



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:55 PM UTC

PDB ID : 1E0T / pdb_00001e0t
Title : R292D mutant of E. coli pyruvate kinase
Authors : Fortin, R.; Mattevi, A.
Deposited on : 2000-04-10
Resolution : 1.80 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

<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

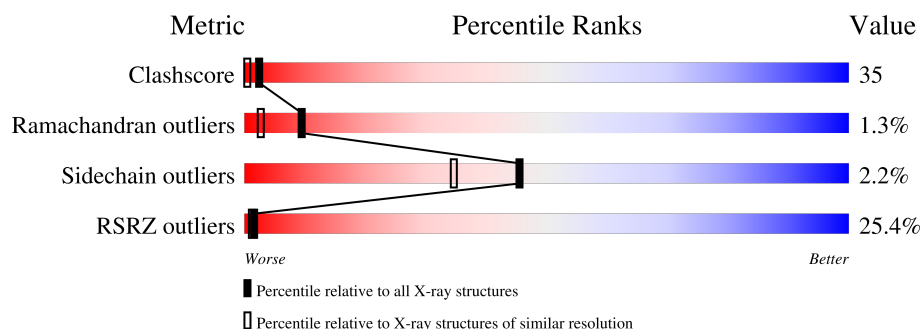
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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))
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	A	470	
1	B	470	
1	C	470	
1	D	470	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	B	702	-	-	X	-
2	SO4	C	703	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13374 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 Pyruvate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	0	0
			3307	2060	568	657	22			
1	B	446	Total	C	N	O	S	0	0	0
			3307	2060	568	657	22			
1	C	446	Total	C	N	O	S	0	0	0
			3307	2060	568	657	22			
1	D	446	Total	C	N	O	S	0	0	0
			3307	2060	568	657	22			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	MET	GLN	engineered mutation	UNP A0A0A0G552
A	292	ASP	ARG	engineered mutation	UNP A0A0A0G552
B	279	MET	GLN	engineered mutation	UNP A0A0A0G552
B	292	ASP	ARG	engineered mutation	UNP A0A0A0G552
C	279	MET	GLN	engineered mutation	UNP A0A0A0G552
C	292	ASP	ARG	engineered mutation	UNP A0A0A0G552
D	279	MET	GLN	engineered mutation	UNP A0A0A0G552
D	292	ASP	ARG	engineered mutation	UNP A0A0A0G552

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

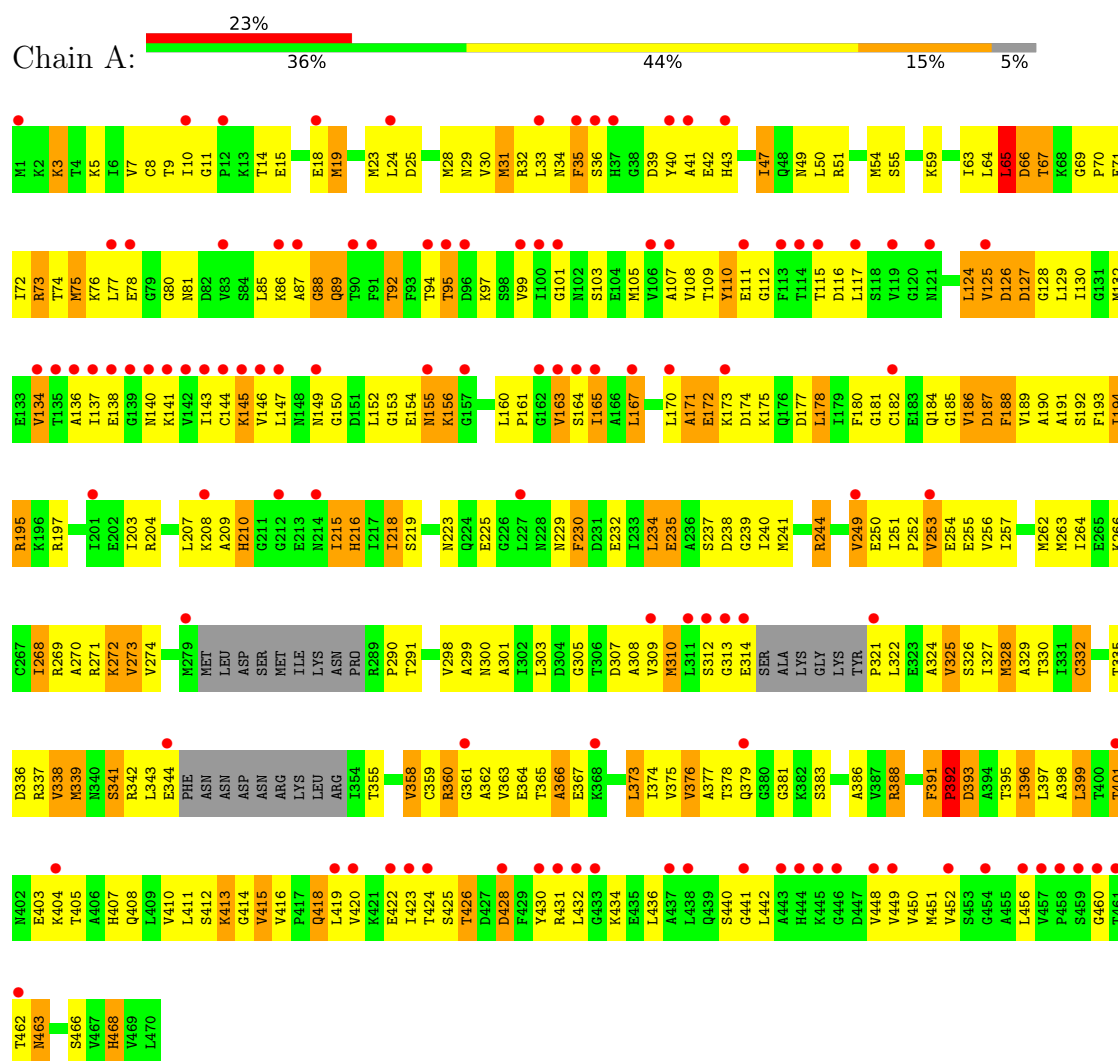
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	24	Total	O	0	0
			24	24		
3	B	35	Total	O	0	0
			35	35		
3	C	29	Total	O	0	0
			29	29		
3	D	38	Total	O	0	0
			38	38		

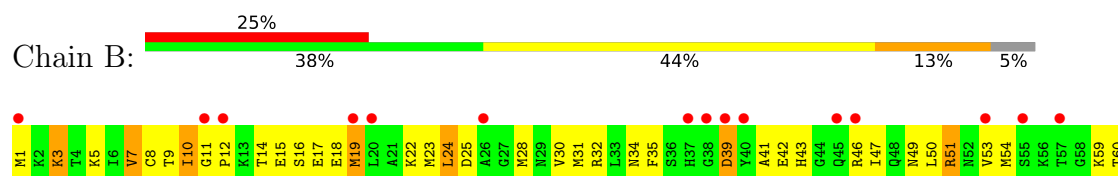
3 Residue-property plots

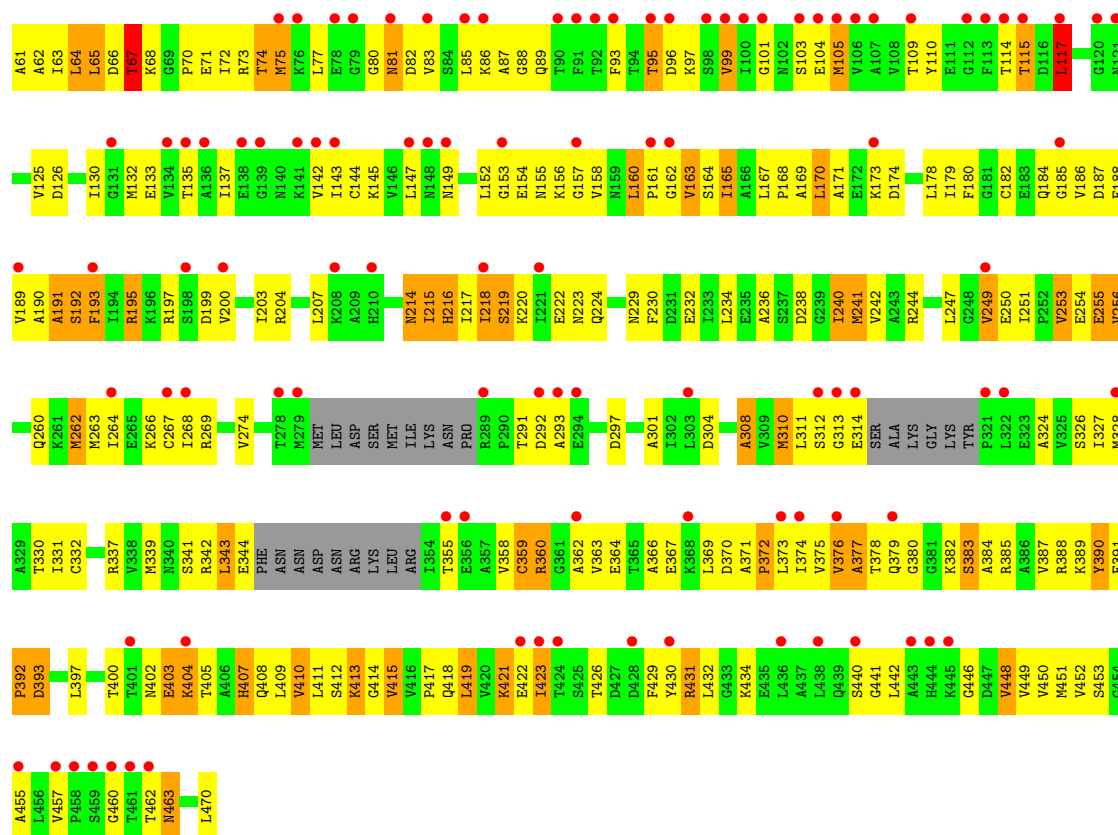
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Pyruvate kinase

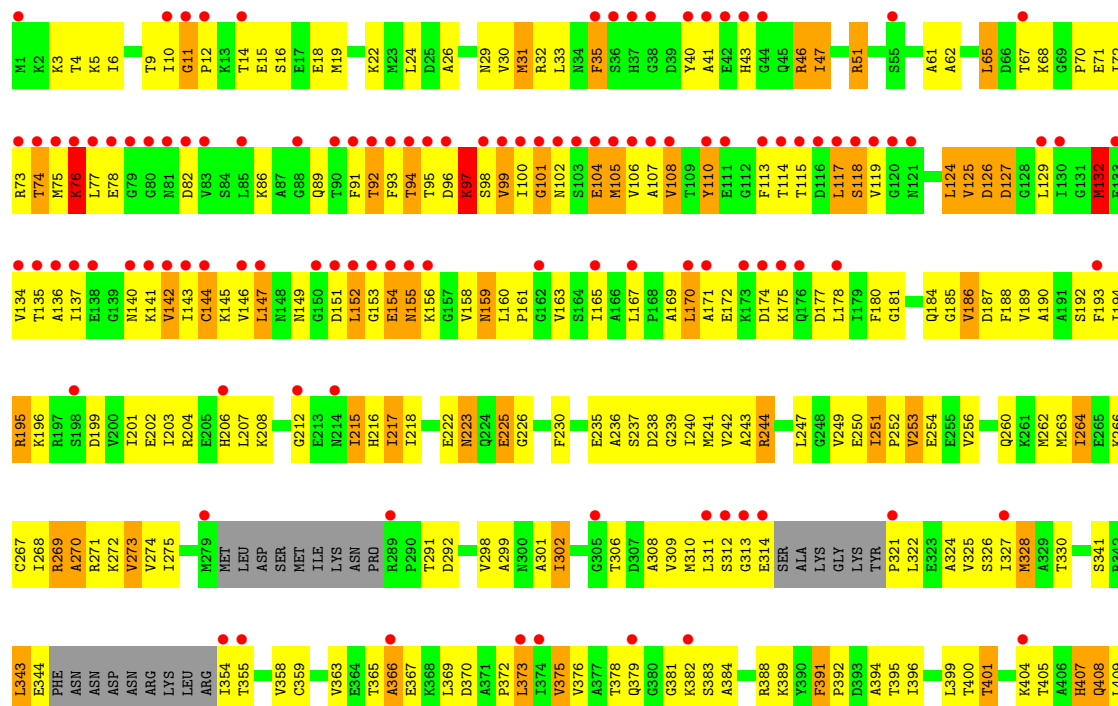


• Molecule 1: Pyruvate kinase



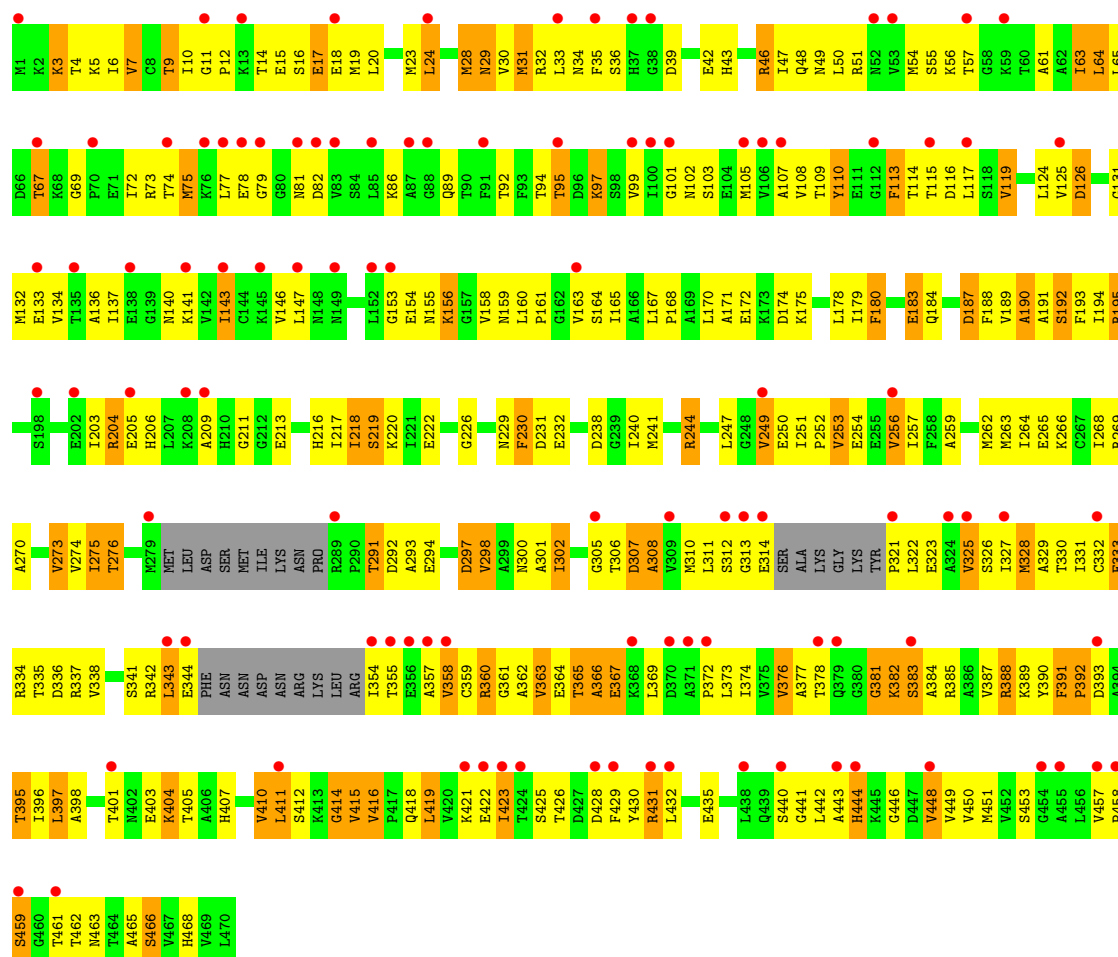


● Molecule 1: Pyruvate kinase





● Molecule 1: Pyruvate kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.47Å 129.34Å 240.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 1.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.3 (15.00-1.80) 95.6 (15.00-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.88 (at 2.81Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.246 , 0.315 0.242 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	25.1	Xtrriage
Anisotropy	0.776	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 88.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	13374	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.41 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.7480e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.89	0/3337	2.20	157/4507 (3.5%)
1	B	0.91	0/3337	2.14	145/4507 (3.2%)
1	C	0.92	0/3337	2.20	139/4507 (3.1%)
1	D	0.92	1/3337 (0.0%)	2.24	170/4507 (3.8%)
All	All	0.91	1/13348 (0.0%)	2.20	611/18028 (3.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	358	VAL	CA-CB	-5.61	1.48	1.54

