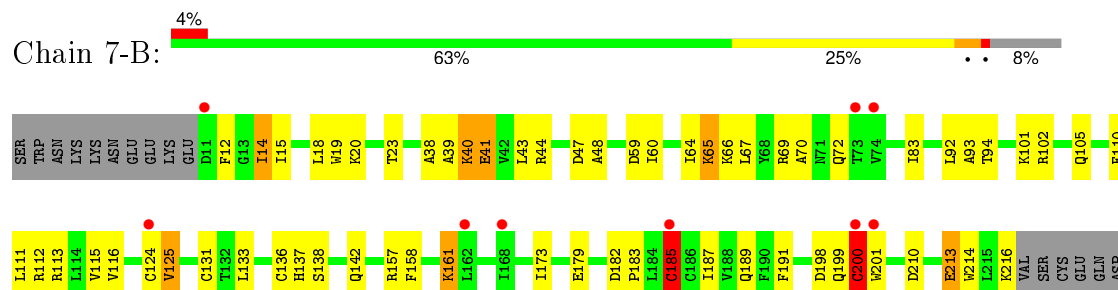
- Molecule 1: Glycolipid transfer-like protein



- Molecule 1: Glycolipid transfer-like protein



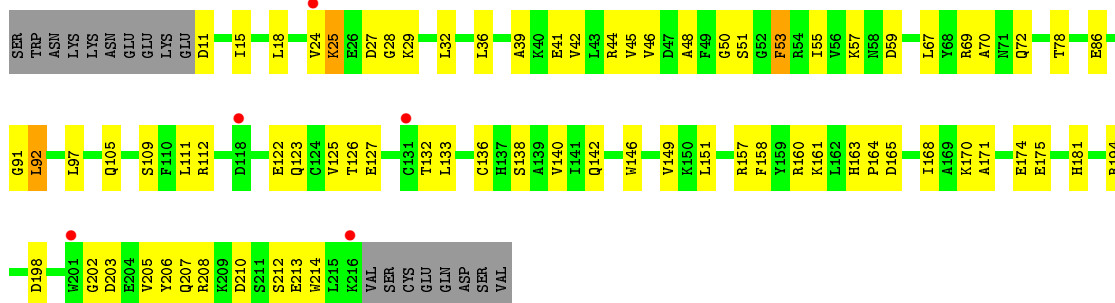
- Molecule 1: Glycolipid transfer-like protein



SER
VAL

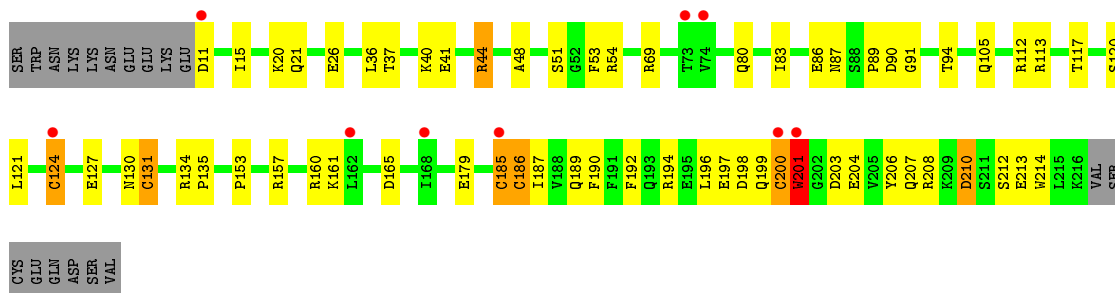
- Molecule 1: Glycolipid transfer-like protein

Chain 8-A: 



- Molecule 1: Glycolipid transfer-like protein

Chain 8-B: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	118.44Å 48.20Å 89.41Å 90.00° 115.06° 90.00°	Depositor
Resolution (Å)	41.99 – 1.38 43.96 – 1.38	Depositor EDS
% Data completeness (in resolution range)	98.8 (41.99-1.38) 99.0 (43.96-1.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.08 (at 1.38Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.166 , 0.202 0.170 , 0.205	Depositor DCC
R_{free} test set	4669 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	16.9	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 93176 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	29856	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 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	1-A	0.77	1/1711 (0.1%)	0.83	1/2315 (0.0%)
1	1-B	0.73	1/1711 (0.1%)	0.77	1/2315 (0.0%)
1	2-A	0.72	0/1711	0.82	0/2315
1	2-B	0.78	1/1711 (0.1%)	0.80	1/2315 (0.0%)
1	3-A	0.73	0/1711	0.80	0/2315
1	3-B	0.78	2/1711 (0.1%)	0.86	1/2315 (0.0%)
1	4-A	0.74	0/1711	0.86	3/2315 (0.1%)
1	4-B	0.76	0/1711	0.81	2/2315 (0.1%)
1	5-A	0.78	0/1711	0.91	4/2315 (0.2%)
1	5-B	0.82	1/1711 (0.1%)	0.89	4/2315 (0.2%)
1	6-A	0.81	0/1711	0.91	1/2315 (0.0%)
1	6-B	0.78	0/1711	0.88	2/2315 (0.1%)
1	7-A	0.80	1/1711 (0.1%)	0.86	0/2315
1	7-B	0.79	0/1711	0.90	2/2315 (0.1%)
1	8-A	0.76	0/1711	0.85	2/2315 (0.1%)
1	8-B	0.88	3/1711 (0.2%)	0.90	2/2315 (0.1%)
All	All	0.78	10/27376 (0.0%)	0.85	26/37040 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	2-A	0	1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5-B	200	CYS	CB-SG	10.14	1.99	1.82
1	8-B	124	CYS	CB-SG	-8.95	1.67	1.82
1	8-B	131	CYS	CB-SG	-8.78	1.67	1.82
1	8-B	186	CYS	CB-SG	-6.94	1.70	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1-A	124	CYS	CB-SG	-6.82	1.70	1.82
1	3-B	124	CYS	CB-SG	-6.55	1.71	1.82
1	7-A	185	CYS	CB-SG	6.24	1.92	1.82
1	1-B	185	CYS	CB-SG	-5.89	1.72	1.81
1	2-B	200	CYS	CB-SG	5.44	1.91	1.82
1	3-B	131	CYS	CB-SG	-5.01	1.73	1.81

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5-B	200	CYS	CA-CB-SG	9.89	131.80	114.00
1	5-A	102	ARG	NE-CZ-NH1	-7.92	116.34	120.30
1	8-B	201	TRP	CA-CB-CG	-7.11	100.20	113.70
1	5-B	112	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	4-A	113	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	6-B	200	CYS	N-CA-C	6.46	128.45	111.00
1	4-B	101	LYS	CD-CE-NZ	6.22	126.00	111.70
1	3-B	155	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	7-B	185	CYS	CA-CB-SG	-6.14	102.95	114.00
1	7-B	200	CYS	CA-CB-SG	-6.13	102.97	114.00
1	5-A	188	VAL	CG1-CB-CG2	-6.12	101.10	110.90
1	4-A	113	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	1-B	112	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	8-A	92	LEU	CB-CG-CD2	5.74	120.76	111.00
1	5-B	200	CYS	N-CA-CB	-5.71	100.31	110.60
1	4-A	194	ARG	NE-CZ-NH1	-5.64	117.48	120.30
1	1-A	182	ASP	CB-CG-OD1	5.50	123.25	118.30
1	8-A	194	ARG	NE-CZ-NH1	-5.41	117.59	120.30
1	4-B	208	ARG	NE-CZ-NH1	-5.31	117.65	120.30
1	8-B	112	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	2-B	102	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	5-A	194	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	6-B	112	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	6-A	134	ARG	C-N-CD	5.19	139.29	128.40
1	5-A	79	LEU	CB-CG-CD1	-5.08	102.37	111.00
1	5-B	155	ARG	NE-CZ-NH1	-5.03	117.79	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2-A	129	TYR	Sidechain

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	1674	0	1701	90	0
1	1-B	1674	0	1701	66	0
1	2-A	1674	0	1701	80	0
1	2-B	1674	0	1701	76	0
1	3-A	1674	0	1701	71	0
1	3-B	1674	0	1701	84	0
1	4-A	1674	0	1701	77	0
1	4-B	1674	0	1701	94	0
1	5-A	1674	0	1701	55	0
1	5-B	1674	0	1701	55	0
1	6-A	1674	0	1701	64	0
1	6-B	1674	0	1701	62	0
1	7-A	1674	0	1701	83	0
1	7-B	1674	0	1701	63	0
1	8-A	1674	0	1701	66	0
1	8-B	1674	0	1701	59	0
2	1-A	201	0	0	19	0
2	1-B	183	0	0	10	0
2	2-A	206	0	0	19	0
2	2-B	178	0	0	9	0
2	3-A	212	0	0	22	0
2	3-B	172	0	0	17	0
2	4-A	202	0	0	21	0
2	4-B	182	0	0	11	0
2	5-A	201	0	0	16	0
2	5-B	183	0	0	12	0
2	6-A	202	0	0	16	0
2	6-B	182	0	0	8	0
2	7-A	204	0	0	22	0
2	7-B	180	0	0	15	0
2	8-A	206	0	0	15	0
2	8-B	178	0	0	13	0
All	All	29856	0	27216	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 21.

