



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 09:42 PM UTC

PDB ID : 5YEI / pdb_00005yei
Title : Mechanistic insight into the regulation of *Pseudomonas aeruginosa* aspartate kinase
Authors : Li, C.; Yang, M.; Liu, L.; Peng, C.; Li, T.; He, L.; Song, Y.; Zhu, Y.; Bao, R.
Deposited on : 2017-09-17
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

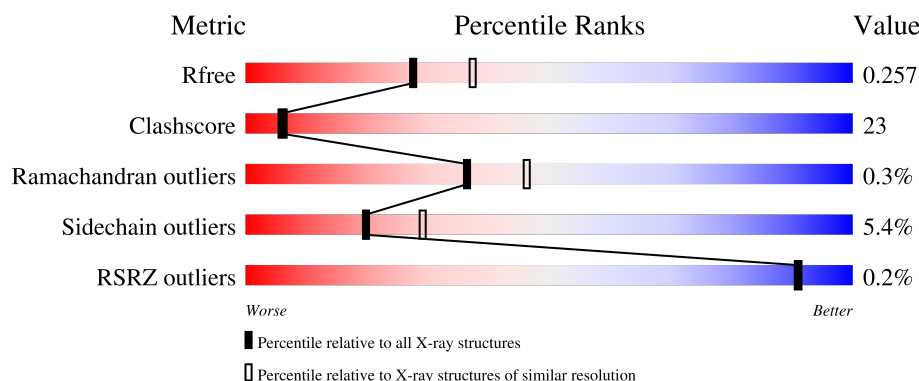
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	164	
1	D	164	
1	F	164	
1	H	164	
2	A	412	

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Mol	Chain	Length	Quality of chain
2	C	412	
2	E	412	
2	G	412	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	THR	F	501	-	-	X	-
3	THR	G	503	-	-	X	-
4	LYS	C	502	-	-	X	-
4	LYS	G	502	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16949 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.

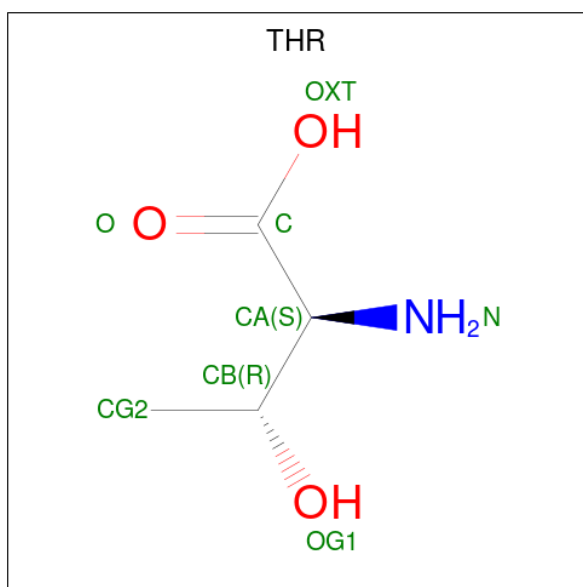
- Molecule 1 is a protein called Aspartokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	156	Total	C	N	O	S	0	0	0
			1178	743	204	227	4			
1	B	156	Total	C	N	O	S	0	0	0
			1178	743	204	227	4			
1	F	151	Total	C	N	O	S	0	0	0
			1145	722	199	220	4			
1	H	156	Total	C	N	O	S	0	0	0
			1178	743	204	227	4			

- Molecule 2 is a protein called Aspartokinase.

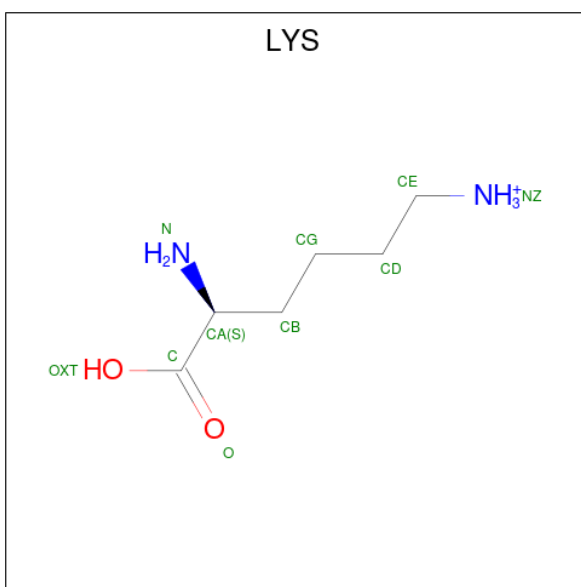
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	397	Total	C	N	O	S	0	0	0
			2993	1879	526	577	11			
2	G	397	Total	C	N	O	S	0	0	0
			2993	1879	526	577	11			
2	A	397	Total	C	N	O	S	0	0	0
			2993	1879	526	577	11			
2	E	397	Total	C	N	O	S	0	0	0
			2993	1879	526	577	11			

- Molecule 3 is THREONINE (CCD ID: THR) (formula: C₄H₉NO₃).



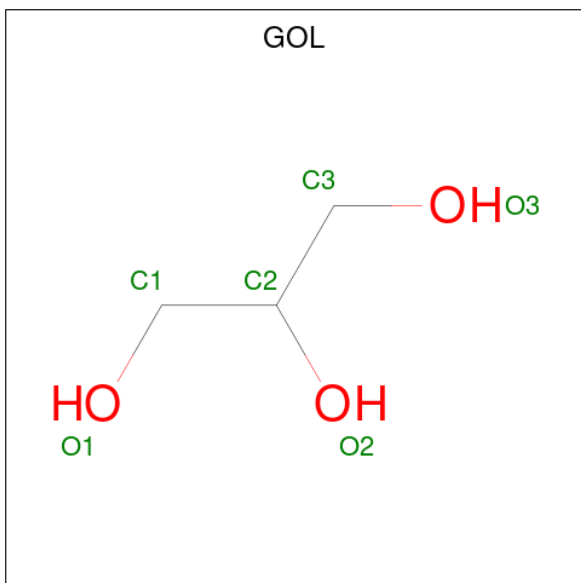
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	C	N	O	0	0
			8	4	1	3		
3	B	1	Total	C	N	O	0	0
			8	4	1	3		
3	F	1	Total	C	N	O	0	0
			8	4	1	3		
3	F	1	Total	C	N	O	0	0
			8	4	1	3		
3	C	1	Total	C	N	O	0	0
			8	4	1	3		
3	H	1	Total	C	N	O	0	0
			8	4	1	3		
3	G	1	Total	C	N	O	0	0
			8	4	1	3		
3	A	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 4 is LYSINE (CCD ID: LYS) (formula: C₆H₁₅N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			10	6	2	2		
4	G	1	Total	C	N	O	0	0
			10	6	2	2		
4	A	1	Total	C	N	O	0	0
			10	6	2	2		
4	E	1	Total	C	N	O	0	0
			10	6	2	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0

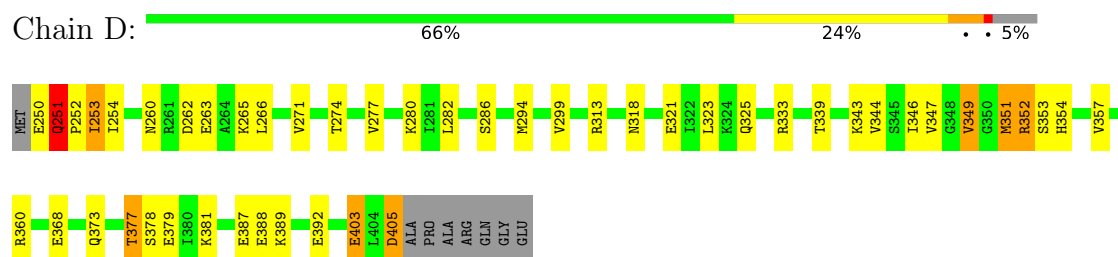
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	13	Total O 13 13	0	0
6	B	13	Total O 13 13	0	0
6	F	7	Total O 7 7	0	0
6	C	36	Total O 36 36	0	0
6	H	10	Total O 10 10	0	0
6	G	34	Total O 34 34	0	0
6	A	42	Total O 42 42	0	0
6	E	21	Total O 21 21	0	0