All (611) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	ARG	N-CA-C	13.00	129.14	113.28
1	D	250	GLU	N-CA-C	12.18	127.92	113.18
1	D	273	VAL	N-CA-C	11.86	124.88	109.58
1	C	169	ALA	N-CA-C	-11.64	98.59	111.28
1	D	75	MET	CA-C-O	11.28	124.48	117.94
1	C	110	TYR	N-CA-C	11.25	128.68	107.75
1	C	194	ILE	CB-CA-C	-11.25	99.09	111.35
1	D	75	MET	N-CA-C	10.71	117.57	108.78
1	C	46	ARG	N-CA-C	-10.23	99.82	110.97
1	B	253	VAL	CB-CA-C	-10.21	98.36	112.14
1	C	328	MET	N-CA-C	-10.10	100.27	111.28
1	C	384	ALA	N-CA-C	-9.95	100.52	111.36
1	A	428	ASP	N-CA-C	-9.77	100.59	111.14
1	C	195	ARG	N-CA-C	9.75	125.37	113.38
1	A	393	ASP	N-CA-C	-9.65	99.04	112.45
1	D	253	VAL	CB-CA-C	-9.62	99.44	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	459	SER	N-CA-CB	9.54	123.91	110.17
1	D	328	MET	N-CA-C	-9.46	99.76	111.11
1	C	170	LEU	N-CA-C	9.30	124.11	108.20
1	B	256	VAL	N-CA-C	9.23	119.28	110.42
1	A	128	GLY	N-CA-C	-8.96	103.56	115.21
1	B	373	LEU	N-CA-CB	-8.96	97.40	111.56
1	D	244	ARG	N-CA-C	8.92	121.91	111.02
1	D	307	ASP	N-CA-C	-8.88	100.77	111.69
1	C	309	VAL	CA-C-N	-8.87	108.88	122.81
1	C	309	VAL	C-N-CA	-8.87	108.88	122.81
1	C	110	TYR	CA-C-O	8.81	130.36	120.84
1	C	373	LEU	N-CA-CB	-8.81	96.50	111.21
1	D	74	THR	CA-C-N	-8.75	113.59	123.04
1	D	74	THR	C-N-CA	-8.75	113.59	123.04
1	A	415	VAL	CB-CA-C	-8.72	100.09	110.91
1	A	216	HIS	N-CA-CB	8.67	124.27	110.23
1	B	404	LYS	N-CA-C	-8.56	101.52	111.03
1	D	259	ALA	N-CA-C	-8.54	102.06	111.36
1	D	226	GLY	N-CA-C	-8.46	102.25	112.49
1	A	456	LEU	CD1-CG-CD2	-8.45	92.21	110.80
1	D	384	ALA	N-CA-C	-8.43	102.18	111.36
1	A	271	ARG	CB-CA-C	8.41	122.17	110.06
1	D	308	ALA	N-CA-C	8.35	123.26	109.06
1	A	361	GLY	O-C-N	8.32	130.16	122.18
1	C	366	ALA	N-CA-C	-8.25	102.24	111.07
1	B	236	ALA	N-CA-C	8.22	123.09	112.89
1	A	141	LYS	N-CA-C	8.21	122.63	109.24
1	B	372	PRO	CA-C-N	-8.21	108.41	121.87
1	B	372	PRO	C-N-CA	-8.21	108.41	121.87
1	A	230	PHE	N-CA-C	8.19	121.24	111.33
1	C	215	ILE	CA-C-N	-8.13	109.80	121.42
1	C	215	ILE	C-N-CA	-8.13	109.80	121.42
1	A	69	GLY	CA-C-N	8.09	127.98	120.21
1	A	69	GLY	C-N-CA	8.09	127.98	120.21
1	D	110	TYR	N-CA-C	8.06	122.17	107.99
1	D	256	VAL	N-CA-C	8.05	118.14	110.42
1	D	125	VAL	N-CA-C	7.99	119.79	108.36
1	A	401	THR	N-CA-C	-7.99	103.68	113.50
1	C	99	VAL	N-CA-C	7.98	119.76	109.30
1	A	182	CYS	N-CA-C	-7.95	102.56	111.07
1	A	219	SER	N-CA-C	7.90	121.52	108.96
1	A	145	LYS	N-CA-C	-7.90	96.37	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	75	MET	CA-CB-CG	-7.89	98.33	114.10
1	D	24	LEU	N-CA-C	-7.86	102.71	111.82
1	C	35	PHE	CB-CA-C	7.84	125.01	110.11
1	A	250	GLU	N-CA-C	7.84	122.95	113.23
1	B	419	LEU	N-CA-C	-7.83	98.89	110.48
1	D	29	ASN	CA-C-N	-7.83	111.44	122.71
1	D	29	ASN	C-N-CA	-7.83	111.44	122.71
1	A	366	ALA	N-CA-C	-7.82	101.72	111.11
1	C	455	ALA	CA-C-N	7.77	133.18	122.07
1	C	455	ALA	C-N-CA	7.77	133.18	122.07
1	A	358	VAL	O-C-N	7.76	129.51	121.91
1	D	195	ARG	N-CA-C	7.74	123.41	113.88
1	A	134	VAL	CB-CA-C	-7.74	101.42	111.25
1	C	391	PHE	CA-C-O	7.68	125.77	120.47
1	D	404	LYS	N-CA-C	-7.65	102.63	110.97
1	D	292	ASP	N-CA-CB	-7.64	98.60	110.06
1	D	158	VAL	N-CA-C	7.62	119.26	108.36
1	C	343	LEU	N-CA-C	7.61	120.65	111.82
1	A	80	GLY	N-CA-C	-7.59	103.39	115.08
1	C	237	SER	N-CA-C	7.58	121.58	110.59
1	A	365	THR	CB-CA-C	-7.53	98.28	110.79
1	C	189	VAL	CA-C-N	-7.53	113.05	122.84
1	C	189	VAL	C-N-CA	-7.53	113.05	122.84
1	B	204	ARG	N-CA-C	-7.53	103.08	111.28
1	C	186	VAL	CA-C-N	7.53	130.98	120.29
1	C	186	VAL	C-N-CA	7.53	130.98	120.29
1	B	80	GLY	N-CA-C	-7.51	103.42	114.61
1	C	401	THR	N-CA-C	-7.51	104.27	113.50
1	B	249	VAL	CB-CA-C	-7.48	101.10	111.65
1	C	98	SER	CB-CA-C	-7.48	98.14	110.85
1	B	393	ASP	N-CA-C	-7.47	103.12	112.90
1	A	249	VAL	CB-CA-C	-7.46	99.99	112.16
1	A	300	ASN	OD1-CG-ND2	-7.45	115.15	122.60
1	D	180	PHE	N-CA-C	-7.42	103.13	111.07
1	A	377	ALA	CA-C-N	-7.42	110.05	122.29
1	A	377	ALA	C-N-CA	-7.42	110.05	122.29
1	A	218	ILE	CB-CA-C	-7.40	100.85	110.98
1	B	195	ARG	N-CA-C	7.40	123.44	113.97
1	C	3	LYS	N-CA-C	-7.39	104.88	114.04
1	D	30	VAL	CA-C-N	-7.38	112.95	122.77
1	D	30	VAL	C-N-CA	-7.38	112.95	122.77
1	D	415	VAL	CB-CA-C	-7.38	101.10	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	328	MET	N-CA-C	-7.37	103.23	111.71
1	A	35	PHE	CB-CA-C	7.35	124.53	110.27
1	D	29	ASN	N-CA-C	-7.33	105.25	114.56
1	B	343	LEU	N-CA-C	7.33	120.71	111.69
1	A	215	ILE	CA-C-N	-7.32	111.26	122.09
1	A	215	ILE	C-N-CA	-7.32	111.26	122.09
1	B	173	LYS	N-CA-C	-7.32	104.23	113.01
1	B	192	SER	N-CA-C	7.31	121.75	110.20
1	A	111	GLU	N-CA-C	7.29	120.10	111.71
1	B	310	MET	N-CA-C	7.26	121.49	109.95
1	A	186	VAL	CA-C-N	7.23	130.56	120.29
1	A	186	VAL	C-N-CA	7.23	130.56	120.29
1	A	15	GLU	N-CA-C	7.22	121.32	112.23
1	D	441	GLY	N-CA-C	-7.21	105.88	115.40
1	D	115	THR	N-CA-C	7.20	119.13	111.28
1	D	398	ALA	N-CA-C	7.18	120.43	108.73
1	B	67	THR	N-CA-C	7.15	120.86	110.28
1	D	275	ILE	O-C-N	7.14	130.96	123.03
1	C	382	LYS	N-CA-C	7.14	119.67	111.11
1	B	250	GLU	N-CA-C	7.09	122.10	113.17
1	A	66	ASP	O-C-N	7.09	131.28	123.27
1	A	125	VAL	N-CA-C	7.08	119.25	108.71
1	D	189	VAL	N-CA-C	-7.07	97.30	107.77
1	C	299	ALA	CA-C-N	-7.06	110.26	120.29
1	C	299	ALA	C-N-CA	-7.06	110.26	120.29
1	C	389	LYS	N-CA-C	7.06	118.98	111.28
1	D	365	THR	CB-CA-C	-7.04	98.88	110.85
1	B	448	VAL	N-CA-C	-7.03	99.68	109.45
1	B	392	PRO	CB-CA-C	-7.02	102.41	111.39
1	D	97	LYS	N-CA-C	7.00	119.77	111.71
1	B	199	ASP	N-CA-C	-7.00	103.58	111.14
1	B	332	CYS	CA-C-N	-6.99	110.36	120.29
1	B	332	CYS	C-N-CA	-6.99	110.36	120.29
1	A	332	CYS	CA-C-N	-6.98	110.93	120.28
1	A	332	CYS	C-N-CA	-6.98	110.93	120.28
1	C	142	VAL	N-CA-CB	6.97	120.46	111.67
1	A	415	VAL	N-CA-C	6.96	118.60	108.58
1	C	417	PRO	CB-CA-C	-6.94	101.86	110.95
1	A	441	GLY	N-CA-C	-6.93	106.25	115.40
1	D	331	ILE	N-CA-C	-6.92	103.46	111.00
1	D	211	GLY	N-CA-C	-6.90	105.80	115.32
1	A	253	VAL	CB-CA-C	-6.88	103.07	111.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	24	LEU	N-CA-C	-6.87	103.79	111.28
1	D	99	VAL	N-CA-C	6.87	118.65	109.37
1	D	57	THR	CB-CA-C	-6.86	98.14	110.35
1	A	167	LEU	CA-C-N	6.83	128.38	119.84
1	A	167	LEU	C-N-CA	6.83	128.38	119.84
1	B	460	GLY	N-CA-C	-6.83	106.33	115.21
1	B	61	ALA	N-CA-C	-6.83	98.14	108.52
1	D	358	VAL	CB-CA-C	-6.79	103.32	111.81
1	C	6	ILE	CB-CA-C	-6.79	100.71	110.83
1	B	110	TYR	N-CA-C	6.79	119.94	107.99
1	C	74	THR	N-CA-C	-6.77	99.56	110.32
1	A	47	ILE	CB-CA-C	-6.77	101.30	112.26
1	C	264	ILE	N-CA-C	6.74	117.49	110.62
1	B	412	SER	CA-C-N	-6.73	110.59	120.75
1	B	412	SER	C-N-CA	-6.73	110.59	120.75
1	C	441	GLY	N-CA-C	-6.73	106.41	115.36
1	A	30	VAL	CB-CA-C	-6.71	99.67	110.28
1	A	65	LEU	N-CA-C	-6.70	96.09	108.02
1	B	367	GLU	N-CA-C	6.70	118.67	111.36
1	A	290	PRO	N-CA-C	6.70	122.87	111.68
1	D	444	HIS	CA-CB-CG	-6.69	107.11	113.80
1	D	388	ARG	N-CA-C	6.69	119.40	111.71
1	C	204	ARG	N-CA-C	-6.67	103.94	111.07
1	D	209	ALA	N-CA-C	-6.65	104.42	112.54
1	C	149	ASN	N-CA-C	6.62	119.90	109.96
1	D	168	PRO	CA-C-N	6.61	129.13	120.28
1	D	168	PRO	C-N-CA	6.61	129.13	120.28
1	B	158	VAL	N-CA-C	6.60	118.55	108.71
1	A	262	MET	CA-CB-CG	6.60	127.29	114.10
1	D	466	SER	N-CA-CB	-6.59	99.43	110.57
1	D	273	VAL	CA-C-N	-6.59	112.61	122.70
1	D	273	VAL	C-N-CA	-6.59	112.61	122.70
1	C	193	PHE	N-CA-C	6.58	120.59	111.90
1	D	357	ALA	CA-C-N	-6.56	112.50	120.70
1	D	357	ALA	C-N-CA	-6.56	112.50	120.70
1	D	461	THR	CB-CA-C	-6.56	101.04	110.62
1	C	194	ILE	N-CA-C	6.54	116.89	108.12
1	A	145	LYS	CB-CG-CD	6.54	126.33	111.30
1	A	171	ALA	N-CA-C	-6.53	102.11	110.53
1	B	417	PRO	N-CA-C	6.52	120.35	111.22
1	D	392	PRO	CA-C-O	-6.52	114.13	121.43
1	C	71	GLU	CB-CA-C	-6.51	98.14	109.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	403	GLU	N-CA-C	6.49	118.44	111.36
1	A	391	PHE	CA-C-N	6.48	127.94	119.84
1	A	391	PHE	C-N-CA	6.48	127.94	119.84
1	D	435	GLU	N-CA-C	-6.48	103.83	111.03
1	B	99	VAL	N-CA-C	6.47	122.79	109.34
1	B	222	GLU	N-CA-C	6.47	122.25	113.97
1	C	145	LYS	CA-C-N	-6.46	112.19	120.98
1	C	145	LYS	C-N-CA	-6.46	112.19	120.98
1	D	273	VAL	N-CA-CB	6.45	120.19	110.13
1	A	234	LEU	CA-C-N	6.44	129.15	120.65
1	A	234	LEU	C-N-CA	6.44	129.15	120.65
1	D	275	ILE	CB-CA-C	-6.43	102.09	110.84
1	D	383	SER	N-CA-C	6.42	120.22	112.38
1	D	366	ALA	N-CA-C	-6.41	104.21	111.07
1	D	3	LYS	N-CA-C	-6.40	106.05	114.31
1	D	397	LEU	CB-CA-C	-6.40	100.54	110.78
1	C	97	LYS	N-CA-C	6.40	120.18	112.38
1	C	407	HIS	CA-C-O	-6.39	113.71	120.55
1	B	10	ILE	N-CA-C	6.39	118.23	108.71
1	C	129	LEU	CA-C-N	-6.39	113.49	122.75
1	C	129	LEU	C-N-CA	-6.39	113.49	122.75
1	B	125	VAL	N-CA-C	6.38	117.11	108.17
1	C	407	HIS	O-C-N	6.38	129.89	122.17
1	A	305	GLY	N-CA-C	6.36	125.33	115.72
1	C	271	ARG	CB-CA-C	6.35	123.03	110.65
1	A	412	SER	N-CA-C	6.34	120.22	110.20
1	B	170	LEU	N-CA-C	6.34	119.47	108.76
1	C	291	THR	N-CA-C	-6.33	101.57	110.50
1	B	223	ASN	N-CA-CB	-6.33	100.74	111.31
1	D	195	ARG	CA-C-O	6.33	126.39	119.24
1	B	65	LEU	CA-C-N	-6.33	114.27	123.00
1	B	65	LEU	C-N-CA	-6.33	114.27	123.00
1	D	270	ALA	CA-C-N	-6.33	113.22	122.40
1	D	270	ALA	C-N-CA	-6.33	113.22	122.40
1	A	215	ILE	CA-C-O	-6.32	113.84	121.04
1	D	300	ASN	N-CA-C	6.31	118.97	111.71
1	D	307	ASP	CB-CA-C	-6.31	99.16	110.70
1	B	384	ALA	N-CA-C	-6.30	104.49	111.36
1	D	423	ILE	N-CA-C	-6.30	96.24	109.34
1	D	401	THR	N-CA-C	-6.29	105.43	113.23
1	B	421	LYS	N-CA-C	6.28	118.13	111.28
1	A	186	VAL	N-CA-C	-6.28	100.73	109.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	276	THR	N-CA-C	6.26	118.91	108.20
1	B	331	ILE	N-CA-C	-6.25	104.19	111.00
1	D	218	ILE	CB-CA-C	-6.25	102.56	111.31
1	C	308	ALA	O-C-N	6.24	130.47	123.48
1	A	325	VAL	CB-CA-C	-6.24	103.71	111.70
1	A	396	ILE	CB-CA-C	-6.24	103.33	111.25
1	D	393	ASP	N-CA-C	-6.24	104.73	112.90
1	C	115	THR	N-CA-C	6.22	117.94	111.03
1	D	306	THR	O-C-N	-6.22	115.16	122.81
1	B	241	MET	CA-C-N	6.22	130.25	122.48
1	B	241	MET	C-N-CA	6.22	130.25	122.48
1	C	410	VAL	N-CA-C	-6.17	103.34	111.05
1	D	204	ARG	N-CA-C	-6.17	104.25	110.97
1	B	234	LEU	N-CA-C	-6.17	103.50	111.02
1	B	68	LYS	N-CA-C	-6.16	103.88	111.40
1	D	9	THR	N-CA-C	-6.16	99.17	108.96
1	C	273	VAL	CB-CA-C	-6.15	103.15	111.63
1	D	419	LEU	CB-CA-C	6.14	119.91	109.53
1	C	275	ILE	CA-C-N	-6.13	114.47	123.05
1	C	275	ILE	C-N-CA	-6.13	114.47	123.05
1	A	31	MET	CA-C-N	-6.13	114.04	122.93
1	A	31	MET	C-N-CA	-6.13	114.04	122.93
1	D	410	VAL	N-CA-C	-6.12	103.44	111.09
1	C	250	GLU	N-CA-C	6.12	120.88	113.17
1	D	393	ASP	N-CA-CB	6.11	119.50	110.33
1	D	387	VAL	O-C-N	6.09	128.11	121.83
1	A	172	GLU	N-CA-C	-6.08	104.74	111.36
1	C	451	MET	CA-CB-CG	-6.06	101.97	114.10
1	A	55	SER	CB-CA-C	-6.05	101.12	110.81
1	D	46	ARG	N-CA-CB	-6.05	100.98	110.06
1	B	185	GLY	O-C-N	-6.05	117.06	122.57
1	B	292	ASP	CB-CA-C	-6.05	101.13	110.81
1	A	182	CYS	CA-C-O	-6.05	114.47	120.82
1	A	363	VAL	N-CA-C	6.04	116.21	110.53
1	D	28	MET	N-CA-C	6.04	118.75	110.24
1	D	187	ASP	N-CA-C	6.04	119.11	111.69
1	C	47	ILE	CB-CA-C	-6.03	104.00	112.14
1	C	365	THR	CB-CA-C	-6.03	99.48	110.63
1	B	115	THR	N-CA-C	6.02	118.33	111.11
1	C	309	VAL	O-C-N	-6.02	116.55	122.93
1	B	99	VAL	CB-CA-C	-6.01	101.43	111.29
1	D	343	LEU	N-CA-C	6.01	119.08	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	302	ILE	CB-CA-C	6.00	119.89	112.02
1	A	153	GLY	N-CA-C	-6.00	103.10	112.58
1	D	302	ILE	N-CA-C	-6.00	104.89	110.53
1	A	244	ARG	N-CA-C	5.99	117.48	111.07
1	B	7	VAL	CB-CA-C	-5.99	102.21	110.96
1	B	383	SER	CA-C-N	-5.99	111.78	120.29
1	B	383	SER	C-N-CA	-5.99	111.78	120.29
1	D	391	PHE	CB-CA-C	-5.99	105.08	110.71
1	C	125	VAL	N-CA-C	5.98	117.95	108.87
1	B	207	LEU	CA-C-O	5.97	126.83	119.97
1	B	217	ILE	CA-C-N	5.96	130.33	122.95
1	B	217	ILE	C-N-CA	5.96	130.33	122.95
1	C	465	ALA	CA-C-N	-5.95	111.53	121.89
1	C	465	ALA	C-N-CA	-5.95	111.53	121.89
1	D	192	SER	N-CA-C	5.95	119.28	110.48
1	A	418	GLN	N-CA-CB	5.94	120.57	110.71
1	C	163	VAL	CB-CA-C	-5.94	103.08	111.28
1	C	94	THR	CA-C-N	5.93	131.52	121.14
1	C	94	THR	C-N-CA	5.93	131.52	121.14
1	B	371	ALA	CA-C-N	5.93	125.63	119.64
1	B	371	ALA	C-N-CA	5.93	125.63	119.64
1	C	416	VAL	CB-CA-C	-5.93	100.58	111.36
1	D	103	SER	N-CA-C	5.92	119.98	112.87
1	B	34	ASN	N-CA-C	5.92	118.41	107.99
1	D	395	THR	CA-C-N	-5.92	115.32	122.90
1	D	395	THR	C-N-CA	-5.92	115.32	122.90
1	A	291	THR	N-CA-C	-5.92	101.65	110.23
1	B	130	ILE	CB-CA-C	-5.91	102.08	110.12
1	A	89	GLN	CB-CA-C	-5.90	97.58	109.68
1	B	260	GLN	N-CA-C	-5.90	104.92	111.36
1	D	48	GLN	CB-CA-C	-5.90	100.99	110.79
1	B	267	CYS	N-CA-CB	5.90	118.54	109.98
1	A	360	ARG	CB-CA-C	-5.90	101.62	110.88
1	D	265	GLU	CA-CB-CG	5.90	125.89	114.10
1	B	160	LEU	CB-CA-C	-5.89	104.52	110.65
1	D	411	LEU	CA-C-N	5.89	129.23	120.87
1	D	411	LEU	C-N-CA	5.89	129.23	120.87
1	A	110	TYR	N-CA-C	5.88	119.21	107.62