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:200:CYS:O	1:B:200:CYS:SG	1.98	1.21
1:B:102:ARG:HG2	1:B:200:CYS:SG	1.82	1.17
1:B:210:ASP:OD2	1:B:213:GLU:HB2	1.44	1.14
1:A:57:LYS:HD3	2:B:298:HOH:O	1.48	1.11
1:A:46:VAL:HG13	1:A:53:PHE:HB3	1.30	1.11
1:B:50:GLY:HA3	2:B:275:HOH:O	1.49	1.11
1:A:112:ARG:HD3	1:A:206:TYR:HB2	1.40	1.03
1:B:48:ALA:HA	1:B:161:LYS:HG2	1.34	1.03
1:B:11:ASP:O	1:B:14:ILE:HG22	1.58	1.02
1:B:105:GLN:HE21	1:B:207:GLN:HE22	1.06	1.02
1:A:140:VAL:HG22	2:A:316:HOH:O	1.60	1.02
1:B:134:ARG:HD3	2:B:352:HOH:O	1.61	1.00
1:A:18:LEU:HD23	1:A:21:GLN:HE22	1.28	0.96
1:B:210:ASP:OD1	1:B:213:GLU:HB2	1.66	0.96
1:A:27:ASP:HB3	2:A:387:HOH:O	1.65	0.95
1:B:185:CYS:SG	2:B:280:HOH:O	2.24	0.95
1:A:46:VAL:HG11	1:A:57:LYS:HB2	1.44	0.95
1:B:210:ASP:HB2	1:B:213:GLU:HB2	1.49	0.94
1:A:27:ASP:HB3	2:A:378:HOH:O	1.65	0.94
1:B:40:LYS:HG3	1:B:64:ILE:HG21	1.49	0.94
1:A:105:GLN:HE21	1:A:207:GLN:HE22	1.04	0.93
1:B:102:ARG:HG2	1:B:200:CYS:SG	2.09	0.92
1:A:46:VAL:HG11	1:A:57:LYS:HB2	1.49	0.92
1:A:55:ILE:HD13	2:B:230:HOH:O	1.69	0.92
1:B:102:ARG:HG2	1:B:200:CYS:SG	2.10	0.92
1:A:18:LEU:HD23	1:A:21:GLN:NE2	1.84	0.91
1:B:101:LYS:HE2	1:B:197:GLU:OE2	1.71	0.91
1:A:92:LEU:HD13	2:A:280:HOH:O	1.68	0.91
1:A:140:VAL:HG22	2:A:316:HOH:O	1.70	0.90
1:A:126:THR:HG23	1:A:146:TRP:CH2	2.06	0.90
1:B:113:ARG:HB2	1:B:124:CYS:SG	2.12	0.90
1:B:12:PHE:HD1	1:B:44:ARG:HD2	1.36	0.90
1:A:184:LEU:HD23	1:A:206:TYR:HE2	1.37	0.89
1:A:210:ASP:HB3	1:A:213:GLU:HB2	1.55	0.89
1:A:57:LYS:HD3	2:A:296:HOH:O	1.72	0.89
1:A:27:ASP:HB3	2:A:378:HOH:O	1.72	0.89
1:B:199:GLN:NE2	2:B:341:HOH:O	2.05	0.89
1:A:205:VAL:HG23	2:A:322:HOH:O	1.73	0.89
1:B:132:THR:O	1:B:200:CYS:HB3	1.73	0.89
1:A:157:ARG:HG2	1:A:161:LYS:HE3	1.52	0.88
1:B:121:LEU:HA	1:B:124:CYS:SG	2.13	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:ARG:HB3	1:B:124:CYS:HB2	1.53	0.88
1:A:105:GLN:HE21	1:A:207:GLN:NE2	1.71	0.87
1:A:111:LEU:O	1:A:115:VAL:HG13	1.74	0.87
1:A:27:ASP:HB3	2:A:382:HOH:O	1.71	0.87
1:A:46:VAL:CG1	1:A:53:PHE:HB3	2.04	0.87
1:B:116:VAL:HG23	1:B:117:THR:HG23	1.57	0.87
1:B:105:GLN:HE21	1:B:207:GLN:NE2	1.73	0.86
1:B:66:LYS:HG2	1:B:69:ARG:HH22	1.40	0.86
1:A:185:CYS:SG	2:A:368:HOH:O	2.34	0.85
1:A:70:ALA:HB2	1:A:92:LEU:HB3	1.59	0.85
1:A:134:ARG:HD3	2:A:291:HOH:O	1.75	0.85
1:A:105:GLN:HE21	1:A:207:GLN:HE22	1.24	0.85
1:B:120:SER:O	1:B:124:CYS:SG	2.35	0.85
1:B:214:TRP:HA	2:B:384:HOH:O	1.76	0.85
1:B:113:ARG:HB2	1:B:124:CYS:SG	2.16	0.84
1:B:134:ARG:HD3	2:B:353:HOH:O	1.75	0.84
1:B:111:LEU:HD22	1:B:173:ILE:HD12	1.58	0.84
1:B:66:LYS:HG2	1:B:69:ARG:NH2	1.93	0.84
1:A:86:GLU:OE1	1:A:91:GLY:HA3	1.78	0.83
1:B:29:LYS:HD3	1:B:80:GLN:HB2	1.61	0.83
1:A:160:ARG:HD2	2:A:358:HOH:O	1.76	0.83
1:B:27:ASP:OD2	1:B:29:LYS:HE2	1.79	0.83
1:A:162:LEU:CD1	1:A:173:ILE:HD11	2.07	0.82
1:A:57:LYS:HD3	2:A:302:HOH:O	1.78	0.82
1:A:92:LEU:CD1	2:A:280:HOH:O	2.25	0.82
1:B:139:ALA:O	2:B:401:HOH:O	1.98	0.82
1:A:131:CYS:SG	2:A:422:HOH:O	2.38	0.82
1:A:125:VAL:HG11	1:A:149:VAL:HG22	1.58	0.82
1:A:195:GLU:OE1	2:A:289:HOH:O	1.97	0.81
1:A:105:GLN:HE21	1:A:207:GLN:HE22	1.26	0.81
1:B:111:LEU:O	1:B:115:VAL:HG22	1.80	0.81
1:B:210:ASP:OD2	1:B:213:GLU:CB	2.29	0.81
1:B:182:ASP:OD1	2:B:247:HOH:O	1.98	0.81
1:A:119:LYS:HD3	1:A:123:GLN:HE21	1.45	0.81
1:B:214:TRP:HD1	2:B:241:HOH:O	1.62	0.80
1:B:160:ARG:HB2	1:B:166:LEU:HD21	1.62	0.80
1:B:48:ALA:HA	1:B:161:LYS:HG2	1.64	0.80
1:B:113:ARG:HB2	1:B:124:CYS:HB2	1.62	0.80
1:A:44:ARG:HG2	1:A:44:ARG:HH21	1.46	0.80
1:A:167:ASN:O	2:A:250:HOH:O	2.00	0.79
1:A:55:ILE:O	1:A:59:ASP:HB2	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:GLN:O	1:B:200:CYS:HB3	1.82	0.79
1:B:36:LEU:HD21	1:B:67:LEU:HD13	1.63	0.79
1:A:46:VAL:HG12	2:A:243:HOH:O	1.82	0.79
1:A:46:VAL:HG13	1:A:53:PHE:HB3	1.63	0.79
1:B:131:CYS:SG	2:B:383:HOH:O	2.40	0.79
1:A:31:PRO:HB2	1:A:34:PRO:HG2	1.63	0.78
1:B:31:PRO:HD2	2:B:288:HOH:O	1.81	0.78
1:A:15:ILE:HG13	1:A:41:GLU:HB3	1.65	0.78
1:B:157:ARG:HG3	1:B:157:ARG:HH11	1.48	0.78
1:A:140:VAL:CG2	2:A:318:HOH:O	2.32	0.78
1:B:112:ARG:HH21	1:B:113:ARG:CG	1.97	0.78
1:B:48:ALA:HA	1:B:161:LYS:HG2	1.66	0.78
1:A:165:ASP:OD2	2:A:363:HOH:O	2.02	0.78
1:A:131:CYS:SG	2:A:349:HOH:O	2.42	0.78
1:B:198:ASP:OD1	2:B:263:HOH:O	2.02	0.77
1:A:210:ASP:HB3	1:A:213:GLU:CB	2.15	0.77
1:B:113:ARG:CB	1:B:124:CYS:SG	2.72	0.77
1:A:156:GLU:OE2	2:A:394:HOH:O	2.02	0.77
1:B:112:ARG:O	1:B:116:VAL:HG22	1.84	0.77
1:B:98:LEU:O	1:B:102:ARG:HG3	1.85	0.77
1:B:101:LYS:CE	1:B:197:GLU:OE2	2.33	0.76
1:A:131:CYS:SG	2:A:424:HOH:O	2.42	0.76
1:A:140:VAL:CG2	2:A:316:HOH:O	2.30	0.76
1:A:46:VAL:HG11	1:A:57:LYS:HB2	1.65	0.76
1:B:113:ARG:CB	1:B:124:CYS:HB2	2.15	0.76
1:B:132:THR:HG22	1:B:133:LEU:N	1.99	0.76
1:B:208:ARG:HD2	1:B:213:GLU:HG2	1.67	0.76
1:A:33:GLU:HB2	1:A:34:PRO:HD3	1.68	0.76
1:B:37:THR:HA	1:B:40:LYS:CE	2.15	0.76
1:B:156:GLU:HG3	1:B:166:LEU:HD11	1.66	0.76
1:B:48:ALA:O	1:B:161:LYS:HE3	1.85	0.76
1:B:201:TRP:O	2:B:256:HOH:O	2.03	0.75
1:A:174:GLU:HG2	1:A:214:TRP:HH2	1.51	0.75
1:A:198:ASP:OD1	2:A:402:HOH:O	2.04	0.75
1:A:29:LYS:HB3	1:A:78:THR:HG21	1.67	0.75
1:A:146:TRP:O	1:A:150:LYS:HD2	1.87	0.75
1:A:130:ASN:OD1	1:A:134:ARG:HD2	1.87	0.74
1:B:213:GLU:OE1	1:B:216:LYS:HG3	1.87	0.74
1:B:11:ASP:O	1:B:14:ILE:HG22	1.87	0.74
1:A:41:GLU:OE1	1:A:44:ARG:CZ	2.35	0.74
1:A:140:VAL:HG21	1:B:21:GLN:OE1	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:CYS:SG	1:B:187:ILE:N	2.60	0.74
1:A:50:GLY:HA3	2:A:236:HOH:O	1.86	0.74
1:A:185:CYS:SG	2:A:367:HOH:O	2.45	0.74
1:B:83:ILE:HD11	1:B:94:THR:HA	1.70	0.74
1:B:157:ARG:HG2	1:B:161:LYS:HE2	1.70	0.74
1:B:192:PHE:O	2:B:392:HOH:O	2.06	0.73
1:A:44:ARG:NH1	2:A:384:HOH:O	2.19	0.73
1:B:101:LYS:O	1:B:105:GLN:HG3	1.88	0.73
1:B:216:LYS:HB3	1:B:216:LYS:NZ	2.03	0.73
1:B:59:ASP:OD1	2:B:237:HOH:O	2.06	0.73
1:A:140:VAL:HG22	2:A:318:HOH:O	1.89	0.73
1:B:18:LEU:HD12	1:B:41:GLU:HG2	1.70	0.73
1:A:92:LEU:HD12	1:A:92:LEU:H	1.53	0.73
1:B:114:LEU:HD11	1:B:155:ARG:HG3	1.70	0.72
1:B:101:LYS:HD3	1:B:187:ILE:HG22	1.71	0.72
1:A:46:VAL:HG13	1:A:53:PHE:CB	2.14	0.72
1:A:117:THR:HG21	1:A:119:LYS:HE3	1.72	0.71
1:B:11:ASP:O	1:B:14:ILE:HG22	1.90	0.71
1:B:114:LEU:N	1:B:124:CYS:SG	2.63	0.71
1:B:76:ALA:HB1	1:B:81:GLU:HB3	1.71	0.71
1:A:21:GLN:HG3	2:A:303:HOH:O	1.88	0.71
1:A:125:VAL:HG11	1:A:149:VAL:HG22	1.72	0.71
1:B:200:CYS:O	1:B:201:TRP:CD2	2.44	0.71
1:A:105:GLN:NE2	1:A:207:GLN:HE22	1.86	0.71
1:B:155:ARG:NH1	1:B:155:ARG:HB2	2.06	0.71
1:B:47:ASP:OD1	2:B:305:HOH:O	2.07	0.70
1:B:110:PHE:CD1	1:B:124:CYS:SG	2.81	0.70
1:B:33:GLU:HB2	1:B:34:PRO:HD3	1.72	0.70
1:A:101:LYS:HD3	1:A:188:VAL:HA	1.73	0.70
1:A:69:ARG:HA	1:A:72:GLN:HG3	1.71	0.70
1:A:31:PRO:HB2	1:A:34:PRO:HD2	1.70	0.70
1:B:119:LYS:HD2	1:B:123:GLN:NE2	2.07	0.70
1:A:27:ASP:HB3	2:A:381:HOH:O	1.91	0.70
1:A:92:LEU:HD12	1:A:92:LEU:N	2.07	0.70
1:B:101:LYS:HZ2	1:B:105:GLN:HE22	1.39	0.70
1:B:110:PHE:CZ	1:B:114:LEU:HD22	2.26	0.70
1:A:162:LEU:HD13	1:A:173:ILE:HD11	1.73	0.70
1:B:101:LYS:NZ	1:B:105:GLN:HE22	1.89	0.70
1:A:71:ASN:O	1:A:72:GLN:HG3	1.91	0.70
1:A:123:GLN:O	1:A:127:GLU:HG3	1.90	0.70
1:B:47:ASP:OD1	2:B:299:HOH:O	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:PHE:CD2	1:B:79:LEU:HD11	2.26	0.69
1:B:121:LEU:CA	1:B:124:CYS:SG	2.80	0.69
1:B:72:GLN:NE2	2:B:382:HOH:O	2.23	0.69
1:A:59:ASP:O	2:A:319:HOH:O	2.10	0.69
1:B:12:PHE:HE1	1:B:45:VAL:HG22	1.57	0.69
1:A:48:ALA:O	1:A:161:LYS:HD2	1.91	0.69
1:B:105:GLN:HE21	1:B:207:GLN:HE22	1.41	0.69
1:B:72:GLN:NE2	2:B:379:HOH:O	2.24	0.69
1:B:214:TRP:HD1	2:B:242:HOH:O	1.73	0.69
1:B:189:GLN:HG3	2:B:399:HOH:O	1.93	0.69
1:A:178:ILE:HD11	1:A:215:LEU:HD11	1.74	0.69
1:B:106:PHE:HB2	1:B:132:THR:OG1	1.93	0.69
1:B:102:ARG:HG2	1:B:200:CYS:SG	2.33	0.69
1:A:18:LEU:HA	1:A:21:GLN:HE21	1.57	0.68
1:B:105:GLN:NE2	1:B:207:GLN:HE22	1.87	0.68
1:A:201:TRP:HB2	2:A:332:HOH:O	1.92	0.68
1:B:18:LEU:HB3	1:B:38:ALA:HB2	1.76	0.68
1:B:113:ARG:HB2	1:B:124:CYS:SG	2.33	0.68
1:B:27:ASP:OD1	1:B:29:LYS:HG3	1.92	0.68
1:A:69:ARG:NH1	2:A:375:HOH:O	2.27	0.68
1:A:77:GLU:HG2	1:A:78:THR:HG23	1.76	0.68
1:A:65:LYS:HB3	2:A:385:HOH:O	1.93	0.68
1:A:195:GLU:OE2	2:A:376:HOH:O	2.11	0.68
1:A:46:VAL:HG12	2:A:242:HOH:O	1.92	0.68
1:B:113:ARG:HB2	1:B:124:CYS:CB	2.23	0.68
1:A:59:ASP:HB3	2:A:319:HOH:O	1.94	0.68
1:A:133:LEU:HA	1:A:136:CYS:SG	2.33	0.68
1:B:133:LEU:HA	1:B:136:CYS:SG	2.34	0.68
1:A:18:LEU:HD12	1:A:41:GLU:HG3	1.75	0.67
1:A:59:ASP:HB3	2:A:322:HOH:O	1.93	0.67
1:B:37:THR:HA	1:B:40:LYS:HE3	1.76	0.67
1:B:72:GLN:NE2	2:B:381:HOH:O	2.26	0.67
1:A:159:TYR:OH	2:A:244:HOH:O	2.11	0.67
1:A:37:THR:OG1	2:A:282:HOH:O	2.12	0.67
1:A:146:TRP:O	1:A:150:LYS:HD2	1.94	0.67
1:A:122:GLU:O	1:A:125:VAL:HG12	1.95	0.67
1:A:198:ASP:OD2	2:A:305:HOH:O	2.11	0.67
1:B:37:THR:HA	1:B:40:LYS:HE2	1.76	0.67
1:A:105:GLN:HE21	1:A:207:GLN:HE22	1.43	0.67
1:A:212:SER:OG	2:A:269:HOH:O	2.12	0.67
1:A:70:ALA:CB	1:A:93:ALA:HB2	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:LEU:HD12	1:A:41:GLU:HG2	1.76	0.67
1:A:55:ILE:HB	2:A:229:HOH:O	1.94	0.67
1:A:110:PHE:CE1	1:A:125:VAL:HG23	2.30	0.67
1:B:175:GLU:OE1	2:B:319:HOH:O	2.13	0.66
1:A:194:ARG:HD3	2:A:369:HOH:O	1.94	0.66
1:B:126:THR:HG23	1:B:146:TRP:CZ3	2.30	0.66
1:B:101:LYS:CD	1:B:187:ILE:HG22	2.25	0.66
1:B:132:THR:O	1:B:200:CYS:CB	2.42	0.66
1:A:113:ARG:HD3	1:A:127:GLU:HB2	1.78	0.66
1:B:70:ALA:HB2	1:B:92:LEU:HD23	1.77	0.66
1:A:59:ASP:HB3	2:A:320:HOH:O	1.95	0.66
1:A:125:VAL:HG11	1:A:149:VAL:HG22	1.77	0.66
1:B:32:LEU:N	1:B:78:THR:HA	2.11	0.66
1:A:205:VAL:HG23	2:A:321:HOH:O	1.94	0.66
1:A:116:VAL:HG12	2:A:263:HOH:O	1.96	0.66
1:B:47:ASP:OD1	2:B:305:HOH:O	2.13	0.66
1:A:18:LEU:CD1	1:A:41:GLU:HG3	2.26	0.66
1:A:78:THR:HG23	2:A:316:HOH:O	1.96	0.66
1:A:102:ARG:HG2	1:A:200:CYS:SG	2.35	0.66
1:A:163:HIS:ND1	1:A:164:PRO:HD2	2.10	0.66
1:A:132:THR:HG22	1:A:202:GLY:HA2	1.78	0.66
1:A:69:ARG:O	2:A:389:HOH:O	2.13	0.66
1:B:59:ASP:OD2	2:B:326:HOH:O	2.14	0.66
1:A:165:ASP:OD2	2:A:364:HOH:O	2.13	0.65
1:A:33:GLU:HB2	1:A:34:PRO:HD3	1.77	0.65
1:B:14:ILE:HG22	1:B:44:ARG:NH1	2.11	0.65
1:A:83:ILE:CD1	1:A:94:THR:HA	2.27	0.65
1:B:36:LEU:HD22	1:B:64:ILE:HG23	1.78	0.65
1:B:111:LEU:O	1:B:115:VAL:HG22	1.97	0.65
1:B:12:PHE:HA	1:B:44:ARG:HH11	1.61	0.65
1:A:185:CYS:SG	2:A:364:HOH:O	2.53	0.65
1:B:40:LYS:CG	1:B:64:ILE:HG21	2.25	0.65
1:A:98:LEU:O	1:A:102:ARG:HG3	1.97	0.65
1:B:111:LEU:HD13	1:B:173:ILE:HD13	1.78	0.65
1:B:210:ASP:OD2	1:B:213:GLU:HB2	1.97	0.65
1:A:146:TRP:O	1:A:150:LYS:HD2	1.96	0.65
1:B:190:PHE:HA	2:B:399:HOH:O	1.97	0.65
1:A:59:ASP:O	2:A:322:HOH:O	2.14	0.65
1:A:160:ARG:HD2	2:A:357:HOH:O	1.96	0.64
1:B:27:ASP:CG	1:B:29:LYS:HE2	2.17	0.64
1:B:112:ARG:HA	1:B:115:VAL:CG2	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:GLU:CD	1:A:93:ALA:HB3	2.18	0.64
1:A:67:LEU:HG	1:A:96:ALA:HB3	1.79	0.64
1:B:101:LYS:HZ1	1:B:197:GLU:CD	2.01	0.64
1:B:109:SER:HB3	1:B:203:ASP:HB2	1.80	0.64
1:A:69:ARG:NH1	2:A:374:HOH:O	2.29	0.64
1:B:55:ILE:HD13	1:B:144:VAL:HG12	1.78	0.64
1:B:174:GLU:HG3	1:B:214:TRP:CZ2	2.32	0.64
1:A:101:LYS:HD2	1:A:188:VAL:HA	1.80	0.64
1:B:201:TRP:HB2	2:B:254:HOH:O	1.98	0.64
1:B:83:ILE:HD12	1:B:94:THR:OG1	1.98	0.64
1:A:150:LYS:HE3	1:A:150:LYS:N	2.13	0.64
1:B:174:GLU:HG3	1:B:214:TRP:HZ2	1.62	0.64
1:B:20:LYS:HG2	1:B:179:GLU:CD	2.19	0.64
1:B:87:ASN:HA	1:B:194:ARG:NH2	2.13	0.63
1:A:24:VAL:CG1	1:A:28:GLY:HA2	2.28	0.63
1:B:112:ARG:NH1	2:B:248:HOH:O	2.23	0.63
1:A:78:THR:CG2	2:A:316:HOH:O	2.46	0.63
1:B:86:GLU:OE1	1:B:91:GLY:HA3	1.98	0.63
1:A:160:ARG:HG3	1:A:166:LEU:HD21	1.80	0.63
1:B:182:ASP:OD2	2:B:310:HOH:O	2.15	0.63
1:A:171:ALA:O	1:A:175:GLU:HG3	1.97	0.63
1:A:76:ALA:HB1	1:A:81:GLU:HB3	1.79	0.63
1:A:208:ARG:HD3	1:A:213:GLU:HG2	1.80	0.63
1:B:32:LEU:C	1:B:32:LEU:HD23	2.18	0.63
1:A:174:GLU:HG2	1:A:214:TRP:CH2	2.34	0.63
1:A:114:LEU:HD11	1:A:155:ARG:HG3	1.81	0.63
1:B:199:GLN:OE1	1:B:199:GLN:HA	1.99	0.63
1:A:20:LYS:O	1:A:23:THR:HG22	1.99	0.63
1:B:110:PHE:CD1	1:B:124:CYS:SG	2.91	0.63
1:A:27:ASP:HB3	2:A:380:HOH:O	1.98	0.63
1:A:60:ILE:HD11	1:A:103:ALA:HB1	1.81	0.63
1:A:201:TRP:CD1	2:A:328:HOH:O	2.50	0.63
1:A:25:LYS:HB3	2:A:380:HOH:O	1.98	0.63
1:A:35:PHE:CG	1:A:79:LEU:HD11	2.34	0.62
1:A:201:TRP:O	2:A:239:HOH:O	2.15	0.62
1:A:132:THR:HG22	1:A:202:GLY:HA2	1.81	0.62
1:A:131:CYS:HB3	2:A:430:HOH:O	1.98	0.62
1:A:55:ILE:HD11	2:B:233:HOH:O	2.00	0.62
1:B:37:THR:HG23	1:B:40:LYS:NZ	2.14	0.62
1:B:157:ARG:NH1	1:B:157:ARG:HG3	2.14	0.62