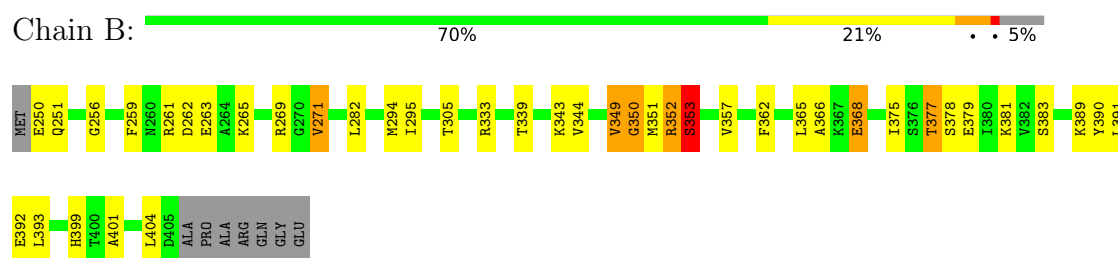
3 Residue-property plots

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

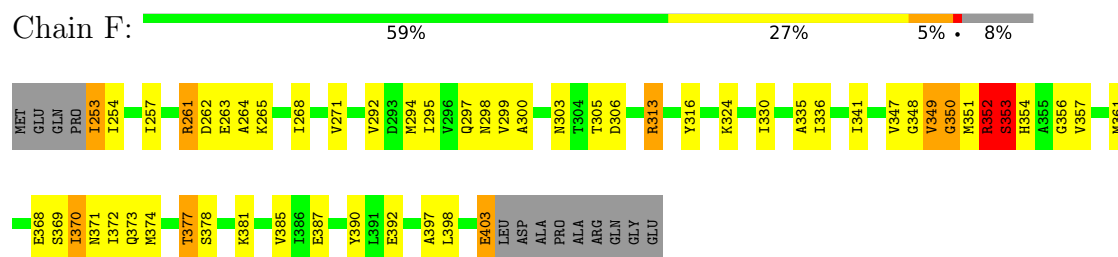
• Molecule 1: Aspartokinase



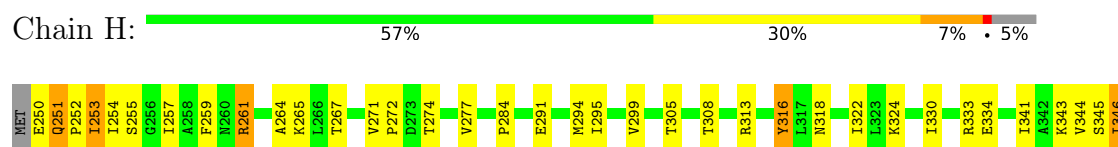
• Molecule 1: Aspartokinase



• Molecule 1: Aspartokinase



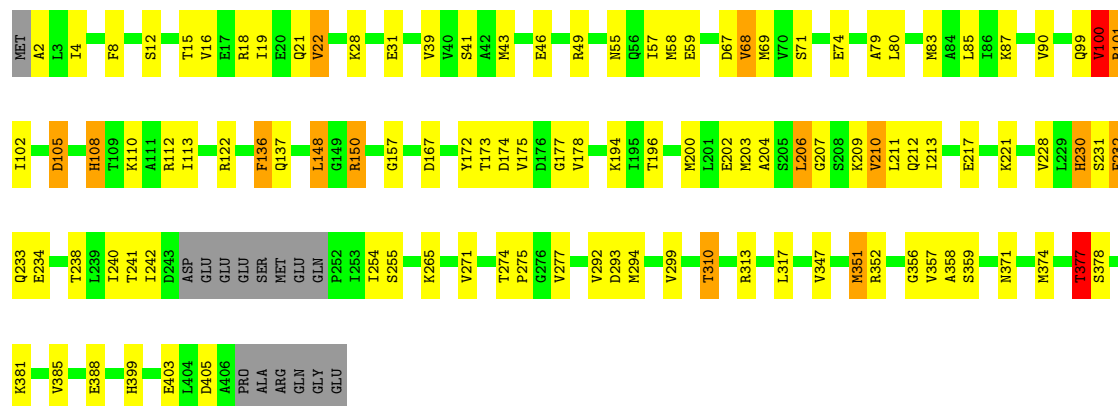
• Molecule 1: Aspartokinase





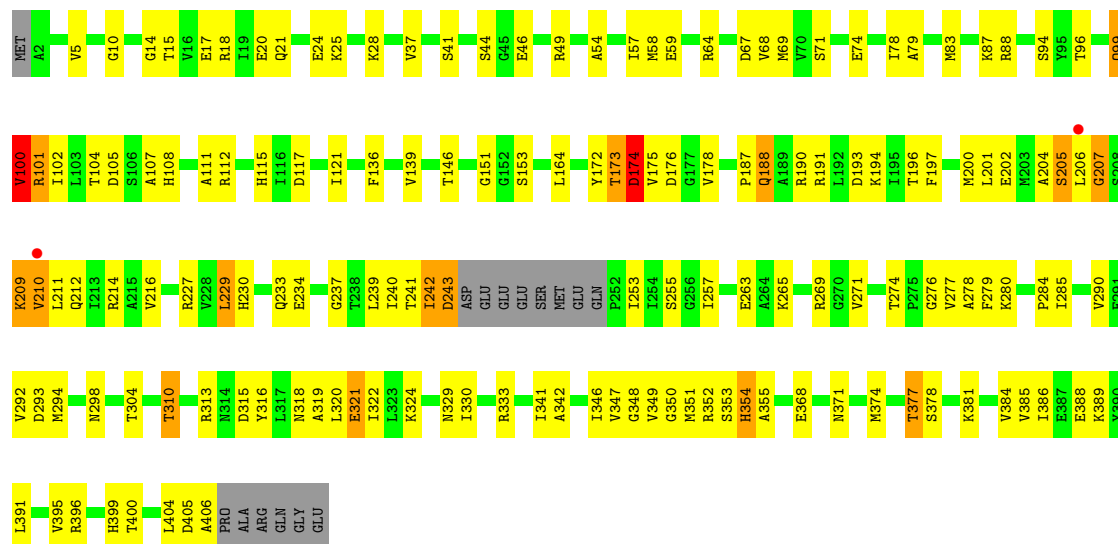
• Molecule 2: Aspartokinase

Chain C: 70% 23%



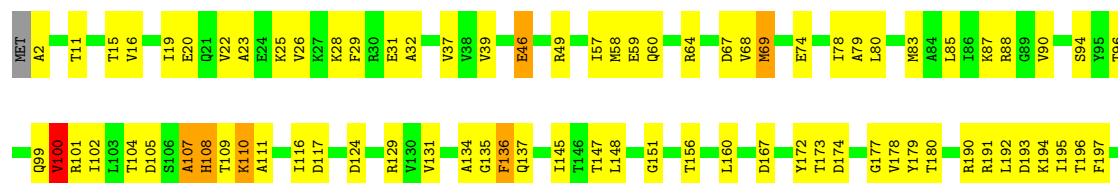
• Molecule 2: Aspartokinase

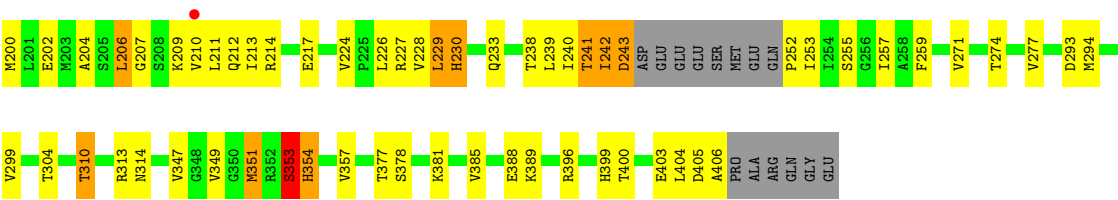
Chain G: 59% 33%



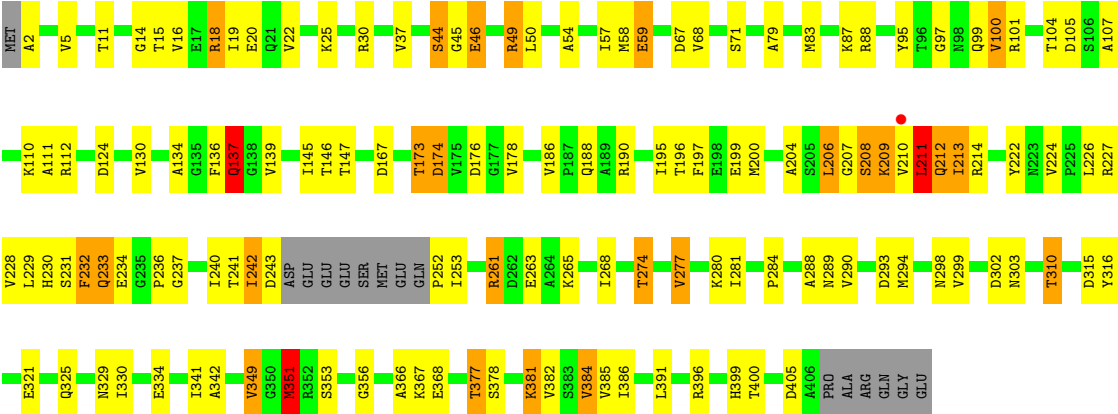
• Molecule 2: Aspartokinase

Chain A: 63% 29%





● Molecule 2: Aspartokinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.46Å 171.79Å 88.93Å 90.00° 90.29° 90.00°	Depositor
Resolution (Å)	40.09 – 2.30 40.09 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.7 (40.09-2.30) 96.8 (40.09-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.10.1-2155_1692	Depositor
R, R_{free}	0.222 , 0.257 0.223 , 0.257	Depositor DCC
R_{free} test set	5273 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	37.5	Xtriage
Anisotropy	0.420	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.267 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	16949	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	B	0.96	0/1193	0.99	8/1618 (0.5%)
1	D	0.87	0/1193	1.06	9/1618 (0.6%)
1	F	1.04	0/1159	1.09	11/1570 (0.7%)
1	H	1.21	0/1193	1.19	11/1618 (0.7%)
2	A	1.13	5/3028 (0.2%)	1.10	23/4102 (0.6%)
2	C	0.99	3/3028 (0.1%)	1.05	17/4102 (0.4%)
2	E	1.11	2/3028 (0.1%)	1.12	26/4102 (0.6%)
2	G	1.20	7/3028 (0.2%)	1.15	26/4102 (0.6%)
All	All	1.09	17/16850 (0.1%)	1.10	131/22832 (0.6%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	347	VAL	C-O	-7.18	1.16	1.24
2	G	349	VAL	CA-C	-6.72	1.45	1.53
2	C	254	ILE	C-O	-6.34	1.17	1.24
2	A	224	VAL	CA-C	-5.94	1.48	1.53
2	A	241	THR	C-O	-5.90	1.18	1.24
2	E	134	ALA	N-CA	-5.89	1.38	1.46
2	G	350	GLY	C-O	-5.77	1.15	1.24
2	E	224	VAL	CA-C	5.71	1.57	1.53
2	C	377	THR	C-O	-5.58	1.16	1.23
2	A	257	ILE	C-O	-5.47	1.18	1.24
2	C	4	ILE	C-O	-5.42	1.18	1.24
2	G	102	ILE	N-CA	-5.39	1.39	1.46
2	G	115	HIS	C-O	-5.22	1.17	1.23
2	A	107	ALA	N-CA	-5.16	1.40	1.46
2	A	134	ALA	N-CA	-5.08	1.39	1.46
2	G	348	GLY	C-O	-5.04	1.17	1.23
2	G	194	LYS	C-O	-5.03	1.17	1.23

All (131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	108	HIS	N-CA-C	15.79	128.49	111.28
1	H	368	GLU	N-CA-C	-14.49	91.84	110.53
1	D	368	GLU	N-CA-C	-11.88	93.36	110.59
2	E	232	PHE	N-CA-C	11.59	125.71	110.88
2	G	207	GLY	N-CA-C	-11.14	98.32	111.36
2	A	108	HIS	N-CA-C	11.08	123.35	111.28
1	B	349	VAL	N-CA-C	11.01	121.85	110.62
2	G	349	VAL	N-CA-C	-10.46	98.39	110.21
1	D	349	VAL	N-CA-C	9.86	120.67	110.62
1	F	353	SER	N-CA-C	9.82	123.92	112.72
2	G	350	GLY	N-CA-C	-9.60	103.27	114.69
2	G	210	VAL	N-CA-C	8.99	119.05	110.42
2	G	377	THR	N-CA-C	8.83	122.30	109.14
1	B	353	SER	N-CA-C	8.37	122.80	112.59
1	F	349	VAL	N-CA-C	8.03	118.81	110.62
2	E	137	GLN	N-CA-C	8.03	121.97	109.52
1	D	351	MET	N-CA-C	7.95	119.94	111.28
2	C	377	THR	N-CA-C	7.82	121.05	109.24
2	C	206	LEU	N-CA-C	-7.66	103.01	111.36
1	H	353	SER	N-CA-C	7.58	121.84	112.59
2	G	205	SER	N-CA-C	7.58	119.54	111.28
2	E	329	ASN	N-CA-C	7.49	119.53	111.36
1	D	253	ILE	N-CA-C	7.34	118.86	108.36
2	A	354	HIS	N-CA-C	7.31	121.93	110.17
2	E	204	ALA	N-CA-C	7.27	118.85	111.07
2	C	148	LEU	N-CA-C	7.27	119.28	111.36
2	E	349	VAL	N-CA-C	-7.25	102.02	110.21
2	C	351	MET	N-CA-C	-7.15	103.49	111.28
2	E	211	LEU	N-CA-C	-7.15	95.51	108.02
2	A	349	VAL	N-CA-C	-7.14	102.27	110.05
2	C	210	VAL	N-CA-C	7.09	117.23	110.42
2	E	377	THR	N-CA-C	6.99	119.80	109.24
1	F	350	GLY	N-CA-C	-6.95	96.72	113.18
2	G	174	ASP	N-CA-C	6.93	118.84	111.28
2	A	69	MET	N-CA-C	6.90	118.59	111.14
2	A	230	HIS	N-CA-C	-6.88	100.30	110.48
2	C	100	VAL	CA-C-N	6.85	134.62	121.54
2	C	100	VAL	C-N-CA	6.85	134.62	121.54
2	G	108	HIS	CA-C-N	-6.82	110.83	122.56
2	G	108	HIS	C-N-CA	-6.82	110.83	122.56
1	H	404	LEU	CA-C-N	-6.72	109.60	121.70
1	H	404	LEU	C-N-CA	-6.72	109.60	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	234	GLU	N-CA-C	-6.68	104.00	111.28
2	E	100	VAL	CA-C-N	6.62	134.19	121.54
2	E	100	VAL	C-N-CA	6.62	134.19	121.54
1	F	352	ARG	N-CA-C	6.54	118.41	111.28
2	E	173	THR	N-CA-C	6.52	116.67	108.45
2	A	351	MET	N-CA-C	-6.51	104.18	111.28
2	G	101	ARG	N-CA-CB	6.39	121.30	110.49
2	G	329	ASN	N-CA-C	6.39	118.25	111.28
2	E	99	GLN	N-CA-C	6.37	118.30	111.36
2	A	99	GLN	N-CA-C	6.32	117.83	111.07
2	E	213	ILE	N-CA-C	-6.30	104.81	113.00
2	G	100	VAL	CA-C-N	6.29	133.55	121.54
2	G	100	VAL	C-N-CA	6.29	133.55	121.54
2	G	316	TYR	N-CA-C	6.27	117.78	111.07
2	C	232	PHE	N-CA-C	6.27	119.95	112.93
2	E	316	TYR	N-CA-C	6.26	117.76	111.07
1	H	377	THR	N-CA-C	6.25	119.21	109.52
2	C	136	PHE	CB-CA-C	6.15	122.67	111.06
2	A	353	SER	N-CA-C	6.14	118.06	111.36
2	G	255	SER	N-CA-C	6.12	118.03	111.36
2	G	99	GLN	N-CA-C	6.09	118.00	111.36
2	C	234	GLU	N-CA-C	-6.03	104.79	111.36
2	A	100	VAL	CA-C-N	6.01	133.02	121.54
2	A	100	VAL	C-N-CA	6.01	133.02	121.54
1	H	380	ILE	N-CA-C	5.98	117.85	112.17
1	H	316	TYR	N-CA-C	5.96	117.45	111.07
2	E	174	ASP	N-CA-C	5.96	120.39	113.18
1	B	368	GLU	CA-C-N	-5.95	113.08	122.95
1	B	368	GLU	C-N-CA	-5.95	113.08	122.95
2	E	356	GLY	N-CA-C	5.88	123.48	115.30
2	E	381	LYS	N-CA-C	5.88	119.06	109.06
2	A	224	VAL	CA-C-O	5.83	122.38	119.12
1	F	336	ILE	CB-CG1-CD1	5.82	126.02	113.80
1	F	303	ASN	N-CA-C	5.81	119.68	112.24
2	A	148	LEU	N-CA-C	5.81	117.61	111.28
2	E	351	MET	N-CA-C	-5.79	105.05	111.36
2	C	100	VAL	O-C-N	5.78	127.78	121.83
2	A	204	ALA	N-CA-C	5.76	117.56	111.28
2	E	100	VAL	O-C-N	5.73	127.73	121.83
2	E	334	GLU	N-CA-C	5.72	116.83	108.14
1	F	356	GLY	N-CA-C	5.72	119.41	112.49
2	C	255	SER	N-CA-C	5.67	117.54	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	105	ASP	N-CA-CB	-5.66	102.63	110.38
2	A	96	THR	N-CA-C	-5.64	103.25	110.53
1	D	388	GLU	N-CA-C	5.63	117.42	111.28
2	A	255	SER	N-CA-C	5.62	117.49	111.36
1	H	251	GLN	CA-C-N	-5.58	114.21	119.85
1	H	251	GLN	C-N-CA	-5.58	114.21	119.85
1	H	370	ILE	N-CA-C	5.57	115.87	107.80
2	G	101	ARG	CA-CB-CG	-5.56	102.98	114.10
2	A	179	TYR	N-CA-C	5.54	118.72	110.52
2	G	175	VAL	N-CA-C	5.52	116.07	110.05
1	F	330	ILE	N-CA-C	5.44	118.22	112.83
2	G	274	THR	CA-C-N	-5.41	114.19	119.76
2	G	274	THR	C-N-CA	-5.41	114.19	119.76
2	G	204	ALA	N-CA-C	5.38	117.15	111.28
2	G	173	THR	N-CA-C	5.37	115.22	108.45
2	A	111	ALA	N-CA-C	5.37	118.02	110.23
1	F	336	ILE	CA-CB-CG1	5.31	119.43	110.40
2	G	354	HIS	N-CA-C	5.29	118.34	110.52
2	E	208	SER	N-CA-C	5.26	115.23	108.34
2	C	403	GLU	N-CA-C	5.25	118.83	111.74
2	C	99	GLN	N-CA-C	5.24	117.07	111.36
1	B	251	GLN	CA-C-N	-5.23	114.37	119.76
1	B	251	GLN	C-N-CA	-5.23	114.37	119.76
2	E	44	SER	N-CA-C	5.16	117.82	110.24
1	D	333	ARG	N-CA-C	5.15	116.71	111.14
2	A	174	ASP	N-CA-C	5.14	116.97	111.36
2	C	4	ILE	N-CA-C	5.13	115.50	108.12
2	A	136	PHE	CB-CA-C	5.12	119.82	111.26
2	E	274	THR	CA-C-N	-5.12	114.49	119.76
2	E	274	THR	C-N-CA	-5.12	114.49	119.76
2	G	368	GLU	CA-C-N	-5.10	112.83	122.27
2	G	368	GLU	C-N-CA	-5.10	112.83	122.27
2	E	330	ILE	N-CA-C	5.10	118.66	112.80
1	B	350	GLY	N-CA-C	-5.09	101.11	113.18
2	E	367	LYS	CD-CE-NZ	-5.09	95.62	111.90
1	D	353	SER	N-CA-C	5.08	118.51	112.72
2	A	46	GLU	N-CA-C	5.06	116.88	111.36
1	D	251	GLN	CA-C-N	-5.06	114.56	119.78
1	D	251	GLN	C-N-CA	-5.06	114.56	119.78
2	C	230	HIS	N-CA-C	-5.05	103.01	110.48
1	H	345	SER	N-CA-C	5.05	117.34	109.52
1	F	351	MET	CA-C-N	5.04	127.03	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	351	MET	C-N-CA	5.04	127.03	120.28
1	B	256	GLY	N-CA-C	5.02	117.90	110.42
2	E	224	VAL	O-C-N	5.01	125.11	121.55
2	A	104	THR	CA-C-N	5.00	130.46	121.06
2	A	104	THR	C-N-CA	5.00	130.46	121.06