1	D	382	LYS	N-CA-C	5.88	118.19	111.02
1	C	31	MET	CB-CA-C	-5.88	100.67	110.19
1	C	452	VAL	CB-CA-C	-5.87	101.50	110.95
1	A	413	LYS	CD-CE-NZ	5.87	130.67	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	332	CYS	CA-C-N	-5.86	112.47	120.44
1	D	332	CYS	C-N-CA	-5.86	112.47	120.44
1	D	249	VAL	CB-CA-C	-5.85	104.15	112.22
1	D	405	THR	CA-C-N	-5.85	111.42	120.31
1	D	405	THR	C-N-CA	-5.85	111.42	120.31
1	A	392	PRO	CB-CA-C	-5.84	101.92	111.56
1	D	117	LEU	CA-CB-CG	5.84	136.75	116.30
1	D	326	SER	N-CA-C	5.84	117.64	111.28
1	B	95	THR	N-CA-C	-5.84	106.14	113.20
1	B	253	VAL	N-CA-C	5.84	116.57	110.62
1	B	360	ARG	N-CA-C	-5.82	104.85	111.14
1	D	238	ASP	N-CA-C	-5.82	106.15	113.72
1	C	41	ALA	CA-C-N	5.82	128.33	120.65
1	C	41	ALA	C-N-CA	5.82	128.33	120.65
1	D	361	GLY	CA-C-N	5.82	129.55	120.82
1	D	361	GLY	C-N-CA	5.82	129.55	120.82
1	C	302	ILE	CA-C-O	-5.82	114.68	120.85
1	A	332	CYS	N-CA-C	-5.82	104.31	111.40
1	C	144	CYS	N-CA-C	5.81	118.02	109.24
1	D	55	SER	N-CA-C	-5.81	103.93	111.02
1	D	17	GLU	N-CA-C	-5.81	105.08	111.82
1	B	191	ALA	N-CA-C	5.80	119.37	110.20
1	B	240	ILE	CA-CB-CG1	5.77	120.21	110.40
1	A	460	GLY	N-CA-C	-5.76	107.69	115.36
1	D	412	SER	N-CA-C	5.75	118.79	110.28
1	C	271	ARG	N-CA-CB	-5.75	105.20	113.65
1	B	415	VAL	CB-CA-C	-5.75	103.70	111.63
1	C	435	GLU	CB-CA-C	-5.75	101.08	110.85
1	C	269	ARG	NE-CZ-NH2	5.74	124.37	119.20
1	C	170	LEU	CA-C-O	5.74	126.51	120.54
1	D	416	VAL	CB-CA-C	-5.74	100.92	111.36
1	A	419	LEU	N-CA-C	-5.74	100.32	109.96
1	B	291	THR	N-CA-C	-5.73	102.42	110.50
1	C	193	PHE	CB-CA-C	5.72	120.65	111.66
1	D	298	VAL	O-C-N	5.72	129.72	122.57
1	D	360	ARG	O-C-N	5.72	128.18	122.12
1	C	154	GLU	N-CA-C	5.71	118.93	110.48
1	A	360	ARG	CA-C-N	-5.69	113.62	119.94
1	A	360	ARG	C-N-CA	-5.69	113.62	119.94
1	B	72	ILE	CB-CA-C	-5.69	102.20	110.63
1	D	291	THR	N-CA-C	-5.69	101.86	110.28
1	A	127	ASP	N-CA-C	5.68	122.91	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	ILE	CB-CA-C	-5.68	103.19	110.98
1	B	81	ASN	N-CA-C	5.67	119.49	109.96
1	D	418	GLN	N-CA-CB	5.67	119.68	110.32
1	D	363	VAL	CB-CA-C	-5.67	104.39	112.22
1	A	363	VAL	CA-C-O	5.67	127.34	121.05
1	D	219	SER	N-CA-C	5.67	118.46	109.96
1	A	401	THR	CA-C-N	5.66	129.93	121.72
1	A	401	THR	C-N-CA	5.66	129.93	121.72
1	B	410	VAL	CA-C-O	5.65	126.62	120.57
1	D	117	LEU	CB-CA-C	5.64	124.30	111.71
1	C	292	ASP	CB-CA-C	-5.63	100.22	110.63
1	B	262	MET	CA-CB-CG	5.63	125.35	114.10
1	C	202	GLU	O-C-N	-5.63	115.64	122.22
1	B	224	GLN	CA-C-O	-5.62	114.88	120.90
1	B	390	TYR	CA-CB-CG	-5.62	103.78	113.90
1	D	115	THR	CB-CA-C	-5.61	101.47	110.79
1	D	205	GLU	N-CA-C	5.61	122.76	110.80
1	A	3	LYS	CA-C-N	-5.61	113.79	122.09
1	A	3	LYS	C-N-CA	-5.61	113.79	122.09
1	B	308	ALA	N-CA-C	5.61	117.92	109.23
1	A	173	LYS	N-CA-C	-5.61	105.32	111.82
1	B	182	CYS	N-CA-CB	5.61	118.11	109.98
1	B	255	GLU	N-CA-C	5.60	120.23	112.90
1	B	229	ASN	CA-CB-CG	-5.59	107.01	112.60
1	A	216	HIS	CB-CA-C	-5.59	100.31	109.53
1	B	234	LEU	N-CA-CB	5.58	118.30	109.82
1	D	61	ALA	CA-C-N	-5.58	112.95	123.27
1	D	61	ALA	C-N-CA	-5.58	112.95	123.27
1	C	195	ARG	CB-CA-C	-5.57	99.96	109.65
1	B	8	CYS	CA-CB-SG	-5.57	101.60	114.40
1	C	236	ALA	N-CA-C	5.56	119.17	112.38
1	B	216	HIS	O-C-N	5.56	129.55	123.04
1	B	51	ARG	CB-CG-CD	5.56	124.09	111.30
1	D	46	ARG	CA-C-O	5.56	126.64	120.63
1	A	210	HIS	CB-CA-C	-5.56	99.36	110.42
1	A	64	LEU	CB-CA-C	5.55	118.81	109.48
1	A	273	VAL	N-CA-CB	5.55	120.20	110.49
1	D	82	ASP	CB-CA-C	-5.55	101.01	109.89
1	C	118	SER	CB-CA-C	-5.55	101.06	109.99
1	D	381	GLY	N-CA-C	-5.54	108.00	115.21
1	B	193	PHE	CA-C-N	-5.54	113.44	120.98
1	B	193	PHE	C-N-CA	-5.54	113.44	120.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	153	GLY	N-CA-C	-5.54	103.83	112.58
1	C	373	LEU	N-CA-C	5.54	116.38	108.74
1	C	217	ILE	CA-C-N	5.53	130.63	123.11
1	C	217	ILE	C-N-CA	5.53	130.63	123.11
1	B	308	ALA	CA-C-N	5.53	130.23	123.10
1	B	308	ALA	C-N-CA	5.53	130.23	123.10
1	A	180	PHE	N-CA-C	-5.53	105.25	111.28
1	B	359	CYS	N-CA-C	5.52	117.38	111.36
1	A	187	ASP	CA-C-O	-5.52	114.57	120.42
1	D	419	LEU	N-CA-C	-5.52	101.48	110.20
1	B	165	ILE	N-CA-CB	-5.51	104.71	110.72
1	B	169	ALA	CA-C-N	-5.51	114.25	122.74
1	B	169	ALA	C-N-CA	-5.51	114.25	122.74
1	C	407	HIS	N-CA-CB	5.51	118.28	110.13
1	A	425	SER	CB-CA-C	-5.50	101.05	110.95
1	B	441	GLY	N-CA-C	-5.50	108.34	115.59
1	D	367	GLU	N-CA-C	5.50	117.35	111.36
1	D	333	GLU	CB-CA-C	5.50	119.58	110.90
1	C	186	VAL	N-CA-C	-5.49	102.50	109.80
1	C	76	LYS	N-CA-C	5.49	119.18	109.96
1	B	301	ALA	N-CA-C	-5.49	105.22	111.14
1	A	103	SER	N-CA-C	5.48	119.06	112.38
1	C	425	SER	CB-CA-C	-5.47	100.45	110.62
1	A	124	LEU	N-CA-C	5.46	117.66	107.99
1	D	31	MET	CA-CB-CG	-5.46	103.17	114.10
1	B	214	ASN	N-CA-C	5.46	119.93	113.16
1	B	215	ILE	CB-CA-C	-5.46	104.05	111.15
1	D	360	ARG	N-CA-C	-5.46	105.33	111.28
1	D	7	VAL	CB-CA-C	-5.46	103.51	110.98
1	A	49	ASN	CA-C-N	-5.46	112.54	120.29
1	A	49	ASN	C-N-CA	-5.46	112.54	120.29
1	B	418	GLN	N-CA-CB	5.45	119.78	110.57
1	D	56	LYS	N-CA-C	5.45	122.41	110.80
1	D	247	LEU	N-CA-C	-5.44	104.99	111.69
1	A	342	ARG	N-CA-C	-5.44	96.11	107.37
1	A	338	VAL	CA-C-N	-5.44	113.26	122.67
1	A	338	VAL	C-N-CA	-5.44	113.26	122.67
1	B	223	ASN	N-CA-C	5.44	116.53	108.86
1	D	358	VAL	N-CA-CB	-5.44	104.69	110.62
1	A	373	LEU	CA-C-N	-5.43	117.80	122.96
1	A	373	LEU	C-N-CA	-5.43	117.80	122.96
1	D	194	ILE	CB-CA-C	5.43	117.43	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	225	GLU	CA-C-N	-5.42	113.97	119.98
1	C	225	GLU	C-N-CA	-5.42	113.97	119.98
1	A	163	VAL	N-CA-C	5.42	120.60	109.34
1	D	425	SER	CB-CA-C	-5.42	100.56	111.17
1	B	180	PHE	N-CA-C	-5.41	105.46	111.36
1	C	114	THR	CA-C-O	5.41	126.28	120.55
1	A	341	SER	CA-C-N	-5.40	113.96	122.76
1	A	341	SER	C-N-CA	-5.40	113.96	122.76
1	C	124	LEU	CA-C-O	5.40	126.16	120.33
1	D	325	VAL	CA-C-N	-5.39	113.05	120.28
1	D	325	VAL	C-N-CA	-5.39	113.05	120.28
1	A	19	MET	N-CA-CB	-5.39	102.26	110.07
1	B	35	PHE	CB-CA-C	5.39	120.97	110.57
1	A	272	LYS	N-CA-C	5.38	118.88	110.32
1	B	117	LEU	CA-CB-CG	5.38	135.12	116.30
1	C	11	GLY	CA-C-N	5.38	126.56	119.84
1	C	11	GLY	C-N-CA	5.38	126.56	119.84
1	D	450	VAL	CB-CA-C	5.38	118.57	111.21
1	A	268	ILE	CB-CA-C	-5.37	105.01	111.88
1	A	229	ASN	N-CA-C	-5.37	106.60	112.72
1	A	426	THR	CB-CA-C	-5.36	101.84	110.74
1	B	105	MET	N-CA-CB	-5.34	103.44	111.56
1	A	164	SER	N-CA-C	-5.34	100.02	108.73
1	A	388	ARG	N-CA-C	5.34	118.59	111.75
1	B	145	LYS	CA-C-N	-5.34	113.72	120.98
1	B	145	LYS	C-N-CA	-5.34	113.72	120.98
1	C	413	LYS	N-CA-C	5.34	117.97	110.23
1	C	226	GLY	N-CA-C	-5.34	106.33	112.73
1	C	466	SER	N-CA-CB	-5.33	101.86	110.71
1	C	270	ALA	N-CA-C	5.33	119.53	113.19
1	D	357	ALA	O-C-N	5.32	127.78	122.08
1	C	262	MET	CA-C-N	-5.32	113.21	120.44
1	C	262	MET	C-N-CA	-5.32	113.21	120.44
1	C	151	ASP	N-CA-C	5.32	117.41	108.96
1	A	75	MET	CA-CB-CG	-5.31	103.47	114.10
1	C	101	GLY	CA-C-N	5.31	131.68	121.54
1	C	101	GLY	C-N-CA	5.31	131.68	121.54
1	A	8	CYS	CB-CA-C	-5.31	99.83	109.38
1	A	273	VAL	CB-CA-C	-5.31	104.31	111.63
1	A	223	ASN	N-CA-C	5.30	115.36	107.88
1	D	323	GLU	N-CA-C	-5.30	105.67	111.82
1	A	376	VAL	CA-C-N	-5.30	115.41	122.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	376	VAL	C-N-CA	-5.30	115.41	122.72
1	D	146	VAL	CB-CA-C	5.30	118.04	111.15
1	A	92	THR	N-CA-C	5.29	117.59	109.07
1	A	182	CYS	CA-CB-SG	5.29	126.58	114.40
1	B	218	ILE	CB-CA-C	-5.29	104.56	111.81
1	C	159	ASN	CA-C-N	-5.29	115.54	122.74
1	C	159	ASN	C-N-CA	-5.29	115.54	122.74
1	C	31	MET	CA-C-O	-5.29	114.70	120.36
1	D	153	GLY	N-CA-C	-5.29	104.53	112.89
1	B	337	ARG	CA-CB-CG	5.29	124.67	114.10
1	D	323	GLU	CA-C-N	-5.28	112.79	120.29
1	D	323	GLU	C-N-CA	-5.28	112.79	120.29
1	D	160	LEU	CA-C-O	-5.28	114.94	120.38
1	B	72	ILE	N-CA-C	-5.28	100.72	108.11
1	C	104	GLU	CA-C-N	-5.27	112.29	122.09
1	C	104	GLU	C-N-CA	-5.27	112.29	122.09
1	D	105	MET	N-CA-CB	-5.26	103.57	111.56
1	D	4	THR	N-CA-CB	5.25	118.09	109.95
1	A	270	ALA	CA-C-N	-5.24	117.17	126.45
1	A	270	ALA	C-N-CA	-5.24	117.17	126.45
1	D	448	VAL	CA-C-N	-5.24	113.94	122.33
1	D	448	VAL	C-N-CA	-5.24	113.94	122.33
1	B	446	GLY	CA-C-N	-5.24	113.92	121.42
1	B	446	GLY	C-N-CA	-5.24	113.92	121.42
1	A	156	LYS	CA-C-N	5.23	125.98	120.43
1	A	156	LYS	C-N-CA	5.23	125.98	120.43
1	D	143	ILE	CB-CA-C	-5.23	104.35	111.15
1	D	113	PHE	N-CA-C	5.22	116.97	111.28
1	A	339	MET	N-CA-C	-5.22	102.73	110.46
1	B	64	LEU	N-CA-C	5.22	117.75	109.24
1	D	446	GLY	N-CA-C	-5.22	108.87	115.08
1	C	4	THR	CA-C-N	-5.22	114.88	122.65
1	C	4	THR	C-N-CA	-5.22	114.88	122.65
1	D	6	ILE	CB-CA-C	-5.21	103.75	110.84
1	B	423	ILE	N-CA-C	-5.21	98.50	109.34
1	A	155	ASN	CA-C-N	-5.20	113.17	122.07
1	A	155	ASN	C-N-CA	-5.20	113.17	122.07
1	A	273	VAL	CA-C-N	-5.20	115.21	122.75
1	A	273	VAL	C-N-CA	-5.20	115.21	122.75
1	A	414	GLY	CA-C-N	-5.20	115.66	122.37
1	A	414	GLY	C-N-CA	-5.20	115.66	122.37
1	B	41	ALA	CA-C-N	5.20	127.70	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	41	ALA	C-N-CA	5.20	127.70	120.63
1	C	92	THR	N-CA-C	5.20	117.54	108.76
1	C	366	ALA	O-C-N	5.20	127.42	122.07
1	C	132	MET	N-CA-CB	5.19	120.48	111.39
1	A	310	MET	N-CA-C	5.19	118.46	110.42
1	A	188	PHE	CB-CA-C	-5.18	99.31	110.45
1	A	235	GLU	O-C-N	5.18	127.42	122.03
1	B	74	THR	N-CA-C	-5.18	102.81	110.48
1	D	292	ASP	CB-CG-OD1	5.18	130.31	118.40
1	B	219	SER	CA-CB-OG	5.17	121.45	111.10
1	A	41	ALA	N-CA-C	5.17	116.99	111.36
1	D	297	ASP	CB-CA-C	5.17	120.19	110.63
1	D	137	ILE	CB-CA-C	-5.16	102.83	111.29
1	B	407	HIS	O-C-N	5.16	128.41	122.17
1	B	397	LEU	CA-C-N	-5.16	115.61	122.72
1	B	397	LEU	C-N-CA	-5.16	115.61	122.72
1	C	92	THR	N-CA-CB	-5.16	101.88	110.80
1	C	375	VAL	CB-CA-C	-5.15	103.43	111.26
1	A	24	LEU	N-CA-C	-5.15	105.75	111.36
1	C	244	ARG	N-CA-C	5.14	116.58	110.97
1	C	251	ILE	CB-CA-C	-5.14	102.00	111.36
1	C	270	ALA	CA-C-N	-5.14	115.98	125.02
1	C	270	ALA	C-N-CA	-5.14	115.98	125.02
1	B	377	ALA	N-CA-C	-5.14	101.90	110.17
1	D	119	VAL	N-CA-CB	5.14	116.83	110.05
1	A	309	VAL	CA-CB-CG1	5.13	119.13	110.40
1	A	399	LEU	CA-C-O	5.13	126.03	120.43
1	D	183	GLU	CB-CG-CD	-5.13	103.88	112.60
1	C	82	ASP	CA-C-N	-5.13	115.06	122.45
1	C	82	ASP	C-N-CA	-5.13	115.06	122.45
1	D	116	ASP	CA-C-N	-5.13	111.81	121.66
1	D	116	ASP	C-N-CA	-5.13	111.81	121.66
1	B	137	ILE	N-CA-C	-5.13	101.58	108.35
1	B	203	ILE	CB-CA-C	-5.13	105.22	112.14
1	B	376	VAL	CA-C-N	-5.13	113.92	122.64
1	B	376	VAL	C-N-CA	-5.13	113.92	122.64
1	C	223	ASN	N-CA-C	5.12	115.93	108.14
1	A	99	VAL	N-CA-C	5.12	116.28	109.37
1	B	75	MET	N-CA-C	5.11	121.69	110.80
1	B	304	ASP	CB-CA-C	-5.11	99.63	110.31
1	C	273	VAL	CA-C-N	-5.10	115.35	122.75
1	C	273	VAL	C-N-CA	-5.10	115.35	122.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	173	LYS	CA-CB-CG	5.10	124.30	114.10
1	B	238	ASP	CA-C-O	5.10	124.66	119.05
1	D	172	GLU	CA-CB-CG	-5.10	103.91	114.10
1	A	195	ARG	CB-CA-C	-5.09	99.94	109.72
1	A	239	GLY	CA-C-N	-5.09	116.41	122.11
1	A	239	GLY	C-N-CA	-5.09	116.41	122.11
1	D	222	GLU	CA-C-N	-5.09	113.10	121.80
1	D	222	GLU	C-N-CA	-5.09	113.10	121.80
1	A	81	ASN	N-CA-C	5.09	118.50	109.96
1	A	178	LEU	CA-C-N	-5.09	113.49	120.46
1	A	178	LEU	C-N-CA	-5.09	113.49	120.46
1	D	428	ASP	N-CA-C	-5.09	105.74	111.28
1	D	190	ALA	CA-C-O	-5.08	115.26	120.54
1	B	240	ILE	O-C-N	5.08	128.67	122.58
1	D	298	VAL	CA-C-O	-5.07	114.44	120.78
1	C	24	LEU	N-CA-C	-5.07	105.75	111.28
1	C	448	VAL	N-CA-C	-5.07	101.11	108.97
1	B	39	ASP	CA-C-N	-5.07	112.98	120.28
1	B	39	ASP	C-N-CA	-5.07	112.98	120.28
1	B	409	LEU	N-CA-C	5.07	118.56	112.38
1	B	97	LYS	N-CA-C	5.07	117.70	111.82
1	B	163	VAL	N-CA-C	5.06	116.53	109.80
1	B	3	LYS	CB-CA-C	-5.05	100.84	109.03
1	A	328	MET	CA-C-N	-5.05	113.76	120.63
1	A	328	MET	C-N-CA	-5.05	113.76	120.63
1	D	230	PHE	N-CA-C	5.05	119.66	111.37
1	B	403	GLU	CA-C-N	-5.05	113.76	120.63
1	B	403	GLU	C-N-CA	-5.05	113.76	120.63
1	D	376	VAL	CB-CA-C	-5.05	104.02	111.80
1	A	73	ARG	N-CA-C	5.04	117.34	109.52
1	D	63	ILE	CA-C-O	5.04	125.25	120.25
1	A	24	LEU	CD1-CG-CD2	-5.04	99.71	110.80
1	B	19	MET	CA-C-N	5.04	126.98	120.44
1	B	19	MET	C-N-CA	5.04	126.98	120.44
1	C	47	ILE	N-CA-C	5.03	115.75	110.62
1	C	408	GLN	N-CA-C	5.03	116.45	111.07
1	A	144	CYS	N-CA-C	5.03	116.83	109.24
1	A	468	HIS	N-CA-C	5.02	117.34	108.75
1	D	389	LYS	CB-CG-CD	-5.02	99.75	111.30
1	B	387	VAL	N-CA-C	5.01	115.73	110.62
1	B	413	LYS	N-CA-C	5.01	117.17	110.35
1	A	130	ILE	CB-CA-C	-5.01	103.01	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1	MET	CB-CG-SD	5.01	127.73	112.70
1	D	18	GLU	O-C-N	5.01	127.23	122.07
1	C	155	ASN	CA-C-N	-5.01	114.13	122.64
1	C	155	ASN	C-N-CA	-5.01	114.13	122.64
1	C	416	VAL	CA-C-N	5.00	124.98	120.03
1	C	416	VAL	C-N-CA	5.00	124.98	120.03
1	D	329	ALA	CA-C-O	-5.00	115.57	120.82

