



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:19 PM UTC

PDB ID : 1PKL / pdb_00001pkl
Title : THE STRUCTURE OF LEISHMANIA PYRUVATE KINASE
Authors : Rigden, D.J.; Phillips, S.E.V.; Michels, P.A.M.; Fothergill-Gilmore, L.A.
Deposited on : 1998-09-15
Resolution : 2.35 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

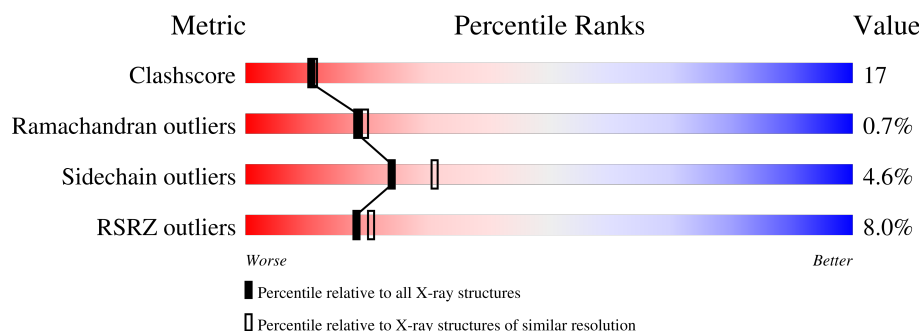
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	499	13% 65% 30% ..
1	B	499	6% 69% 26% ..
1	C	499	3% 64% 31% ..
1	D	499	16% 65% 30% ..
1	E	499	12% 66% 29% ..
1	F	499	5% 69% 27% ..

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Mol	Chain	Length	Quality of chain
1	G	499	6% 72% 24% .
1	H	499	3% 69% 26% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 32986 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 PROTEIN (PYRUVATE KINASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	0	0	0
			3740	2330	659	725	26			
1	B	489	Total	C	N	O	S	0	0	0
			3725	2321	655	723	26			
1	C	492	Total	C	N	O	S	0	0	0
			3748	2334	660	728	26			
1	D	493	Total	C	N	O	S	0	0	0
			3758	2340	663	729	26			
1	E	493	Total	C	N	O	S	0	0	0
			3758	2340	663	729	26			
1	F	491	Total	C	N	O	S	0	0	0
			3740	2330	659	725	26			
1	H	492	Total	C	N	O	S	0	0	0
			3748	2334	660	728	26			
1	G	498	Total	C	N	O	S	0	0	0
			3777	2351	666	734	26			

There are 32 discrepancies between the modelled and reference sequences:

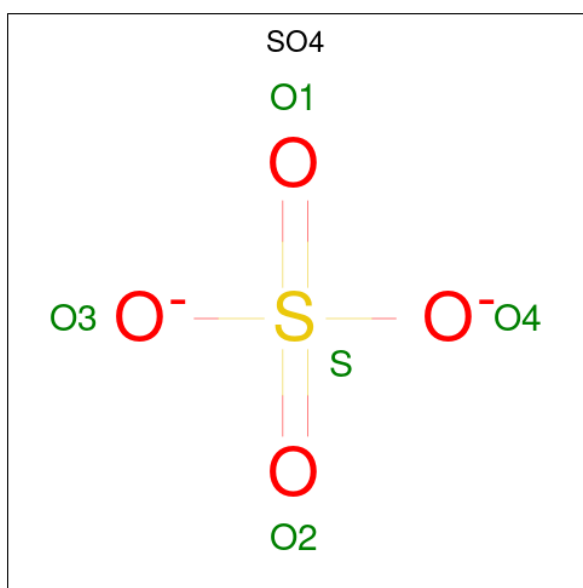
Chain	Residue	Modelled	Actual	Comment	Reference
A	382	SER	GLY	conflict	UNP Q27686
A	389	TYR	SER	conflict	UNP Q27686
A	404	ARG	ALA	conflict	UNP Q27686
A	405	SER	GLY	conflict	UNP Q27686
B	382	SER	GLY	conflict	UNP Q27686
B	389	TYR	SER	conflict	UNP Q27686
B	404	ARG	ALA	conflict	UNP Q27686
B	405	SER	GLY	conflict	UNP Q27686
C	382	SER	GLY	conflict	UNP Q27686
C	389	TYR	SER	conflict	UNP Q27686
C	404	ARG	ALA	conflict	UNP Q27686
C	405	SER	GLY	conflict	UNP Q27686
D	382	SER	GLY	conflict	UNP Q27686