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1178	0	1194	44	0
1	D	1178	0	1194	38	0
1	F	1145	0	1168	67	0
1	H	1178	0	1194	75	0
2	A	2993	0	3069	125	0
2	C	2993	0	3067	150	0
2	E	2993	0	3069	157	0
2	G	2993	0	3068	199	0
3	A	8	0	6	1	0
3	B	8	0	6	0	0
3	C	8	0	6	1	0
3	D	8	0	6	3	0
3	F	16	0	12	4	0
3	G	8	0	6	11	0
3	H	8	0	6	2	0
4	A	10	0	12	4	0
4	C	10	0	12	39	0
4	E	10	0	12	4	0
4	G	10	0	12	7	0
5	E	12	0	16	0	0
5	G	6	0	8	1	0
6	A	42	0	0	5	0
6	B	13	0	0	4	0
6	C	36	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	13	0	0	3	0
6	E	21	0	0	3	0
6	F	7	0	0	3	0
6	G	34	0	0	5	0
6	H	10	0	0	1	0
All	All	16949	0	17143	775	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 23.

All (775) 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)
2:G:277:VAL:CG1	3:G:503:THR:HG23	1.10	1.58
2:C:358:ALA:N	4:C:502:LYS:HG3	1.18	1.45
2:C:358:ALA:H	4:C:502:LYS:CG	1.27	1.44
2:G:277:VAL:CG1	3:G:503:THR:CG2	1.97	1.41
2:C:87:LYS:NZ	2:A:57:ILE:O	1.59	1.33
2:G:188:GLN:CG	2:G:406:ALA:O	1.80	1.29
2:G:277:VAL:HG13	3:G:503:THR:CG2	1.60	1.28
2:A:2:ALA:HB1	2:A:167:ASP:OD2	1.24	1.28
1:H:253:ILE:CD1	1:H:405:ASP:OD2	1.82	1.26
6:B:605:HOH:O	1:F:261:ARG:HD3	1.37	1.24
2:G:277:VAL:HG12	3:G:503:THR:CG2	1.64	1.23
2:C:357:VAL:N	4:C:502:LYS:HG2	1.55	1.20
1:F:253:ILE:CD1	1:F:403:GLU:HG2	1.69	1.19
2:C:356:GLY:C	4:C:502:LYS:HG2	1.69	1.17
2:C:46:GLU:OE1	2:C:49:ARG:NH1	1.77	1.16
2:C:357:VAL:H	4:C:502:LYS:CB	1.58	1.16
1:B:261:ARG:H	1:F:261:ARG:NH2	1.42	1.15
1:F:253:ILE:HD13	1:F:403:GLU:HG2	1.25	1.15
2:E:197:PHE:CD2	2:E:242:ILE:HG12	1.83	1.14
2:G:351:MET:CE	4:G:502:LYS:HE3	1.80	1.11
2:G:57:ILE:HD11	2:E:16:VAL:HG13	1.19	1.09
2:G:188:GLN:HG3	2:G:406:ALA:O	0.93	1.09
2:C:357:VAL:N	4:C:502:LYS:CG	2.16	1.08
2:A:351:MET:CE	4:A:501:LYS:HE3	1.83	1.08
2:E:15:THR:HG22	2:E:18:ARG:HB2	1.34	1.08
2:G:278:ALA:N	3:G:503:THR:HG22	1.68	1.07
1:H:253:ILE:HD11	1:H:405:ASP:CG	1.80	1.06
2:E:229:LEU:CD2	2:E:237:GLY:HA3	1.86	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:399:HIS:HD2	2:C:405:ASP:OD1	1.36	1.06
2:C:358:ALA:N	4:C:502:LYS:CG	1.95	1.05
2:C:357:VAL:N	4:C:502:LYS:CB	2.20	1.04
1:B:351:MET:HG2	1:B:379:GLU:HG3	1.36	1.04
1:H:253:ILE:HD11	1:H:405:ASP:OD2	0.85	1.03
2:G:57:ILE:CD1	2:E:16:VAL:HG13	1.88	1.03
2:E:351:MET:CE	4:E:503:LYS:HE3	1.89	1.03
2:E:229:LEU:HD23	2:E:237:GLY:HA3	1.37	1.02
2:E:197:PHE:HD2	2:E:242:ILE:HG12	1.21	1.01
2:G:214:ARG:H	2:G:214:ARG:HD3	1.27	1.00
2:G:277:VAL:HG13	3:G:503:THR:HG23	1.19	1.00
2:E:15:THR:HG23	2:E:18:ARG:H	1.27	0.99
2:E:261:ARG:HG2	6:E:608:HOH:O	1.61	0.99
2:G:351:MET:HE1	4:G:502:LYS:HE3	1.43	0.98
1:F:253:ILE:HD12	1:F:254:ILE:H	1.29	0.98
1:H:377:THR:HG21	2:G:294:MET:HA	1.45	0.98
2:E:178:VAL:HG13	2:E:206:LEU:CD1	1.94	0.97
2:A:136:PHE:CZ	2:A:147:THR:OG1	2.16	0.97
2:G:57:ILE:O	2:E:87:LYS:NZ	1.97	0.96
2:G:212:GLN:HB3	2:G:214:ARG:CZ	1.96	0.96
1:H:351:MET:HE2	1:H:379:GLU:HG3	1.48	0.95
2:C:357:VAL:H	4:C:502:LYS:HB2	1.29	0.95
2:G:278:ALA:H	3:G:503:THR:HG22	1.26	0.95
2:G:211:LEU:HD21	2:G:216:VAL:CG2	1.96	0.95
2:C:2:ALA:HB1	2:C:167:ASP:OD2	1.68	0.94
2:C:359:SER:H	4:C:502:LYS:HE3	1.31	0.93
1:B:261:ARG:H	1:F:261:ARG:HH22	0.96	0.93
2:G:321:GLU:OE2	2:G:324:LYS:HE2	1.69	0.92
2:G:227:ARG:CD	2:G:229:LEU:HD21	1.99	0.92
2:C:356:GLY:HA2	4:C:502:LYS:HE2	1.49	0.92
2:G:277:VAL:HG13	3:G:503:THR:HG21	1.51	0.91
2:E:178:VAL:HG13	2:E:206:LEU:HD12	1.49	0.90
2:G:284:PRO:HB2	2:G:322:ILE:HD11	1.52	0.89
2:G:64:ARG:HG2	6:G:617:HOH:O	1.74	0.87
1:F:253:ILE:HD12	1:F:403:GLU:HG2	1.55	0.87
2:C:67:ASP:OD2	2:C:108:HIS:O	1.93	0.87
1:F:377:THR:HG21	2:E:294:MET:HA	1.57	0.86
2:C:19:ILE:O	2:C:22:VAL:HG23	1.75	0.86
2:C:359:SER:N	4:C:502:LYS:HE3	1.91	0.86
1:H:252:PRO:O	1:H:403:GLU:CD	2.18	0.86
2:G:58:MET:HG2	2:E:87:LYS:HZ3	1.38	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:GLU:N	1:D:360:ARG:HH21	1.72	0.85
1:F:253:ILE:HD12	1:F:254:ILE:N	1.91	0.85
2:A:294:MET:H	2:A:310:THR:HG22	1.41	0.85
1:B:377:THR:HG21	2:A:294:MET:HA	1.59	0.85
2:A:190:ARG:NH2	2:A:404:LEU:O	2.10	0.85
2:E:208:SER:O	2:E:211:LEU:O	1.95	0.84
2:E:351:MET:HE2	4:E:503:LYS:HE3	1.58	0.83
2:G:41:SER:HA	2:G:74:GLU:HG3	1.59	0.83
2:G:200:MET:HE2	2:G:240:ILE:CD1	2.08	0.83
1:B:261:ARG:N	1:F:261:ARG:NH2	2.27	0.82
2:G:212:GLN:HE21	2:G:214:ARG:HH12	1.27	0.82
2:E:49:ARG:HD2	2:E:49:ARG:C	2.02	0.82
2:G:351:MET:HE3	4:G:502:LYS:HE3	1.60	0.82
2:C:28:LYS:O	2:C:31:GLU:HG2	1.80	0.82
1:D:260:ASN:ND2	1:H:261:ARG:NH2	2.27	0.82
2:C:359:SER:H	4:C:502:LYS:CE	1.92	0.82
2:E:197:PHE:CE2	2:E:242:ILE:HG12	2.15	0.82
2:C:357:VAL:HB	4:C:502:LYS:HB3	1.61	0.81
2:G:211:LEU:HD21	2:G:216:VAL:HG23	1.61	0.81
2:A:351:MET:HE2	4:A:501:LYS:HE3	1.60	0.81
2:C:274:THR:CG2	2:C:275:PRO:HD2	2.11	0.81
1:H:284:PRO:HB2	1:H:322:ILE:HD11	1.63	0.80
2:G:321:GLU:OE2	2:G:324:LYS:CE	2.29	0.80
2:G:178:VAL:HG21	2:G:200:MET:HE1	1.61	0.80
1:F:253:ILE:HD13	1:F:403:GLU:CG	2.11	0.80
2:C:399:HIS:CD2	2:C:405:ASP:OD1	2.29	0.80
1:H:267:THR:HG23	1:H:308:THR:HG22	1.62	0.80
1:B:261:ARG:N	1:F:261:ARG:HH22	1.78	0.80
2:G:196:THR:HA	2:G:241:THR:O	1.81	0.80
2:G:214:ARG:HD3	2:G:214:ARG:N	1.97	0.79
1:B:294:MET:HE2	1:B:343:LYS:CD	2.12	0.79
2:G:351:MET:HE3	4:G:502:LYS:HB2	1.63	0.78
2:C:358:ALA:CA	4:C:502:LYS:HG3	2.13	0.78
6:B:605:HOH:O	1:F:261:ARG:CD	2.08	0.78
2:A:57:ILE:HG22	2:A:58:MET:HG3	1.65	0.78
1:D:403:GLU:OE1	1:D:403:GLU:HA	1.83	0.77
2:G:173:THR:OG1	2:G:210:VAL:HG21	1.84	0.77
2:C:19:ILE:HA	2:C:22:VAL:CG2	2.14	0.77
2:E:229:LEU:CD2	2:E:237:GLY:CA	2.62	0.77
1:D:351:MET:HG2	1:D:379:GLU:HG3	1.65	0.77
2:G:277:VAL:HG12	3:G:503:THR:HG23	0.78	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:209:LYS:O	2:A:212:GLN:OE1	2.03	0.77
2:G:68:VAL:CG2	2:E:79:ALA:HB2	2.14	0.77
2:C:293:ASP:HB3	2:C:310:THR:HG22	1.67	0.76
2:G:187:PRO:HG2	6:G:618:HOH:O	1.85	0.76
2:G:57:ILE:CD1	2:E:16:VAL:CG1	2.63	0.76
2:E:231:SER:HB2	2:E:232:PHE:CE1	2.21	0.76
2:E:15:THR:CG2	2:E:18:ARG:H	1.99	0.76
2:G:104:THR:HG21	2:G:146:THR:OG1	1.85	0.76
2:C:274:THR:O	3:C:501:THR:HA	1.86	0.75
2:A:151:GLY:HA3	2:A:212:GLN:HG3	1.68	0.75
1:F:254:ILE:O	1:F:254:ILE:HD12	1.86	0.75
2:C:87:LYS:NZ	2:A:58:MET:HG2	2.01	0.75
2:C:68:VAL:HG22	2:A:79:ALA:HB2	1.68	0.74
2:E:104:THR:HG21	2:E:146:THR:OG1	1.87	0.74
2:G:200:MET:HE2	2:G:240:ILE:HD11	1.68	0.74
2:G:399:HIS:ND1	2:G:405:ASP:OD1	2.19	0.74
1:B:250:GLU:HA	1:B:401:ALA:O	1.88	0.74
2:G:211:LEU:C	2:G:211:LEU:HD23	2.13	0.74
2:A:274:THR:O	3:A:502:THR:HA	1.87	0.74
2:E:197:PHE:CE2	2:E:242:ILE:CG1	2.71	0.74
2:E:200:MET:HE2	2:E:240:ILE:CD1	2.16	0.74
2:C:178:VAL:HG23	2:C:206:LEU:HG	1.71	0.73
2:G:212:GLN:HE21	2:G:212:GLN:HA	1.53	0.73
2:E:212:GLN:HA	2:E:212:GLN:OE1	1.88	0.73
2:E:178:VAL:CG1	2:E:206:LEU:HD12	2.18	0.73
2:G:173:THR:OG1	2:G:210:VAL:CG2	2.37	0.73
1:D:271:VAL:CG1	1:D:277:VAL:HG11	2.19	0.73
2:G:278:ALA:N	3:G:503:THR:CG2	2.49	0.72
2:E:261:ARG:CG	6:E:608:HOH:O	2.27	0.72
2:C:196:THR:HA	2:C:241:THR:O	1.89	0.72
2:E:15:THR:CG2	2:E:18:ARG:HB2	2.17	0.72
1:F:295:ILE:H	2:E:377:THR:HG21	1.54	0.72
2:C:274:THR:HG23	2:C:275:PRO:HD2	1.71	0.72