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3307	0	3346	241	0
1	B	3307	0	3346	224	0
1	C	3307	0	3346	260	1
1	D	3307	0	3346	214	1
2	A	5	0	0	0	0
2	B	5	0	0	2	0
2	C	5	0	0	3	0
2	D	5	0	0	1	0
3	A	24	0	0	4	0
3	B	35	0	0	11	0
3	C	29	0	0	13	0
3	D	38	0	0	7	0
All	All	13374	0	13384	934	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 35.

All (934) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:VAL:HG12	1:A:165:ILE:HD12	1.36	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:LEU:HD23	1:B:63:ILE:HD11	1.38	1.06
1:C:170:LEU:HD11	1:C:178:LEU:HD12	1.40	1.04
1:C:92:THR:HB	1:C:105:MET:HB2	1.38	1.02
1:C:409:LEU:HB2	3:C:2024:HOH:O	1.57	1.01
1:C:170:LEU:HD13	1:C:175:LYS:HG2	1.43	0.99
1:C:95:THR:HB	1:C:140:ASN:HB2	1.40	0.99
1:C:355:THR:HG23	1:C:462:THR:HB	1.48	0.95
1:A:31:MET:HE3	1:A:33:LEU:HD21	1.50	0.94
1:C:132:MET:HA	1:C:147:LEU:HD22	1.52	0.92
1:C:132:MET:CA	1:C:147:LEU:HD22	2.01	0.91
1:B:67:THR:HG22	1:B:192:SER:HB2	1.50	0.90
1:C:241:MET:CE	1:C:310:MET:HE1	2.03	0.87
1:B:241:MET:CE	1:B:310:MET:HE1	2.05	0.87
1:A:193:PHE:CD2	1:A:195:ARG:HD2	2.10	0.86
1:B:268:ILE:HD13	1:B:391:PHE:CZ	2.11	0.85
1:B:241:MET:HE2	1:B:310:MET:HE1	1.58	0.85
1:C:170:LEU:CD2	1:C:174:ASP:HB3	2.06	0.85
1:C:14:THR:HA	1:C:19:MET:HG2	1.57	0.85
1:D:86:LYS:O	1:D:89:GLN:HG2	1.76	0.85
1:D:10:ILE:HG22	1:D:46:ARG:HD2	1.59	0.84
1:C:170:LEU:HD22	1:C:174:ASP:HB3	1.60	0.83
1:D:124:LEU:HD12	1:D:161:PRO:HD3	1.61	0.83
1:D:72:ILE:HG23	1:D:110:TYR:HB3	1.58	0.83
1:C:31:MET:HE3	1:C:33:LEU:HD21	1.61	0.83
1:D:154:GLU:O	1:D:156:LYS:HE2	1.77	0.83
1:C:117:LEU:HD11	1:C:160:LEU:HD22	1.61	0.82
1:B:25:ASP:OD1	1:B:59:LYS:NZ	2.12	0.82
1:C:124:LEU:HD11	1:C:161:PRO:HG3	1.62	0.81
1:A:75:MET:HG3	1:A:107:ALA:O	1.81	0.81
1:A:404:LYS:O	1:A:408:GLN:HG3	1.81	0.81
1:D:230:PHE:CE2	1:D:263:MET:HG2	2.16	0.80
1:C:154:GLU:HA	3:C:2010:HOH:O	1.81	0.80
1:C:241:MET:HE1	1:C:310:MET:HE1	1.63	0.80
1:D:264:ILE:O	1:D:268:ILE:HG13	1.81	0.80
1:C:76:LYS:HE3	3:C:2002:HOH:O	1.81	0.80
1:C:326:SER:O	1:C:330:THR:HG23	1.81	0.80
1:C:75:MET:HB2	3:C:2003:HOH:O	1.81	0.80
1:D:355:THR:HG23	1:D:462:THR:HB	1.65	0.79
1:C:411:LEU:HG	3:C:2025:HOH:O	1.82	0.79
1:A:373:LEU:HD12	1:A:395:THR:O	1.83	0.78
1:A:193:PHE:CE2	1:A:195:ARG:HD2	2.19	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:VAL:HG21	1:B:470:LEU:HD11	1.64	0.77
1:C:187:ASP:HA	1:C:404:LYS:HE3	1.67	0.77
1:D:10:ILE:HG12	1:D:31:MET:HG3	1.65	0.77
1:A:324:ALA:O	1:A:327:ILE:HG22	1.85	0.76
1:C:78:GLU:HG3	1:C:101:GLY:O	1.84	0.76
1:C:132:MET:N	1:C:147:LEU:HD22	2.00	0.76
1:C:170:LEU:HD11	1:C:178:LEU:CD1	2.15	0.76
1:B:10:ILE:CD1	1:B:23:MET:HE1	2.14	0.76
1:B:11:GLY:HA2	1:B:46:ARG:NH1	1.99	0.76
1:B:326:SER:O	1:B:330:THR:HG23	1.86	0.76
1:A:10:ILE:HG12	1:A:31:MET:HG3	1.67	0.76
1:C:134:VAL:HA	1:C:144:CYS:SG	2.26	0.76
1:D:124:LEU:HD11	1:D:161:PRO:HG3	1.68	0.76
1:B:167:LEU:HB3	1:B:168:PRO:HD2	1.68	0.75
1:D:7:VAL:HG11	1:D:310:MET:HE2	1.67	0.75
1:A:165:ILE:HG22	1:A:167:LEU:H	1.51	0.75
1:C:170:LEU:HD21	1:C:178:LEU:HD11	1.67	0.75
1:C:430:TYR:O	1:C:434:LYS:HG3	1.86	0.75
1:B:67:THR:CG2	1:B:192:SER:HB2	2.15	0.75
1:B:230:PHE:CE2	1:B:263:MET:HG2	2.21	0.75
1:C:171:ALA:HB3	1:C:174:ASP:CG	2.12	0.74
1:A:208:LYS:HD2	3:A:2014:HOH:O	1.88	0.74
1:C:273:VAL:HG12	3:C:2019:HOH:O	1.86	0.74
1:D:167:LEU:O	1:D:195:ARG:NH2	2.21	0.74
1:C:11:GLY:HA2	1:C:46:ARG:NH1	2.03	0.73
1:B:268:ILE:HD13	1:B:391:PHE:HZ	1.52	0.73
1:C:77:LEU:HG	1:C:154:GLU:HG2	1.70	0.73
1:A:23:MET:HB3	1:A:28:MET:HE2	1.69	0.73
1:B:17:GLU:HG2	1:B:49:ASN:HB3	1.70	0.73
1:C:378:THR:OG1	2:C:703:SO4:O1	2.05	0.73
1:B:50:LEU:HD23	1:B:63:ILE:CD1	2.18	0.72
1:D:78:GLU:HG3	1:D:101:GLY:O	1.89	0.72
1:A:3:LYS:NZ	1:A:393:ASP:O	2.17	0.72
1:C:264:ILE:O	1:C:268:ILE:HG13	1.88	0.72
1:C:75:MET:CE	1:C:97:LYS:HG2	2.19	0.72
1:A:254:GLU:OE1	1:A:254:GLU:N	2.22	0.72
1:A:110:TYR:CD1	1:A:167:LEU:HD21	2.24	0.72
1:A:170:LEU:HD22	1:A:174:ASP:HB3	1.71	0.72
1:A:171:ALA:N	1:A:174:ASP:HB2	2.05	0.72
1:D:165:ILE:HG22	1:D:167:LEU:H	1.55	0.71
1:A:167:LEU:O	1:A:195:ARG:NH2	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:TYR:CD1	1:C:167:LEU:HD21	2.25	0.71
1:D:14:THR:HA	1:D:19:MET:HG2	1.70	0.71
1:D:276:THR:HG21	1:D:301:ALA:CB	2.21	0.71
1:A:51:ARG:NH2	1:A:184:GLN:O	2.23	0.71
1:D:276:THR:HG21	1:D:301:ALA:HB1	1.73	0.71
1:B:430:TYR:O	1:B:434:LYS:HG3	1.89	0.70
1:D:426:THR:HG22	1:D:430:TYR:CE2	2.26	0.70
1:B:67:THR:HG22	1:B:192:SER:CB	2.21	0.70
1:C:94:THR:CG2	1:C:107:ALA:HA	2.22	0.70
1:B:49:ASN:O	1:B:53:VAL:HG23	1.92	0.70
1:A:431:ARG:HD3	1:A:432:LEU:N	2.07	0.70
1:C:181:GLY:O	1:C:185:GLY:N	2.25	0.70
1:B:355:THR:HG23	1:B:462:THR:HB	1.72	0.70
1:A:273:VAL:HG21	1:A:411:LEU:HD23	1.73	0.70
1:C:241:MET:HE2	1:C:310:MET:HE1	1.72	0.70
1:B:253:VAL:HG23	1:B:254:GLU:H	1.57	0.69
1:D:383:SER:HB3	1:D:462:THR:OG1	1.92	0.69
1:D:124:LEU:HB2	1:D:159:ASN:HB2	1.74	0.69
1:A:23:MET:CB	1:A:28:MET:HE2	2.23	0.69
1:D:193:PHE:CD2	1:D:195:ARG:HD2	2.29	0.68
1:A:203:ILE:O	1:A:207:LEU:HG	1.93	0.68
1:A:204:ARG:NH1	3:A:2012:HOH:O	2.24	0.68
1:C:153:GLY:O	1:C:156:LYS:HG2	1.92	0.68
1:B:70:PRO:HB2	1:B:167:LEU:HD13	1.73	0.68
1:A:189:VAL:HG23	1:A:215:ILE:HG21	1.74	0.68
1:A:75:MET:CE	1:A:97:LYS:HA	2.24	0.68
1:B:358:VAL:HG21	1:B:463:ASN:HA	1.75	0.68
1:B:380:GLY:N	2:B:702:SO4:O2	2.22	0.68
1:C:124:LEU:CD1	1:C:161:PRO:HG3	2.24	0.68
1:D:219:SER:HB2	1:D:240:ILE:HD13	1.75	0.68
1:B:15:GLU:HB3	1:B:46:ARG:HD3	1.76	0.67
1:C:119:VAL:HG13	1:C:134:VAL:O	1.94	0.67
1:D:188:PHE:CD1	1:D:216:HIS:HB2	2.29	0.67
1:A:181:GLY:O	1:A:185:GLY:N	2.28	0.67
1:B:268:ILE:HG21	1:B:391:PHE:HE1	1.57	0.67
1:C:253:VAL:HG23	1:C:254:GLU:OE1	1.95	0.67
1:A:388:ARG:HB2	1:A:396:ILE:CD1	2.25	0.67
1:A:75:MET:HE1	1:A:97:LYS:CA	2.25	0.67
1:C:391:PHE:N	1:C:392:PRO:HD3	2.10	0.67
1:C:378:THR:HA	2:C:703:SO4:O1	1.95	0.66
1:A:87:ALA:N	1:A:149:ASN:OD1	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:SER:HB3	1:A:442:LEU:HG	1.77	0.66
1:B:18:GLU:O	1:B:22:LYS:HG3	1.95	0.66
1:B:253:VAL:HG23	1:B:254:GLU:N	2.08	0.66
1:D:132:MET:HA	1:D:147:LEU:HG	1.75	0.66
1:D:312:SER:O	1:D:314:GLU:N	2.29	0.66
1:B:241:MET:HE2	1:B:310:MET:CE	2.25	0.66
1:C:321:PRO:HD2	1:C:322:LEU:H	1.59	0.66
1:A:43:HIS:O	1:A:47:ILE:HG13	1.94	0.66
1:D:94:THR:HG23	1:D:107:ALA:HB2	1.78	0.66
1:C:94:THR:HG23	1:C:107:ALA:HA	1.75	0.66
1:D:67:THR:HG22	1:D:192:SER:HB2	1.78	0.66
1:D:360:ARG:NH2	1:D:364:GLU:OE1	2.27	0.66
1:A:86:LYS:O	1:A:89:GLN:HG2	1.94	0.65
1:C:95:THR:HB	1:C:140:ASN:CB	2.24	0.65
1:C:170:LEU:HD22	1:C:174:ASP:CB	2.25	0.65
1:B:11:GLY:O	1:B:15:GLU:N	2.29	0.65
1:C:373:LEU:HD12	1:C:395:THR:O	1.95	0.65
1:A:171:ALA:HB3	1:A:174:ASP:CG	2.22	0.65
1:B:268:ILE:HD13	1:B:391:PHE:CE1	2.32	0.65
1:C:207:LEU:O	1:C:212:GLY:N	2.28	0.65
1:A:163:VAL:HG12	1:A:165:ILE:CD1	2.20	0.65
1:D:273:VAL:HG12	1:D:307:ASP:CG	2.22	0.65
1:A:94:THR:HG23	1:A:107:ALA:HB2	1.79	0.65
1:D:47:ILE:O	1:D:51:ARG:HG2	1.97	0.65
1:D:65:LEU:HD23	1:D:65:LEU:C	2.22	0.65
1:D:124:LEU:HD12	1:D:161:PRO:CD	2.27	0.65
1:A:171:ALA:H	1:A:174:ASP:HB2	1.62	0.64
1:A:75:MET:HE1	1:A:97:LYS:HA	1.80	0.64
1:A:374:ILE:O	1:A:376:VAL:HG23	1.97	0.64
1:B:379:GLN:N	2:B:702:SO4:O2	2.29	0.64
1:D:39:ASP:OD1	1:D:42:GLU:HG3	1.98	0.64
1:D:69:GLY:HA2	1:D:174:ASP:OD2	1.97	0.64
1:C:93:PHE:HB2	1:C:142:VAL:HB	1.79	0.64
1:A:163:VAL:CG1	1:A:165:ILE:HD12	2.22	0.64
1:D:67:THR:HG21	3:D:2014:HOH:O	1.96	0.64
1:A:253:VAL:HG23	1:A:254:GLU:H	1.62	0.64
1:C:373:LEU:HA	1:C:394:ALA:HB1	1.80	0.64
1:C:415:VAL:HG12	1:C:416:VAL:N	2.11	0.64
1:B:117:LEU:HD13	1:B:160:LEU:HD13	1.80	0.64
1:B:372:PRO:HD2	1:B:448:VAL:O	1.97	0.64
1:C:117:LEU:HD13	1:C:160:LEU:HD13	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:LEU:N	1:C:154:GLU:OE2	2.28	0.64
1:A:326:SER:O	1:A:330:THR:HG23	1.98	0.64
1:A:73:ARG:O	1:A:108:VAL:HA	1.98	0.63
1:B:342:ARG:HD2	1:B:391:PHE:CD1	2.33	0.63
1:D:12:PRO:HD3	1:D:46:ARG:HH12	1.61	0.63
1:A:170:LEU:HD11	1:A:178:LEU:HD12	1.80	0.63
1:D:16:SER:OG	1:D:19:MET:HB2	1.99	0.63
1:A:329:ALA:O	1:A:332:CYS:N	2.30	0.63
1:C:10:ILE:HG22	1:C:11:GLY:N	2.13	0.63
1:C:235:GLU:O	1:C:272:LYS:NZ	2.31	0.63
1:A:186:VAL:O	1:A:215:ILE:HG12	1.99	0.63
1:A:132:MET:HA	1:A:147:LEU:HG	1.80	0.63
1:A:170:LEU:HD11	1:A:178:LEU:CD1	2.28	0.63
1:B:10:ILE:HG12	1:B:31:MET:HG3	1.81	0.63
1:B:64:LEU:HD21	1:B:190:ALA:HB2	1.80	0.63
1:D:124:LEU:CD1	1:D:161:PRO:HG3	2.29	0.63
1:D:133:GLU:HG2	3:D:2009:HOH:O	1.99	0.62
1:A:257:ILE:HD11	3:A:2017:HOH:O	1.99	0.62
1:B:240:ILE:O	1:B:274:VAL:HA	2.00	0.62
1:C:170:LEU:CD1	1:C:175:LYS:HG2	2.25	0.62
1:D:72:ILE:HG23	1:D:110:TYR:CB	2.27	0.62
1:B:114:THR:OG1	1:B:115:THR:N	2.28	0.62
1:B:174:ASP:O	1:B:178:LEU:HG	2.00	0.62
1:C:65:LEU:C	1:C:65:LEU:HD23	2.24	0.62
1:A:78:GLU:HG3	1:A:101:GLY:O	1.99	0.62
1:B:65:LEU:C	1:B:65:LEU:HD23	2.25	0.62
1:A:388:ARG:HD3	1:A:388:ARG:C	2.25	0.61
1:B:5:LYS:HG3	1:B:410:VAL:O	2.00	0.61
1:D:159:ASN:CG	1:D:249:VAL:HG11	2.26	0.61
1:C:242:VAL:HG22	1:C:263:MET:HE3	1.82	0.61
1:B:87:ALA:N	1:B:149:ASN:OD1	2.29	0.61
1:C:75:MET:HE2	1:C:97:LYS:HG2	1.82	0.61
1:C:76:LYS:O	1:C:101:GLY:N	2.29	0.61
1:C:449:VAL:HG21	1:C:470:LEU:HD11	1.83	0.61
1:B:216:HIS:ND1	3:B:2017:HOH:O	2.24	0.61
1:D:321:PRO:O	1:D:325:VAL:HG23	2.01	0.61
1:B:391:PHE:N	1:B:392:PRO:HD3	2.16	0.61
1:C:312:SER:O	1:C:314:GLU:N	2.34	0.61
1:A:253:VAL:HG23	1:A:254:GLU:N	2.16	0.61
1:D:126:ASP:HB2	1:D:156:LYS:HG3	1.82	0.61
1:D:94:THR:HG23	1:D:107:ALA:CB	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:195:ARG:O	1:D:229:ASN:ND2	2.31	0.60
1:A:47:ILE:O	1:A:51:ARG:HG3	2.02	0.60
1:A:92:THR:HG23	1:A:143:ILE:HD13	1.81	0.60
1:D:373:LEU:HD12	1:D:395:THR:O	2.01	0.60
1:A:321:PRO:HD2	1:A:322:LEU:H	1.65	0.60
1:B:297:ASP:OD1	3:B:2027:HOH:O	2.16	0.60
1:B:379:GLN:O	1:B:405:THR:HG21	2.01	0.60
1:D:170:LEU:HD23	3:D:2014:HOH:O	2.02	0.60
1:B:244:ARG:HD2	1:B:256:VAL:CG1	2.31	0.60
1:B:388:ARG:HD3	1:B:388:ARG:C	2.27	0.60
1:D:165:ILE:N	1:D:165:ILE:HD12	2.17	0.60
1:D:342:ARG:HD2	1:D:391:PHE:CD1	2.36	0.60
1:D:126:ASP:CB	1:D:156:LYS:HG3	2.31	0.60
1:D:244:ARG:HD2	1:D:256:VAL:CG1	2.32	0.60
1:C:132:MET:HB3	1:C:146:VAL:HA	1.83	0.60
1:C:172:GLU:HA	1:C:172:GLU:OE1	2.01	0.60
1:D:297:ASP:OD1	3:D:2029:HOH:O	2.16	0.60
1:A:75:MET:HE1	1:A:97:LYS:HB3	1.84	0.59
1:B:230:PHE:CE2	1:B:263:MET:CG	2.85	0.59
1:B:171:ALA:O	1:B:174:ASP:N	2.35	0.59
1:D:302:ILE:HB	1:D:335:THR:HG21	1.85	0.59
1:B:312:SER:O	1:B:314:GLU:N	2.36	0.59
1:D:443:ALA:C	1:D:444:HIS:CD2	2.80	0.59
1:B:403:GLU:HG2	1:B:419:LEU:HD22	1.84	0.59
1:B:51:ARG:HA	1:B:54:MET:HE2	1.85	0.59
1:C:170:LEU:HD23	1:C:174:ASP:HB3	1.81	0.59
1:A:241:MET:CE	1:A:310:MET:HE1	2.32	0.59
1:B:241:MET:HE1	1:B:310:MET:HE1	1.81	0.59
1:C:152:LEU:HD12	1:C:153:GLY:O	2.02	0.59
1:D:51:ARG:NH2	1:D:184:GLN:O	2.36	0.59
1:B:10:ILE:CG1	1:B:31:MET:HG3	2.33	0.59
1:B:67:THR:HG22	1:B:192:SER:H	1.68	0.59
1:B:312:SER:C	1:B:314:GLU:H	2.11	0.59
1:D:92:THR:HG23	1:D:143:ILE:HD13	1.84	0.59
1:C:77:LEU:HG	1:C:154:GLU:CG	2.32	0.59
1:A:321:PRO:O	1:A:325:VAL:HG23	2.02	0.58
1:B:67:THR:CG2	1:B:192:SER:H	2.16	0.58
1:C:136:ALA:HB3	1:C:143:ILE:HB	1.85	0.58
1:D:31:MET:HE3	1:D:33:LEU:HD21	1.85	0.58
1:C:195:ARG:O	1:C:225:GLU:HG2	2.02	0.58
1:A:75:MET:HE1	1:A:97:LYS:CB	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:302:ILE:O	1:D:305:GLY:N	2.34	0.58
1:D:422:GLU:HG3	1:D:423:ILE:N	2.19	0.58
1:A:73:ARG:NH1	1:A:155:ASN:O	2.36	0.58
1:B:343:LEU:O	1:B:360:ARG:HD2	2.03	0.58
1:D:253:VAL:HG23	1:D:254:GLU:N	2.18	0.58
1:B:10:ILE:HD11	1:B:23:MET:HE1	1.84	0.58
1:D:231:ASP:OD1	1:D:266:LYS:NZ	2.35	0.58
1:A:422:GLU:HG3	1:A:423:ILE:N	2.19	0.58
1:A:216:HIS:HB3	1:A:238:ASP:CB	2.34	0.58
1:C:452:VAL:HG12	1:C:453:SER:N	2.18	0.58
1:A:3:LYS:HZ1	1:A:393:ASP:C	2.07	0.58
1:B:171:ALA:O	1:B:174:ASP:HB2	2.04	0.58
1:B:449:VAL:CG2	1:B:470:LEU:HD11	2.34	0.58
1:C:388:ARG:HB2	1:C:396:ILE:CD1	2.34	0.57
1:D:262:MET:SD	1:D:266:LYS:HE3	2.44	0.57
1:A:124:LEU:CD1	1:A:161:PRO:HG3	2.34	0.57
1:A:452:VAL:CG1	1:A:462:THR:HG21	2.35	0.57
1:C:170:LEU:HD13	1:C:175:LYS:CG	2.29	0.57
1:D:15:GLU:HB3	1:D:46:ARG:HD3	1.85	0.57
1:A:67:THR:O	1:A:192:SER:OG	2.23	0.57
1:B:117:LEU:HD11	1:B:160:LEU:HD22	1.86	0.57
1:B:391:PHE:N	1:B:392:PRO:CD	2.66	0.57
1:B:422:GLU:HG3	1:B:423:ILE:N	2.19	0.57
1:C:67:THR:O	1:C:192:SER:OG	2.21	0.57
1:C:230:PHE:CE1	1:C:263:MET:HG2	2.40	0.57
1:B:413:LYS:O	1:B:415:VAL:N	2.37	0.57
1:C:10:ILE:CG1	1:C:31:MET:HG3	2.34	0.57
1:A:10:ILE:CG1	1:A:31:MET:HG3	2.35	0.57
1:C:10:ILE:HG13	1:C:31:MET:HG3	1.87	0.57
1:A:378:THR:OG1	1:A:381:GLY:HA2	2.05	0.57
1:B:132:MET:HA	1:B:147:LEU:HG	1.85	0.57
1:B:403:GLU:HG2	1:B:419:LEU:CD2	2.35	0.57
1:D:75:MET:CE	1:D:97:LYS:HA	2.35	0.57
1:A:171:ALA:H	1:A:174:ASP:CB	2.17	0.57
1:A:187:ASP:HA	1:A:404:LYS:HE3	1.87	0.57
1:A:195:ARG:HB3	1:A:225:GLU:HG2	1.86	0.57
1:C:30:VAL:HG22	1:C:62:ALA:HB3	1.86	0.57
1:C:35:PHE:CZ	1:C:43:HIS:CD2	2.92	0.57
1:C:241:MET:HE2	1:C:310:MET:CE	2.34	0.56
1:C:274:VAL:HG13	1:C:274:VAL:O	2.03	0.56
1:D:253:VAL:HG23	1:D:254:GLU:H	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:434:LYS:CG	1:B:451:MET:HE1	2.36	0.56
1:C:240:ILE:CG2	1:C:241:MET:N	2.65	0.56
1:C:431:ARG:HD3	1:C:432:LEU:N	2.21	0.56
1:D:343:LEU:O	1:D:360:ARG:HD2	2.05	0.56
1:B:9:THR:HA	1:B:32:ARG:HB3	1.85	0.56
1:B:65:LEU:HD23	1:B:66:ASP:N	2.20	0.56
1:D:312:SER:C	1:D:314:GLU:H	2.13	0.56
1:C:417:PRO:HB3	3:C:2024:HOH:O	2.06	0.56
1:A:73:ARG:O	1:A:109:THR:N	2.37	0.56
1:C:400:THR:O	1:C:420:VAL:N	2.36	0.56
1:D:440:SER:C	1:D:442:LEU:H	2.14	0.56
1:A:466:SER:OG	1:A:468:HIS:NE2	2.38	0.56
1:B:51:ARG:NH2	1:B:184:GLN:O	2.39	0.56
1:C:73:ARG:HD3	1:C:155:ASN:OD1	2.06	0.56
1:C:195:ARG:HB3	1:C:225:GLU:CD	2.30	0.56