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Chain	Residue	Modelled	Actual	Comment	Reference
D	389	TYR	SER	conflict	UNP Q27686
D	404	ARG	ALA	conflict	UNP Q27686
D	405	SER	GLY	conflict	UNP Q27686
E	382	SER	GLY	conflict	UNP Q27686
E	389	TYR	SER	conflict	UNP Q27686
E	404	ARG	ALA	conflict	UNP Q27686
E	405	SER	GLY	conflict	UNP Q27686
F	382	SER	GLY	conflict	UNP Q27686
F	389	TYR	SER	conflict	UNP Q27686
F	404	ARG	ALA	conflict	UNP Q27686
F	405	SER	GLY	conflict	UNP Q27686
H	382	SER	GLY	conflict	UNP Q27686
H	389	TYR	SER	conflict	UNP Q27686
H	404	ARG	ALA	conflict	UNP Q27686
H	405	SER	GLY	conflict	UNP Q27686
G	382	SER	GLY	conflict	UNP Q27686
G	389	TYR	SER	conflict	UNP Q27686
G	404	ARG	ALA	conflict	UNP Q27686
G	405	SER	GLY	conflict	UNP Q27686

- 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		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		

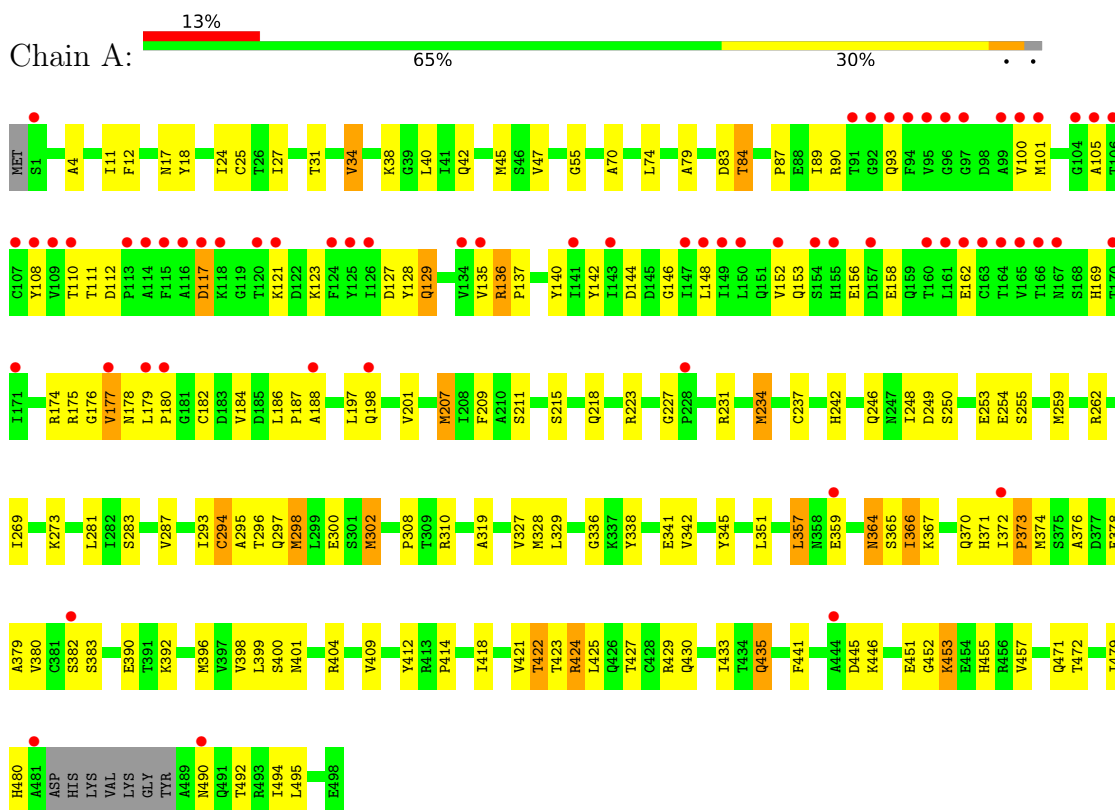
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	315	Total	O	0	0
			315	315		
3	B	366	Total	O	0	0
			366	366		
3	C	453	Total	O	0	0
			453	453		
3	D	244	Total	O	0	0
			244	244		
3	E	386	Total	O	0	0
			386	386		
3	F	399	Total	O	0	0
			399	399		
3	H	400	Total	O	0	0
			400	400		
3	G	389	Total	O	0	0
			389	389		