1:B:379:GLU:HB2	2:A:202:GLU:OE2	1.88	0.72
1:D:262:ASP:OD1	1:D:313:ARG:HB2	1.90	0.72
2:G:87:LYS:HE3	2:E:57:ILE:CD1	2.20	0.72
2:G:212:GLN:HE21	2:G:214:ARG:NH1	1.87	0.71
1:F:324:LYS:HE2	1:F:335:ALA:O	1.89	0.71
2:G:83:MET:HE1	2:E:54:ALA:HB1	1.71	0.71
2:E:173:THR:OG1	2:E:210:VAL:HG21	1.91	0.71
2:E:49:ARG:HD2	2:E:49:ARG:O	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:349:VAL:HG13	1:D:357:VAL:HG21	1.71	0.71
3:D:501:THR:O	6:D:601:HOH:O	2.08	0.70
2:G:284:PRO:CB	2:G:322:ILE:HD11	2.19	0.70
2:A:136:PHE:CE1	2:A:147:THR:OG1	2.40	0.70
2:E:15:THR:HG22	2:E:18:ARG:CB	2.18	0.70
2:G:79:ALA:HB2	2:E:68:VAL:CG2	2.21	0.70
2:A:252:PRO:HA	6:A:620:HOH:O	1.90	0.69
2:C:194:LYS:HZ1	2:C:241:THR:HG23	1.57	0.69
2:G:294:MET:H	2:G:310:THR:HG22	1.57	0.69
1:B:294:MET:HE2	1:B:343:LYS:HD2	1.73	0.69
2:G:87:LYS:NZ	2:E:58:MET:HA	2.07	0.69
2:E:173:THR:OG1	2:E:174:ASP:N	2.23	0.69
1:B:269:ARG:HH22	1:B:333:ARG:HH21	1.40	0.69
2:G:242:ILE:HD12	2:G:242:ILE:H	1.57	0.69
1:B:294:MET:HE2	1:B:343:LYS:HD3	1.74	0.68
2:E:15:THR:CG2	2:E:18:ARG:HD3	2.22	0.68
2:C:16:VAL:HG13	2:A:57:ILE:HD11	1.75	0.68
2:C:357:VAL:H	4:C:502:LYS:HB3	1.52	0.68
2:A:19:ILE:O	2:A:22:VAL:HG22	1.93	0.68
1:D:392:GLU:CD	1:D:392:GLU:H	2.01	0.68
1:F:350:GLY:HA3	1:F:352:ARG:NH1	2.08	0.68
1:H:295:ILE:H	2:G:377:THR:HG21	1.57	0.68
2:G:197:PHE:CE2	2:G:242:ILE:HG13	2.29	0.68
2:A:25:LYS:NZ	2:A:233:GLN:HB2	2.09	0.68
2:A:59:GLU:HG2	2:A:60:GLN:N	2.08	0.68
2:E:196:THR:HA	2:E:241:THR:O	1.92	0.68
2:E:342:ALA:HB1	2:E:391:LEU:HD12	1.76	0.68
1:B:392:GLU:CD	1:B:392:GLU:H	2.00	0.68
1:F:294:MET:HA	2:E:377:THR:HG21	1.76	0.68
1:H:291:GLU:OE2	2:G:353:SER:O	2.12	0.68
2:G:87:LYS:HE3	2:E:57:ILE:HD11	1.76	0.68
2:G:197:PHE:HE2	2:G:242:ILE:HG13	1.58	0.68
2:G:293:ASP:HB3	2:G:310:THR:HG22	1.75	0.67
1:H:274:THR:O	3:H:501:THR:HA	1.94	0.67
2:E:293:ASP:HB3	2:E:310:THR:HG22	1.76	0.67
2:C:358:ALA:N	4:C:502:LYS:HG2	2.02	0.67
2:G:227:ARG:HD3	2:G:229:LEU:HD21	1.76	0.67
2:G:200:MET:HE2	2:G:240:ILE:HD13	1.76	0.67
2:A:207:GLY:HA3	2:A:213:ILE:HD11	1.76	0.67
2:E:293:ASP:HB3	2:E:310:THR:CG2	2.25	0.67
2:G:96:THR:HG23	2:G:99:GLN:H	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:151:GLY:HA3	2:G:212:GLN:HG3	1.76	0.66
2:G:293:ASP:HB3	2:G:310:THR:CG2	2.24	0.66
2:G:209:LYS:HG3	2:G:210:VAL:N	2.07	0.66
2:E:399:HIS:ND1	2:E:405:ASP:OD1	2.24	0.66
1:D:254:ILE:HD13	1:D:346:ILE:HG23	1.75	0.66
2:G:212:GLN:NE2	2:G:214:ARG:HH22	1.93	0.66
2:E:95:TYR:OH	2:E:124:ASP:OD2	2.07	0.66
2:E:263:GLU:OE1	2:E:310:THR:HG21	1.94	0.66
1:B:295:ILE:H	2:A:377:THR:HG21	1.61	0.66
2:C:274:THR:CG2	2:C:275:PRO:CD	2.72	0.66
2:E:25:LYS:NZ	2:E:233:GLN:HB3	2.09	0.66
2:E:277:VAL:O	2:E:281:ILE:HG13	1.95	0.66
2:G:212:GLN:NE2	2:G:214:ARG:HH12	1.94	0.66
1:H:399:HIS:HD2	1:H:404:LEU:HD13	1.61	0.66
2:A:59:GLU:CD	2:A:59:GLU:H	2.03	0.66
1:B:378:SER:OG	2:A:202:GLU:OE1	2.14	0.65
1:D:379:GLU:HB2	2:C:202:GLU:OE2	1.96	0.65
2:C:274:THR:HG22	2:C:275:PRO:HD2	1.77	0.65
2:E:229:LEU:HD21	2:E:237:GLY:HA3	1.78	0.65
1:F:298:ASN:OD1	1:F:299:VAL:N	2.26	0.65
2:G:227:ARG:CG	2:G:229:LEU:HD21	2.26	0.65
2:A:351:MET:HE3	4:A:501:LYS:HE3	1.74	0.65
1:H:351:MET:HE2	1:H:379:GLU:CG	2.23	0.65
1:F:348:GLY:HA2	6:F:603:HOH:O	1.95	0.65
2:G:57:ILE:HD11	2:E:16:VAL:CG1	2.11	0.65
1:F:292:VAL:O	4:E:503:LYS:HG2	1.97	0.65
2:C:46:GLU:CD	2:C:49:ARG:HH11	2.05	0.65
2:E:200:MET:HE2	2:E:240:ILE:HD11	1.77	0.65
1:D:377:THR:HG21	2:C:294:MET:HA	1.79	0.65
2:G:214:ARG:H	2:G:214:ARG:CD	2.08	0.65
2:A:68:VAL:HG22	2:A:145:ILE:HD12	1.78	0.65
2:A:293:ASP:HB3	2:A:310:THR:CG2	2.28	0.64
2:A:25:LYS:HE3	2:A:29:PHE:HE1	1.62	0.64
2:E:136:PHE:CZ	2:E:147:THR:HB	2.33	0.64
2:C:194:LYS:NZ	2:C:241:THR:HG23	2.12	0.64
2:C:207:GLY:HA3	2:C:213:ILE:HD11	1.80	0.64
1:H:251:GLN:C	1:H:403:GLU:OE2	2.41	0.64
2:C:79:ALA:CB	2:A:69:MET:HG3	2.28	0.64
2:C:173:THR:OG1	2:C:174:ASP:N	2.29	0.64
2:E:5:VAL:HG22	2:E:37:VAL:HB	1.80	0.64
2:E:105:ASP:HB2	2:E:112:ARG:H	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:242:ILE:O	2:E:243:ASP:HB2	1.97	0.64
2:A:210:VAL:HG13	2:A:211:LEU:N	2.11	0.64
2:E:15:THR:HG22	2:E:18:ARG:HD3	1.79	0.63
2:C:87:LYS:HZ3	2:A:57:ILE:C	1.86	0.63
2:A:241:THR:OG1	2:A:242:ILE:N	2.29	0.63
2:C:2:ALA:CB	2:C:167:ASP:OD2	2.44	0.63
2:C:71:SER:O	2:C:137:GLN:NE2	2.31	0.63
1:H:253:ILE:HG23	1:H:253:ILE:O	1.99	0.63
1:H:404:LEU:HD12	1:H:404:LEU:N	2.13	0.62
2:E:197:PHE:CD2	2:E:242:ILE:CG1	2.73	0.62
1:B:259:PHE:CD2	1:B:391:LEU:HD21	2.35	0.62
2:G:20:GLU:CD	2:E:57:ILE:HD13	2.24	0.62
1:B:294:MET:HA	2:A:377:THR:HG21	1.81	0.62
2:G:212:GLN:CD	2:G:214:ARG:HH22	2.08	0.62
1:H:252:PRO:HG3	1:H:360:ARG:HD3	1.82	0.62
2:G:212:GLN:HA	2:G:212:GLN:NE2	2.13	0.62
2:G:320:LEU:O	2:G:324:LYS:HG3	2.00	0.61
2:A:110:LYS:HD2	6:A:630:HOH:O	2.00	0.61
2:E:351:MET:HE1	2:E:382:VAL:HG23	1.82	0.61
1:B:259:PHE:HD2	1:B:391:LEU:HD21	1.64	0.61
2:E:200:MET:HE2	2:E:240:ILE:HD13	1.81	0.61
2:E:288:ALA:O	2:E:289:ASN:HB2	2.00	0.61
2:C:357:VAL:C	4:C:502:LYS:CG	2.73	0.61
2:A:67:ASP:OD1	2:A:147:THR:HG22	1.99	0.61
2:A:213:ILE:O	2:A:217:GLU:HG3	2.01	0.61
2:E:229:LEU:HD23	2:E:237:GLY:CA	2.22	0.61
2:G:59:GLU:CD	2:G:59:GLU:H	2.07	0.61
2:G:188:GLN:HG3	2:G:406:ALA:C	2.05	0.61
2:G:87:LYS:NZ	2:E:58:MET:CG	2.64	0.61
2:E:263:GLU:OE1	2:E:310:THR:CG2	2.49	0.61
2:C:173:THR:OG1	2:C:210:VAL:HG21	2.00	0.61
1:H:378:SER:OG	2:G:202:GLU:OE1	2.19	0.61
2:E:197:PHE:HE2	2:E:242:ILE:CG1	2.14	0.61
2:A:67:ASP:OD2	2:A:108:HIS:O	2.19	0.60
2:C:356:GLY:C	4:C:502:LYS:CG	2.59	0.60
1:H:252:PRO:HB3	1:H:360:ARG:NH1	2.16	0.60
2:A:227:ARG:HG2	2:A:229:LEU:CD1	2.32	0.60
2:C:79:ALA:HB3	2:A:69:MET:CG	2.30	0.60
1:H:252:PRO:O	1:H:403:GLU:OE2	2.20	0.60
2:A:313:ARG:HH12	2:A:388:GLU:CD	2.09	0.60
1:D:378:SER:OG	2:C:202:GLU:OE1	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:46:GLU:OE1	2:A:49:ARG:NH1	2.34	0.60
2:A:242:ILE:O	2:A:243:ASP:HB2	2.01	0.60
1:F:348:GLY:CA	6:F:603:HOH:O	2.48	0.60
2:G:284:PRO:C	2:G:322:ILE:HD11	2.27	0.60
2:E:197:PHE:HE2	2:E:242:ILE:HG13	1.67	0.60
2:C:357:VAL:CB	4:C:502:LYS:HB3	2.32	0.60
1:D:280:LYS:NZ	6:D:602:HOH:O	2.33	0.60
2:G:227:ARG:HG2	2:G:229:LEU:CD2	2.31	0.60
2:A:178:VAL:CG1	2:A:238:THR:HG21	2.32	0.60
1:H:252:PRO:HG3	1:H:360:ARG:CD	2.31	0.59
2:G:104:THR:OG1	2:G:111:ALA:HB1	2.02	0.59
1:H:250:GLU:CB	1:H:403:GLU:HB3	2.31	0.59
2:C:19:ILE:C	2:C:22:VAL:HG23	2.26	0.59
2:C:174:ASP:O	2:C:230:HIS:ND1	2.34	0.59
2:C:274:THR:HG22	2:C:275:PRO:CD	2.33	0.59
2:A:197:PHE:CD2	2:A:242:ILE:HG23	2.38	0.59
2:E:178:VAL:HG21	2:E:200:MET:HE1	1.85	0.59
2:G:285:ILE:HD13	2:G:322:ILE:HD13	1.84	0.59
1:H:403:GLU:O	1:H:403:GLU:HG2	2.01	0.59
2:E:207:GLY:HA3	2:E:213:ILE:HD11	1.84	0.59
2:E:294:MET:HE1	2:E:385:VAL:CG2	2.33	0.59
1:D:250:GLU:N	1:D:360:ARG:NH2	2.49	0.58
2:E:104:THR:OG1	2:E:111:ALA:HB1	2.03	0.58
1:F:261:ARG:H	1:F:261:ARG:NE	2.01	0.58
2:A:190:ARG:NH2	2:A:406:ALA:HB3	2.17	0.58
1:B:261:ARG:HD3	1:F:262:ASP:OD2	2.03	0.58
2:G:227:ARG:HG2	2:G:229:LEU:HD21	1.84	0.58
2:C:19:ILE:HA	2:C:22:VAL:HG23	1.85	0.58
2:A:59:GLU:HG2	2:A:60:GLN:H	1.68	0.58