1:B:29:LYS:HA	1:B:80:GLN:NE2	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:PHE:CG	1:B:79:LEU:HD11	2.35	0.62
1:A:198:ASP:HB2	2:A:228:HOH:O	1.99	0.62
1:B:111:LEU:HD22	1:B:173:ILE:HG21	1.80	0.62
1:B:25:LYS:HG3	1:B:29:LYS:O	2.00	0.61
1:A:70:ALA:CB	1:A:92:LEU:HB3	2.30	0.61
1:A:17:ILE:HG22	1:A:21:GLN:NE2	2.16	0.61
1:A:46:VAL:HG21	1:A:60:ILE:HD12	1.83	0.61
1:B:182:ASP:HB2	2:B:229:HOH:O	2.00	0.61
1:A:11:ASP:OD2	1:A:44:ARG:NH1	2.31	0.61
1:B:102:ARG:NH1	1:B:136:CYS:SG	2.73	0.61
1:A:29:LYS:NZ	2:A:408:HOH:O	2.34	0.61
1:A:112:ARG:HD2	1:A:214:TRP:HB2	1.82	0.61
1:B:31:PRO:HA	1:B:78:THR:HG22	1.81	0.61
1:A:140:VAL:CG2	2:A:316:HOH:O	2.48	0.61
1:A:11:ASP:OD2	1:A:11:ASP:N	2.34	0.61
1:B:32:LEU:H	1:B:78:THR:HA	1.63	0.61
1:A:67:LEU:HG	1:A:96:ALA:CB	2.31	0.61
1:B:120:SER:C	1:B:124:CYS:SG	2.79	0.61
1:A:210:ASP:HB3	1:A:213:GLU:HB2	1.83	0.61
1:A:162:LEU:CD1	1:A:173:ILE:HD11	2.30	0.61
1:B:161:LYS:HE3	2:B:283:HOH:O	2.01	0.61
1:A:18:LEU:HD22	1:A:37:THR:HG22	1.83	0.61
1:A:121:LEU:O	1:A:125:VAL:HG23	2.01	0.60
1:B:105:GLN:HA	1:B:105:GLN:OE1	2.00	0.60
1:B:111:LEU:HD22	1:B:173:ILE:CG2	2.30	0.60
1:A:63:ASN:HB3	1:A:100:LEU:HD13	1.82	0.60
1:A:112:ARG:NH2	1:A:113:ARG:HG2	2.16	0.60
1:B:29:LYS:HB3	1:B:78:THR:HG21	1.83	0.60
1:A:14:ILE:HG23	1:A:41:GLU:HG3	1.82	0.60
1:B:106:PHE:HA	1:B:132:THR:HG21	1.82	0.60
1:A:29:LYS:NZ	2:A:419:HOH:O	2.34	0.60
1:B:97:LEU:HD11	1:B:187:ILE:HD13	1.82	0.60
1:B:106:PHE:HB2	1:B:132:THR:OG1	2.00	0.60
1:A:165:ASP:HB3	1:A:168:ILE:HD12	1.82	0.60
1:A:140:VAL:HG23	2:A:318:HOH:O	1.98	0.60
1:B:101:LYS:O	1:B:105:GLN:HG3	2.02	0.60
1:A:65:LYS:NZ	2:A:338:HOH:O	2.34	0.60
1:B:167:ASN:O	2:B:362:HOH:O	2.16	0.60
1:B:156:GLU:HG2	1:B:160:ARG:HH12	1.67	0.60
1:A:33:GLU:HB2	1:A:34:PRO:HD3	1.82	0.60
1:A:63:ASN:O	1:A:96:ALA:HB1	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:ALA:CB	1:B:93:ALA:HB2	2.32	0.60
1:B:157:ARG:HA	1:B:160:ARG:HH12	1.66	0.60
1:A:65:LYS:HB3	2:A:387:HOH:O	2.00	0.60
1:A:83:ILE:HG23	1:A:94:THR:OG1	2.02	0.60
1:B:157:ARG:HA	1:B:160:ARG:NH1	2.17	0.60
1:A:89:PRO:HA	1:A:94:THR:HG21	1.83	0.60
1:B:204:GLU:O	1:B:208:ARG:HG3	2.02	0.60
1:B:29:LYS:HD3	1:B:80:GLN:CB	2.31	0.60
1:A:183:PRO:O	1:A:187:ILE:HG13	2.02	0.60
1:B:157:ARG:HG3	1:B:157:ARG:HH11	1.67	0.60
1:A:83:ILE:HD11	1:A:94:THR:HA	1.82	0.60
1:A:70:ALA:HB1	1:A:93:ALA:HB2	1.82	0.59
1:B:14:ILE:HG13	1:B:18:LEU:HG	1.84	0.59
1:B:197:GLU:CD	1:B:200:CYS:HB3	2.22	0.59
1:A:86:GLU:OE1	1:A:93:ALA:HB3	2.01	0.59
1:B:101:LYS:HG2	1:B:105:GLN:HE21	1.67	0.59
1:A:151:LEU:HD22	1:B:26:GLU:HB2	1.85	0.59
1:A:45:VAL:HG11	1:A:111:LEU:HD11	1.84	0.59
1:A:131:CYS:SG	2:A:259:HOH:O	2.55	0.59
1:A:109:SER:HB2	1:A:203:ASP:HB2	1.84	0.59
1:B:12:PHE:CE1	1:B:45:VAL:HG22	2.37	0.59
1:B:176:PHE:CZ	1:B:180:LEU:HD22	2.37	0.59
1:A:43:LEU:HD22	1:A:57:LYS:HD2	1.84	0.59
1:B:105:GLN:HE21	1:B:207:GLN:HE22	1.48	0.59
1:B:67:LEU:HG	1:B:96:ALA:CB	2.32	0.59
1:B:155:ARG:HH11	1:B:155:ARG:CB	2.16	0.59
1:B:198:ASP:O	1:B:198:ASP:OD1	2.21	0.59
1:A:105:GLN:HE21	1:A:207:GLN:NE2	1.96	0.59
1:A:201:TRP:O	2:A:240:HOH:O	2.17	0.59
1:B:48:ALA:O	1:B:161:LYS:CE	2.51	0.59
1:A:205:VAL:HG23	2:A:324:HOH:O	2.03	0.59
1:B:162:LEU:CD1	1:B:173:ILE:HD11	2.33	0.59
1:B:112:ARG:HH21	1:B:113:ARG:HG3	1.67	0.59
1:A:68:TYR:O	2:A:272:HOH:O	2.16	0.59
1:B:169:ALA:O	1:B:173:ILE:HG12	2.03	0.59
1:A:140:VAL:HG21	1:B:21:GLN:OE1	2.03	0.59
1:A:113:ARG:HB2	1:A:124:CYS:SG	2.42	0.59
1:A:99:TRP:CH2	1:A:136:CYS:SG	2.96	0.59
1:A:190:PHE:CE1	1:A:194:ARG:HD3	2.38	0.58
1:A:160:ARG:NH1	1:A:164:PRO:O	2.36	0.58
1:B:119:LYS:HD3	1:B:123:GLN:HG2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:LYS:HE3	2:B:279:HOH:O	2.03	0.58
1:B:203:ASP:HB3	1:B:206:TYR:HB3	1.84	0.58
1:B:17:ILE:HG22	1:B:21:GLN:NE2	2.17	0.58
1:A:46:VAL:HG11	1:A:57:LYS:HB2	1.85	0.58
1:B:184:LEU:O	1:B:188:VAL:HG23	2.02	0.58
1:A:150:LYS:HE3	1:A:150:LYS:N	2.17	0.58
1:A:17:ILE:HG23	2:A:303:HOH:O	2.03	0.58
1:A:126:THR:HG23	1:A:146:TRP:CZ3	2.38	0.58
1:B:44:ARG:HG3	2:B:371:HOH:O	2.03	0.58
1:A:40:LYS:HD2	2:A:314:HOH:O	2.02	0.58
1:A:33:GLU:HG2	2:A:245:HOH:O	2.03	0.58
1:B:22:VAL:HG12	1:B:183:PRO:HB3	1.86	0.58
1:A:116:VAL:HG23	1:A:117:THR:HG23	1.85	0.58
1:A:136:CYS:SG	1:A:200:CYS:HB2	2.42	0.58
1:B:19:TRP:CE2	1:B:38:ALA:HB1	2.38	0.58
1:A:27:ASP:OD2	1:A:29:LYS:HG2	2.03	0.58
1:A:110:PHE:CE1	1:A:125:VAL:CG2	2.86	0.58
1:A:184:LEU:HD23	1:A:206:TYR:CE2	2.28	0.58
1:B:157:ARG:O	1:B:161:LYS:HD3	2.03	0.58
1:B:133:LEU:HB3	1:B:137:HIS:CE1	2.38	0.58
1:A:27:ASP:CB	2:A:382:HOH:O	2.41	0.58
1:B:80:GLN:HA	1:B:190:PHE:CZ	2.37	0.58
1:A:63:ASN:CB	1:A:100:LEU:HD13	2.34	0.58
1:B:115:VAL:HG23	1:B:116:VAL:H	1.69	0.58
1:A:70:ALA:HB2	1:A:92:LEU:CB	2.32	0.58
1:A:71:ASN:OD1	1:A:82:LEU:HD13	2.04	0.58
1:B:113:ARG:NH1	1:B:127:GLU:HB3	2.18	0.58
1:A:35:PHE:CD2	1:A:79:LEU:HD11	2.39	0.58
1:B:216:LYS:HB3	1:B:216:LYS:HZ3	1.67	0.58
1:B:31:PRO:HG2	2:B:259:HOH:O	2.03	0.58
1:A:25:LYS:HB3	2:A:381:HOH:O	2.03	0.58
1:A:51:SER:OG	1:A:151:LEU:HD13	2.04	0.57
1:A:113:ARG:HD3	1:A:127:GLU:HB2	1.86	0.57
1:A:174:GLU:OE2	2:A:265:HOH:O	2.17	0.57
1:B:112:ARG:NH2	1:B:113:ARG:HG2	2.18	0.57
1:B:161:LYS:HD2	2:B:284:HOH:O	2.03	0.57
1:B:17:ILE:HG22	1:B:21:GLN:HE21	1.69	0.57
1:B:33:GLU:HB2	1:B:34:PRO:HD3	1.86	0.57
1:A:25:LYS:HD2	1:A:25:LYS:N	2.18	0.57
1:A:48:ALA:O	1:A:161:LYS:HD2	2.05	0.57
1:A:12:PHE:HE1	1:A:45:VAL:HG22	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ASP:HB2	2:A:228:HOH:O	2.03	0.57
1:A:35:PHE:CD2	1:A:79:LEU:HD11	2.40	0.57
1:A:113:ARG:HD3	1:A:127:GLU:HB2	1.87	0.57
1:B:205:VAL:HG23	2:B:278:HOH:O	2.05	0.57
1:A:46:VAL:HG21	1:A:60:ILE:HD12	1.85	0.57
1:A:109:SER:HB2	1:A:203:ASP:HB2	1.87	0.57
1:A:160:ARG:HG3	1:A:166:LEU:CD2	2.35	0.57
1:A:198:ASP:OD1	1:A:199:GLN:HG3	2.05	0.57
1:B:112:ARG:O	1:B:116:VAL:HG22	2.05	0.57
1:B:33:GLU:HB2	1:B:34:PRO:HD3	1.87	0.57
1:A:109:SER:CB	1:A:203:ASP:HB2	2.35	0.57
1:A:78:THR:OG1	1:A:81:GLU:HB2	2.05	0.57
1:B:12:PHE:CD1	1:B:44:ARG:HD2	2.28	0.57
1:A:46:VAL:CG1	1:A:57:LYS:HB2	2.27	0.56
1:B:113:ARG:HB3	1:B:124:CYS:SG	2.44	0.56
1:B:127:GLU:OE2	2:B:404:HOH:O	2.17	0.56
1:B:36:LEU:HD21	1:B:67:LEU:HD13	1.86	0.56
1:A:55:ILE:HD13	2:B:230:HOH:O	2.05	0.56
1:B:208:ARG:HD2	1:B:213:GLU:HG2	1.88	0.56
1:B:101:LYS:HZ2	1:B:105:GLN:NE2	2.03	0.56
1:A:23:THR:HG22	2:A:311:HOH:O	2.05	0.56
1:B:198:ASP:OD2	2:B:301:HOH:O	2.18	0.56
1:B:177:LEU:HD22	1:B:206:TYR:CE1	2.39	0.56
1:B:112:ARG:HH21	1:B:113:ARG:HG2	1.67	0.56
1:A:160:ARG:HG3	1:A:166:LEU:CD2	2.35	0.56
1:A:160:ARG:HG3	1:A:166:LEU:HD21	1.87	0.56
1:B:130:ASN:HA	1:B:134:ARG:HB2	1.87	0.56
1:A:55:ILE:CD1	2:B:230:HOH:O	2.37	0.56
1:B:102:ARG:HB3	1:B:133:LEU:HD23	1.88	0.56
1:B:112:ARG:HG3	1:B:214:TRP:CE3	2.40	0.56
1:A:24:VAL:HG11	1:A:186:CYS:SG	2.46	0.56
1:B:32:LEU:H	1:B:78:THR:HA	1.71	0.56
1:A:98:LEU:HB2	1:A:191:PHE:CE2	2.41	0.56
1:B:112:ARG:NH2	1:B:113:ARG:CG	2.69	0.56
1:B:119:LYS:HB3	1:B:123:GLN:HB3	1.87	0.56
1:A:49:PHE:HE2	1:A:52:GLY:HA3	1.72	0.55
1:A:11:ASP:OD2	1:A:11:ASP:N	2.38	0.55
1:A:204:GLU:O	1:A:208:ARG:HG3	2.06	0.55
1:A:181:HIS:NE2	1:A:206:TYR:O	2.39	0.55
1:A:46:VAL:HG11	1:A:57:LYS:CB	2.28	0.55
1:A:102:ARG:NH1	1:A:136:CYS:SG	2.80	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:VAL:CG1	1:A:57:LYS:HB2	2.30	0.55
1:A:25:LYS:H	1:A:25:LYS:HD2	1.72	0.55
1:B:157:ARG:HG3	1:B:157:ARG:HH11	1.71	0.55
1:B:55:ILE:HD13	1:B:144:VAL:CG1	2.36	0.55
1:A:150:LYS:N	1:A:150:LYS:HE3	2.20	0.55
1:A:121:LEU:HD22	1:A:152:ALA:HB1	1.88	0.55
1:B:110:PHE:CE2	1:B:114:LEU:HD22	2.41	0.55
1:A:50:GLY:O	1:A:53:PHE:N	2.36	0.55
1:B:132:THR:HG22	1:B:202:GLY:HA2	1.89	0.55
1:A:66:LYS:HD3	2:A:264:HOH:O	2.07	0.55
1:A:70:ALA:CB	1:A:93:ALA:HB2	2.36	0.55
1:A:27:ASP:HB3	2:A:380:HOH:O	2.06	0.55
1:B:157:ARG:HH11	1:B:157:ARG:HG3	1.72	0.55
1:B:160:ARG:HB2	1:B:160:ARG:NH1	2.21	0.55
1:B:121:LEU:C	1:B:121:LEU:HD23	2.27	0.55
1:A:18:LEU:HA	1:A:21:GLN:NE2	2.21	0.55
1:A:156:GLU:O	1:A:160:ARG:HG3	2.06	0.55
1:A:109:SER:HB2	1:A:203:ASP:HB2	1.89	0.54
1:B:167:ASN:HD22	1:B:167:ASN:N	2.04	0.54
1:A:196:LEU:HD21	2:A:341:HOH:O	2.06	0.54
1:A:160:ARG:NH1	1:A:166:LEU:HD11	2.23	0.54
1:B:32:LEU:HD23	1:B:32:LEU:C	2.28	0.54
1:A:80:GLN:OE1	1:A:80:GLN:N	2.37	0.54
1:A:116:VAL:HG23	1:A:117:THR:N	2.22	0.54
1:B:186:CYS:SG	1:B:187:ILE:N	2.81	0.54
1:A:21:GLN:HG3	2:A:304:HOH:O	2.06	0.54
1:A:205:VAL:HG23	2:A:324:HOH:O	2.07	0.54
1:A:121:LEU:HD22	1:A:152:ALA:HB1	1.89	0.54
1:A:117:THR:O	2:A:283:HOH:O	2.19	0.54
1:B:79:LEU:O	1:B:83:ILE:HG12	2.07	0.54
1:B:101:LYS:HB3	1:B:101:LYS:HZ3	1.72	0.54
1:A:115:VAL:HG12	1:A:159:TYR:OH	2.07	0.54
1:A:134:ARG:NH1	2:A:349:HOH:O	2.27	0.54
1:B:132:THR:HG22	1:B:133:LEU:HG	1.90	0.54
1:A:32:LEU:HD23	1:A:32:LEU:C	2.28	0.54
1:A:140:VAL:HG23	2:A:317:HOH:O	2.07	0.54
1:B:105:GLN:HE21	1:B:207:GLN:HE22	1.55	0.54
1:B:201:TRP:HZ3	2:B:271:HOH:O	1.90	0.53
1:B:165:ASP:OD1	1:B:167:ASN:HB2	2.08	0.53
1:B:174:GLU:HG3	1:B:214:TRP:CH2	2.42	0.53
1:B:44:ARG:HG3	2:B:365:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:PHE:CE1	1:B:124:CYS:SG	3.01	0.53
1:A:18:LEU:CD1	1:A:41:GLU:HG2	2.37	0.53
1:A:18:LEU:HD12	1:A:41:GLU:CG	2.38	0.53
1:A:14:ILE:HD12	1:A:17:ILE:HB	1.90	0.53
1:A:132:THR:HG22	1:A:202:GLY:HA2	1.89	0.53
1:B:198:ASP:C	1:B:198:ASP:OD1	2.46	0.53
1:A:140:VAL:HG23	2:A:316:HOH:O	2.08	0.53
1:A:160:ARG:HG3	1:A:166:LEU:HD21	1.91	0.53
1:A:102:ARG:HG2	1:A:200:CYS:CB	2.38	0.53
1:A:150:LYS:N	1:A:150:LYS:HE3	2.23	0.53
1:B:111:LEU:CB	1:B:177:LEU:HD11	2.38	0.53
1:A:12:PHE:O	1:A:15:ILE:HG22	2.09	0.53
1:B:55:ILE:HG21	1:B:144:VAL:HG11	1.90	0.53
1:A:51:SER:N	2:A:336:HOH:O	2.40	0.53
1:B:134:ARG:HD2	1:B:146:TRP:HZ2	1.74	0.53
1:B:112:ARG:HA	1:B:115:VAL:HG22	1.88	0.53
1:A:63:ASN:HD22	1:A:96:ALA:HA	1.72	0.53
1:B:157:ARG:HD3	2:B:386:HOH:O	2.07	0.53
1:B:105:GLN:HG2	1:B:207:GLN:NE2	2.24	0.53
1:B:26:GLU:HB3	2:B:367:HOH:O	2.09	0.53
1:A:160:ARG:CZ	1:A:166:LEU:HG	2.39	0.53
1:A:160:ARG:HA	1:A:163:HIS:O	2.08	0.53
1:B:198:ASP:OD1	1:B:199:GLN:HG2	2.09	0.53
1:B:155:ARG:HH11	1:B:155:ARG:HB2	1.73	0.53
1:B:114:LEU:CD1	1:B:155:ARG:HG3	2.38	0.53
1:B:113:ARG:O	1:B:117:THR:HG23	2.08	0.53
1:B:46:VAL:HG22	1:B:107:ILE:HD11	1.91	0.53
1:A:31:PRO:HB2	1:A:34:PRO:CG	2.38	0.53
1:A:105:GLN:HE21	1:A:207:GLN:NE2	2.07	0.53
1:B:71:ASN:OD1	1:B:82:LEU:HD13	2.10	0.53
1:A:126:THR:HG23	1:A:146:TRP:HH2	1.68	0.52
1:A:165:ASP:OD2	2:A:362:HOH:O	2.18	0.52
1:B:41:GLU:OE2	1:B:44:ARG:CZ	2.57	0.52
1:B:27:ASP:OD1	1:B:29:LYS:HE2	2.09	0.52
1:B:124:CYS:SG	1:B:125:VAL:N	2.82	0.52
1:B:55:ILE:HG21	1:B:144:VAL:HG11	1.90	0.52
1:A:29:LYS:NZ	2:A:413:HOH:O	2.41	0.52
1:B:204:GLU:O	1:B:208:ARG:HG3	2.09	0.52
1:B:119:LYS:O	1:B:155:ARG:NH2	2.35	0.52
1:B:201:TRP:O	2:B:253:HOH:O	2.19	0.52
1:A:86:GLU:CD	1:A:91:GLY:HA3	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:PRO:HA	1:B:78:THR:HA	1.90	0.52
1:B:102:ARG:NH2	1:B:197:GLU:OE2	2.39	0.52
1:B:182:ASP:HB2	2:B:229:HOH:O	2.09	0.52
1:B:67:LEU:HG	1:B:96:ALA:HB1	1.92	0.52
1:A:29:LYS:HD2	1:A:80:GLN:HB2	1.90	0.52
1:B:162:LEU:HD13	1:B:173:ILE:HD11	1.90	0.52
1:B:162:LEU:HD13	1:B:173:ILE:HD11	1.91	0.52
1:B:118:ASP:OD2	2:B:232:HOH:O	2.19	0.52
1:A:55:ILE:HG12	2:B:233:HOH:O	2.09	0.52
1:B:160:ARG:HD2	2:B:361:HOH:O	2.10	0.52
1:B:12:PHE:O	1:B:15:ILE:HG22	2.10	0.52
1:A:170:LYS:NZ	2:A:288:HOH:O	2.43	0.52
1:B:115:VAL:HG23	1:B:116:VAL:HG13	1.91	0.52
1:B:101:LYS:CG	1:B:187:ILE:HG22	2.40	0.52
1:B:27:ASP:N	2:B:370:HOH:O	2.43	0.52
1:B:112:ARG:HG3	1:B:214:TRP:CE3	2.44	0.52
1:A:122:GLU:O	1:A:125:VAL:HB	2.09	0.52
1:B:185:CYS:SG	2:B:365:HOH:O	2.59	0.52
1:B:32:LEU:N	1:B:78:THR:HA	2.25	0.52
1:B:18:LEU:HD12	1:B:41:GLU:HG2	1.91	0.52
1:B:87:ASN:HA	1:B:194:ARG:HH21	1.72	0.52
1:A:101:LYS:NZ	1:A:197:GLU:OE1	2.38	0.52
1:B:66:LYS:HG2	1:B:69:ARG:NH2	2.25	0.52
1:A:92:LEU:H	1:A:92:LEU:CD1	2.20	0.52
1:B:121:LEU:O	1:B:121:LEU:HD23	2.09	0.52
1:A:98:LEU:HB2	1:A:191:PHE:HE2	1.74	0.52
1:B:58:ASN:OD1	2:B:318:HOH:O	2.19	0.52
1:B:83:ILE:CD1	1:B:94:THR:HA	2.37	0.52
1:B:55:ILE:HD12	1:B:56:VAL:HG23	1.92	0.52
1:A:60:ILE:HG12	1:A:103:ALA:CB	2.39	0.51
1:B:69:ARG:HH11	1:B:69:ARG:HG3	1.76	0.51
1:B:214:TRP:CD1	1:B:215:LEU:HD23	2.45	0.51
1:B:204:GLU:O	1:B:208:ARG:HG3	2.10	0.51
1:A:67:LEU:HD21	1:A:97:LEU:HB2	1.92	0.51
1:B:101:LYS:NZ	1:B:105:GLN:NE2	2.57	0.51
1:A:140:VAL:HG23	2:A:322:HOH:O	2.10	0.51
1:B:64:ILE:O	1:B:65:LYS:C	2.48	0.51
1:A:110:PHE:HD1	1:A:124:CYS:SG	2.33	0.51
1:B:167:ASN:O	2:B:363:HOH:O	2.19	0.51
1:B:109:SER:CB	1:B:203:ASP:HB2	2.40	0.51