1:A:72:ILE:HG23	1:A:110:TYR:HB3	1.88	0.55
1:A:341:SER:HA	1:A:391:PHE:O	2.05	0.55
1:A:360:ARG:NH2	1:A:364:GLU:OE1	2.39	0.55
1:B:240:ILE:HG23	1:B:241:MET:N	2.21	0.55
1:C:388:ARG:C	1:C:388:ARG:HD3	2.31	0.55
1:D:94:THR:CG2	1:D:107:ALA:HB2	2.35	0.55
1:D:171:ALA:HB3	1:D:174:ASP:CG	2.31	0.55
1:D:358:VAL:HG21	1:D:463:ASN:HA	1.88	0.55
1:D:359:CYS:O	1:D:363:VAL:HG23	2.06	0.55
1:B:81:ASN:HA	3:B:2004:HOH:O	2.06	0.55
1:C:369:LEU:O	1:C:370:ASP:HB2	2.06	0.55
1:D:10:ILE:CG1	1:D:31:MET:HG3	2.36	0.55
1:B:242:VAL:HG22	1:B:263:MET:HE3	1.89	0.55
1:B:440:SER:C	1:B:442:LEU:H	2.14	0.55
1:C:195:ARG:N	1:C:195:ARG:HD3	2.22	0.55
1:A:18:GLU:N	1:A:18:GLU:OE1	2.40	0.55
1:A:165:ILE:HD12	1:A:165:ILE:N	2.22	0.55
1:C:244:ARG:HD2	1:C:256:VAL:HG12	1.89	0.55
1:A:358:VAL:HG21	1:A:463:ASN:HA	1.88	0.55
1:C:363:VAL:O	1:C:366:ALA:HB3	2.06	0.55
1:D:19:MET:O	1:D:23:MET:HG2	2.07	0.55
1:A:430:TYR:O	1:A:434:LYS:HG3	2.07	0.54
1:B:39:ASP:OD1	1:B:42:GLU:HG3	2.07	0.54
1:B:82:ASP:N	3:B:2004:HOH:O	2.28	0.54
1:B:96:ASP:OD2	1:B:99:VAL:HG23	2.07	0.54
1:D:140:ASN:OD1	1:D:141:LYS:HE2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:THR:HA	1:A:19:MET:HG2	1.89	0.54
1:A:303:LEU:HA	1:A:339:MET:HE3	1.89	0.54
1:A:379:GLN:O	1:A:405:THR:HG21	2.07	0.54
1:D:178:LEU:HD12	1:D:206:HIS:CD2	2.43	0.54
1:D:327:ILE:HG23	1:D:328:MET:N	2.21	0.54
1:A:312:SER:O	1:A:314:GLU:N	2.40	0.54
1:B:404:LYS:HE2	3:B:2032:HOH:O	2.07	0.54
1:C:70:PRO:HB2	1:C:167:LEU:HD12	1.89	0.54
1:D:190:ALA:HA	1:D:218:ILE:HB	1.89	0.54
1:A:50:LEU:O	1:A:54:MET:HG3	2.07	0.54
1:A:92:THR:O	1:A:105:MET:HG3	2.07	0.54
1:B:73:ARG:N	1:B:109:THR:OG1	2.39	0.54
1:D:154:GLU:HA	3:D:2011:HOH:O	2.06	0.54
1:B:74:THR:C	1:B:75:MET:HG3	2.30	0.54
1:B:327:ILE:HD11	1:D:253:VAL:HG21	1.89	0.54
1:C:124:LEU:HD11	1:C:161:PRO:CG	2.34	0.54
1:D:163:VAL:HG12	1:D:164:SER:N	2.22	0.54
1:A:378:THR:OG1	1:A:381:GLY:CA	2.56	0.54
1:C:216:HIS:CD2	1:C:408:GLN:NE2	2.76	0.54
1:A:10:ILE:HG22	1:A:11:GLY:N	2.23	0.54
1:A:341:SER:HB3	1:A:367:GLU:OE2	2.07	0.54
1:B:383:SER:HB3	1:B:462:THR:OG1	2.08	0.54
1:C:110:TYR:CE1	1:C:167:LEU:CD2	2.91	0.54
1:A:448:VAL:HG12	1:A:449:VAL:N	2.22	0.54
1:B:161:PRO:O	1:B:163:VAL:N	2.41	0.54
1:C:105:MET:HG3	1:C:106:VAL:N	2.22	0.54
1:D:5:LYS:HA	1:D:29:ASN:OD1	2.08	0.54
1:D:274:VAL:HG13	1:D:274:VAL:O	2.07	0.54
1:B:359:CYS:O	1:B:363:VAL:HG23	2.08	0.54
1:B:382:LYS:O	1:B:385:ARG:HB2	2.08	0.54
1:C:463:ASN:O	1:D:466:SER:HA	2.08	0.54
1:B:135:THR:OG1	1:B:143:ILE:HG22	2.08	0.53
1:C:73:ARG:O	1:C:108:VAL:HG12	2.07	0.53
1:A:39:ASP:OD1	1:A:42:GLU:HG3	2.08	0.53
1:B:12:PRO:HD3	1:B:46:ARG:HH12	1.73	0.53
1:A:422:GLU:CG	1:A:423:ILE:N	2.71	0.53
1:A:216:HIS:HB3	1:A:238:ASP:HB2	1.88	0.53
1:A:431:ARG:HD3	1:A:431:ARG:C	2.33	0.53
1:B:426:THR:HG22	1:B:430:TYR:CE2	2.43	0.53
1:C:77:LEU:H	1:C:154:GLU:CD	2.17	0.53
1:B:431:ARG:HD3	1:B:432:LEU:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:LEU:HD21	1:B:190:ALA:CB	2.39	0.53
1:B:324:ALA:O	1:B:327:ILE:HG22	2.08	0.53
1:C:324:ALA:O	1:C:327:ILE:HG22	2.08	0.53
1:D:378:THR:OG1	1:D:381:GLY:N	2.41	0.53
1:A:237:SER:O	1:A:272:LYS:NZ	2.31	0.53
1:A:355:THR:HG23	1:A:462:THR:HB	1.89	0.53
1:C:153:GLY:C	1:C:156:LYS:HE2	2.33	0.53
1:A:25:ASP:OD1	1:A:59:LYS:NZ	2.24	0.53
1:A:383:SER:HB3	1:A:462:THR:OG1	2.09	0.53
1:B:268:ILE:CD1	1:B:391:PHE:HZ	2.22	0.53
1:B:434:LYS:HG2	1:B:451:MET:HE1	1.90	0.53
1:C:312:SER:C	1:C:314:GLU:H	2.15	0.53
1:C:165:ILE:HG22	1:C:167:LEU:H	1.75	0.52
1:D:34:ASN:OD1	1:D:36:SER:HB2	2.08	0.52
1:A:240:ILE:CG2	1:A:241:MET:N	2.71	0.52
1:B:11:GLY:HA2	1:B:46:ARG:HH11	1.73	0.52
1:C:422:GLU:HG3	1:C:423:ILE:N	2.25	0.52
1:A:124:LEU:HD11	1:A:161:PRO:CG	2.40	0.52
1:B:377:ALA:HB2	1:B:429:PHE:CE1	2.45	0.52
1:D:391:PHE:N	1:D:392:PRO:CD	2.71	0.52
1:B:19:MET:O	1:B:23:MET:HG3	2.08	0.52
1:C:466:SER:OG	1:C:468:HIS:NE2	2.42	0.52
1:A:268:ILE:HD13	1:A:391:PHE:CE1	2.44	0.52
1:A:416:VAL:HG12	1:A:416:VAL:O	2.10	0.52
1:C:302:ILE:HA	1:C:306:THR:HG22	1.92	0.52
1:C:383:SER:HB3	1:C:462:THR:OG1	2.08	0.52
1:D:50:LEU:HD23	1:D:63:ILE:HD11	1.90	0.52
1:D:65:LEU:C	1:D:65:LEU:CD2	2.82	0.52
1:A:75:MET:HE2	1:A:97:LYS:HA	1.92	0.52
1:A:94:THR:CG2	1:A:107:ALA:HB2	2.40	0.52
1:A:388:ARG:HB2	1:A:396:ILE:HD12	1.91	0.52
1:B:191:ALA:O	1:B:220:LYS:HB2	2.10	0.52
1:B:411:LEU:HD12	1:B:411:LEU:O	2.09	0.52
1:C:75:MET:HE1	1:C:97:LYS:HG2	1.91	0.52
1:D:230:PHE:CD2	1:D:263:MET:HG2	2.44	0.52
1:A:397:LEU:HD12	1:A:416:VAL:O	2.10	0.52
1:B:244:ARG:HD2	1:B:256:VAL:HG12	1.92	0.52
1:C:251:ILE:HB	1:C:252:PRO:HD2	1.91	0.52
1:D:431:ARG:HD3	1:D:432:LEU:N	2.25	0.52
1:A:77:LEU:HD23	1:A:101:GLY:HA3	1.91	0.52
1:B:87:ALA:C	1:B:89:GLN:H	2.18	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:ALA:HA	1:B:450:VAL:HG21	1.91	0.52
1:A:312:SER:C	1:A:314:GLU:H	2.18	0.51
1:A:359:CYS:SG	1:A:386:ALA:HB1	2.50	0.51
1:A:440:SER:C	1:A:442:LEU:H	2.18	0.51
1:B:253:VAL:HG21	1:D:327:ILE:HD11	1.92	0.51
1:C:372:PRO:HD2	1:C:448:VAL:O	2.10	0.51
1:D:321:PRO:HD2	1:D:322:LEU:H	1.74	0.51
1:A:244:ARG:HD2	1:A:256:VAL:CG1	2.40	0.51
1:A:426:THR:HG22	1:A:430:TYR:CE2	2.46	0.51
1:C:110:TYR:O	1:C:113:PHE:HB2	2.11	0.51
1:C:152:LEU:HD12	1:C:152:LEU:C	2.35	0.51
1:C:175:LYS:HB3	1:C:206:HIS:CE1	2.46	0.51
1:D:9:THR:HA	1:D:32:ARG:HB3	1.92	0.51
1:A:401:THR:HG22	1:A:420:VAL:O	2.11	0.51
1:B:363:VAL:HG21	1:B:390:TYR:HB2	1.93	0.51
1:A:440:SER:HB3	1:A:442:LEU:CG	2.40	0.51
1:B:10:ILE:HD12	1:B:23:MET:HE1	1.90	0.51
1:D:43:HIS:O	1:D:46:ARG:HB3	2.10	0.51
1:D:385:ARG:O	1:D:388:ARG:N	2.44	0.51
1:B:264:ILE:O	1:B:268:ILE:HG13	2.10	0.51
1:D:422:GLU:CG	1:D:423:ILE:N	2.74	0.51
1:A:136:ALA:HB3	1:A:143:ILE:HB	1.92	0.51
1:D:430:TYR:HD1	1:D:451:MET:SD	2.34	0.51
1:A:95:THR:HB	1:A:140:ASN:HB2	1.92	0.51
1:A:126:ASP:HB3	1:A:129:LEU:HB3	1.93	0.51
1:B:249:VAL:HG12	1:B:249:VAL:O	2.11	0.51
1:C:110:TYR:CD1	1:C:167:LEU:CD2	2.94	0.51
1:D:119:VAL:HG13	1:D:134:VAL:O	2.10	0.51
1:A:398:ALA:C	1:A:399:LEU:HD12	2.35	0.50
1:B:10:ILE:CD1	1:B:23:MET:CE	2.87	0.50
1:D:291:THR:O	1:D:294:GLU:HB2	2.10	0.50
1:B:167:LEU:O	1:B:195:ARG:NH2	2.45	0.50
1:A:124:LEU:HD11	1:A:161:PRO:HG3	1.94	0.50
1:A:366:ALA:HA	1:A:450:VAL:HG21	1.93	0.50
1:B:77:LEU:N	1:B:154:GLU:HG2	2.27	0.50
1:C:10:ILE:CG2	1:C:11:GLY:N	2.74	0.50
1:D:365:THR:HG22	1:D:369:LEU:HD12	1.91	0.50
1:B:5:LYS:HB2	1:B:308:ALA:HB2	1.93	0.50
1:C:373:LEU:CA	1:C:394:ALA:HB1	2.40	0.50
1:A:7:VAL:HG11	1:A:310:MET:CE	2.42	0.50
1:B:160:LEU:HB2	1:B:165:ILE:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:359:CYS:O	1:C:363:VAL:HG23	2.12	0.50
1:D:94:THR:HG22	1:D:107:ALA:HA	1.93	0.50
1:A:74:THR:OG1	1:A:156:LYS:N	2.42	0.50
1:A:298:VAL:O	1:A:301:ALA:N	2.45	0.50
1:B:187:ASP:HA	1:B:404:LYS:HE3	1.92	0.50
1:C:127:ASP:C	1:C:249:VAL:HG13	2.36	0.50
1:C:426:THR:HG22	1:C:430:TYR:CE2	2.47	0.50
1:A:7:VAL:HG11	1:A:310:MET:HE2	1.93	0.50
1:B:62:ALA:HA	3:B:2011:HOH:O	2.11	0.50
1:A:422:GLU:CG	1:A:423:ILE:H	2.25	0.50
1:B:251:ILE:HD11	1:B:256:VAL:HG22	1.94	0.50
1:B:327:ILE:CG2	1:B:328:MET:N	2.75	0.50
1:C:391:PHE:N	1:C:392:PRO:CD	2.75	0.50
1:B:422:GLU:CG	1:B:423:ILE:N	2.75	0.49
1:C:78:GLU:HG3	1:C:100:ILE:HG22	1.93	0.49
1:A:327:ILE:CG2	1:A:328:MET:N	2.75	0.49
1:B:67:THR:HG22	1:B:192:SER:N	2.26	0.49
1:B:214:ASN:O	1:B:408:GLN:NE2	2.44	0.49
1:C:119:VAL:HG13	1:C:135:THR:CA	2.42	0.49
1:D:336:ASP:O	1:D:338:VAL:N	2.45	0.49
1:C:430:TYR:HD1	1:C:451:MET:SD	2.35	0.49
1:D:110:TYR:O	1:D:113:PHE:HB2	2.12	0.49
1:D:293:ALA:O	1:D:297:ASP:HB2	2.12	0.49
1:A:5:LYS:HB2	1:A:308:ALA:HB2	1.95	0.49
1:B:9:THR:OG1	1:B:32:ARG:HD3	2.12	0.49
1:B:31:MET:HE1	1:B:47:ILE:HA	1.94	0.49
1:D:254:GLU:N	1:D:254:GLU:OE1	2.34	0.49
1:D:377:ALA:HB2	1:D:429:PHE:CE1	2.48	0.49
1:B:3:LYS:NZ	1:B:393:ASP:O	2.45	0.49
1:B:189:VAL:HG23	1:B:215:ILE:HG21	1.95	0.49
1:C:30:VAL:HG21	1:C:411:LEU:HD13	1.95	0.49
1:C:222:GLU:O	1:C:223:ASN:HB3	2.13	0.49
1:C:240:ILE:HG23	1:C:241:MET:N	2.28	0.49
1:A:426:THR:CG2	1:A:430:TYR:CE2	2.96	0.49
1:B:74:THR:O	1:B:155:ASN:HA	2.13	0.49
1:B:255:GLU:OE2	1:D:334:ARG:NE	2.39	0.49
1:C:94:THR:CG2	1:C:107:ALA:CA	2.91	0.49
1:D:75:MET:HE1	1:D:97:LYS:HA	1.94	0.49
1:D:382:LYS:HB2	2:D:704:SO4:O1	2.12	0.49
1:D:415:VAL:HG12	1:D:416:VAL:N	2.27	0.49
1:A:50:LEU:HD23	1:A:63:ILE:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:VAL:HG23	1:A:215:ILE:CG2	2.42	0.49
1:A:268:ILE:HD13	1:A:391:PHE:CZ	2.47	0.49
1:C:94:THR:HG22	1:C:107:ALA:HA	1.92	0.49
1:C:171:ALA:N	1:C:174:ASP:HB2	2.28	0.49
1:C:449:VAL:CG2	1:C:470:LEU:HD11	2.41	0.49
1:D:73:ARG:O	1:D:108:VAL:HA	2.12	0.49
1:A:112:GLY:O	1:A:115:THR:HB	2.12	0.49
1:A:171:ALA:O	1:A:174:ASP:HB2	2.12	0.49
1:B:274:VAL:HG13	1:B:274:VAL:O	2.13	0.49
1:B:360:ARG:NH2	1:B:364:GLU:OE1	2.42	0.49
1:C:378:THR:CG2	1:C:381:GLY:HA2	2.43	0.49
1:D:94:THR:CG2	1:D:107:ALA:HA	2.43	0.49
1:D:163:VAL:CG1	1:D:164:SER:N	2.76	0.49
1:A:35:PHE:CE1	1:A:65:LEU:HG	2.48	0.49
1:A:235:GLU:O	1:A:272:LYS:NZ	2.45	0.49
1:B:421:LYS:O	1:B:422:GLU:HB2	2.13	0.49
1:C:119:VAL:HG13	1:C:135:THR:HA	1.95	0.49
1:C:170:LEU:HD22	1:C:174:ASP:C	2.38	0.49
1:D:241:MET:HE2	1:D:310:MET:HE1	1.95	0.49
1:A:241:MET:HE2	1:A:310:MET:HE1	1.95	0.48
1:C:43:HIS:O	1:C:47:ILE:HG13	2.12	0.48
1:C:207:LEU:HD13	1:C:215:ILE:HG21	1.95	0.48
1:A:32:ARG:HD2	1:A:310:MET:HE2	1.95	0.48
1:D:343:LEU:O	1:D:344:GLU:O	2.32	0.48
1:A:117:LEU:HG	1:A:134:VAL:HG21	1.95	0.48
1:D:388:ARG:HD3	1:D:388:ARG:C	2.38	0.48
1:B:253:VAL:HG23	1:B:254:GLU:OE1	2.13	0.48
1:C:239:GLY:O	1:C:240:ILE:HG12	2.13	0.48
1:A:65:LEU:HD23	1:A:66:ASP:N	2.29	0.48
1:B:86:LYS:O	1:B:89:GLN:HG2	2.13	0.48
1:C:354:ILE:HG21	1:C:354:ILE:HD13	1.48	0.48
1:D:230:PHE:CE2	1:D:263:MET:CG	2.93	0.48
1:B:10:ILE:HD11	1:B:23:MET:CE	2.43	0.48
1:C:105:MET:CG	1:C:106:VAL:N	2.74	0.48
1:C:327:ILE:CG2	1:C:328:MET:N	2.76	0.48
1:C:378:THR:CA	2:C:703:SO4:O1	2.60	0.48
1:D:95:THR:HB	1:D:140:ASN:HB2	1.95	0.48
1:B:83:VAL:HG11	1:B:103:SER:N	2.28	0.48
1:C:51:ARG:NH2	1:C:184:GLN:O	2.44	0.48
1:A:422:GLU:CD	1:A:423:ILE:H	2.22	0.48
1:C:407:HIS:O	1:C:410:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:GLU:CD	1:D:102:ASN:HB3	2.38	0.48
1:D:327:ILE:CG2	1:D:328:MET:N	2.76	0.48
1:A:88:GLY:N	1:A:146:VAL:O	2.47	0.48
1:A:124:LEU:HD12	1:A:161:PRO:HG3	1.96	0.48
1:A:424:THR:HG23	1:A:428:ASP:OD2	2.14	0.48
1:B:7:VAL:HG11	1:B:310:MET:HE2	1.95	0.48
1:C:125:VAL:O	1:C:126:ASP:O	2.30	0.48
1:D:131:GLY:C	1:D:132:MET:HG3	2.39	0.48
1:D:449:VAL:N	1:D:468:HIS:O	2.46	0.48
1:A:251:ILE:HD12	1:A:255:GLU:HB2	1.96	0.48
1:B:86:LYS:HA	1:B:149:ASN:OD1	2.14	0.48
1:B:269:ARG:HA	1:B:389:LYS:HE3	1.96	0.48
1:C:110:TYR:CE1	1:C:167:LEU:HD23	2.49	0.48
1:C:132:MET:N	1:C:147:LEU:CD2	2.75	0.48
1:C:158:VAL:HG12	1:C:159:ASN:N	2.29	0.48
1:A:327:ILE:HG23	1:A:328:MET:N	2.29	0.47
1:B:193:PHE:CD2	1:B:195:ARG:HD2	2.49	0.47
1:C:35:PHE:HB3	1:C:177:ASP:OD2	2.14	0.47
1:C:254:GLU:H	1:C:254:GLU:CD	2.21	0.47
1:D:251:ILE:HB	1:D:252:PRO:HD2	1.96	0.47
1:A:73:ARG:HD3	1:A:155:ASN:OD1	2.14	0.47
1:B:200:VAL:HG22	1:B:219:SER:OG	2.14	0.47
1:C:440:SER:C	1:C:442:LEU:H	2.21	0.47
1:D:192:SER:HA	1:D:220:LYS:HD3	1.96	0.47
1:A:65:LEU:HD23	1:A:65:LEU:C	2.40	0.47
1:B:16:SER:OG	1:B:19:MET:HB2	2.14	0.47
1:B:167:LEU:HB3	1:B:168:PRO:CD	2.41	0.47
1:D:390:TYR:C	1:D:392:PRO:HD3	2.40	0.47
1:A:75:MET:HB2	3:A:2010:HOH:O	2.15	0.47
1:D:175:LYS:O	1:D:179:ILE:HG13	2.14	0.47
1:A:34:ASN:C	1:A:36:SER:H	2.22	0.47
1:A:197:ARG:HB2	1:A:232:GLU:CD	2.40	0.47
1:B:7:VAL:CG1	1:B:32:ARG:HB2	2.44	0.47
1:B:343:LEU:O	1:B:344:GLU:O	2.32	0.47
1:B:422:GLU:HG3	1:B:423:ILE:H	1.79	0.47
1:C:244:ARG:CD	1:C:256:VAL:HG12	2.44	0.47
1:A:249:VAL:HG12	1:A:249:VAL:O	2.13	0.47
1:B:422:GLU:CG	1:B:423:ILE:H	2.28	0.47
1:C:273:VAL:HG11	3:C:2025:HOH:O	2.14	0.47
1:C:378:THR:HG21	1:C:381:GLY:HA2	1.95	0.47
1:D:298:VAL:O	1:D:301:ALA:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:LEU:C	1:A:65:LEU:CD2	2.88	0.47
1:A:132:MET:HG2	1:A:146:VAL:HA	1.97	0.47
1:A:399:LEU:HD21	1:A:436:LEU:HD12	1.96	0.47
1:B:452:VAL:HG12	1:B:453:SER:N	2.29	0.47
1:C:92:THR:HA	1:C:142:VAL:O	2.15	0.47
1:C:102:ASN:OD1	1:C:104:GLU:N	2.40	0.47
1:C:244:ARG:HD2	1:C:256:VAL:CG1	2.44	0.47
1:C:401:THR:HA	1:C:420:VAL:O	2.14	0.47
1:D:391:PHE:N	1:D:392:PRO:HD3	2.29	0.47
1:A:244:ARG:HG3	1:A:244:ARG:HH11	1.80	0.47
1:D:266:LYS:HG2	1:D:269:ARG:HH12	1.79	0.47
1:A:10:ILE:CG2	1:A:11:GLY:N	2.77	0.47
1:A:124:LEU:CD1	1:A:161:PRO:CG	2.92	0.47
1:A:415:VAL:HG12	1:A:416:VAL:N	2.29	0.47
1:C:26:ALA:HB3	1:C:325:VAL:HG11	1.96	0.47
1:B:11:GLY:O	1:B:14:THR:N	2.39	0.47
1:C:72:ILE:HG12	1:C:110:TYR:HB3	1.96	0.47
1:C:86:LYS:O	1:C:89:GLN:HG2	2.15	0.47
1:C:195:ARG:HD3	1:C:195:ARG:H	1.79	0.47
1:B:5:LYS:HA	1:B:5:LYS:HD3	1.76	0.46
1:B:440:SER:C	1:B:442:LEU:N	2.73	0.46
1:C:18:GLU:O	1:C:22:LYS:HG3	2.15	0.46
1:C:32:ARG:HD2	1:C:310:MET:HE2	1.96	0.46
1:C:378:THR:OG1	1:C:381:GLY:CA	2.63	0.46
1:B:293:ALA:O	1:B:297:ASP:HB2	2.15	0.46
1:B:369:LEU:HA	1:B:369:LEU:HD23	1.71	0.46
1:D:342:ARG:HD2	1:D:391:PHE:CE1	2.51	0.46
1:D:407:HIS:O	1:D:410:VAL:HG23	2.15	0.46
1:B:240:ILE:CG2	1:B:241:MET:N	2.76	0.46
1:B:67:THR:HG21	3:B:2010:HOH:O	2.15	0.46
1:B:126:ASP:CG	1:B:156:LYS:HG3	2.40	0.46
1:C:5:LYS:HA	1:C:29:ASN:OD1	2.16	0.46
1:C:379:GLN:O	1:C:405:THR:HG21	2.15	0.46
1:C:422:GLU:CG	1:C:423:ILE:N	2.77	0.46
1:D:191:ALA:CB	1:D:203:ILE:CD1	2.93	0.46
1:A:125:VAL:HG12	1:A:126:ASP:N	2.29	0.46
1:B:77:LEU:HD11	1:B:152:LEU:HG	1.97	0.46
1:B:327:ILE:HD12	1:B:327:ILE:HA	1.73	0.46
1:C:165:ILE:O	1:C:195:ARG:NH2	2.49	0.46
1:C:375:VAL:HG12	1:C:376:VAL:N	2.29	0.46
1:A:422:GLU:HG3	1:A:423:ILE:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:LEU:HD23	1:D:28:MET:HE3	1.98	0.46
1:D:187:ASP:HA	1:D:404:LYS:HE3	1.97	0.46