2:G:68:VAL:HG23	2:E:79:ALA:HB2	1.86	0.58
2:C:105:ASP:HB2	2:C:112:ARG:H	1.68	0.58
2:G:351:MET:HE1	4:G:502:LYS:CE	2.26	0.58
1:D:265:LYS:HE3	2:C:299:VAL:HG11	1.85	0.57
1:D:405:ASP:OD2	2:C:221:LYS:HE2	2.04	0.57
2:C:79:ALA:HB3	2:A:69:MET:HG3	1.86	0.57
2:E:294:MET:H	2:E:310:THR:HG22	1.69	0.57
2:G:87:LYS:NZ	2:E:58:MET:HG2	2.19	0.57
2:A:173:THR:HG21	2:A:210:VAL:HG21	1.85	0.57
2:E:174:ASP:C	2:E:230:HIS:CD2	2.82	0.57
2:G:191:ARG:NH2	2:G:193:ASP:OD1	2.37	0.57
2:C:178:VAL:CG1	2:C:238:THR:HG21	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:253:ILE:CD1	1:H:405:ASP:CG	2.57	0.57
2:C:113:ILE:HD11	2:C:148:LEU:CD1	2.35	0.56
1:H:392:GLU:H	1:H:392:GLU:CD	2.12	0.56
1:F:305:THR:HG23	1:F:306:ASP:O	2.04	0.56
2:G:206:LEU:O	2:G:207:GLY:C	2.45	0.56
2:G:242:ILE:O	2:G:243:ASP:HB2	2.04	0.56
2:A:15:THR:O	2:A:19:ILE:HG13	2.05	0.56
1:H:389:LYS:HG3	1:H:390:TYR:CD1	2.40	0.56
1:H:389:LYS:HG3	1:H:390:TYR:CE1	2.40	0.56
2:G:351:MET:CE	4:G:502:LYS:CE	2.70	0.56
6:B:605:HOH:O	1:F:261:ARG:HG2	2.06	0.56
2:G:174:ASP:O	2:G:230:HIS:ND1	2.38	0.56
2:G:58:MET:CG	2:E:87:LYS:HZ3	2.15	0.56
1:F:347:VAL:HG12	1:F:348:GLY:N	2.21	0.56
1:F:352:ARG:HG3	1:F:353:SER:OG	2.06	0.56
2:G:200:MET:CE	2:G:240:ILE:HD11	2.36	0.56
2:E:15:THR:HG22	2:E:18:ARG:CD	2.35	0.56
2:A:37:VAL:HG22	2:A:131:VAL:HG22	1.88	0.56
1:H:318:ASN:O	1:H:322:ILE:HG22	2.06	0.56
2:G:178:VAL:CG2	2:G:200:MET:HE1	2.34	0.56
2:G:321:GLU:OE2	2:G:321:GLU:HA	2.06	0.56
1:B:262:ASP:O	1:B:263:GLU:HG2	2.06	0.55
1:H:252:PRO:O	1:H:403:GLU:CG	2.53	0.55
1:H:252:PRO:HD3	1:H:360:ARG:NE	2.21	0.55
3:F:501:THR:HA	2:E:274:THR:O	2.07	0.55
2:C:358:ALA:HB3	4:C:502:LYS:HD2	1.87	0.55
1:D:251:GLN:H	1:D:252:PRO:CD	2.19	0.55
2:G:58:MET:HA	2:E:87:LYS:NZ	2.20	0.55
2:A:16:VAL:O	2:A:20:GLU:HG3	2.07	0.55
2:E:290:VAL:HG13	2:E:315:ASP:HB3	1.89	0.55
2:C:293:ASP:HB3	2:C:310:THR:CG2	2.37	0.55
2:E:378:SER:HB3	2:E:381:LYS:HB3	1.88	0.55
2:G:405:ASP:O	2:G:406:ALA:HB2	2.05	0.55
2:A:293:ASP:HB3	2:A:310:THR:HG22	1.88	0.55
2:E:231:SER:C	2:E:232:PHE:CG	2.85	0.55
2:C:313:ARG:HH22	2:C:388:GLU:CD	2.15	0.55
2:A:191:ARG:NH2	2:A:193:ASP:OD1	2.40	0.55
2:C:67:ASP:CG	2:C:108:HIS:O	2.50	0.55
1:H:372:ILE:O	3:G:503:THR:N	2.39	0.55
2:G:276:GLY:O	2:G:280:LYS:HG3	2.06	0.55
1:B:269:ARG:HH22	1:B:333:ARG:NH2	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:366:ALA:O	1:H:368:GLU:O	2.24	0.54
2:G:104:THR:HG23	2:G:105:ASP:O	2.07	0.54
1:B:265:LYS:HE3	2:A:299:VAL:HG11	1.89	0.54
2:G:57:ILE:HD13	2:E:16:VAL:CG1	2.37	0.54
2:A:180:THR:HG21	2:A:404:LEU:HB3	1.88	0.54
1:D:271:VAL:HG11	1:D:277:VAL:HG11	1.90	0.54
1:B:349:VAL:HG13	1:B:357:VAL:HG21	1.89	0.54
2:C:87:LYS:NZ	2:A:57:ILE:C	2.56	0.54
2:G:374:MET:HB2	2:G:385:VAL:HB	1.89	0.54
1:D:352:ARG:H	1:D:352:ARG:CD	2.18	0.54
2:E:274:THR:O	2:E:277:VAL:HG13	2.07	0.54
2:C:59:GLU:CD	2:C:59:GLU:H	2.16	0.54
1:H:399:HIS:CD2	1:H:404:LEU:HD13	2.41	0.54
2:C:356:GLY:N	4:C:502:LYS:HB2	2.22	0.54
2:A:2:ALA:CB	2:A:167:ASP:OD2	2.21	0.54
2:C:113:ILE:HD11	2:C:148:LEU:HD11	1.90	0.53
2:C:357:VAL:N	4:C:502:LYS:HB3	2.11	0.53
1:H:265:LYS:HB2	1:H:341:ILE:HD13	1.90	0.53
2:G:20:GLU:OE1	2:G:88:ARG:NH1	2.25	0.53
2:C:358:ALA:H	4:C:502:LYS:HG3	0.41	0.53
2:G:105:ASP:HB2	2:G:112:ARG:H	1.73	0.53
1:D:286:SER:HB2	4:C:502:LYS:NZ	2.22	0.53
1:D:352:ARG:H	1:D:352:ARG:HD3	1.73	0.53
2:C:233:GLN:O	2:C:233:GLN:NE2	2.40	0.53
2:C:19:ILE:HD11	2:C:43:MET:HE3	1.91	0.53
2:C:242:ILE:O	2:C:242:ILE:HG23	2.08	0.53
1:H:368:GLU:OE2	1:H:368:GLU:HA	2.08	0.53
2:A:210:VAL:CG1	2:A:211:LEU:N	2.72	0.53
2:E:45:GLY:O	2:E:49:ARG:HB2	2.08	0.53
2:C:274:THR:HG23	2:C:275:PRO:CD	2.36	0.53
1:H:308:THR:HG23	2:G:298:ASN:HD21	1.74	0.53
2:C:357:VAL:CA	4:C:502:LYS:HG2	2.38	0.53
2:A:271:VAL:HG13	2:A:277:VAL:HG11	1.89	0.53
1:D:286:SER:HB2	4:C:502:LYS:HZ3	1.74	0.53
2:C:18:ARG:O	2:C:22:VAL:HG22	2.09	0.53
1:F:372:ILE:N	3:F:501:THR:O	2.29	0.52
2:A:173:THR:OG1	2:A:210:VAL:HG23	2.09	0.52
1:F:265:LYS:HB2	1:F:341:ILE:HD13	1.92	0.52
1:F:350:GLY:CA	1:F:352:ARG:NH1	2.73	0.52
1:F:374:MET:HB2	1:F:385:VAL:HB	1.92	0.52
2:C:16:VAL:HG23	6:C:608:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:212:GLN:HB3	2:G:214:ARG:NH1	2.24	0.52
2:E:104:THR:HG23	2:E:105:ASP:O	2.08	0.52
2:A:100:VAL:HG13	2:A:102:ILE:HG13	1.90	0.52
2:E:396:ARG:O	2:E:400:THR:HG23	2.10	0.52
2:C:351:MET:O	4:C:502:LYS:OXT	2.28	0.52
2:C:357:VAL:CA	4:C:502:LYS:CG	2.87	0.52
2:E:15:THR:HG21	2:E:18:ARG:HD3	1.91	0.52
2:E:174:ASP:O	2:E:230:HIS:CD2	2.63	0.52
1:B:389:LYS:HE3	1:B:390:TYR:CZ	2.43	0.52
3:H:501:THR:N	2:G:371:ASN:OD1	2.43	0.52
1:D:349:VAL:CG1	1:D:357:VAL:HG21	2.40	0.52
2:A:173:THR:OG1	2:A:210:VAL:CG2	2.57	0.52
2:A:357:VAL:N	4:A:501:LYS:OXT	2.43	0.52
1:D:253:ILE:HG23	1:D:253:ILE:O	2.10	0.52
1:H:294:MET:HA	2:G:377:THR:HG21	1.92	0.52
2:C:313:ARG:HH12	2:C:388:GLU:CD	2.18	0.52
1:H:252:PRO:O	1:H:403:GLU:HG2	2.10	0.52
2:G:78:ILE:HD12	2:G:94:SER:HB2	1.92	0.52
2:G:227:ARG:HD2	2:G:229:LEU:HD21	1.88	0.52
1:H:368:GLU:HB3	1:H:393:LEU:HD11	1.91	0.51
2:G:227:ARG:CG	2:G:229:LEU:CD2	2.88	0.51
6:B:605:HOH:O	1:F:261:ARG:CG	2.50	0.51
1:F:254:ILE:HD12	1:F:254:ILE:C	2.35	0.51
2:C:203:MET:HG3	2:C:347:VAL:HG21	1.91	0.51
2:C:209:LYS:O	2:C:212:GLN:NE2	2.42	0.51
2:C:358:ALA:CB	4:C:502:LYS:HG3	2.41	0.51
2:G:151:GLY:HA3	2:G:212:GLN:CG	2.41	0.51
2:E:105:ASP:HB3	2:E:107:ALA:H	1.74	0.51
2:A:194:LYS:HG2	2:A:239:LEU:HB3	1.91	0.51
1:F:354:HIS:CE1	1:F:378:SER:O	2.63	0.51
3:F:501:THR:HB	2:E:277:VAL:HG22	1.91	0.51
2:G:79:ALA:HB2	2:E:68:VAL:HG23	1.92	0.51
2:A:259:PHE:CD1	2:A:259:PHE:C	2.89	0.51
2:C:67:ASP:O	2:C:71:SER:HB3	2.10	0.51
2:G:41:SER:HB3	2:G:153:SER:OG	2.11	0.51
2:E:232:PHE:O	2:E:233:GLN:HG3	2.10	0.51
1:D:294:MET:HE2	1:D:343:LYS:HD2	1.93	0.51
1:H:284:PRO:C	1:H:322:ILE:HD11	2.35	0.51
2:A:107:ALA:HB1	2:A:110:LYS:HE2	1.92	0.51
1:F:368:GLU:HA	1:F:368:GLU:OE2	2.12	0.50
2:G:79:ALA:O	2:G:83:MET:HG3	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:227:ARG:NH2	2:G:239:LEU:HD13	2.25	0.50
2:C:357:VAL:N	4:C:502:LYS:HB2	2.04	0.50
2:E:351:MET:CE	2:E:382:VAL:HG23	2.41	0.50
1:B:381:LYS:HE3	1:B:383:SER:OG	2.11	0.50
1:F:305:THR:CG2	1:F:306:ASP:N	2.74	0.50
1:H:291:GLU:HG3	2:G:355:ALA:HB2	1.94	0.50
2:G:24:GLU:O	2:G:28:LYS:HG3	2.11	0.50
2:E:2:ALA:HB3	2:E:167:ASP:OD2	2.10	0.50
1:D:347:VAL:HG12	1:D:381:LYS:HG2	1.92	0.50
2:C:57:ILE:HG22	2:C:58:MET:HG2	1.94	0.50
2:C:274:THR:HG22	2:C:275:PRO:N	2.26	0.50
1:H:251:GLN:N	1:H:252:PRO:HD2	2.27	0.50
2:G:319:ALA:O	2:G:322:ILE:HG23	2.12	0.50
2:E:199:GLU:HG3	2:E:349:VAL:HG13	1.94	0.50
2:C:68:VAL:CG2	2:A:79:ALA:HB2	2.40	0.50
2:A:192:LEU:HD13	2:A:195:ILE:HG21	1.93	0.50
1:B:271:VAL:HG12	1:B:305:THR:HG22	1.92	0.50
1:F:348:GLY:C	6:F:603:HOH:O	2.55	0.50
2:C:19:ILE:CA	2:C:22:VAL:HG23	2.40	0.50
2:C:356:GLY:CA	4:C:502:LYS:HE2	2.33	0.50
2:A:294:MET:HE1	2:A:385:VAL:CG2	2.42	0.50
1:F:350:GLY:CA	1:F:352:ARG:CZ	2.90	0.49
2:G:319:ALA:HA	2:G:322:ILE:CG2	2.42	0.49
2:C:347:VAL:HG12	2:C:381:LYS:HG3	1.93	0.49
1:H:370:ILE:HD11	1:H:393:LEU:HD12	1.95	0.49
1:H:399:HIS:HD2	1:H:404:LEU:CD1	2.24	0.49