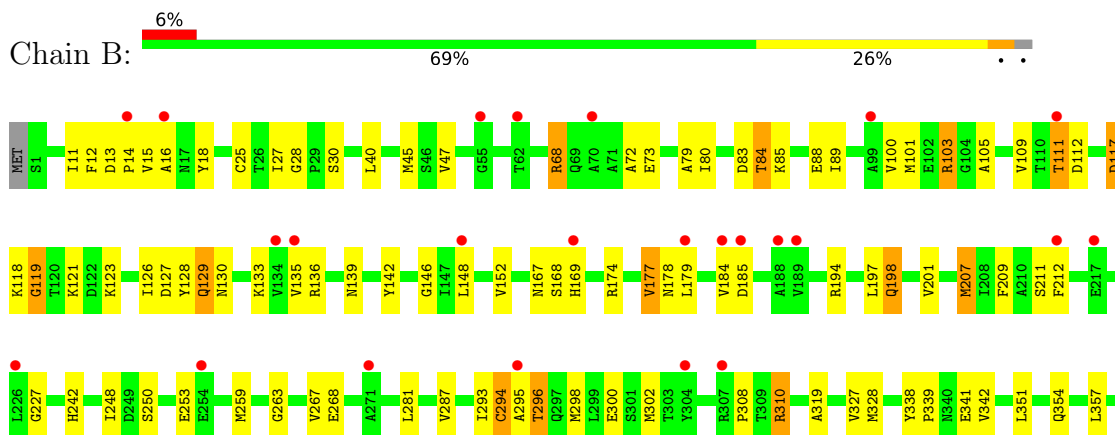
3 Residue-property plots

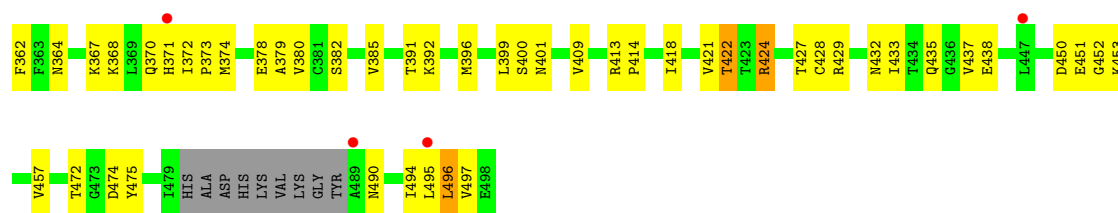
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