1:B:159:TYR:CB	1:B:166:LEU:HD22	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:GLU:OE2	2:B:266:HOH:O	2.19	0.51
1:B:163:HIS:HB3	1:B:169:ALA:HB2	1.92	0.51
1:A:40:LYS:NZ	2:A:331:HOH:O	2.43	0.51
1:A:114:LEU:HD11	1:A:155:ARG:HG3	1.92	0.51
1:B:105:GLN:NE2	1:B:200:CYS:SG	2.84	0.51
1:A:138:SER:O	1:A:142:GLN:HG3	2.09	0.51
1:A:210:ASP:OD1	2:A:425:HOH:O	2.19	0.51
1:B:25:LYS:NZ	2:B:387:HOH:O	2.43	0.51
1:A:42:VAL:HG11	1:A:104:PHE:CE1	2.45	0.51
1:B:41:GLU:CD	2:B:371:HOH:O	2.49	0.51
1:B:125:VAL:CG1	1:B:149:VAL:HG13	2.41	0.51
1:B:15:ILE:HA	1:B:41:GLU:HG2	1.93	0.51
1:B:182:ASP:HB2	1:B:183:PRO:HD3	1.91	0.51
1:A:121:LEU:CD2	1:A:152:ALA:HB1	2.40	0.51
1:A:23:THR:HG22	2:A:311:HOH:O	2.10	0.51
1:A:12:PHE:CE1	1:A:45:VAL:HG22	2.46	0.51
1:A:15:ILE:HD11	1:A:42:VAL:HG22	1.93	0.51
1:B:165:ASP:OD2	2:B:390:HOH:O	2.20	0.51
1:A:208:ARG:HD2	1:A:213:GLU:HG2	1.92	0.51
1:B:59:ASP:OD2	2:B:325:HOH:O	2.19	0.51
1:A:129:TYR:CD2	1:A:134:ARG:HB2	2.46	0.51
1:B:97:LEU:HB3	1:B:191:PHE:HZ	1.75	0.51
1:A:140:VAL:HG21	1:B:21:GLN:OE1	2.10	0.50
1:B:134:ARG:N	1:B:135:PRO:HD2	2.25	0.50
1:B:110:PHE:CE1	1:B:124:CYS:SG	3.00	0.50
1:A:92:LEU:HD12	2:A:266:HOH:O	2.10	0.50
1:B:112:ARG:O	1:B:116:VAL:HG22	2.11	0.50
1:B:48:ALA:HA	1:B:161:LYS:CG	2.37	0.50
1:B:216:LYS:HB2	1:B:216:LYS:NZ	2.25	0.50
1:B:160:ARG:HD2	2:B:361:HOH:O	2.10	0.50
1:A:18:LEU:HD12	1:A:41:GLU:HG3	1.93	0.50
1:A:24:VAL:HG12	1:A:28:GLY:HA2	1.94	0.50
1:A:19:TRP:CE2	1:A:38:ALA:HB1	2.46	0.50
1:B:180:LEU:HD21	1:B:184:LEU:HD22	1.92	0.50
1:A:140:VAL:HG22	2:A:316:HOH:O	2.10	0.50
1:A:24:VAL:O	1:A:25:LYS:O	2.29	0.50
1:A:123:GLN:CD	2:A:287:HOH:O	2.48	0.50
1:B:126:THR:HG23	1:B:146:TRP:HZ3	1.76	0.50
1:B:37:THR:HA	1:B:40:LYS:HE3	1.94	0.50
1:B:203:ASP:O	1:B:207:GLN:HG3	2.12	0.50
1:A:55:ILE:HG12	2:A:229:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:GLU:HB2	1:B:34:PRO:HD3	1.93	0.50
1:B:22:VAL:HA	2:B:294:HOH:O	2.11	0.50
1:A:140:VAL:CG2	1:B:21:GLN:OE1	2.60	0.50
1:A:44:ARG:CG	1:A:44:ARG:HH21	2.18	0.50
1:A:160:ARG:HG3	1:A:166:LEU:CD2	2.42	0.50
1:A:57:LYS:HD2	2:A:337:HOH:O	2.11	0.50
1:A:46:VAL:HG13	1:A:53:PHE:CB	2.37	0.50
1:A:121:LEU:HD12	1:A:155:ARG:HA	1.94	0.50
1:A:165:ASP:HB3	1:A:168:ILE:HD12	1.93	0.50
1:B:46:VAL:O	1:B:49:PHE:HB2	2.12	0.50
1:B:127:GLU:HA	1:B:130:ASN:HB2	1.93	0.50
1:B:155:ARG:NH1	1:B:155:ARG:CB	2.74	0.50
1:B:172:LYS:HD3	1:B:175:GLU:OE1	2.12	0.50
1:A:69:ARG:NH2	2:A:408:HOH:O	2.34	0.50
1:B:189:GLN:O	1:B:192:PHE:HB2	2.12	0.50
1:A:32:LEU:HD23	1:A:32:LEU:C	2.33	0.50
1:A:210:ASP:HA	2:A:425:HOH:O	2.12	0.49
1:A:43:LEU:HD21	1:A:61:ALA:H	1.76	0.49
1:B:200:CYS:O	1:B:200:CYS:SG	2.70	0.49
1:A:173:ILE:O	1:A:176:PHE:HB3	2.13	0.49
1:A:69:ARG:NH2	2:A:404:HOH:O	2.32	0.49
1:B:20:LYS:HG2	1:B:179:GLU:CD	2.33	0.49
1:A:21:GLN:O	1:A:23:THR:HG23	2.13	0.49
1:B:107:ILE:O	1:B:111:LEU:HG	2.13	0.49
1:B:19:TRP:CD1	1:B:38:ALA:HB1	2.48	0.49
1:A:89:PRO:HD3	2:A:324:HOH:O	2.13	0.49
1:B:208:ARG:HD2	1:B:213:GLU:HG2	1.94	0.49
1:A:167:ASN:ND2	2:A:363:HOH:O	2.44	0.49
1:B:32:LEU:HB2	1:B:78:THR:C	2.33	0.49
1:B:16:VAL:O	1:B:20:LYS:HG3	2.13	0.49
1:B:44:ARG:O	1:B:47:ASP:HB2	2.12	0.49
1:B:33:GLU:CB	1:B:34:PRO:HD3	2.41	0.49
1:B:19:TRP:CD1	1:B:38:ALA:HB1	2.48	0.49
1:B:184:LEU:O	1:B:188:VAL:HG23	2.13	0.49
1:A:57:LYS:HD3	1:A:57:LYS:C	2.33	0.49
1:A:141:ILE:HG13	2:A:288:HOH:O	2.11	0.49
1:B:101:LYS:HD2	1:B:188:VAL:HA	1.94	0.49
1:A:151:LEU:CD2	1:B:26:GLU:HB2	2.43	0.49
1:A:151:LEU:CD2	1:B:26:GLU:HB2	2.42	0.49
1:B:64:ILE:O	1:B:67:LEU:N	2.45	0.49
1:B:83:ILE:HD12	1:B:94:THR:HG23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:ARG:NH2	1:A:92:LEU:HD11	2.28	0.49
1:B:138:SER:OG	1:B:141:ILE:HD12	2.12	0.49
1:A:69:ARG:HA	1:A:72:GLN:HG3	1.94	0.48
1:B:112:ARG:HG3	1:B:214:TRP:HE3	1.77	0.48
1:B:55:ILE:CD1	1:B:56:VAL:HG23	2.43	0.48
1:B:94:THR:HG23	1:B:196:LEU:HD13	1.95	0.48
1:A:143:LYS:HG3	2:A:355:HOH:O	2.13	0.48
1:B:25:LYS:HA	2:B:316:HOH:O	2.12	0.48
1:B:119:LYS:HD3	1:B:123:GLN:NE2	2.28	0.48
1:B:35:PHE:CD2	1:B:79:LEU:HD11	2.48	0.48
1:A:150:LYS:N	1:A:150:LYS:HE3	2.28	0.48
1:B:134:ARG:H	1:B:135:PRO:HD2	1.77	0.48
1:A:86:GLU:OE1	1:A:91:GLY:HA3	2.13	0.48
1:A:181:HIS:CE1	1:A:208:ARG:O	2.67	0.48
1:B:106:PHE:CA	1:B:132:THR:HG21	2.43	0.48
1:B:122:GLU:O	1:B:125:VAL:HG12	2.13	0.48
1:B:197:GLU:OE1	1:B:200:CYS:HB3	2.12	0.48
1:B:101:LYS:HG3	1:B:187:ILE:CG2	2.43	0.48
1:A:24:VAL:HG13	1:A:29:LYS:O	2.13	0.48
1:A:189:GLN:HB3	2:A:253:HOH:O	2.13	0.48
1:A:140:VAL:HG21	1:B:21:GLN:CD	2.34	0.48
1:B:175:GLU:HG3	2:B:296:HOH:O	2.12	0.48
1:A:14:ILE:HD12	1:A:17:ILE:HB	1.95	0.48
1:A:157:ARG:O	1:A:161:LYS:HG3	2.14	0.48
1:A:43:LEU:HD21	1:A:61:ALA:N	2.27	0.48
1:A:163:HIS:ND1	1:A:164:PRO:CD	2.77	0.48
1:A:181:HIS:CD2	1:A:206:TYR:O	2.66	0.48
1:A:40:LYS:HA	1:A:64:ILE:HD13	1.95	0.48
1:B:48:ALA:HB3	1:B:158:PHE:CE1	2.48	0.48
1:A:27:ASP:CB	2:A:380:HOH:O	2.59	0.48
1:A:140:VAL:O	1:A:144:VAL:HG23	2.14	0.48
1:A:66:LYS:HG3	2:A:395:HOH:O	2.13	0.48
1:B:60:ILE:HD11	1:B:103:ALA:HB1	1.95	0.48
1:A:66:LYS:HD2	2:A:292:HOH:O	2.13	0.48
1:B:101:LYS:HG3	1:B:187:ILE:HG22	1.95	0.48
1:B:210:ASP:OD2	1:B:213:GLU:N	2.46	0.48
1:A:114:LEU:HA	1:A:124:CYS:SG	2.53	0.48
1:B:14:ILE:HA	1:B:17:ILE:HD12	1.95	0.48
1:A:55:ILE:HD13	2:B:230:HOH:O	2.13	0.48
1:B:110:PHE:O	1:B:124:CYS:SG	2.71	0.48
1:A:87:ASN:OD1	1:A:194:ARG:NH2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:LYS:NZ	1:B:123:GLN:NE2	2.62	0.48
1:A:135:PRO:HB3	2:A:303:HOH:O	2.13	0.48
1:B:33:GLU:HB2	1:B:34:PRO:HD3	1.95	0.48
1:A:44:ARG:NH2	1:A:44:ARG:HG2	2.23	0.48
1:A:102:ARG:HB3	1:A:133:LEU:HD23	1.96	0.47
1:A:87:ASN:HA	1:A:194:ARG:NH2	2.29	0.47
1:B:49:PHE:CZ	1:B:110:PHE:CD2	3.01	0.47
1:A:111:LEU:HB2	1:A:177:LEU:HD21	1.96	0.47
1:B:20:LYS:HG3	1:B:179:GLU:HG3	1.95	0.47
1:B:132:THR:HG22	1:B:202:GLY:HA2	1.96	0.47
1:A:55:ILE:HD13	2:B:230:HOH:O	2.14	0.47
1:B:12:PHE:HA	1:B:44:ARG:HH11	1.80	0.47
1:B:102:ARG:HA	1:B:105:GLN:OE1	2.14	0.47
1:A:71:ASN:OD1	1:A:82:LEU:HD13	2.15	0.47
1:B:119:LYS:HZ3	1:B:123:GLN:NE2	2.12	0.47
1:A:15:ILE:HG13	1:A:41:GLU:CB	2.40	0.47
1:A:163:HIS:CE1	1:A:164:PRO:HD2	2.49	0.47
1:B:106:PHE:HA	1:B:132:THR:HG21	1.96	0.47
1:A:138:SER:OG	1:A:140:VAL:HG12	2.14	0.47
1:B:48:ALA:O	1:B:161:LYS:NZ	2.46	0.47
1:A:26:GLU:N	2:A:381:HOH:O	2.46	0.47
1:B:15:ILE:HG13	1:B:41:GLU:HB3	1.96	0.47
1:B:157:ARG:NH1	1:B:157:ARG:HG3	2.29	0.47
1:B:83:ILE:HD12	1:B:94:THR:HA	1.96	0.47
1:B:119:LYS:NZ	1:B:127:GLU:OE2	2.39	0.47
1:B:134:ARG:N	1:B:135:PRO:HD2	2.30	0.47
1:B:111:LEU:HD22	1:B:173:ILE:HD12	1.95	0.47
1:A:112:ARG:O	1:A:116:VAL:HG22	2.14	0.47
1:B:63:ASN:OD1	1:B:96:ALA:HA	2.14	0.47
1:B:98:LEU:HD21	1:B:102:ARG:NH2	2.30	0.47
1:B:111:LEU:O	1:B:115:VAL:HG22	2.15	0.47
1:A:134:ARG:N	1:A:135:PRO:HD2	2.29	0.47
1:A:160:ARG:HA	1:A:163:HIS:O	2.15	0.47
1:A:54:ARG:HD2	1:B:182:ASP:OD2	2.14	0.47
1:A:18:LEU:HD12	1:A:41:GLU:HG3	1.96	0.47
1:A:170:LYS:O	1:A:174:GLU:HG3	2.14	0.47
1:A:157:ARG:O	1:A:161:LYS:HG3	2.15	0.47
1:B:121:LEU:CD1	1:B:158:PHE:HB2	2.44	0.47
1:B:19:TRP:CE2	1:B:38:ALA:HB1	2.50	0.47
1:A:49:PHE:HE1	1:A:125:VAL:HG21	1.80	0.47
1:A:101:LYS:HD2	1:A:188:VAL:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:PHE:HD1	1:B:44:ARG:CD	2.18	0.47
1:A:69:ARG:HH21	1:A:92:LEU:CD1	2.27	0.47
1:A:129:TYR:OH	1:A:142:GLN:HA	2.15	0.47
1:B:213:GLU:HG3	1:B:213:GLU:O	2.14	0.47
1:A:160:ARG:HG2	1:A:160:ARG:HH11	1.79	0.47
1:B:47:ASP:OD1	2:B:304:HOH:O	2.20	0.47
1:B:132:THR:CG2	1:B:133:LEU:N	2.71	0.47
1:B:134:ARG:N	1:B:135:PRO:HD2	2.29	0.47
1:A:76:ALA:HB1	1:A:81:GLU:HB3	1.96	0.47
1:A:178:ILE:HG23	1:A:211:SER:HB2	1.97	0.47
1:B:216:LYS:HB2	2:B:395:HOH:O	2.15	0.47
1:A:69:ARG:HA	1:A:72:GLN:HG3	1.96	0.47
1:A:145:PHE:O	1:A:148:GLY:N	2.48	0.46
1:A:109:SER:CB	1:A:203:ASP:HB2	2.45	0.46
1:B:34:PRO:HB2	2:B:293:HOH:O	2.14	0.46
1:B:103:ALA:O	1:B:106:PHE:HB3	2.15	0.46
1:A:129:TYR:CD2	1:A:134:ARG:HB2	2.51	0.46
1:B:22:VAL:HG21	1:B:35:PHE:HA	1.96	0.46
1:A:30:VAL:HG23	1:A:80:GLN:HE22	1.80	0.46
1:B:101:LYS:HD2	1:B:188:VAL:HA	1.96	0.46
1:B:19:TRP:CE2	1:B:38:ALA:HB1	2.50	0.46
1:A:204:GLU:OE2	2:A:366:HOH:O	2.20	0.46
1:B:116:VAL:HG23	1:B:117:THR:HG22	1.97	0.46
1:B:36:LEU:O	1:B:40:LYS:HG3	2.15	0.46
1:A:33:GLU:CB	1:A:34:PRO:HD3	2.43	0.46
1:A:19:TRP:NE1	1:A:38:ALA:HB1	2.29	0.46
1:A:163:HIS:CD2	1:A:168:ILE:HG21	2.50	0.46
1:B:132:THR:HA	1:B:200:CYS:HB2	1.95	0.46
1:A:204:GLU:OE1	1:A:208:ARG:NH2	2.42	0.46
1:B:182:ASP:HB2	2:B:229:HOH:O	2.14	0.46
1:B:112:ARG:CA	1:B:115:VAL:HG22	2.45	0.46
1:A:105:GLN:HG2	1:A:207:GLN:NE2	2.31	0.46
1:A:105:GLN:HE21	1:A:207:GLN:HE22	1.63	0.46
1:A:60:ILE:CD1	1:A:103:ALA:HB1	2.44	0.46
1:A:110:PHE:HA	1:A:128:ALA:HB2	1.97	0.46
1:B:121:LEU:C	1:B:121:LEU:HD23	2.36	0.46
1:B:216:LYS:HB2	1:B:216:LYS:NZ	2.31	0.46
1:B:156:GLU:HG3	1:B:166:LEU:CD1	2.41	0.46
1:A:40:LYS:HG3	2:A:286:HOH:O	2.14	0.46
1:B:84:ILE:HG12	1:B:194:ARG:CZ	2.46	0.46
1:A:147:GLY:O	1:A:150:LYS:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:TYR:CZ	1:B:134:ARG:HA	2.51	0.46
1:A:33:GLU:CB	1:A:34:PRO:HD3	2.46	0.46
1:A:55:ILE:HG21	1:A:145:PHE:HD1	1.81	0.46
1:A:151:LEU:HD22	2:A:402:HOH:O	2.16	0.46
1:A:112:ARG:HG3	1:A:214:TRP:CE3	2.51	0.46
1:A:151:LEU:HD11	2:B:316:HOH:O	2.16	0.46
1:B:48:ALA:HA	1:B:161:LYS:HG2	1.97	0.46
1:A:110:PHE:CD1	1:A:125:VAL:HG22	2.51	0.46
1:A:160:ARG:NH1	1:A:166:LEU:HD11	2.31	0.46
1:B:162:LEU:CD1	1:B:173:ILE:HD11	2.46	0.46
1:A:81:GLU:HB2	2:A:311:HOH:O	2.16	0.46
1:A:194:ARG:HB2	1:A:196:LEU:HG	1.97	0.46
1:A:86:GLU:OE1	1:A:94:THR:OG1	2.31	0.46
1:A:18:LEU:HD13	1:A:41:GLU:HG3	1.95	0.46
1:B:177:LEU:HD22	1:B:206:TYR:CE1	2.51	0.46
1:A:40:LYS:NZ	2:A:325:HOH:O	2.48	0.46
1:A:198:ASP:OD1	1:A:199:GLN:HG3	2.16	0.46
1:B:111:LEU:CD1	1:B:173:ILE:HD13	2.44	0.46
1:A:55:ILE:HD13	1:A:55:ILE:HA	1.72	0.46
1:A:65:LYS:HE3	1:B:215:LEU:HD13	1.97	0.46
1:A:110:PHE:HE1	1:A:125:VAL:HG23	1.80	0.46
1:B:31:PRO:HG2	2:B:262:HOH:O	2.16	0.46
1:B:213:GLU:OE1	1:B:213:GLU:HA	2.16	0.46
1:B:213:GLU:HA	1:B:216:LYS:HZ2	1.81	0.46
1:B:32:LEU:HB2	1:B:78:THR:C	2.36	0.45
1:B:31:PRO:HB2	1:B:34:PRO:HG2	1.97	0.45
1:A:18:LEU:HD22	1:A:37:THR:CG2	2.45	0.45
1:B:79:LEU:O	1:B:83:ILE:HG12	2.16	0.45
1:A:59:ASP:HB3	2:A:322:HOH:O	2.14	0.45
1:B:159:TYR:HB2	1:B:166:LEU:HD22	1.98	0.45
1:B:52:GLY:C	1:B:54:ARG:N	2.70	0.45
1:A:121:LEU:HB3	2:A:417:HOH:O	2.15	0.45
1:B:44:ARG:NH2	2:B:371:HOH:O	2.49	0.45
1:B:143:LYS:HG3	2:B:355:HOH:O	2.17	0.45
1:B:197:GLU:CD	1:B:200:CYS:HB3	2.36	0.45
1:B:40:LYS:HG2	1:B:64:ILE:HD13	1.97	0.45
1:A:111:LEU:HD13	1:A:173:ILE:HG23	1.98	0.45
1:A:83:ILE:HD12	1:A:94:THR:HA	1.99	0.45
1:A:71:ASN:HB3	2:A:306:HOH:O	2.16	0.45
1:A:110:PHE:CD1	1:A:124:CYS:SG	3.07	0.45
1:A:139:ALA:O	1:A:143:LYS:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ASP:OD1	1:A:167:ASN:HB2	2.17	0.45
1:B:43:LEU:HD21	1:B:60:ILE:HB	1.98	0.45
1:B:153:PRO:HB3	1:B:157:ARG:HD3	1.98	0.45
1:A:173:ILE:O	1:A:177:LEU:HG	2.16	0.45
1:B:36:LEU:O	1:B:40:LYS:HG3	2.17	0.45
1:B:216:LYS:HZ2	1:B:216:LYS:HB2	1.82	0.45
1:B:116:VAL:HG23	1:B:117:THR:HG23	1.99	0.45
1:A:201:TRP:HD1	2:A:328:HOH:O	1.96	0.45
1:A:151:LEU:HD22	2:A:402:HOH:O	2.17	0.45
1:A:160:ARG:HH11	1:A:160:ARG:HG3	1.82	0.45
1:B:39:ALA:O	1:B:41:GLU:N	2.50	0.45
1:A:49:PHE:HE1	1:A:125:VAL:HG21	1.81	0.45
1:A:56:VAL:HG23	1:A:145:PHE:HE1	1.82	0.45
1:A:29:LYS:HB3	1:A:78:THR:CG2	2.41	0.45
1:B:214:TRP:HD1	2:B:242:HOH:O	1.99	0.45
1:B:131:CYS:SG	1:B:131:CYS:O	2.73	0.45
1:A:119:LYS:O	1:A:155:ARG:NH2	2.46	0.45
1:B:205:VAL:HG23	2:B:277:HOH:O	2.16	0.45
1:A:49:PHE:HE2	1:A:52:GLY:HA3	1.81	0.45
1:A:69:ARG:HH21	1:B:167:ASN:HB3	1.81	0.45
1:B:192:PHE:HE2	2:B:254:HOH:O	1.99	0.45
1:B:80:GLN:N	1:B:80:GLN:OE1	2.46	0.44
1:B:160:ARG:HD2	2:B:354:HOH:O	2.17	0.44
1:A:69:ARG:NH1	1:A:92:LEU:HD21	2.32	0.44
1:B:115:VAL:HG23	1:B:116:VAL:HG13	1.99	0.44
1:B:70:ALA:HB3	1:B:93:ALA:HB2	1.99	0.44
1:A:140:VAL:HG22	1:B:21:GLN:HG2	1.98	0.44
1:A:194:ARG:NH1	2:A:370:HOH:O	2.46	0.44
1:B:101:LYS:HE3	1:B:197:GLU:HG3	1.99	0.44
1:A:31:PRO:C	1:A:34:PRO:HD2	2.38	0.44
1:A:69:ARG:CZ	2:A:340:HOH:O	2.65	0.44
1:B:130:ASN:OD1	1:B:134:ARG:HD3	2.17	0.44
1:B:18:LEU:HD13	1:B:37:THR:HG22	1.99	0.44
1:A:113:ARG:CB	1:A:124:CYS:HB3	2.47	0.44
1:B:112:ARG:HD3	1:B:206:TYR:HB2	2.00	0.44
1:B:49:PHE:CZ	1:B:110:PHE:CE2	3.06	0.44
1:A:43:LEU:HD21	1:A:60:ILE:HB	2.00	0.44
1:B:35:PHE:CG	1:B:79:LEU:HD11	2.52	0.44
1:B:67:LEU:HD21	1:B:97:LEU:HB2	2.00	0.44
1:B:57:LYS:HG2	2:B:303:HOH:O	2.17	0.44
1:B:113:ARG:HD3	1:B:127:GLU:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:LYS:HG2	1:B:179:GLU:OE1	2.16	0.44