2:G:188:GLN:CD	2:G:406:ALA:O	2.51	0.49
2:G:378:SER:HB3	2:G:381:LYS:HB3	1.93	0.49
1:F:392:GLU:CD	1:F:392:GLU:H	2.19	0.49
2:G:46:GLU:OE1	2:G:49:ARG:NH1	2.45	0.49
1:H:271:VAL:HG22	1:H:272:PRO:HD2	1.95	0.49
2:E:252:PRO:HG3	6:E:619:HOH:O	2.12	0.49
2:A:197:PHE:CE2	2:A:242:ILE:HG23	2.48	0.49
1:B:259:PHE:HA	1:B:343:LYS:O	2.13	0.49
2:C:55:ASN:HA	2:C:58:MET:O	2.12	0.49
1:H:389:LYS:CG	1:H:390:TYR:CE1	2.96	0.49
2:G:389:LYS:HB3	6:G:604:HOH:O	2.13	0.49
2:G:271:VAL:O	2:G:304:THR:HA	2.13	0.49
2:G:396:ARG:O	2:G:400:THR:HG23	2.12	0.49
1:F:361:MET:HG3	1:F:398:LEU:HD21	1.94	0.49
1:F:347:VAL:CG1	1:F:348:GLY:N	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:58:MET:HE3	2:A:87:LYS:CG	2.43	0.48
1:B:378:SER:HB2	2:A:378:SER:HB2	1.94	0.48
2:G:190:ARG:HD2	2:G:406:ALA:HB3	1.95	0.48
2:A:59:GLU:CD	2:A:59:GLU:N	2.71	0.48
2:A:64:ARG:HG2	6:A:619:HOH:O	2.14	0.48
1:B:350:GLY:CA	1:B:352:ARG:HH11	2.27	0.48
1:F:350:GLY:HA2	1:F:352:ARG:NH2	2.29	0.48
2:C:200:MET:HE2	2:C:240:ILE:HD11	1.94	0.48
2:G:100:VAL:O	2:G:117:ASP:HB2	2.12	0.48
2:E:241:THR:OG1	2:E:242:ILE:N	2.46	0.48
2:E:366:ALA:O	2:E:368:GLU:O	2.31	0.48
2:A:59:GLU:CG	2:A:60:GLN:N	2.76	0.48
2:A:378:SER:HB3	2:A:381:LYS:HB3	1.95	0.48
1:B:392:GLU:CD	1:B:392:GLU:N	2.69	0.48
2:C:194:LYS:NZ	2:C:241:THR:CG2	2.76	0.48
2:G:212:GLN:NE2	2:G:214:ARG:NH2	2.60	0.48
2:E:229:LEU:HD21	2:E:236:PRO:C	2.38	0.48
2:C:172:TYR:HD2	2:C:231:SER:HA	1.79	0.48
2:C:177:GLY:HA2	2:C:228:VAL:HG23	1.94	0.48
2:G:211:LEU:C	2:G:211:LEU:CD2	2.85	0.48
2:G:54:ALA:HB1	2:E:83:MET:HE1	1.96	0.48
2:C:58:MET:HE3	2:A:87:LYS:HG2	1.96	0.48
2:G:172:TYR:CE2	2:G:229:LEU:HD12	2.48	0.48
2:C:39:VAL:HG21	2:C:157:GLY:HA2	1.96	0.48
1:H:333:ARG:O	1:H:334:GLU:HB3	2.14	0.48
2:G:227:ARG:HD3	2:G:229:LEU:CD2	2.44	0.48
2:A:135:GLY:HA2	2:A:156:THR:HG21	1.95	0.48
2:C:204:ALA:O	2:C:207:GLY:N	2.47	0.48
2:G:333:ARG:NH1	6:G:603:HOH:O	2.43	0.48
2:A:25:LYS:HZ2	2:A:233:GLN:HB2	1.76	0.48
2:A:347:VAL:HG12	2:A:381:LYS:HG3	1.95	0.48
2:E:57:ILE:HD12	2:E:57:ILE:O	2.14	0.48
2:C:357:VAL:C	4:C:502:LYS:HG2	2.37	0.47
2:G:96:THR:HG22	2:G:99:GLN:HG3	1.96	0.47
2:G:121:ILE:HG21	2:G:164:LEU:HD21	1.96	0.47
2:G:211:LEU:CD2	2:G:216:VAL:CG2	2.82	0.47
1:F:300:ALA:HB2	1:F:305:THR:OG1	2.14	0.47
2:C:377:THR:HG23	2:C:378:SER:N	2.28	0.47
2:E:229:LEU:HD21	2:E:236:PRO:O	2.13	0.47
2:C:378:SER:HB3	2:C:381:LYS:HB3	1.96	0.47
2:G:212:GLN:CG	2:G:214:ARG:NH2	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:253:ILE:HD12	2:A:253:ILE:HA	1.79	0.47
1:D:299:VAL:HG11	2:C:265:LYS:HE3	1.97	0.47
1:F:368:GLU:HB2	1:F:370:ILE:HG13	1.96	0.47
2:C:28:LYS:C	2:C:31:GLU:HG2	2.40	0.47
2:G:17:GLU:OE2	2:G:17:GLU:HA	2.14	0.47
2:G:68:VAL:HG22	2:E:79:ALA:HB2	1.96	0.47
2:A:173:THR:O	2:A:230:HIS:HA	2.13	0.47
2:A:192:LEU:HD13	2:A:195:ILE:CG2	2.44	0.47
2:G:173:THR:OG1	2:G:174:ASP:N	2.47	0.47
3:D:501:THR:N	2:C:371:ASN:OD1	2.47	0.47
1:H:259:PHE:HA	1:H:343:LYS:O	2.15	0.47
2:G:41:SER:HA	2:G:74:GLU:CG	2.37	0.47
2:A:227:ARG:HG2	2:A:229:LEU:HD11	1.96	0.47
2:G:176:ASP:O	2:G:237:GLY:HA2	2.15	0.47
2:A:177:GLY:HA2	2:A:228:VAL:HG23	1.96	0.47
1:F:297:GLN:CG	1:F:305:THR:HG21	2.45	0.47
1:H:251:GLN:N	1:H:252:PRO:CD	2.78	0.47
2:E:16:VAL:O	2:E:20:GLU:HG3	2.15	0.47
2:C:57:ILE:HG22	2:C:58:MET:CG	2.45	0.47
1:H:347:VAL:HG23	1:H:381:LYS:HG2	1.97	0.46
2:A:80:LEU:HA	2:A:83:MET:HE2	1.96	0.46
2:E:107:ALA:HB1	2:E:110:LYS:HG3	1.97	0.46
1:B:261:ARG:H	1:F:261:ARG:HH21	1.51	0.46
2:A:178:VAL:HG23	2:A:206:LEU:HG	1.97	0.46
2:E:222:TYR:CD1	2:E:222:TYR:N	2.83	0.46
1:H:250:GLU:C	1:H:252:PRO:HD2	2.40	0.46
2:G:212:GLN:CD	2:G:214:ARG:NH2	2.72	0.46
2:G:265:LYS:HB3	2:G:341:ILE:HD13	1.97	0.46
1:D:321:GLU:O	1:D:325:GLN:HG2	2.15	0.46
2:E:351:MET:HE3	4:E:503:LYS:HE3	1.88	0.46
1:H:404:LEU:N	1:H:404:LEU:CD1	2.79	0.46
2:A:20:GLU:HB3	2:A:88:ARG:HH22	1.80	0.46
2:A:353:SER:HB2	2:A:354:HIS:ND1	2.31	0.46
2:E:68:VAL:HG12	2:E:145:ILE:HB	1.98	0.46
2:E:107:ALA:O	2:E:111:ALA:N	2.48	0.46
2:C:294:MET:HE1	2:C:385:VAL:CG2	2.46	0.46
2:E:15:THR:HG23	2:E:18:ARG:N	2.11	0.46
2:E:46:GLU:O	2:E:50:LEU:HG	2.15	0.46
2:E:302:ASP:O	2:E:303:ASN:HB2	2.15	0.46
2:E:227:ARG:NH1	2:E:236:PRO:O	2.44	0.46
1:B:352:ARG:HG2	1:B:353:SER:OG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:263:GLU:OE1	2:G:310:THR:HG21	2.16	0.46
2:E:234:GLU:CD	2:E:234:GLU:C	2.84	0.46
1:F:262:ASP:C	1:F:263:GLU:HG2	2.41	0.45
2:C:79:ALA:HB3	2:A:69:MET:HG2	1.97	0.45
2:G:20:GLU:HB3	2:G:88:ARG:NH2	2.31	0.45
2:A:136:PHE:CE2	2:A:147:THR:OG1	2.64	0.45
2:E:195:ILE:O	2:E:240:ILE:HA	2.15	0.45
1:B:362:PHE:CZ	1:B:375:ILE:HD13	2.51	0.45
1:F:305:THR:HG23	1:F:306:ASP:N	2.32	0.45
2:G:212:GLN:HE21	2:G:212:GLN:CA	2.20	0.45
2:G:212:GLN:NE2	2:G:212:GLN:CA	2.73	0.45
1:F:373:GLN:HG3	1:F:385:VAL:HG12	1.98	0.45
2:G:190:ARG:NH2	2:G:404:LEU:HA	2.31	0.45
2:E:228:VAL:HG23	2:E:228:VAL:O	2.15	0.45
2:A:78:ILE:HD12	2:A:94:SER:HB2	1.97	0.45
2:A:196:THR:HA	2:A:241:THR:O	2.16	0.45
1:B:377:THR:CG2	2:A:294:MET:HA	2.36	0.45
2:C:122:ARG:HE	2:C:122:ARG:HB3	1.58	0.45
2:G:342:ALA:HB1	2:G:391:LEU:HD12	1.99	0.45
2:G:69:MET:HE2	2:G:69:MET:HB3	1.83	0.45
2:G:210:VAL:HG13	2:G:211:LEU:N	2.32	0.45
2:G:253:ILE:HD12	2:G:253:ILE:HA	1.76	0.45
2:G:271:VAL:HG13	2:G:277:VAL:HG21	1.99	0.45
2:E:25:LYS:HZ3	2:E:233:GLN:HB3	1.79	0.45
1:F:378:SER:HB3	1:F:381:LYS:HG3	1.97	0.45
2:C:377:THR:CG2	2:C:378:SER:N	2.79	0.45
2:G:67:ASP:O	2:G:71:SER:HB3	2.16	0.45
2:C:150:ARG:HD2	2:C:150:ARG:HA	1.70	0.45
2:C:317:LEU:HD23	2:C:317:LEU:C	2.42	0.45
2:G:242:ILE:HG22	2:G:243:ASP:N	2.32	0.45
2:E:226:LEU:O	2:E:240:ILE:N	2.34	0.45
2:E:231:SER:O	2:E:232:PHE:CD2	2.70	0.45
2:C:28:LYS:HA	2:C:31:GLU:CD	2.42	0.45
2:G:290:VAL:HG13	2:G:315:ASP:HB3	1.99	0.45
2:E:288:ALA:HB3	2:E:290:VAL:HG23	1.99	0.45
1:F:261:ARG:H	1:F:261:ARG:HE	1.63	0.45
1:F:262:ASP:OD1	1:F:313:ARG:HB2	2.17	0.45
2:E:265:LYS:HB3	2:E:341:ILE:HD13	1.99	0.45
2:E:280:LYS:O	2:E:284:PRO:HD2	2.17	0.45
1:F:257:ILE:HD11	1:F:398:LEU:HB3	1.99	0.44
2:C:359:SER:HB2	4:C:502:LYS:HE2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:350:GLY:HA2	1:F:352:ARG:CZ	2.48	0.44
1:H:351:MET:HE2	1:H:351:MET:HB3	1.77	0.44
2:E:212:GLN:C	2:E:214:ARG:N	2.74	0.44
2:E:268:ILE:HG21	2:E:281:ILE:HD13	1.99	0.44
1:D:274:THR:O	3:D:501:THR:HA	2.18	0.44
1:D:377:THR:CG2	2:C:294:MET:HA	2.48	0.44
2:C:174:ASP:C	2:C:230:HIS:HD1	2.25	0.44
2:G:212:GLN:HB3	2:G:214:ARG:NH2	2.30	0.44
1:F:349:VAL:HG11	1:F:354:HIS:CD2	2.53	0.44
2:C:100:VAL:HG13	2:C:102:ILE:HG13	2.00	0.44
2:A:57:ILE:HG22	2:A:58:MET:CG	2.43	0.44
2:E:209:LYS:HA	2:E:212:GLN:OE1	2.17	0.44
1:D:251:GLN:H	1:D:252:PRO:HD3	1.83	0.44
2:A:271:VAL:O	2:A:304:THR:HA	2.18	0.44
2:G:15:THR:OG1	2:G:18:ARG:CG	2.66	0.44
2:A:200:MET:HE2	2:A:240:ILE:HD11	1.98	0.44
1:F:297:GLN:HG3	1:F:305:THR:CG2	2.48	0.44
2:A:314:ASN:CG	6:A:614:HOH:O	2.60	0.44
1:D:354:HIS:HB2	2:C:292:VAL:O	2.17	0.44
1:B:282:LEU:HD12	1:B:282:LEU:HA	1.80	0.44
1:F:253:ILE:CD1	1:F:254:ILE:N	2.73	0.44
1:F:264:ALA:HB1	1:F:316:TYR:CD1	2.53	0.44
2:C:174:ASP:OD1	2:C:175:VAL:N	2.51	0.44