1:B:93:PHE:HB2	1:B:142:VAL:HB	1.98	0.46
1:B:230:PHE:CE2	1:B:263:MET:SD	3.09	0.46
1:A:5:LYS:HG3	1:A:410:VAL:O	2.16	0.46
1:A:165:ILE:CD1	1:A:165:ILE:N	2.78	0.46
1:A:195:ARG:O	1:A:225:GLU:HG2	2.16	0.46
1:A:244:ARG:HD2	1:A:256:VAL:HG12	1.98	0.46
1:D:372:PRO:HD2	1:D:448:VAL:O	2.15	0.46
1:B:10:ILE:HG22	1:B:11:GLY:N	2.31	0.46
1:B:15:GLU:CB	1:B:46:ARG:HD3	2.46	0.46
1:B:85:LEU:O	1:B:149:ASN:HA	2.15	0.46
1:B:104:GLU:O	3:B:2007:HOH:O	2.20	0.46
1:C:78:GLU:OE1	3:C:2004:HOH:O	2.21	0.46
1:B:133:GLU:O	1:B:144:CYS:HB3	2.16	0.46
1:C:11:GLY:CA	1:C:46:ARG:NH1	2.76	0.46
1:B:43:HIS:O	1:B:46:ARG:HB3	2.16	0.45
1:C:31:MET:HE3	1:C:33:LEU:CD2	2.39	0.45
1:D:156:LYS:HD3	1:D:156:LYS:HA	1.55	0.45
1:D:230:PHE:CD1	1:D:230:PHE:C	2.94	0.45
1:D:354:ILE:O	1:D:358:VAL:HG23	2.16	0.45
1:D:363:VAL:O	1:D:367:GLU:HG3	2.16	0.45
1:A:5:LYS:HA	1:A:29:ASN:OD1	2.16	0.45
1:D:253:VAL:HG23	1:D:254:GLU:OE1	2.16	0.45
1:A:171:ALA:H	1:A:174:ASP:CG	2.23	0.45
1:C:190:ALA:HA	1:C:218:ILE:HB	1.97	0.45
1:C:254:GLU:OE1	1:C:254:GLU:N	2.33	0.45
1:C:343:LEU:O	1:C:344:GLU:O	2.35	0.45
1:D:444:HIS:CD2	1:D:444:HIS:N	2.84	0.45
1:C:93:PHE:HA	1:C:106:VAL:O	2.16	0.45
1:C:266:LYS:HG2	1:C:269:ARG:HH12	1.81	0.45
1:C:358:VAL:HG21	1:C:463:ASN:HA	1.98	0.45
1:A:110:TYR:OH	1:A:116:ASP:OD2	2.27	0.45
1:A:241:MET:HE1	1:A:310:MET:HE1	1.97	0.45
1:C:154:GLU:O	1:C:155:ASN:HB3	2.17	0.45
1:D:422:GLU:CG	1:D:423:ILE:H	2.29	0.45
1:A:171:ALA:O	1:A:175:LYS:HG3	2.17	0.45
1:B:24:LEU:HD23	1:B:28:MET:HE3	1.99	0.45
1:B:179:ILE:O	1:B:179:ILE:HG22	2.16	0.45
1:B:362:ALA:O	1:B:366:ALA:HB2	2.17	0.45
1:C:113:PHE:CD2	1:C:142:VAL:HG21	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:GLU:CB	1:D:46:ARG:HD3	2.46	0.45
1:D:17:GLU:HG2	1:D:49:ASN:HB3	1.98	0.45
1:A:407:HIS:O	1:A:410:VAL:HG23	2.16	0.45
1:B:310:MET:HG2	1:B:311:LEU:N	2.32	0.45
1:C:16:SER:OG	1:C:19:MET:HB2	2.16	0.45
1:C:217:ILE:O	1:C:238:ASP:HB2	2.17	0.45
1:D:10:ILE:HG13	1:D:31:MET:SD	2.57	0.45
1:D:216:HIS:ND1	3:D:2020:HOH:O	2.36	0.45
1:D:275:ILE:HA	1:D:308:ALA:O	2.17	0.45
1:D:416:VAL:O	1:D:416:VAL:HG12	2.16	0.45
1:A:240:ILE:HG23	1:A:241:MET:N	2.32	0.45
1:A:440:SER:HB3	1:A:442:LEU:CD1	2.47	0.45
1:B:216:HIS:CE1	3:B:2017:HOH:O	2.69	0.45
1:C:12:PRO:HA	1:C:15:GLU:OE2	2.17	0.45
1:C:344:GLU:N	3:C:2022:HOH:O	2.48	0.45
1:D:124:LEU:CD1	1:D:161:PRO:CG	2.95	0.45
1:A:362:ALA:O	1:A:366:ALA:HB2	2.17	0.45
1:C:65:LEU:C	1:C:65:LEU:CD2	2.88	0.45
1:C:91:PHE:HE2	1:C:106:VAL:HG12	1.82	0.45
1:C:216:HIS:CD2	1:C:408:GLN:HE22	2.35	0.45
1:C:443:ALA:C	1:C:444:HIS:CG	2.95	0.45
1:D:240:ILE:CG2	1:D:241:MET:N	2.80	0.45
1:D:443:ALA:C	1:D:444:HIS:CG	2.95	0.45
1:B:47:ILE:O	1:B:51:ARG:HG2	2.16	0.44
1:B:70:PRO:O	1:B:71:GLU:HG3	2.17	0.44
1:B:419:LEU:HD12	1:B:419:LEU:HA	1.53	0.44
1:C:35:PHE:HE2	1:C:40:TYR:CE1	2.35	0.44
1:A:171:ALA:CB	1:A:174:ASP:CG	2.90	0.44
1:A:191:ALA:CB	1:A:194:ILE:HD11	2.46	0.44
1:A:307:ASP:HA	1:A:413:LYS:HB2	1.99	0.44
1:D:219:SER:HB2	1:D:240:ILE:CD1	2.45	0.44
1:D:327:ILE:O	1:D:328:MET:C	2.60	0.44
1:B:366:ALA:HA	1:B:450:VAL:CG2	2.48	0.44
1:B:426:THR:CG2	1:B:430:TYR:CE2	3.00	0.44
1:D:20:LEU:O	1:D:23:MET:HB2	2.17	0.44
1:D:50:LEU:O	1:D:54:MET:HG3	2.17	0.44
1:A:70:PRO:C	1:A:71:GLU:HG3	2.42	0.44
1:A:172:GLU:HA	1:A:172:GLU:OE1	2.17	0.44
1:C:170:LEU:O	1:C:175:LYS:HE3	2.17	0.44
1:D:374:ILE:O	1:D:376:VAL:HG23	2.18	0.44
1:D:422:GLU:HG3	1:D:423:ILE:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ILE:C	1:A:138:GLU:HG3	2.42	0.44
1:A:193:PHE:O	1:A:195:ARG:HD3	2.17	0.44
1:B:77:LEU:H	1:B:154:GLU:CD	2.25	0.44
1:D:15:GLU:HB3	1:D:46:ARG:CD	2.48	0.44
1:D:77:LEU:H	1:D:154:GLU:HG2	1.83	0.44
1:D:77:LEU:N	1:D:154:GLU:HG2	2.32	0.44
1:A:170:LEU:CD1	1:A:178:LEU:HD12	2.46	0.44
1:A:466:SER:HA	1:B:463:ASN:O	2.17	0.44
1:C:203:ILE:O	1:C:207:LEU:HG	2.18	0.44
1:C:260:GLN:O	1:C:264:ILE:HG13	2.18	0.44
1:D:42:GLU:O	1:D:46:ARG:HB2	2.17	0.44
1:D:75:MET:HE1	1:D:97:LYS:CA	2.48	0.44
1:D:448:VAL:O	1:D:449:VAL:HG23	2.17	0.44
1:C:96:ASP:CG	1:C:99:VAL:HG23	2.42	0.44
1:C:188:PHE:CD2	1:C:216:HIS:HB2	2.53	0.44
1:D:9:THR:OG1	1:D:32:ARG:HD3	2.18	0.44
1:B:132:MET:CA	1:B:147:LEU:HG	2.48	0.44
1:B:242:VAL:HG12	1:B:244:ARG:HG2	1.99	0.44
1:B:311:LEU:HA	1:B:311:LEU:HD23	1.73	0.44
1:C:165:ILE:HD12	1:C:165:ILE:N	2.32	0.44
1:D:114:THR:HG21	1:D:140:ASN:HA	2.00	0.44
1:D:421:LYS:O	1:D:422:GLU:HB2	2.18	0.44
1:A:89:GLN:O	1:A:89:GLN:HG3	2.12	0.44
1:A:391:PHE:N	1:A:392:PRO:CD	2.81	0.44
1:B:63:ILE:HG22	1:B:186:VAL:HG12	2.00	0.44
1:B:64:LEU:HD23	1:B:65:LEU:C	2.43	0.44
1:B:197:ARG:HB2	1:B:232:GLU:CD	2.42	0.44
1:C:74:THR:O	1:C:155:ASN:HA	2.18	0.44
1:D:77:LEU:HA	1:D:77:LEU:HD23	1.50	0.44
1:D:204:ARG:HA	1:D:217:ILE:HD11	1.99	0.44
1:A:452:VAL:CG1	1:A:462:THR:CG2	2.96	0.43
1:B:73:ARG:HG2	1:B:157:GLY:HA2	2.00	0.43
1:C:253:VAL:H	1:C:253:VAL:HG22	1.42	0.43
1:C:321:PRO:O	1:C:325:VAL:HG23	2.18	0.43
1:D:10:ILE:CG2	1:D:46:ARG:HD2	2.37	0.43
1:D:12:PRO:HA	1:D:15:GLU:OE2	2.18	0.43
1:D:73:ARG:NH1	1:D:155:ASN:O	2.51	0.43
1:A:5:LYS:HA	1:A:5:LYS:HD3	1.85	0.43
1:A:191:ALA:HB2	1:A:203:ILE:CD1	2.48	0.43
1:A:375:VAL:C	1:A:376:VAL:HG23	2.42	0.43
1:A:434:LYS:HG3	1:A:451:MET:HE1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:ALA:HA	1:B:218:ILE:HB	2.00	0.43
1:B:366:ALA:CA	1:B:450:VAL:HG21	2.48	0.43
1:C:140:ASN:OD1	1:C:141:LYS:HE2	2.18	0.43
1:C:369:LEU:HA	1:C:369:LEU:HD23	1.68	0.43
1:C:415:VAL:CG1	1:C:416:VAL:N	2.80	0.43
1:A:77:LEU:HD11	1:A:152:LEU:HG	1.99	0.43
1:A:132:MET:CA	1:A:147:LEU:HG	2.48	0.43
1:A:298:VAL:O	1:A:301:ALA:HB3	2.17	0.43
1:B:161:PRO:C	1:B:163:VAL:H	2.26	0.43
1:C:91:PHE:CE2	1:C:106:VAL:HG12	2.53	0.43
1:C:170:LEU:CD2	1:C:174:ASP:CB	2.88	0.43
1:C:178:LEU:O	1:C:181:GLY:N	2.51	0.43
1:C:196:LYS:HZ3	1:C:199:ASP:CG	2.26	0.43
1:C:419:LEU:HD12	1:C:419:LEU:HA	1.75	0.43
1:A:7:VAL:CG1	1:A:310:MET:HE2	2.49	0.43
1:B:262:MET:HE3	1:B:262:MET:HB3	1.68	0.43
1:C:9:THR:HA	1:C:32:ARG:HB3	1.99	0.43
1:D:403:GLU:HG2	1:D:419:LEU:CD2	2.49	0.43
1:A:230:PHE:CE2	1:A:263:MET:HG2	2.54	0.43
1:A:312:SER:C	1:A:314:GLU:N	2.77	0.43
1:B:64:LEU:HA	1:B:188:PHE:O	2.19	0.43
1:B:455:ALA:H	1:B:457:VAL:HG22	1.83	0.43
1:C:137:ILE:HA	1:C:141:LYS:O	2.19	0.43
1:C:186:VAL:O	1:C:404:LYS:NZ	2.47	0.43
1:B:339:MET:HE2	1:B:339:MET:HB3	1.88	0.43
1:C:136:ALA:O	1:C:143:ILE:N	2.44	0.43
1:C:207:LEU:HD13	1:C:215:ILE:CG2	2.49	0.43
1:C:440:SER:HB3	1:C:442:LEU:HG	2.01	0.43
1:A:244:ARG:HG3	1:A:244:ARG:NH1	2.33	0.43
1:A:298:VAL:HG12	1:A:299:ALA:N	2.34	0.43
1:B:65:LEU:C	1:B:65:LEU:CD2	2.92	0.43
1:B:83:VAL:O	1:B:83:VAL:HG23	2.19	0.43
1:B:310:MET:CG	1:B:311:LEU:N	2.82	0.43
1:C:40:TYR:HB3	1:C:180:PHE:CE2	2.53	0.43
1:C:61:ALA:HA	1:C:410:VAL:HG11	2.01	0.43
1:C:77:LEU:H	1:C:154:GLU:HG2	1.84	0.43
1:C:94:THR:HA	1:C:140:ASN:O	2.19	0.43
1:A:23:MET:HB2	1:A:28:MET:CE	2.49	0.43
1:D:3:LYS:HB3	1:D:414:GLY:CA	2.49	0.43
1:D:35:PHE:HZ	1:D:180:PHE:CE2	2.37	0.43
1:D:124:LEU:HD11	1:D:161:PRO:CG	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:154:GLU:O	1:D:156:LYS:CE	2.59	0.43
1:A:188:PHE:CD2	1:A:218:ILE:HD11	2.54	0.42
1:A:241:MET:HE2	1:A:310:MET:CE	2.49	0.42
1:C:18:GLU:H	1:C:18:GLU:CD	2.27	0.42
1:C:67:THR:CG2	1:C:68:LYS:N	2.78	0.42
1:D:396:ILE:HB	1:D:415:VAL:HA	2.01	0.42
1:B:375:VAL:HG12	1:B:376:VAL:N	2.33	0.42
1:B:434:LYS:HG3	1:B:451:MET:HE1	1.99	0.42
1:C:77:LEU:N	1:C:154:GLU:HG2	2.34	0.42
1:C:399:LEU:HD21	1:C:436:LEU:HD12	2.00	0.42
1:D:5:LYS:HB2	1:D:308:ALA:HB2	2.00	0.42
1:D:244:ARG:CD	1:D:256:VAL:CG1	2.96	0.42
1:A:23:MET:CB	1:A:28:MET:CE	2.94	0.42
1:A:170:LEU:HD23	1:A:170:LEU:HA	1.83	0.42
1:B:117:LEU:CD1	1:B:160:LEU:HD13	2.49	0.42
1:B:247:LEU:O	1:B:251:ILE:HG12	2.19	0.42
1:B:431:ARG:HD3	1:B:431:ARG:C	2.45	0.42
1:D:188:PHE:CD1	1:D:216:HIS:CB	3.01	0.42
1:D:415:VAL:CG1	1:D:416:VAL:N	2.81	0.42
1:D:457:VAL:HA	1:D:458:PRO:HD3	1.84	0.42
1:A:31:MET:HE3	1:A:33:LEU:CD2	2.34	0.42
1:A:378:THR:OG1	1:A:381:GLY:N	2.52	0.42
1:C:78:GLU:CG	1:C:100:ILE:HG22	2.49	0.42
1:C:298:VAL:O	1:C:301:ALA:N	2.52	0.42
1:C:327:ILE:HD12	1:C:327:ILE:HA	1.75	0.42
1:D:440:SER:C	1:D:442:LEU:N	2.77	0.42
1:A:23:MET:HB2	1:A:28:MET:HE2	1.99	0.42
1:A:126:ASP:O	1:A:129:LEU:N	2.38	0.42
1:A:234:LEU:O	1:A:234:LEU:HG	2.15	0.42
1:A:436:LEU:HA	1:A:436:LEU:HD23	1.74	0.42
1:C:94:THR:HG22	1:C:106:VAL:O	2.19	0.42
1:C:135:THR:OG1	1:C:136:ALA:N	2.53	0.42
1:C:251:ILE:HB	1:C:252:PRO:CD	2.49	0.42
1:C:341:SER:HB3	1:C:367:GLU:OE2	2.20	0.42
1:C:436:LEU:O	1:C:439:GLN:N	2.52	0.42
1:D:311:LEU:HD23	1:D:311:LEU:HA	1.43	0.42
1:A:34:ASN:C	1:A:36:SER:N	2.77	0.42
1:C:244:ARG:NH1	1:C:260:GLN:OE1	2.43	0.42
1:A:76:LYS:HA	1:A:154:GLU:OE2	2.19	0.42
1:A:85:LEU:N	1:A:150:GLY:O	2.41	0.42
1:A:191:ALA:HB1	1:A:194:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:416:VAL:O	1:C:416:VAL:HG12	2.19	0.42
1:D:170:LEU:HD22	1:D:174:ASP:HB3	2.01	0.42
1:B:369:LEU:O	1:B:370:ASP:HB2	2.18	0.42
1:A:327:ILE:HA	1:A:327:ILE:HD12	1.69	0.42
1:A:434:LYS:HB3	1:A:434:LYS:HE2	1.89	0.42
1:B:23:MET:CB	1:B:28:MET:HE2	2.50	0.42
1:B:312:SER:C	1:B:314:GLU:N	2.73	0.42
1:C:94:THR:N	1:C:106:VAL:O	2.51	0.42
1:C:253:VAL:HG23	1:C:254:GLU:H	1.84	0.42
1:C:267:CYS:O	1:C:270:ALA:HB3	2.19	0.42
1:D:64:LEU:HA	1:D:188:PHE:O	2.20	0.42
1:D:73:ARG:HB2	1:D:109:THR:HG21	2.02	0.42
1:D:75:MET:HE1	1:D:97:LYS:CB	2.50	0.42
1:D:257:ILE:HD12	1:D:257:ILE:HA	1.80	0.42
1:A:63:ILE:HD13	1:A:63:ILE:HG21	1.79	0.42
1:A:195:ARG:HD3	1:A:195:ARG:N	2.34	0.42
1:B:64:LEU:HD23	1:B:64:LEU:C	2.45	0.42
1:B:402:ASN:OD1	1:B:404:LYS:N	2.53	0.42
1:B:462:THR:O	1:B:463:ASN:HB3	2.20	0.42
1:C:135:THR:HG1	1:C:143:ILE:C	2.24	0.42
1:C:463:ASN:OD1	1:C:463:ASN:C	2.62	0.42
1:A:5:LYS:O	1:A:308:ALA:HA	2.20	0.41
1:A:388:ARG:HB2	1:A:396:ILE:HD11	1.99	0.41
1:C:134:VAL:HG22	1:C:144:CYS:SG	2.59	0.41
1:C:431:ARG:HD3	1:C:431:ARG:C	2.45	0.41
1:D:35:PHE:CZ	1:D:43:HIS:CD2	3.07	0.41
1:B:10:ILE:HD12	1:B:10:ILE:HG23	1.77	0.41
1:B:266:LYS:HG2	1:B:269:ARG:HH12	1.85	0.41
1:C:73:ARG:O	1:C:108:VAL:HA	2.20	0.41
1:C:327:ILE:HG23	1:C:328:MET:N	2.35	0.41
1:B:74:THR:HG1	1:B:156:LYS:H	1.66	0.41
1:B:170:LEU:HD23	3:B:2010:HOH:O	2.19	0.41
1:C:434:LYS:HE2	1:C:434:LYS:HB3	1.82	0.41
1:D:136:ALA:HB3	1:D:143:ILE:HB	2.02	0.41
1:D:341:SER:HA	1:D:391:PHE:O	2.20	0.41
1:A:336:ASP:C	1:A:338:VAL:H	2.27	0.41
1:C:77:LEU:H	1:C:154:GLU:CG	2.32	0.41
1:C:321:PRO:CD	1:C:322:LEU:H	2.31	0.41
1:C:422:GLU:CG	1:C:423:ILE:H	2.33	0.41
1:D:5:LYS:HG3	1:D:411:LEU:O	2.21	0.41
1:D:165:ILE:N	1:D:165:ILE:CD1	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:229:ASN:O	1:D:232:GLU:HG2	2.19	0.41
1:D:268:ILE:HD13	1:D:391:PHE:CZ	2.55	0.41
1:A:35:PHE:CD1	1:A:65:LEU:HG	2.56	0.41
1:A:163:VAL:CG1	1:A:165:ILE:CD1	2.92	0.41
1:A:252:PRO:HB2	1:A:255:GLU:HG2	2.03	0.41
1:B:10:ILE:CG2	1:B:11:GLY:N	2.84	0.41
1:C:435:GLU:HG2	3:C:2028:HOH:O	2.20	0.41
1:D:5:LYS:HG3	1:D:410:VAL:O	2.19	0.41
1:D:343:LEU:HD23	1:D:343:LEU:HA	1.70	0.41
1:A:335:THR:O	1:A:339:MET:HG3	2.21	0.41
1:D:11:GLY:HA2	1:D:46:ARG:NH1	2.35	0.41
1:D:180:PHE:O	1:D:183:GLU:HB2	2.21	0.41
1:D:362:ALA:O	1:D:366:ALA:HB2	2.21	0.41
1:D:451:MET:O	1:D:465:ALA:HA	2.20	0.41
1:A:343:LEU:O	1:A:344:GLU:O	2.39	0.41
1:C:422:GLU:CD	1:C:423:ILE:H	2.29	0.41
1:D:165:ILE:HD12	1:D:165:ILE:H	1.82	0.41
1:D:373:LEU:HD11	1:D:397:LEU:HB2	2.01	0.41
1:A:9:THR:OG1	1:A:32:ARG:HD3	2.21	0.41
1:A:125:VAL:CG1	1:A:126:ASP:N	2.82	0.41
1:A:190:ALA:HA	1:A:218:ILE:O	2.21	0.41
1:A:355:THR:O	1:A:359:CYS:SG	2.77	0.41
1:A:448:VAL:C	1:A:449:VAL:HG23	2.45	0.41
1:B:73:ARG:HD3	1:B:155:ASN:OD1	2.20	0.41
1:B:163:VAL:CG1	1:B:164:SER:N	2.84	0.41
1:B:244:ARG:CD	1:B:256:VAL:HG12	2.51	0.41
1:D:231:ASP:HB2	3:D:2022:HOH:O	2.19	0.41
1:A:39:ASP:OD1	1:A:39:ASP:C	2.63	0.41
1:B:77:LEU:H	1:B:154:GLU:HG2	1.86	0.41
1:B:187:ASP:OD2	3:B:2011:HOH:O	2.21	0.41
1:B:374:ILE:HA	1:B:450:VAL:O	2.21	0.41
1:C:110:TYR:HD1	1:C:167:LEU:HD21	1.80	0.41
1:C:113:PHE:HD2	1:C:142:VAL:HG21	1.85	0.41
1:C:201:ILE:HD12	1:C:201:ILE:HG23	1.92	0.41
1:C:310:MET:HG2	1:C:311:LEU:N	2.36	0.41
1:D:229:ASN:O	1:D:230:PHE:C	2.62	0.41
1:D:403:GLU:HG2	1:D:419:LEU:HD22	2.03	0.41
1:A:74:THR:O	1:A:155:ASN:HA	2.21	0.41
1:A:208:LYS:C	1:A:210:HIS:H	2.29	0.41
1:A:264:ILE:O	1:A:268:ILE:HG13	2.20	0.41
1:B:404:LYS:O	1:B:407:HIS:N	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:ILE:HG23	1:C:218:ILE:HD12	1.75	0.41
1:D:395:THR:HG22	1:D:396:ILE:N	2.35	0.41
1:A:40:TYR:HE1	1:A:177:ASP:OD1	2.04	0.40
1:B:11:GLY:CA	1:B:46:ARG:HH11	2.33	0.40
1:B:378:THR:O	1:B:400:THR:HB	2.21	0.40
1:B:422:GLU:CD	1:B:423:ILE:H	2.29	0.40
1:C:243:ALA:O	1:C:247:LEU:HB2	2.21	0.40
1:A:35:PHE:CD1	1:A:65:LEU:HD21	2.56	0.40
1:A:143:ILE:HD12	1:A:143:ILE:HG23	1.91	0.40
1:A:398:ALA:O	1:A:418:GLN:N	2.54	0.40
1:B:101:GLY:HA2	1:B:105:MET:O	2.21	0.40
1:B:434:LYS:HB3	1:B:434:LYS:HE2	1.82	0.40
1:B:452:VAL:CG1	1:B:453:SER:N	2.84	0.40
1:C:321:PRO:CD	1:C:322:LEU:N	2.84	0.40
1:C:436:LEU:HD23	1:C:436:LEU:HA	1.77	0.40
1:D:79:GLY:C	1:D:81:ASN:N	2.77	0.40
1:B:341:SER:HA	1:B:391:PHE:O	2.21	0.40
1:C:70:PRO:HB2	1:C:167:LEU:CD1	2.50	0.40
1:C:426:THR:CG2	1:C:430:TYR:CE2	3.04	0.40
1:D:403:GLU:O	1:D:404:LYS:C	2.61	0.40
1:A:240:ILE:O	1:A:274:VAL:HA	2.21	0.40
1:A:266:LYS:HG2	1:A:269:ARG:HH12	1.87	0.40
1:A:321:PRO:CD	1:A:322:LEU:H	2.30	0.40
1:A:434:LYS:CG	1:A:451:MET:HE1	2.51	0.40
1:B:30:VAL:HG12	1:B:31:MET:N	2.35	0.40
1:C:170:LEU:HD21	1:C:178:LEU:CD1	2.44	0.40
1:C:273:VAL:CG1	3:C:2025:HOH:O	2.68	0.40
1:C:417:PRO:HD3	3:C:2024:HOH:O	2.21	0.40
1:D:124:LEU:CD1	1:D:161:PRO:CD	2.99	0.40
1:D:132:MET:N	1:D:147:LEU:HD12	2.36	0.40
1:D:132:MET:CA	1:D:147:LEU:HG	2.47	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:LYS:NZ	1:D:213:GLU:OE2[4_446]	2.14	0.06