1:A:17:ILE:HG22	1:A:21:GLN:HE21	1.81	0.44
1:B:76:ALA:HB1	1:B:81:GLU:HB3	1.99	0.44
1:A:157:ARG:HB2	1:A:157:ARG:HE	1.56	0.44
1:A:156:GLU:H	1:A:156:GLU:CD	2.21	0.44
1:B:134:ARG:HB3	1:B:135:PRO:HD3	1.98	0.44
1:B:160:ARG:HD2	2:B:359:HOH:O	2.17	0.44
1:A:35:PHE:CG	1:A:79:LEU:HD11	2.53	0.44
1:A:119:LYS:CD	1:A:123:GLN:HE21	2.23	0.44
1:A:110:PHE:CE1	1:A:114:LEU:HD22	2.53	0.44
1:A:109:SER:OG	1:A:203:ASP:HB2	2.18	0.44
1:A:184:LEU:O	1:A:188:VAL:HG23	2.17	0.44
1:A:151:LEU:HD11	2:B:315:HOH:O	2.17	0.44
1:B:43:LEU:O	1:B:44:ARG:C	2.55	0.44
1:B:35:PHE:CD2	1:B:79:LEU:HD21	2.53	0.44
1:A:204:GLU:OE1	1:A:208:ARG:NH2	2.49	0.44
1:B:100:LEU:HD11	1:B:104:PHE:CZ	2.53	0.44
1:B:200:CYS:O	1:B:201:TRP:CE3	2.70	0.44
1:A:48:ALA:HB3	1:A:158:PHE:CE1	2.53	0.44
1:A:182:ASP:N	1:A:183:PRO:HD2	2.33	0.44
1:A:125:VAL:CG1	1:A:149:VAL:HG22	2.40	0.44
1:B:173:ILE:HA	1:B:173:ILE:HD13	1.84	0.44
1:A:67:LEU:HD23	1:A:67:LEU:HA	1.74	0.44
1:A:66:LYS:NZ	2:A:396:HOH:O	2.29	0.44
1:B:56:VAL:HG12	1:B:60:ILE:HD12	1.99	0.44
1:B:121:LEU:O	1:B:124:CYS:HB3	2.18	0.44
1:A:121:LEU:O	1:A:124:CYS:HB3	2.18	0.44
1:B:161:LYS:HE3	1:B:161:LYS:HB2	1.80	0.44
1:B:12:PHE:CD1	1:B:44:ARG:HG2	2.52	0.44
1:A:54:ARG:HH12	1:B:23:THR:HA	1.82	0.44
1:B:112:ARG:O	1:B:116:VAL:HG22	2.18	0.44
1:A:41:GLU:OE1	1:A:44:ARG:NE	2.50	0.44
1:A:80:GLN:HG3	1:A:190:PHE:CE2	2.53	0.44
1:A:18:LEU:HD23	1:A:18:LEU:HA	1.90	0.44
1:A:144:VAL:HG23	2:A:316:HOH:O	2.18	0.43
1:A:145:PHE:O	1:A:146:TRP:C	2.54	0.43
1:B:65:LYS:HG2	1:B:69:ARG:HH12	1.83	0.43
2:A:282:HOH:O	1:B:215:LEU:HD11	2.17	0.43
1:A:29:LYS:HA	1:A:80:GLN:NE2	2.33	0.43
1:B:111:LEU:HB2	1:B:177:LEU:HD11	1.99	0.43
1:B:119:LYS:O	1:B:155:ARG:NH1	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:GLN:HE21	1:A:207:GLN:HE22	1.65	0.43
1:A:157:ARG:O	1:A:161:LYS:HG3	2.18	0.43
1:A:76:ALA:HB1	1:A:81:GLU:HB3	2.00	0.43
1:A:33:GLU:HB2	1:A:34:PRO:HD3	1.99	0.43
1:A:19:TRP:CD1	1:A:38:ALA:HB1	2.52	0.43
1:A:36:LEU:O	1:A:39:ALA:HB3	2.18	0.43
1:A:144:VAL:HG21	1:B:21:GLN:HG2	1.99	0.43
1:A:54:ARG:HD2	1:B:182:ASP:OD2	2.18	0.43
1:A:27:ASP:HB3	2:A:379:HOH:O	2.17	0.43
1:A:101:LYS:NZ	2:A:226:HOH:O	2.36	0.43
1:B:121:LEU:HD22	1:B:153:PRO:O	2.18	0.43
1:A:11:ASP:OD1	1:A:44:ARG:NH1	2.39	0.43
1:B:134:ARG:N	1:B:135:PRO:HD2	2.33	0.43
1:B:187:ILE:O	1:B:191:PHE:HD1	1.99	0.43
1:B:185:CYS:O	1:B:189:GLN:N	2.39	0.43
1:B:160:ARG:NH1	2:B:361:HOH:O	2.52	0.43
1:B:159:TYR:HE1	1:B:173:ILE:HG13	1.83	0.43
1:A:157:ARG:HD3	2:A:410:HOH:O	2.18	0.43
1:A:81:GLU:HB2	2:A:310:HOH:O	2.19	0.43
1:B:115:VAL:HG21	1:B:214:TRP:CZ3	2.54	0.43
1:B:40:LYS:CG	1:B:64:ILE:HD13	2.49	0.43
1:A:183:PRO:O	1:A:187:ILE:HG13	2.19	0.43
1:A:29:LYS:HB2	1:A:78:THR:HG21	2.01	0.43
1:B:37:THR:HG23	1:B:40:LYS:CE	2.48	0.43
1:B:166:LEU:HB3	2:B:360:HOH:O	2.18	0.43
1:A:140:VAL:HG21	1:B:21:GLN:CD	2.38	0.43
1:B:165:ASP:OD2	2:B:387:HOH:O	2.21	0.43
1:B:51:SER:O	1:B:54:ARG:HG3	2.19	0.43
1:A:140:VAL:HG21	1:B:21:GLN:CD	2.39	0.43
1:A:157:ARG:HG2	2:A:275:HOH:O	2.19	0.43
1:A:17:ILE:O	1:A:20:LYS:HB3	2.19	0.43
1:A:202:GLY:HA3	1:A:207:GLN:OE1	2.19	0.43
1:A:116:VAL:HG23	1:A:117:THR:H	1.84	0.43
1:A:70:ALA:HB2	1:A:92:LEU:CG	2.48	0.43
1:B:29:LYS:HD3	1:B:80:GLN:HB2	2.01	0.43
1:B:173:ILE:HD13	1:B:173:ILE:HA	1.88	0.43
1:A:33:GLU:HB2	1:A:34:PRO:CD	2.49	0.43
1:A:139:ALA:O	1:A:143:LYS:HG3	2.19	0.43
1:B:86:GLU:O	1:B:87:ASN:C	2.57	0.43
1:A:181:HIS:CD2	1:A:206:TYR:O	2.72	0.42
1:B:67:LEU:HG	1:B:96:ALA:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ASP:OD2	2:A:387:HOH:O	2.21	0.42
1:B:126:THR:HG23	1:B:146:TRP:CH2	2.54	0.42
1:B:163:HIS:CE1	1:B:165:ASP:HB3	2.53	0.42
1:A:182:ASP:HB2	1:A:183:PRO:HD3	2.01	0.42
1:B:101:LYS:HB3	1:B:101:LYS:NZ	2.33	0.42
1:A:46:VAL:HG21	1:A:60:ILE:CD1	2.49	0.42
1:B:200:CYS:HA	2:B:255:HOH:O	2.19	0.42
1:A:148:GLY:O	1:A:151:LEU:HB2	2.18	0.42
1:B:15:ILE:HG13	1:B:41:GLU:HB3	2.00	0.42
1:B:114:LEU:CA	1:B:124:CYS:SG	3.07	0.42
1:B:54:ARG:HD2	2:B:228:HOH:O	2.19	0.42
1:A:126:THR:HG23	1:A:146:TRP:CH2	2.55	0.42
1:B:86:GLU:OE1	1:B:91:GLY:HA3	2.19	0.42
1:A:49:PHE:CE2	1:A:52:GLY:HA3	2.54	0.42
1:A:27:ASP:CB	2:A:387:HOH:O	2.42	0.42
1:B:25:LYS:HE2	2:B:387:HOH:O	2.20	0.42
1:A:46:VAL:HG13	1:A:53:PHE:HD2	1.84	0.42
1:B:89:PRO:HA	1:B:196:LEU:CD2	2.49	0.42
1:B:11:ASP:O	1:B:44:ARG:HD3	2.19	0.42
1:A:18:LEU:HD12	1:A:41:GLU:HG3	2.00	0.42
1:B:60:ILE:HG23	1:B:100:LEU:CD1	2.49	0.42
1:A:69:ARG:O	1:A:72:GLN:HG3	2.20	0.42
1:B:153:PRO:HG2	1:B:158:PHE:HB2	2.01	0.42
1:A:119:LYS:HB3	1:A:123:GLN:HB3	2.01	0.42
1:A:138:SER:O	1:A:142:GLN:HG3	2.19	0.42
1:B:115:VAL:HG23	1:B:116:VAL:N	2.33	0.42
1:B:210:ASP:C	1:B:212:SER:H	2.23	0.42
1:A:32:LEU:C	1:A:32:LEU:HD23	2.40	0.42
1:B:41:GLU:OE2	1:B:44:ARG:NH2	2.52	0.42
1:A:132:THR:HG22	1:A:202:GLY:HA2	2.01	0.42
1:A:32:LEU:HD23	1:A:32:LEU:C	2.40	0.42
1:A:163:HIS:CE1	1:A:168:ILE:HD12	2.55	0.42
1:B:94:THR:HG23	1:B:196:LEU:HD13	2.02	0.42
1:B:146:TRP:O	1:B:150:LYS:HG3	2.19	0.42
1:A:82:LEU:O	1:A:86:GLU:HG3	2.19	0.42
1:A:19:TRP:CE2	1:A:38:ALA:HB1	2.54	0.42
1:A:162:LEU:HD12	1:A:173:ILE:HD11	2.00	0.42
1:A:44:ARG:HG3	2:A:333:HOH:O	2.19	0.42
1:A:157:ARG:CG	1:A:161:LYS:HE3	2.36	0.42
1:B:11:ASP:O	1:B:14:ILE:HG22	2.19	0.42
1:A:44:ARG:NE	2:A:331:HOH:O	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:ARG:HD2	1:A:124:CYS:O	2.19	0.42
1:B:89:PRO:O	1:B:95:VAL:HG22	2.20	0.42
1:A:204:GLU:CD	1:A:208:ARG:HE	2.23	0.42
1:A:181:HIS:NE2	1:A:208:ARG:O	2.53	0.42
1:A:76:ALA:HA	1:A:81:GLU:OE2	2.20	0.42
1:A:97:LEU:HD11	1:A:187:ILE:HD13	2.02	0.42
1:A:29:LYS:HB3	1:A:78:THR:HG21	2.02	0.42
1:B:111:LEU:HD22	1:B:173:ILE:CD1	2.40	0.42
1:B:210:ASP:CG	1:B:213:GLU:HB2	2.40	0.42
1:B:182:ASP:CB	2:B:229:HOH:O	2.61	0.42
1:B:19:TRP:NE1	1:B:38:ALA:HB1	2.35	0.42
1:B:49:PHE:HZ	1:B:110:PHE:CD2	2.38	0.42
1:A:20:LYS:O	1:A:23:THR:HG23	2.20	0.42
1:B:190:PHE:CE1	1:B:194:ARG:HD3	2.55	0.42
1:A:14:ILE:HG13	1:A:18:LEU:HG	2.02	0.42
1:A:173:ILE:O	1:A:176:PHE:HB3	2.19	0.42
1:A:70:ALA:HB1	1:A:93:ALA:HB2	2.02	0.42
1:B:82:LEU:O	1:B:86:GLU:HG3	2.20	0.42
1:B:60:ILE:HD11	1:B:103:ALA:HB1	2.00	0.42
1:A:133:LEU:O	1:A:136:CYS:HB2	2.20	0.41
1:B:30:VAL:H	1:B:80:GLN:CD	2.23	0.41
1:B:138:SER:O	1:B:142:GLN:HG3	2.20	0.41
1:B:167:ASN:ND2	1:B:167:ASN:N	2.67	0.41
1:A:165:ASP:HB3	1:A:168:ILE:HD12	2.02	0.41
1:A:212:SER:HB3	1:A:215:LEU:CD1	2.50	0.41
1:A:18:LEU:HB3	1:A:38:ALA:HA	2.02	0.41
1:B:47:ASP:CG	2:B:305:HOH:O	2.58	0.41
1:A:196:LEU:HA	1:A:196:LEU:HD23	1.92	0.41
1:B:12:PHE:O	1:B:15:ILE:HG22	2.20	0.41
1:A:25:LYS:HB3	2:A:380:HOH:O	2.18	0.41
1:B:115:VAL:HG21	1:B:214:TRP:HZ3	1.84	0.41
1:B:110:PHE:CE1	1:B:121:LEU:HG	2.55	0.41
1:B:210:ASP:OD1	1:B:210:ASP:N	2.49	0.41
1:A:47:ASP:OD1	1:A:57:LYS:HE3	2.19	0.41
1:A:22:VAL:O	1:A:22:VAL:HG12	2.19	0.41
1:A:112:ARG:O	1:A:116:VAL:HG22	2.20	0.41
1:B:37:THR:HA	1:B:40:LYS:HE3	2.02	0.41
1:A:181:HIS:CE1	1:A:208:ARG:O	2.73	0.41
1:B:71:ASN:OD1	1:B:76:ALA:N	2.52	0.41
1:B:156:GLU:OE2	1:B:160:ARG:NH2	2.52	0.41
1:B:29:LYS:HA	1:B:80:GLN:CD	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:LYS:O	1:B:155:ARG:NH2	2.51	0.41
1:B:180:LEU:HG	1:B:180:LEU:O	2.20	0.41
1:A:170:LYS:O	1:A:174:GLU:HG3	2.19	0.41
1:A:46:VAL:HG21	1:A:60:ILE:CD1	2.48	0.41
1:A:84:ILE:O	1:A:87:ASN:HB2	2.21	0.41
1:A:182:ASP:OD1	1:A:211:SER:HB3	2.20	0.41
1:A:121:LEU:HD23	1:A:121:LEU:C	2.40	0.41
1:B:204:GLU:OE1	1:B:208:ARG:NH2	2.49	0.41
1:A:165:ASP:HB3	1:A:168:ILE:HD12	2.01	0.41
1:B:90:ASP:OD2	1:B:90:ASP:N	2.53	0.41
1:A:165:ASP:HA	2:A:402:HOH:O	2.20	0.41
1:A:18:LEU:HD13	1:A:37:THR:HG22	2.03	0.41
1:B:101:LYS:HG2	1:B:105:GLN:NE2	2.33	0.41
1:A:117:THR:OG1	1:A:119:LYS:HD2	2.21	0.41
1:B:116:VAL:HG11	1:B:214:TRP:CE3	2.55	0.41
1:A:63:ASN:OD1	1:A:96:ALA:O	2.38	0.41
1:B:105:GLN:HE21	1:B:207:GLN:NE2	2.17	0.41
1:A:24:VAL:C	1:A:25:LYS:O	2.58	0.41
1:A:198:ASP:OD1	2:A:394:HOH:O	2.22	0.41
1:B:210:ASP:OD2	1:B:213:GLU:CA	2.68	0.41
1:A:113:ARG:HD3	1:A:127:GLU:CB	2.50	0.41
1:B:111:LEU:HB2	1:B:177:LEU:HD21	2.02	0.41
1:B:161:LYS:HA	1:B:161:LYS:HD3	1.93	0.41
1:A:202:GLY:HA3	1:A:207:GLN:HE22	1.85	0.41
1:A:71:ASN:HB2	1:A:82:LEU:HD22	2.01	0.41
1:A:210:ASP:HB3	1:A:213:GLU:HB2	2.03	0.41
1:B:16:VAL:O	1:B:179:GLU:HG3	2.20	0.41
1:A:135:PRO:O	1:A:199:GLN:NE2	2.54	0.41
1:A:33:GLU:N	1:A:34:PRO:CD	2.83	0.41
1:A:70:ALA:HB2	1:A:92:LEU:HD23	2.02	0.41
1:B:64:ILE:O	1:B:66:LYS:N	2.54	0.41
1:A:94:THR:CG2	1:A:196:LEU:HD13	2.51	0.41
1:B:20:LYS:NZ	2:B:316:HOH:O	2.25	0.41
1:B:11:ASP:OD2	1:B:11:ASP:N	2.53	0.41
1:B:98:LEU:CD1	1:B:197:GLU:HG2	2.51	0.41
1:A:142:GLN:NE2	2:A:353:HOH:O	2.54	0.41
1:A:49:PHE:CE1	1:A:125:VAL:HG21	2.56	0.41
1:A:195:GLU:C	1:A:196:LEU:HD23	2.41	0.41
1:A:195:GLU:O	1:A:196:LEU:HD23	2.20	0.41
1:B:25:LYS:HB2	1:B:29:LYS:HB2	2.03	0.41
1:A:131:CYS:HB2	2:A:264:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:TRP:CD1	1:A:38:ALA:HB1	2.55	0.41
1:A:101:LYS:HD2	1:A:188:VAL:HG22	2.03	0.41
1:A:88:SER:C	1:A:90:ASP:N	2.74	0.41
1:B:132:THR:CG2	1:B:202:GLY:HA2	2.50	0.41
1:A:122:GLU:HG3	1:A:149:VAL:HG13	2.03	0.41
1:A:40:LYS:NZ	2:A:326:HOH:O	2.53	0.41
1:B:216:LYS:HB3	1:B:216:LYS:HZ2	1.81	0.41
1:A:129:TYR:CZ	1:A:134:ARG:HA	2.56	0.41
1:A:22:VAL:HG12	1:A:183:PRO:HB3	2.03	0.41
1:A:183:PRO:O	1:A:187:ILE:HG13	2.21	0.41
1:A:47:ASP:CG	2:A:339:HOH:O	2.59	0.41
1:A:60:ILE:CG1	1:A:103:ALA:HB1	2.51	0.40
1:A:92:LEU:HA	1:A:92:LEU:HD12	1.82	0.40
1:B:157:ARG:O	1:B:161:LYS:HB2	2.21	0.40
1:B:216:LYS:NZ	1:B:216:LYS:CB	2.85	0.40
1:A:20:LYS:HD2	2:A:312:HOH:O	2.21	0.40
1:A:105:GLN:HE21	1:A:207:GLN:HE22	1.68	0.40
1:B:153:PRO:HB2	1:B:157:ARG:HB3	2.02	0.40
1:B:135:PRO:HG2	1:B:200:CYS:HB3	2.02	0.40
1:B:101:LYS:HG2	1:B:105:GLN:OE1	2.22	0.40
1:A:176:PHE:CZ	1:A:180:LEU:HD22	2.55	0.40
1:A:156:GLU:CD	1:A:156:GLU:N	2.75	0.40
1:A:43:LEU:HD11	1:A:61:ALA:HA	2.03	0.40
1:A:100:LEU:HD11	1:A:104:PHE:CZ	2.56	0.40
1:A:18:LEU:HA	1:A:21:GLN:NE2	2.36	0.40
1:B:111:LEU:HB3	1:B:177:LEU:HD11	2.02	0.40
1:B:126:THR:HG23	1:B:146:TRP:CH2	2.56	0.40
1:B:114:LEU:CD2	1:B:158:PHE:CD2	3.04	0.40
1:B:126:THR:HG23	1:B:146:TRP:CH2	2.55	0.40
1:B:101:LYS:O	1:B:105:GLN:NE2	2.53	0.40
1:A:105:GLN:HE21	1:A:207:GLN:NE2	2.20	0.40
1:A:172:LYS:NZ	2:A:255:HOH:O	2.51	0.40
1:A:67:LEU:HD23	1:A:67:LEU:HA	1.86	0.40
1:B:111:LEU:HD13	1:B:173:ILE:HG23	2.03	0.40
1:B:65:LYS:NZ	1:B:65:LYS:HB2	2.36	0.40
1:B:161:LYS:HB2	1:B:161:LYS:HE3	1.94	0.40
1:A:210:ASP:CB	1:A:213:GLU:HB2	2.36	0.40
1:B:113:ARG:NH1	1:B:127:GLU:CB	2.82	0.40
1:B:114:LEU:CD2	1:B:158:PHE:CE2	3.05	0.40
1:B:102:ARG:HB3	1:B:133:LEU:HD21	2.03	0.40
1:B:157:ARG:NH1	1:B:157:ARG:CG	2.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:TRP:HE3	1:A:201:TRP:HA	1.87	0.40
1:A:44:ARG:HH22	1:A:162:LEU:HA	1.86	0.40
1:A:25:LYS:N	2:A:379:HOH:O	2.23	0.40
1:A:170:LYS:NZ	2:A:283:HOH:O	2.49	0.40
1:A:11:ASP:OD2	1:A:11:ASP:N	2.53	0.40
1:B:204:GLU:OE1	1:B:208:ARG:NH2	2.47	0.40
1:B:54:ARG:HD2	2:B:228:HOH:O	2.21	0.40
1:A:131:CYS:O	1:A:131:CYS:SG	2.80	0.40
1:A:46:VAL:HG11	1:A:57:LYS:HB2	2.03	0.40
1:B:41:GLU:OE2	1:B:44:ARG:CZ	2.70	0.40
1:A:36:LEU:HD12	1:A:68:TYR:CE2	2.56	0.40
1:A:177:LEU:HD23	1:A:177:LEU:HA	1.85	0.40
1:B:29:LYS:CD	2:B:387:HOH:O	2.70	0.40
1:A:208:ARG:CB	1:A:213:GLU:HG2	2.52	0.40
1:A:46:VAL:HG11	1:A:57:LYS:HB2	2.04	0.40
1:A:11:ASP:N	1:A:11:ASP:OD2	2.54	0.40
1:A:56:VAL:HG12	1:A:60:ILE:HD12	2.04	0.40
1:B:14:ILE:CG2	1:B:44:ARG:HH12	2.34	0.40
1:B:160:ARG:NE	2:B:390:HOH:O	2.43	0.40
1:B:97:LEU:O	1:B:98:LEU:C	2.58	0.40
1:B:163:HIS:ND1	1:B:164:PRO:HD2	2.37	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	204/224 (91%)	192 (94%)	11 (5%)	1 (0%)	34	10
1	1-B	204/224 (91%)	194 (95%)	8 (4%)	2 (1%)	19	3
1	2-A	204/224 (91%)	192 (94%)	11 (5%)	1 (0%)	34	10
1	2-B	204/224 (91%)	194 (95%)	9 (4%)	1 (0%)	34	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3-A	204/224 (91%)	198 (97%)	6 (3%)	0	100	100
1	3-B	204/224 (91%)	192 (94%)	11 (5%)	1 (0%)	34	10
1	4-A	204/224 (91%)	189 (93%)	11 (5%)	4 (2%)	9	0
1	4-B	204/224 (91%)	199 (98%)	5 (2%)	0	100	100
1	5-A	204/224 (91%)	198 (97%)	6 (3%)	0	100	100
1	5-B	204/224 (91%)	197 (97%)	7 (3%)	0	100	100
1	6-A	204/224 (91%)	200 (98%)	4 (2%)	0	100	100
1	6-B	204/224 (91%)	195 (96%)	9 (4%)	0	100	100
1	7-A	204/224 (91%)	193 (95%)	11 (5%)	0	100	100
1	7-B	204/224 (91%)	195 (96%)	6 (3%)	3 (2%)	13	1
1	8-A	204/224 (91%)	189 (93%)	13 (6%)	2 (1%)	19	3
1	8-B	204/224 (91%)	193 (95%)	10 (5%)	1 (0%)	34	10
All	All	3264/3584 (91%)	3110 (95%)	138 (4%)	16 (0%)	34	10