2:E:67:ASP:OD1	2:E:147:THR:OG1	2.23	0.44
2:E:67:ASP:OD2	2:E:146:THR:HA	2.18	0.44
2:C:356:GLY:CA	4:C:502:LYS:HG2	2.44	0.43
2:E:342:ALA:CB	2:E:391:LEU:HD12	2.45	0.43
2:C:41:SER:HA	2:C:74:GLU:HG3	2.00	0.43
2:C:374:MET:HB2	2:C:385:VAL:HB	2.00	0.43
1:H:368:GLU:HG3	1:H:393:LEU:HD13	2.00	0.43
2:G:389:LYS:N	6:G:604:HOH:O	2.48	0.43
1:F:297:GLN:HG3	1:F:305:THR:HG21	2.01	0.43
2:C:85:LEU:HB3	2:C:90:VAL:HG13	2.00	0.43
1:H:389:LYS:CG	1:H:390:TYR:CD1	3.01	0.43
2:G:15:THR:OG1	2:G:18:ARG:HG2	2.18	0.43
2:A:136:PHE:CG	2:A:136:PHE:O	2.71	0.43
2:E:298:ASN:OD1	2:E:299:VAL:N	2.47	0.43
2:G:83:MET:HE1	2:E:54:ALA:CB	2.45	0.43
2:G:87:LYS:NZ	2:E:58:MET:CA	2.81	0.43
2:A:22:VAL:HG23	2:A:23:ALA:N	2.32	0.43
2:E:14:GLY:HA2	2:E:44:SER:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:59:GLU:CG	2:A:60:GLN:H	2.31	0.43
2:A:197:PHE:HD2	2:A:242:ILE:HG23	1.82	0.43
2:E:253:ILE:HD12	2:E:253:ILE:HA	1.80	0.43
2:C:12:SER:O	2:C:18:ARG:HB3	2.18	0.43
2:C:58:MET:HE2	2:C:58:MET:HB3	1.84	0.43
1:H:272:PRO:O	1:H:277:VAL:HG21	2.17	0.43
2:G:227:ARG:CD	2:G:229:LEU:CD2	2.86	0.43
2:G:253:ILE:HD13	2:G:354:HIS:ND1	2.33	0.43
2:A:100:VAL:O	2:A:117:ASP:HB2	2.19	0.43
1:D:262:ASP:O	1:D:263:GLU:HG2	2.18	0.43
1:H:255:SER:HB3	1:H:348:GLY:HA3	1.99	0.43
2:E:30:ARG:HD3	2:E:130:VAL:CG2	2.48	0.43
2:E:49:ARG:HG3	2:E:49:ARG:NH1	2.33	0.43
2:C:80:LEU:HA	2:C:83:MET:HE2	2.00	0.43
2:G:330:ILE:O	2:G:330:ILE:HG13	2.19	0.43
2:A:28:LYS:HA	2:A:31:GLU:CD	2.44	0.43
1:B:366:ALA:O	1:B:368:GLU:O	2.35	0.43
1:F:254:ILE:C	1:F:254:ILE:CD1	2.91	0.43
1:F:268:ILE:HG12	1:F:271:VAL:CG1	2.49	0.43
1:H:294:MET:HE3	1:H:294:MET:HB2	1.76	0.43
2:A:74:GLU:O	2:A:78:ILE:HG23	2.19	0.43
1:H:257:ILE:HD13	1:H:398:LEU:HB3	2.01	0.43
1:H:313:ARG:O	1:H:313:ARG:HD3	2.19	0.43
2:G:69:MET:HG3	2:E:79:ALA:CB	2.49	0.43
2:G:313:ARG:HH12	2:G:388:GLU:CD	2.27	0.43
2:G:319:ALA:O	2:G:322:ILE:CG2	2.67	0.43
2:C:69:MET:HE2	2:C:69:MET:HB3	1.76	0.42
2:C:19:ILE:CA	2:C:22:VAL:CG2	2.92	0.42
2:C:213:ILE:O	2:C:217:GLU:HG3	2.19	0.42
1:H:346:ILE:HD13	1:H:346:ILE:HA	1.85	0.42
2:G:173:THR:OG1	2:G:210:VAL:HG23	2.14	0.42
1:F:341:ILE:HG22	1:F:373:GLN:HE22	1.84	0.42
1:F:368:GLU:HG3	1:F:397:ALA:HB2	2.01	0.42
1:H:366:ALA:C	1:H:368:GLU:O	2.63	0.42
2:A:28:LYS:O	2:A:31:GLU:HG2	2.20	0.42
2:C:28:LYS:HA	2:C:31:GLU:HG2	2.01	0.42
2:G:257:ILE:HG12	2:G:346:ILE:HG22	2.01	0.42
2:G:319:ALA:HA	2:G:322:ILE:HG22	2.00	0.42
2:A:25:LYS:HE2	2:A:172:TYR:OH	2.20	0.42
1:B:365:LEU:HA	1:B:365:LEU:HD23	1.85	0.42
2:C:178:VAL:HB	2:C:200:MET:HE1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:252:PRO:HB3	1:H:360:ARG:CZ	2.50	0.42
2:E:186:VAL:HG11	2:E:399:HIS:CG	2.54	0.42
1:F:371:ASN:OD1	3:F:501:THR:N	2.53	0.42
2:C:113:ILE:HD11	2:C:148:LEU:HD13	2.02	0.42
1:H:299:VAL:HG11	2:G:265:LYS:HE3	2.01	0.42
2:G:229:LEU:HD23	2:G:237:GLY:HA3	2.01	0.42
2:A:39:VAL:HG11	2:A:160:LEU:HD12	2.01	0.42
1:B:294:MET:CE	1:B:343:LYS:CD	2.92	0.42
1:H:368:GLU:HB2	1:H:370:ILE:HG13	2.01	0.42
2:G:269:ARG:HH11	2:G:269:ARG:HD2	1.71	0.42
2:G:318:ASN:O	2:G:322:ILE:HG22	2.20	0.42
2:E:366:ALA:C	2:E:368:GLU:O	2.63	0.42
2:C:173:THR:O	2:C:230:HIS:HA	2.20	0.42
2:C:232:PHE:CD1	2:C:232:PHE:N	2.83	0.42
2:G:87:LYS:NZ	2:E:58:MET:HG3	2.35	0.42
2:C:15:THR:OG1	2:C:18:ARG:HG2	2.20	0.42
2:C:194:LYS:HZ3	2:C:241:THR:CG2	2.32	0.42
1:H:363:GLU:HB2	2:G:279:PHE:CD1	2.55	0.42
2:G:69:MET:CG	2:E:79:ALA:HB3	2.50	0.42
1:D:282:LEU:HD12	1:D:282:LEU:HA	1.87	0.41
2:G:391:LEU:C	2:G:391:LEU:HD23	2.45	0.41
2:A:22:VAL:O	2:A:26:VAL:HG23	2.19	0.41
1:D:282:LEU:HG	4:C:502:LYS:NZ	2.35	0.41
1:B:261:ARG:NH2	1:B:392:GLU:OE2	2.48	0.41
1:H:377:THR:CG2	2:G:294:MET:HA	2.33	0.41
2:A:136:PHE:O	2:A:136:PHE:CD1	2.72	0.41
2:E:19:ILE:O	2:E:22:VAL:HG22	2.20	0.41
2:C:317:LEU:HD23	2:C:317:LEU:O	2.20	0.41
2:A:31:GLU:HG2	2:A:32:ALA:N	2.34	0.41
2:E:25:LYS:CE	2:E:233:GLN:HB3	2.50	0.41
2:C:87:LYS:CE	2:A:57:ILE:O	2.57	0.41
2:G:188:GLN:CG	2:G:406:ALA:H	2.33	0.41
2:E:104:THR:HG22	2:E:139:VAL:C	2.45	0.41
2:C:101:ARG:HD3	2:C:101:ARG:HA	1.89	0.41
1:H:324:LYS:HD3	6:H:603:HOH:O	2.21	0.41
1:H:370:ILE:HD11	1:H:393:LEU:CD1	2.50	0.41
2:G:14:GLY:HA2	2:G:44:SER:H	1.86	0.41
2:G:20:GLU:HB3	2:G:88:ARG:HH22	1.86	0.41
2:A:178:VAL:HG12	2:A:238:THR:CB	2.50	0.41
2:A:399:HIS:ND1	2:A:405:ASP:OD1	2.46	0.41
2:E:178:VAL:CG1	2:E:206:LEU:CD1	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:351:MET:CE	4:G:502:LYS:HB2	2.42	0.41
2:A:124:ASP:OD1	2:A:129:ARG:NH2	2.43	0.41
2:C:79:ALA:HB2	2:A:68:VAL:HG12	2.02	0.41
4:C:502:LYS:HD3	6:C:601:HOH:O	2.21	0.41
1:H:351:MET:HE1	2:G:201:LEU:O	2.20	0.41
2:A:226:LEU:HD23	2:A:226:LEU:HA	1.84	0.41
1:B:259:PHE:N	1:B:259:PHE:CD1	2.89	0.41
2:A:389:LYS:HB3	6:A:606:HOH:O	2.20	0.41
2:E:384:VAL:HG13	2:E:386:ILE:HG23	2.02	0.41
1:D:318:ASN:HB2	6:D:607:HOH:O	2.20	0.41
1:B:389:LYS:HE3	1:B:390:TYR:OH	2.21	0.41
1:F:387:GLU:HB2	1:F:390:TYR:CD2	2.55	0.41
2:C:8:PHE:CE1	2:C:22:VAL:HG12	2.56	0.41
2:C:351:MET:HE3	6:C:612:HOH:O	2.21	0.41
2:G:10:GLY:N	5:G:501:GOL:O2	2.52	0.41
2:G:190:ARG:HG2	2:G:404:LEU:O	2.21	0.41
2:E:67:ASP:O	2:E:71:SER:HB3	2.20	0.41
2:E:242:ILE:HG22	2:E:243:ASP:H	1.86	0.41
1:B:294:MET:CE	1:B:343:LYS:HD3	2.46	0.41
1:B:295:ILE:N	2:A:377:THR:HG21	2.34	0.41
1:F:295:ILE:N	2:E:377:THR:HG21	2.29	0.41
2:C:210:VAL:HG13	2:C:211:LEU:N	2.35	0.41
1:H:403:GLU:C	1:H:404:LEU:HD12	2.46	0.41
2:G:5:VAL:HG22	2:G:37:VAL:HB	2.02	0.41
2:G:107:ALA:O	2:G:111:ALA:N	2.53	0.41
2:A:39:VAL:CG1	2:A:160:LEU:HD12	2.51	0.41
2:A:116:ILE:HD13	2:A:160:LEU:HD23	2.03	0.41
2:A:214:ARG:HG3	2:A:214:ARG:NH1	2.36	0.41
1:D:266:LEU:HB3	1:D:323:LEU:HD22	2.03	0.40
1:D:282:LEU:HG	4:C:502:LYS:HZ2	1.85	0.40
2:E:229:LEU:CD2	2:E:237:GLY:N	2.84	0.40
1:B:368:GLU:HB3	1:B:393:LEU:HD21	2.01	0.40
2:C:357:VAL:CA	4:C:502:LYS:HB3	2.51	0.40
1:H:264:ALA:HB1	1:H:316:TYR:CD1	2.56	0.40
1:H:354:HIS:HB2	2:G:292:VAL:O	2.21	0.40
2:E:59:GLU:CD	2:E:59:GLU:H	2.29	0.40
2:E:97:GLY:H	2:E:137:GLN:NE2	2.19	0.40
2:G:384:VAL:HG12	2:G:386:ILE:HG23	2.03	0.40
2:A:396:ARG:O	2:A:400:THR:HG23	2.21	0.40
2:E:20:GLU:OE1	2:E:88:ARG:NH1	2.36	0.40
2:E:176:ASP:O	2:E:237:GLY:HA2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:67:ASP:OD2	2:G:146:THR:HA	2.21	0.40
2:C:271:VAL:CG1	2:C:277:VAL:HG11	2.51	0.40
1:H:259:PHE:CD1	1:H:259:PHE:N	2.89	0.40
2:G:25:LYS:HE2	2:G:233:GLN:HB2	2.04	0.40
2:G:57:ILE:HG22	2:G:58:MET:HG3	2.03	0.40
2:G:104:THR:HG22	2:G:139:VAL:C	2.45	0.40
2:G:391:LEU:O	2:G:395:VAL:HG23	2.22	0.40
2:G:404:LEU:HA	2:G:404:LEU:HD23	1.86	0.40
2:A:85:LEU:HB3	2:A:90:VAL:HG13	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	154/164 (94%)	152 (99%)	2 (1%)	0	100	100
1	D	154/164 (94%)	150 (97%)	3 (2%)	1 (1%)	21	27
1	F	149/164 (91%)	147 (99%)	2 (1%)	0	100	100
1	H	154/164 (94%)	151 (98%)	3 (2%)	0	100	100
2	A	393/412 (95%)	388 (99%)	4 (1%)	1 (0%)	36	46
2	C	393/412 (95%)	387 (98%)	4 (1%)	2 (0%)	24	31
2	E	393/412 (95%)	384 (98%)	8 (2%)	1 (0%)	36	46
2	G	393/412 (95%)	385 (98%)	7 (2%)	1 (0%)	36	46
All	All	2183/2304 (95%)	2144 (98%)	33 (2%)	6 (0%)	36	46