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	438/470 (93%)	398 (91%)	32 (7%)	8 (2%)	6	1
1	B	438/470 (93%)	401 (92%)	32 (7%)	5 (1%)	11	3
1	C	438/470 (93%)	398 (91%)	36 (8%)	4 (1%)	14	5
1	D	438/470 (93%)	405 (92%)	28 (6%)	5 (1%)	11	3
All	All	1752/1880 (93%)	1602 (91%)	128 (7%)	22 (1%)	9	3

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	414	GLY
1	C	313	GLY
1	D	313	GLY
1	D	337	ARG
1	A	88	GLY
1	A	127	ASP
1	A	313	GLY
1	B	162	GLY
1	B	313	GLY
1	B	463	ASN
1	C	126	ASP
1	D	414	GLY
1	A	126	ASP
1	A	463	ASN
1	B	88	GLY
1	C	127	ASP
1	A	337	ARG
1	C	414	GLY
1	D	126	ASP
1	D	453	SER
1	A	209	ALA
1	A	194	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	358/389 (92%)	352 (98%)	6 (2%)	53	45
1	B	358/389 (92%)	353 (99%)	5 (1%)	59	52
1	C	358/389 (92%)	345 (96%)	13 (4%)	31	18
1	D	358/389 (92%)	350 (98%)	8 (2%)	45	34
All	All	1432/1556 (92%)	1400 (98%)	32 (2%)	45	34