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	8-A	25	LYS
1	1-B	200	CYS
1	8-A	51	SER
1	8-B	53	PHE
1	1-A	72	GLN
1	1-B	208	ARG
1	3-B	26	GLU
1	4-A	27	ASP
1	4-A	28	GLY
1	4-A	92	LEU
1	2-A	25	LYS
1	2-B	53	PHE
1	7-B	92	LEU
1	7-B	40	LYS
1	7-B	65	LYS
1	4-A	202	GLY

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	181/199 (91%)	176 (97%)	5 (3%)	51	14
1	1-B	181/199 (91%)	179 (99%)	2 (1%)	80	54
1	2-A	181/199 (91%)	178 (98%)	3 (2%)	68	34
1	2-B	181/199 (91%)	178 (98%)	3 (2%)	68	34
1	3-A	181/199 (91%)	177 (98%)	4 (2%)	60	23
1	3-B	181/199 (91%)	176 (97%)	5 (3%)	51	14
1	4-A	181/199 (91%)	176 (97%)	5 (3%)	51	14
1	4-B	181/199 (91%)	176 (97%)	5 (3%)	51	14
1	5-A	181/199 (91%)	181 (100%)	0	100	100
1	5-B	181/199 (91%)	178 (98%)	3 (2%)	68	34
1	6-A	181/199 (91%)	179 (99%)	2 (1%)	80	54
1	6-B	181/199 (91%)	176 (97%)	5 (3%)	51	14
1	7-A	181/199 (91%)	176 (97%)	5 (3%)	51	14
1	7-B	181/199 (91%)	173 (96%)	8 (4%)	35	5
1	8-A	181/199 (91%)	180 (99%)	1 (1%)	90	73
1	8-B	181/199 (91%)	174 (96%)	7 (4%)	39	7
All	All	2896/3184 (91%)	2833 (98%)	63 (2%)	60	23