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	101	ARG

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Mol	Chain	Res	Type
2	G	101	ARG
2	E	101	ARG
2	A	101	ARG
1	D	251	GLN
2	C	105	ASP

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	B	126/133 (95%)	118 (94%)	8 (6%)	16	23
1	D	126/133 (95%)	117 (93%)	9 (7%)	13	19
1	F	123/133 (92%)	113 (92%)	10 (8%)	11	14
1	H	126/133 (95%)	114 (90%)	12 (10%)	8	10
2	A	323/336 (96%)	311 (96%)	12 (4%)	30	45
2	C	323/336 (96%)	313 (97%)	10 (3%)	35	52
2	E	323/336 (96%)	300 (93%)	23 (7%)	13	19
2	G	323/336 (96%)	310 (96%)	13 (4%)	28	42
All	All	1793/1876 (96%)	1696 (95%)	97 (5%)	20	29

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	339	THR
1	D	344	VAL
1	D	352	ARG
1	D	373	GLN
1	D	377	THR
1	D	387	GLU
1	D	389	LYS
1	D	403	GLU
1	D	405	ASP
1	B	271	VAL

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Mol	Chain	Res	Type
1	B	339	THR
1	B	344	VAL
1	B	352	ARG
1	B	353	SER
1	B	377	THR
1	B	399	HIS
1	B	404	LEU
1	F	253	ILE
1	F	261	ARG
1	F	313	ARG
1	F	352	ARG
1	F	353	SER
1	F	357	VAL
1	F	369	SER
1	F	370	ILE
1	F	377	THR
1	F	403	GLU
2	C	21	GLN
2	C	22	VAL
2	C	68	VAL
2	C	100	VAL
2	C	110	LYS
2	C	136	PHE
2	C	150	ARG
2	C	310	THR
2	C	352	ARG
2	C	377	THR
1	H	253	ILE
1	H	254	ILE
1	H	261	ARG
1	H	305	THR
1	H	330	ILE
1	H	344	VAL
1	H	346	ILE
1	H	347	VAL
1	H	351	MET
1	H	369	SER
1	H	377	THR
1	H	393	LEU
2	G	21	GLN
2	G	100	VAL
2	G	136	PHE

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Mol	Chain	Res	Type
2	G	174	ASP
2	G	188	GLN
2	G	205	SER
2	G	209	LYS
2	G	229	LEU
2	G	242	ILE
2	G	243	ASP
2	G	310	THR
2	G	321	GLU
2	G	352	ARG
2	A	11	THR
2	A	100	VAL
2	A	109	THR
2	A	110	LYS
2	A	137	GLN
2	A	206	LEU
2	A	229	LEU
2	A	242	ILE
2	A	243	ASP
2	A	310	THR
2	A	353	SER
2	A	403	GLU
2	E	11	THR
2	E	18	ARG
2	E	46	GLU
2	E	49	ARG
2	E	59	GLU
2	E	100	VAL
2	E	137	GLN
2	E	188	GLN
2	E	190	ARG
2	E	206	LEU
2	E	209	LYS
2	E	211	LEU
2	E	212	GLN
2	E	233	GLN
2	E	242	ILE
2	E	261	ARG
2	E	277	VAL
2	E	310	THR
2	E	321	GLU
2	E	325	GLN

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Mol	Chain	Res	Type
2	E	351	MET
2	E	353	SER
2	E	384	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	340	ASN
1	D	399	HIS
1	B	301	HIS
1	B	340	ASN
2	C	21	GLN
2	C	301	HIS
2	C	318	ASN
2	C	340	ASN
2	C	371	ASN
2	C	373	GLN
2	C	399	HIS
1	H	301	HIS
1	H	340	ASN
1	H	399	HIS
2	G	98	ASN
2	G	188	GLN
2	G	212	GLN
2	G	301	HIS
2	G	340	ASN
2	G	371	ASN
2	A	55	ASN
2	A	99	GLN
2	A	188	GLN
2	A	233	GLN
2	A	312	HIS
2	A	340	ASN
2	A	371	ASN
2	A	373	GLN
2	E	21	GLN
2	E	55	ASN
2	E	98	ASN
2	E	137	GLN
2	E	188	GLN
2	E	325	GLN
2	E	340	ASN

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Mol	Chain	Res	Type
2	E	371	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

15 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	GOL	G	501	-	5,5,5	0.29	0	5,5,5	0.94	0
3	THR	A	502	-	7,7,7	1.43	1 (14%)	8,9,9	0.49	0
3	THR	F	501	-	7,7,7	1.22	0	8,9,9	0.79	0
4	LYS	G	502	-	8,9,9	0.86	0	7,10,10	1.19	1 (14%)
5	GOL	E	502	-	5,5,5	0.20	0	5,5,5	0.43	0
3	THR	F	502	-	7,7,7	1.75	1 (14%)	8,9,9	0.83	0
4	LYS	C	502	-	8,9,9	1.00	0	7,10,10	0.83	0
4	LYS	A	501	-	8,9,9	1.07	0	7,10,10	0.63	0
3	THR	D	501	-	7,7,7	2.16	3 (42%)	8,9,9	1.55	2 (25%)
4	LYS	E	503	-	8,9,9	1.03	0	7,10,10	0.63	0
3	THR	B	501	-	7,7,7	1.76	2 (28%)	8,9,9	0.94	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	THR	C	501	-	7,7,7	1.50	2 (28%)	8,9,9	1.15	0
5	GOL	E	501	-	5,5,5	0.20	0	5,5,5	0.46	0
3	THR	H	501	-	7,7,7	2.35	3 (42%)	8,9,9	1.67	3 (37%)
3	THR	G	503	-	7,7,7	1.29	1 (14%)	8,9,9	0.92	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	G	501	-	-	2/4/4/4	-
3	THR	A	502	-	-	0/8/8/8	-
3	THR	F	501	-	-	0/8/8/8	-
4	LYS	G	502	-	-	3/9/9/9	-
5	GOL	E	502	-	-	0/4/4/4	-
3	THR	F	502	-	-	0/8/8/8	-
4	LYS	C	502	-	-	4/9/9/9	-
4	LYS	A	501	-	-	1/9/9/9	-
3	THR	D	501	-	-	0/8/8/8	-
4	LYS	E	503	-	-	0/9/9/9	-
3	THR	B	501	-	-	2/8/8/8	-
3	THR	C	501	-	-	2/8/8/8	-
5	GOL	E	501	-	-	2/4/4/4	-
3	THR	H	501	-	-	0/8/8/8	-
3	THR	G	503	-	-	2/8/8/8	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	501	THR	CG2-CB	-4.48	1.39	1.51
3	D	501	THR	CG2-CB	-4.30	1.39	1.51
3	F	502	THR	CG2-CB	-3.12	1.42	1.51
3	H	501	THR	CA-C	-2.70	1.47	1.52
3	B	501	THR	CG2-CB	-2.70	1.44	1.51
3	H	501	THR	OXT-C	-2.45	1.22	1.30
3	B	501	THR	CA-N	-2.26	1.41	1.47
3	C	501	THR	CA-N	-2.21	1.41	1.47
3	A	502	THR	OXT-C	-2.17	1.23	1.30
3	C	501	THR	CG2-CB	-2.15	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	503	THR	CG2-CB	-2.14	1.45	1.51
3	D	501	THR	OXT-C	-2.04	1.24	1.30
3	D	501	THR	CA-N	-2.04	1.41	1.47

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	501	THR	C-CA-N	-3.12	102.93	109.49
3	D	501	THR	C-CA-N	-2.91	103.38	109.49
3	H	501	THR	OXT-C-O	2.28	129.24	124.08
4	G	502	LYS	CB-CA-C	2.23	116.37	110.45
3	H	501	THR	O-C-CA	-2.11	114.59	121.72
3	D	501	THR	O-C-CA	-2.01	114.91	121.72

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	502	LYS	C-CA-CB-CG
4	G	502	LYS	N-CA-CB-CG
4	G	502	LYS	C-CA-CB-CG
5	G	501	GOL	C1-C2-C3-O3
5	E	501	GOL	O1-C1-C2-C3
5	E	501	GOL	O1-C1-C2-O2
5	G	501	GOL	O2-C2-C3-O3
4	C	502	LYS	CA-CB-CG-CD
4	C	502	LYS	CE-CD-CG-CB
3	B	501	THR	O-C-CA-CB
3	C	501	THR	O-C-CA-CB
3	G	503	THR	O-C-CA-CB
3	G	503	THR	OXT-C-CA-CB
4	G	502	LYS	CG-CD-CE-NZ
4	A	501	LYS	CG-CD-CE-NZ
4	C	502	LYS	N-CA-CB-CG
3	B	501	THR	OXT-C-CA-CB
3	C	501	THR	OXT-C-CA-CB

There are no ring outliers.

11 monomers are involved in 77 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	501	GOL	1	0
3	A	502	THR	1	0
3	F	501	THR	4	0
4	G	502	LYS	7	0
4	C	502	LYS	39	0
4	A	501	LYS	4	0
3	D	501	THR	3	0
4	E	503	LYS	4	0
3	C	501	THR	1	0
3	H	501	THR	2	0
3	G	503	THR	11	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	B	156/164 (95%)	-1.24	0	100 100	25, 40, 73, 104	0
1	D	156/164 (95%)	-1.15	0	100 100	23, 41, 91, 141	0
1	F	151/164 (92%)	-1.20	0	100 100	30, 52, 86, 122	0
1	H	156/164 (95%)	-1.15	0	100 100	27, 53, 112, 195	0
2	A	397/412 (96%)	-1.20	1 (0%)	90 90	22, 46, 79, 167	0
2	C	397/412 (96%)	-1.19	0	100 100	23, 46, 81, 136	0
2	E	397/412 (96%)	-1.17	1 (0%)	90 90	28, 52, 94, 153	0
2	G	397/412 (96%)	-1.14	2 (0%)	87 87	27, 50, 93, 154	0
All	All	2207/2304 (95%)	-1.18	4 (0%)	91 91	22, 48, 89, 195	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	206	LEU	2.9
2	E	210	VAL	2.6
2	G	210	VAL	2.4
2	A	210	VAL	2.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	THR	F	501	8/8	0.98	0.04	51,58,62,63	0
5	GOL	G	501	6/6	0.98	0.04	62,63,64,65	0
5	GOL	E	501	6/6	0.98	0.03	60,63,66,67	0
5	GOL	E	502	6/6	0.98	0.04	60,63,64,66	0
3	THR	C	501	8/8	0.99	0.05	43,48,51,59	0
3	THR	H	501	8/8	0.99	0.03	34,36,42,43	0
3	THR	G	503	8/8	0.99	0.04	49,60,66,73	0
3	THR	A	502	8/8	0.99	0.04	30,47,48,49	0
4	LYS	C	502	10/10	0.99	0.04	35,48,51,51	0
4	LYS	A	501	10/10	0.99	0.03	24,28,36,39	0
4	LYS	E	503	10/10	0.99	0.03	33,41,46,49	0
3	THR	B	501	8/8	0.99	0.04	38,43,49,53	0
3	THR	D	501	8/8	0.99	0.03	31,33,36,41	0
3	THR	F	502	8/8	0.99	0.04	33,38,40,43	0
4	LYS	G	502	10/10	1.00	0.02	32,39,43,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.