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	LEU
1	A	67	THR
1	A	95	THR
1	A	145	LYS
1	A	160	LEU
1	A	392	PRO
1	B	60	THR
1	B	67	THR
1	B	95	THR
1	B	117	LEU
1	B	431	ARG
1	C	51	ARG
1	C	65	LEU
1	C	76	LYS
1	C	97	LYS
1	C	105	MET
1	C	108	VAL
1	C	117	LEU
1	C	118	SER
1	C	132	MET
1	C	147	LEU
1	C	152	LEU
1	C	253	VAL
1	C	431	ARG

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Mol	Chain	Res	Type
1	D	64	LEU
1	D	67	THR
1	D	95	THR
1	D	156	LYS
1	D	330	THR
1	D	333	GLU
1	D	431	ARG
1	D	459	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	49	ASN
1	A	81	ASN
1	A	206	HIS
1	A	216	HIS
1	A	300	ASN
1	B	48	GLN
1	B	81	ASN
1	B	206	HIS
1	B	214	ASN
1	B	300	ASN
1	C	43	HIS
1	C	81	ASN
1	C	121	ASN
1	C	210	HIS
1	C	216	HIS
1	C	223	ASN
1	C	300	ASN
1	C	407	HIS
1	C	408	GLN
1	C	444	HIS
1	D	43	HIS
1	D	81	ASN
1	D	206	HIS
1	D	210	HIS
1	D	214	ASN
1	D	224	GLN
1	D	300	ASN
1	D	379	GLN
1	D	444	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
2	SO4	A	701	-	4,4,4	1.17	0	6,6,6	1.08	0
2	SO4	D	704	-	4,4,4	1.17	0	6,6,6	1.08	0
2	SO4	B	702	-	4,4,4	1.17	0	6,6,6	1.08	0
2	SO4	C	703	-	4,4,4	1.18	0	6,6,6	1.08	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	704	SO4	1	0
2	B	702	SO4	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	703	SO4	3	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

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	A	446/470 (94%)	1.34	108 (24%) 2 1	12, 27, 59, 87	0
1	B	446/470 (94%)	1.44	117 (26%) 1 1	12, 27, 59, 87	0
1	C	446/470 (94%)	1.61	125 (28%) 1 1	11, 27, 58, 88	0
1	D	446/470 (94%)	1.40	104 (23%) 2 1	11, 27, 59, 88	0
All	All	1784/1880 (94%)	1.45	454 (25%) 1 1	11, 27, 59, 88	0

All (454) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	313	GLY	7.6
1	C	100	ILE	6.3
1	C	153	GLY	6.0
1	C	77	LEU	6.0
1	B	279	MET	5.9
1	B	11	GLY	5.9
1	C	99	VAL	5.8
1	D	314	GLU	5.6
1	C	134	VAL	5.6
1	C	460	GLY	5.6
1	D	147	LEU	5.6
1	A	279	MET	5.5
1	C	41	ALA	5.4
1	D	100	ILE	5.4
1	C	83	VAL	5.3
1	C	101	GLY	5.3
1	C	35	PHE	5.3
1	C	144	CYS	5.1
1	D	313	GLY	5.0
1	C	120	GLY	5.0
1	C	137	ILE	4.9

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Mol	Chain	Res	Type	RSRZ
1	C	155	ASN	4.9
1	C	102	ASN	4.8
1	C	119	VAL	4.8
1	C	95	THR	4.7
1	C	40	TYR	4.7
1	D	424	THR	4.7
1	B	458	PRO	4.6
1	B	313	GLY	4.6
1	B	135	THR	4.6
1	A	137	ILE	4.6
1	B	100	ILE	4.6
1	B	428	ASP	4.6
1	A	428	ASP	4.5
1	B	460	GLY	4.5
1	B	1	MET	4.5
1	C	178	LEU	4.4
1	D	1	MET	4.4
1	C	37	HIS	4.4
1	D	279	MET	4.3
1	C	90	THR	4.3
1	C	142	VAL	4.3
1	D	77	LEU	4.2
1	C	36	SER	4.2
1	B	147	LEU	4.1
1	C	170	LEU	4.1
1	C	80	GLY	4.1
1	C	141	LYS	4.1
1	C	143	ILE	4.1
1	B	101	GLY	4.1
1	A	423	ILE	4.1
1	D	107	ALA	4.1
1	D	461	THR	4.1
1	C	135	THR	4.0
1	C	138	GLU	4.0
1	C	458	PRO	4.0
1	C	314	GLU	4.0
1	C	174	ASP	4.0
1	C	438	LEU	4.0
1	A	100	ILE	4.0
1	D	423	ILE	4.0
1	C	133	GLU	3.9
1	D	393	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	458	PRO	3.9
1	C	115	THR	3.9
1	D	76	LYS	3.9
1	C	152	LEU	3.9
1	C	459	SER	3.9
1	C	105	MET	3.9
1	A	115	THR	3.9
1	B	321	PRO	3.8
1	C	38	GLY	3.8
1	D	312	SER	3.8
1	B	293	ALA	3.8
1	D	38	GLY	3.7
1	A	462	THR	3.7
1	C	81	ASN	3.7
1	A	87	ALA	3.7
1	D	83	VAL	3.7
1	A	96	ASP	3.7
1	A	314	GLU	3.7
1	A	119	VAL	3.7
1	B	107	ALA	3.6
1	C	78	GLU	3.6
1	B	99	VAL	3.6
1	D	105	MET	3.6
1	B	314	GLU	3.6
1	C	76	LYS	3.6
1	C	79	GLY	3.6
1	A	163	VAL	3.6
1	B	37	HIS	3.6
1	C	106	VAL	3.6
1	C	114	THR	3.6
1	C	461	THR	3.6
1	A	101	GLY	3.5
1	D	11	GLY	3.5
1	C	103	SER	3.5
1	A	448	VAL	3.5
1	D	438	LEU	3.5
1	C	91	PHE	3.5
1	A	170	LEU	3.5
1	B	139	GLY	3.5
1	C	98	SER	3.5
1	C	92	THR	3.5
1	D	321	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	423	ILE	3.5
1	D	79	GLY	3.5
1	D	81	ASN	3.4
1	C	75	MET	3.4
1	C	171	ALA	3.4
1	C	456	LEU	3.4
1	A	18	GLU	3.4
1	D	443	ALA	3.4
1	C	104	GLU	3.4
1	A	454	GLY	3.4
1	D	458	PRO	3.4
1	C	110	TYR	3.3
1	B	38	GLY	3.3
1	A	420	VAL	3.3
1	D	117	LEU	3.3
1	C	136	ALA	3.3
1	B	444	HIS	3.3
1	B	79	GLY	3.3
1	A	143	ILE	3.3
1	A	208	LYS	3.3
1	D	457	VAL	3.3
1	C	379	GLN	3.3
1	D	33	LEU	3.3
1	D	18	GLU	3.2
1	C	107	ALA	3.2
1	A	424	THR	3.2
1	B	462	THR	3.2
1	B	117	LEU	3.2
1	C	93	PHE	3.2
1	C	312	SER	3.2
1	C	111	GLU	3.2
1	D	371	ALA	3.2
1	B	90	THR	3.2
1	C	150	GLY	3.2
1	D	428	ASP	3.2
1	C	94	THR	3.1
1	C	173	LYS	3.1
1	B	98	SER	3.1
1	B	438	LEU	3.1
1	C	43	HIS	3.1
1	D	88	GLY	3.1
1	C	154	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	193	PHE	3.1
1	C	327	ILE	3.1
1	D	325	VAL	3.1
1	C	151	ASP	3.0
1	A	77	LEU	3.0
1	B	289	ARG	3.0
1	B	136	ALA	3.0
1	C	175	LYS	3.0
1	C	121	ASN	3.0
1	C	113	PHE	3.0
1	D	459	SER	3.0
1	A	12	PRO	3.0
1	B	12	PRO	3.0
1	C	12	PRO	3.0
1	A	107	ALA	3.0
1	C	279	MET	3.0
1	B	221	ILE	3.0
1	B	138	GLU	3.0
1	B	142	VAL	3.0
1	D	99	VAL	3.0
1	A	461	THR	3.0
1	A	441	GLY	3.0
1	C	214	ASN	3.0
1	C	108	VAL	2.9
1	D	249	VAL	2.9
1	B	379	GLN	2.9
1	B	115	THR	2.9
1	A	321	PRO	2.9
1	A	136	ALA	2.9
1	C	366	ALA	2.9
1	C	156	LYS	2.9
1	C	428	ASP	2.9
1	A	78	GLU	2.9
1	D	101	GLY	2.9
1	D	309	VAL	2.9
1	A	95	THR	2.9
1	D	455	ALA	2.9
1	A	422	GLU	2.9
1	A	438	LEU	2.9
1	C	165	ILE	2.9
1	C	88	GLY	2.9
1	C	140	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	40	TYR	2.8
1	A	379	GLN	2.8
1	A	444	HIS	2.8
1	D	37	HIS	2.8
1	D	324	ALA	2.8
1	C	147	LEU	2.8
1	D	85	LEU	2.8
1	A	106	VAL	2.8
1	B	312	SER	2.8
1	A	139	GLY	2.8
1	A	368	LYS	2.8
1	A	311	LEU	2.8
1	B	373	LEU	2.8
1	B	422	GLU	2.8
1	A	165	ILE	2.8
1	D	67	THR	2.8
1	C	321	PRO	2.8
1	D	448	VAL	2.8
1	A	121	ASN	2.7
1	D	87	ALA	2.7
1	D	135	THR	2.7
1	A	111	GLU	2.7
1	B	430	TYR	2.7
1	A	446	GLY	2.7
1	B	57	THR	2.7
1	B	355	THR	2.7
1	A	147	LEU	2.7
1	A	86	LYS	2.7
1	A	142	VAL	2.7
1	A	460	GLY	2.7
1	C	67	THR	2.7
1	A	419	LEU	2.7
1	C	354	ILE	2.7
1	B	134	VAL	2.7
1	D	106	VAL	2.7
1	D	153	GLY	2.6
1	B	292	ASP	2.6
1	B	92	THR	2.6
1	C	14	THR	2.6
1	D	401	THR	2.6
1	A	36	SER	2.6
1	C	167	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	311	LEU	2.6
1	C	206	HIS	2.6
1	D	143	ILE	2.6
1	A	134	VAL	2.6
1	C	443	ALA	2.6
1	A	145	LYS	2.6
1	B	76	LYS	2.6
1	D	444	HIS	2.6
1	B	436	LEU	2.6
1	B	143	ILE	2.6
1	A	313	GLY	2.6
1	A	361	GLY	2.6
1	D	82	ASP	2.6
1	A	437	ALA	2.6
1	B	208	LYS	2.6
1	D	141	LYS	2.6
1	B	40	TYR	2.6
1	A	35	PHE	2.6
1	D	379	GLN	2.6
1	B	78	GLU	2.6
1	C	374	ILE	2.6
1	A	445	LYS	2.6
1	D	208	LYS	2.6
1	A	457	VAL	2.6
1	A	140	ASN	2.6
1	A	43	HIS	2.5
1	B	91	PHE	2.5
1	A	432	LEU	2.5
1	B	20	LEU	2.5
1	C	85	LEU	2.5
1	C	130	ILE	2.5
1	C	305	GLY	2.5
1	A	459	SER	2.5
1	D	440	SER	2.5
1	D	372	PRO	2.5
1	B	185	GLY	2.5
1	A	10	ILE	2.5
1	D	354	ILE	2.5
1	D	149	ASN	2.5
1	B	455	ALA	2.5
1	C	426	THR	2.5
1	D	429	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	81	ASN	2.5
1	B	103	SER	2.5
1	C	10	ILE	2.5
1	A	138	GLU	2.5
1	B	157	GLY	2.4
1	A	114	THR	2.4
1	A	135	THR	2.4
1	C	74	THR	2.4
1	D	357	ALA	2.4
1	D	378	THR	2.4
1	B	83	VAL	2.4
1	B	106	VAL	2.4
1	B	161	PRO	2.4
1	A	456	LEU	2.4
1	B	459	SER	2.4
1	D	383	SER	2.4
1	D	421	LYS	2.4
1	B	114	THR	2.4
1	B	401	THR	2.4
1	A	431	ARG	2.4
1	A	309	VAL	2.4
1	C	44	GLY	2.4
1	B	19	MET	2.4
1	B	75	MET	2.4
1	B	105	MET	2.4
1	A	164	SER	2.4
1	A	33	LEU	2.4
1	D	411	LEU	2.4
1	B	93	PHE	2.4
1	D	35	PHE	2.4
1	B	95	THR	2.4
1	B	461	THR	2.4
1	D	74	THR	2.4
1	D	70	PRO	2.4
1	A	155	ASN	2.4
1	B	200	VAL	2.4
1	B	249	VAL	2.4
1	B	457	VAL	2.4
1	C	457	VAL	2.4
1	B	368	LYS	2.4
1	B	96	ASP	2.3
1	A	167	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	303	LEU	2.3
1	A	430	TYR	2.3
1	B	109	THR	2.3
1	C	42	GLU	2.3
1	B	268	ILE	2.3
1	A	162	GLY	2.3
1	A	125	VAL	2.3
1	A	312	SER	2.3
1	D	370	ASP	2.3
1	D	431	ARG	2.3
1	B	45	GLN	2.3
1	C	129	LEU	2.3
1	C	176	GLN	2.3
1	D	432	LEU	2.3
1	C	1	MET	2.3
1	C	404	LYS	2.3
1	D	59	LYS	2.3
1	B	104	GLU	2.3
1	A	144	CYS	2.3
1	B	210	HIS	2.3
1	A	91	PHE	2.3
1	B	445	LYS	2.3
1	D	13	LYS	2.3
1	D	145	LYS	2.3
1	D	368	LYS	2.3
1	B	443	ALA	2.3
1	B	153	GLY	2.3
1	B	218	ILE	2.3
1	B	264	ILE	2.3
1	D	356	GLU	2.3
1	D	358	VAL	2.3
1	A	149	ASN	2.3
1	A	1	MET	2.3
1	B	424	THR	2.3
1	C	117	LEU	2.3
1	C	355	THR	2.3
1	A	212	GLY	2.2
1	A	433	GLY	2.2
1	A	443	ALA	2.2
1	C	162	GLY	2.2
1	C	193	PHE	2.2
1	B	376	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	149	ASN	2.2
1	D	52	ASN	2.2
1	D	57	THR	2.2
1	D	289	ARG	2.2
1	A	117	LEU	2.2
1	D	343	LEU	2.2
1	C	118	SER	2.2
1	D	209	ALA	2.2
1	A	173	LYS	2.2
1	A	214	ASN	2.2
1	A	404	LYS	2.2
1	A	253	VAL	2.2
1	A	449	VAL	2.2
1	C	146	VAL	2.2
1	B	356	GLU	2.2
1	D	95	THR	2.2
1	C	373	LEU	2.2
1	D	454	GLY	2.2
1	B	26	ALA	2.2
1	D	327	ILE	2.2
1	B	173	LYS	2.2
1	B	404	LYS	2.2
1	B	294	GLU	2.2
1	D	202	GLU	2.2
1	D	125	VAL	2.2
1	D	256	VAL	2.2
1	B	278	THR	2.2
1	B	440	SER	2.2
1	B	112	GLY	2.2
1	B	120	GLY	2.2
1	A	41	ALA	2.2
1	A	141	LYS	2.2
1	D	422	GLU	2.1
1	C	96	ASP	2.1
1	A	146	VAL	2.1
1	B	189	VAL	2.1
1	C	449	VAL	2.1
1	A	157	GLY	2.1
1	C	289	ARG	2.1
1	D	24	LEU	2.1
1	D	205	GLU	2.1
1	A	113	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	201	ILE	2.1
1	C	82	ASP	2.1
1	C	424	THR	2.1
1	D	115	THR	2.1
1	D	198	SER	2.1
1	B	162	GLY	2.1
1	B	141	LYS	2.1
1	B	267	CYS	2.1
1	D	332	CYS	2.1
1	B	121	ASN	2.1
1	B	322	LEU	2.1
1	B	362	ALA	2.1
1	B	113	PHE	2.1
1	B	374	ILE	2.1
1	B	198	SER	2.1
1	C	55	SER	2.1
1	C	73	ARG	2.1
1	A	94	THR	2.1
1	B	86	LYS	2.1
1	C	382	LYS	2.1
1	C	445	LYS	2.1
1	D	78	GLU	2.1
1	D	344	GLU	2.1
1	D	355	THR	2.1
1	C	212	GLY	2.1
1	D	305	GLY	2.1
1	A	37	HIS	2.1
1	D	53	VAL	2.1
1	A	182	CYS	2.1
1	A	227	LEU	2.1
1	B	85	LEU	2.1
1	C	116	ASP	2.1
1	D	138	GLU	2.0
1	B	55	SER	2.0
1	C	198	SER	2.0
1	A	90	THR	2.0
1	A	401	THR	2.0
1	B	328	MET	2.0
1	B	131	GLY	2.0
1	D	112	GLY	2.0
1	A	83	VAL	2.0
1	A	249	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	24	LEU	2.0
1	D	152	LEU	2.0
1	B	39	ASP	2.0
1	A	344	GLU	2.0
1	D	133	GLU	2.0
1	D	91	PHE	2.0
1	B	148	ASN	2.0
1	C	11	GLY	2.0
1	A	99	VAL	2.0
1	A	452	VAL	2.0
1	B	46	ARG	2.0
1	B	53	VAL	2.0
1	D	163	VAL	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 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($\text{\AA}^2$)	Q<0.9
2	SO4	B	702	5/5	0.83	0.23	18,19,20,22	0
2	SO4	C	703	5/5	0.87	0.25	18,19,20,22	0
2	SO4	D	704	5/5	0.87	0.22	18,19,20,22	0
2	SO4	A	701	5/5	0.92	0.20	18,19,20,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.