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	53	PHE
1	1-A	55	ILE
1	1-A	63	ASN
1	1-A	101	LYS
1	1-A	150	LYS
1	1-B	136	CYS
1	1-B	210	ASP
1	2-A	124	CYS

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Mol	Chain	Res	Type
1	2-A	131	CYS
1	2-A	150	LYS
1	2-B	49	PHE
1	2-B	55	ILE
1	2-B	200	CYS
1	3-A	110	PHE
1	3-A	131	CYS
1	3-A	150	LYS
1	3-A	201	TRP
1	3-B	105	GLN
1	3-B	123	GLN
1	3-B	161	LYS
1	3-B	198	ASP
1	3-B	214	TRP
1	4-A	23	THR
1	4-A	47	ASP
1	4-A	53	PHE
1	4-A	55	ILE
1	4-A	150	LYS
1	4-B	101	LYS
1	4-B	112	ARG
1	4-B	124	CYS
1	4-B	186	CYS
1	4-B	197	GLU
1	5-B	14	ILE
1	5-B	133	LEU
1	5-B	200	CYS
1	6-A	47	ASP
1	6-A	150	LYS
1	6-B	173	ILE
1	6-B	198	ASP
1	6-B	200	CYS
1	6-B	210	ASP
1	6-B	213	GLU
1	7-A	26	GLU
1	7-A	53	PHE
1	7-A	110	PHE
1	7-A	125	VAL
1	7-A	150	LYS
1	7-B	14	ILE
1	7-B	41	GLU
1	7-B	125	VAL

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Mol	Chain	Res	Type
1	7-B	161	LYS
1	7-B	185	CYS
1	7-B	200	CYS
1	7-B	201	TRP
1	7-B	213	GLU
1	8-A	53	PHE
1	8-B	44	ARG
1	8-B	69	ARG
1	8-B	117	THR
1	8-B	185	CYS
1	8-B	200	CYS
1	8-B	201	TRP
1	8-B	210	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	21	GLN
1	1-A	167	ASN
1	1-A	207	GLN
1	1-B	75	HIS
1	1-B	167	ASN
1	1-B	207	GLN
1	2-A	21	GLN
1	2-A	63	ASN
1	2-A	123	GLN
1	2-A	167	ASN
1	2-A	207	GLN
1	2-B	105	GLN
1	2-B	123	GLN
1	2-B	167	ASN
1	2-B	199	GLN
1	2-B	207	GLN
1	3-A	21	GLN
1	3-A	63	ASN
1	3-A	75	HIS
1	3-A	207	GLN
1	3-B	207	GLN
1	4-A	75	HIS
1	4-A	167	ASN
1	4-A	199	GLN
1	4-A	207	GLN

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Mol	Chain	Res	Type
1	4-B	123	GLN
1	4-B	167	ASN
1	5-A	105	GLN
1	5-A	207	GLN
1	5-B	167	ASN
1	5-B	207	GLN
1	6-A	21	GLN
1	6-A	63	ASN
1	6-A	199	GLN
1	6-A	207	GLN
1	6-B	21	GLN
1	6-B	75	HIS
1	6-B	123	GLN
1	6-B	167	ASN
1	6-B	207	GLN
1	7-A	63	ASN
1	7-A	167	ASN
1	7-A	189	GLN
1	7-A	207	GLN
1	7-B	167	ASN
1	7-B	207	GLN
1	8-A	63	ASN
1	8-A	167	ASN
1	8-A	199	GLN
1	8-A	207	GLN
1	8-B	207	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1-A	206/224 (91%)	0.18	5 (2%) 62 63	10, 15, 27, 36	206 (100%)
1	1-B	206/224 (91%)	0.35	9 (4%) 38 37	9, 15, 27, 37	206 (100%)
1	2-A	206/224 (91%)	0.18	5 (2%) 62 63	10, 15, 27, 36	206 (100%)
1	2-B	206/224 (91%)	0.35	9 (4%) 38 37	9, 15, 27, 37	206 (100%)
1	3-A	206/224 (91%)	0.18	5 (2%) 62 63	10, 15, 27, 36	206 (100%)
1	3-B	206/224 (91%)	0.35	9 (4%) 38 37	9, 15, 27, 37	206 (100%)
1	4-A	206/224 (91%)	0.18	5 (2%) 62 63	10, 15, 27, 36	206 (100%)
1	4-B	206/224 (91%)	0.35	9 (4%) 38 37	9, 15, 27, 37	206 (100%)
1	5-A	206/224 (91%)	0.18	5 (2%) 62 63	10, 15, 27, 36	206 (100%)
1	5-B	206/224 (91%)	0.35	9 (4%) 38 37	9, 15, 27, 37	206 (100%)
1	6-A	206/224 (91%)	0.18	5 (2%) 62 63	10, 15, 27, 36	206 (100%)
1	6-B	206/224 (91%)	0.35	9 (4%) 38 37	9, 15, 27, 37	206 (100%)
1	7-A	206/224 (91%)	0.18	5 (2%) 62 63	10, 15, 27, 36	206 (100%)
1	7-B	206/224 (91%)	0.35	9 (4%) 38 37	9, 15, 27, 37	206 (100%)
1	8-A	206/224 (91%)	0.18	5 (2%) 62 63	10, 15, 27, 36	206 (100%)
1	8-B	206/224 (91%)	0.35	9 (4%) 38 37	9, 15, 27, 37	206 (100%)
All	All	3296/3584 (91%)	0.27	112 (3%) 49 48	9, 15, 27, 37	3296 (100%)

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-B	200	CYS	6.6
1	2-B	200	CYS	6.6
1	3-B	200	CYS	6.6
1	4-B	200	CYS	6.6
1	5-B	200	CYS	6.6

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Mol	Chain	Res	Type	RSRZ
1	6-B	200	CYS	6.6
1	7-B	200	CYS	6.6
1	8-B	200	CYS	6.6
1	1-B	11	ASP	4.2
1	2-B	11	ASP	4.2
1	3-B	11	ASP	4.2
1	4-B	11	ASP	4.2
1	5-B	11	ASP	4.2
1	6-B	11	ASP	4.2
1	7-B	11	ASP	4.2
1	8-B	11	ASP	4.2
1	1-B	73	THR	3.8
1	2-B	73	THR	3.8
1	3-B	73	THR	3.8
1	4-B	73	THR	3.8
1	5-B	73	THR	3.8
1	6-B	73	THR	3.8
1	7-B	73	THR	3.8
1	8-B	73	THR	3.8
1	1-A	24	VAL	3.7
1	2-A	24	VAL	3.7
1	3-A	24	VAL	3.7
1	4-A	24	VAL	3.7
1	5-A	24	VAL	3.7
1	6-A	24	VAL	3.7
1	7-A	24	VAL	3.7
1	8-A	24	VAL	3.7
1	1-B	124	CYS	3.7
1	2-B	124	CYS	3.7
1	3-B	124	CYS	3.7
1	4-B	124	CYS	3.7
1	5-B	124	CYS	3.7
1	6-B	124	CYS	3.7
1	7-B	124	CYS	3.7
1	8-B	124	CYS	3.7
1	1-B	185	CYS	3.1
1	2-B	185	CYS	3.1
1	3-B	185	CYS	3.1
1	4-B	185	CYS	3.1
1	5-B	185	CYS	3.1
1	6-B	185	CYS	3.1
1	7-B	185	CYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	8-B	185	CYS	3.1
1	1-B	201	TRP	2.4
1	2-B	201	TRP	2.4
1	3-B	201	TRP	2.4
1	4-B	201	TRP	2.4
1	5-B	201	TRP	2.4
1	6-B	201	TRP	2.4
1	7-B	201	TRP	2.4
1	8-B	201	TRP	2.4
1	1-A	131	CYS	2.3
1	2-A	131	CYS	2.3
1	3-A	131	CYS	2.3
1	4-A	131	CYS	2.3
1	5-A	131	CYS	2.3
1	6-A	131	CYS	2.3
1	7-A	131	CYS	2.3
1	8-A	131	CYS	2.3
1	1-B	74	VAL	2.3
1	2-B	74	VAL	2.3
1	3-B	74	VAL	2.3
1	4-B	74	VAL	2.3
1	5-B	74	VAL	2.3
1	6-B	74	VAL	2.3
1	7-B	74	VAL	2.3
1	8-B	74	VAL	2.3
1	1-A	201	TRP	2.2
1	2-A	201	TRP	2.2
1	3-A	201	TRP	2.2
1	4-A	201	TRP	2.2
1	5-A	201	TRP	2.2
1	6-A	201	TRP	2.2
1	7-A	201	TRP	2.2
1	8-A	201	TRP	2.2
1	1-B	162	LEU	2.1
1	2-B	162	LEU	2.1
1	3-B	162	LEU	2.1
1	4-B	162	LEU	2.1
1	5-B	162	LEU	2.1
1	6-B	162	LEU	2.1
1	7-B	162	LEU	2.1
1	8-B	162	LEU	2.1
1	1-A	118	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	2-A	118	ASP	2.1
1	3-A	118	ASP	2.1
1	4-A	118	ASP	2.1
1	5-A	118	ASP	2.1
1	6-A	118	ASP	2.1
1	7-A	118	ASP	2.1
1	8-A	118	ASP	2.1
1	1-B	168	ILE	2.1
1	2-B	168	ILE	2.1
1	3-B	168	ILE	2.1
1	4-B	168	ILE	2.1
1	5-B	168	ILE	2.1
1	6-B	168	ILE	2.1
1	7-B	168	ILE	2.1
1	8-B	168	ILE	2.1
1	1-A	216	LYS	2.0
1	2-A	216	LYS	2.0
1	3-A	216	LYS	2.0
1	4-A	216	LYS	2.0
1	5-A	216	LYS	2.0
1	6-A	216	LYS	2.0
1	7-A	216	LYS	2.0
1	8-A	216	LYS	2.0

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.