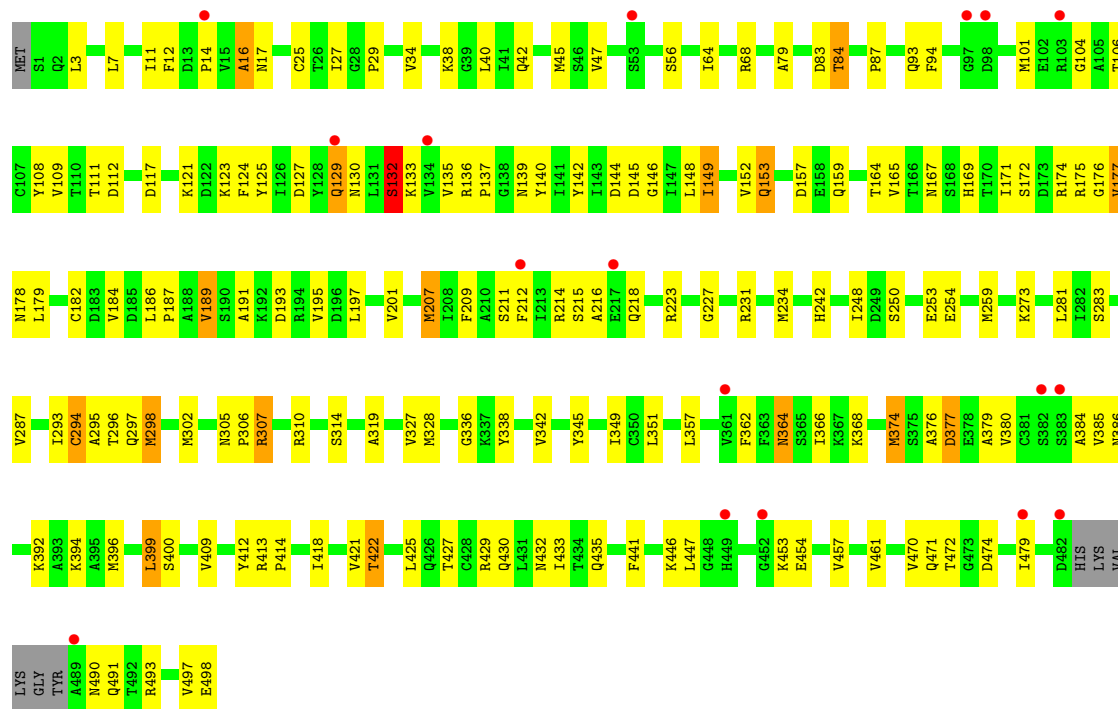


• Molecule 1: PROTEIN (PYRUVATE KINASE)

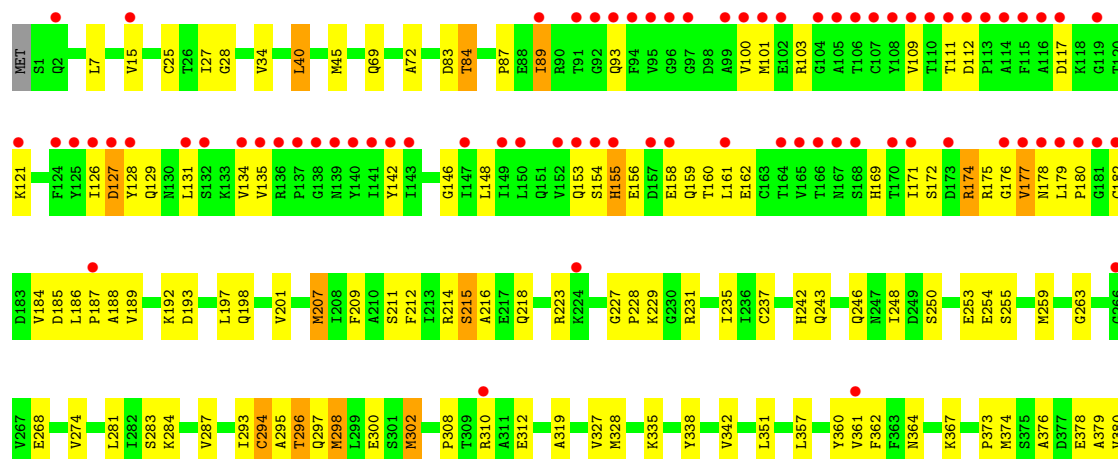


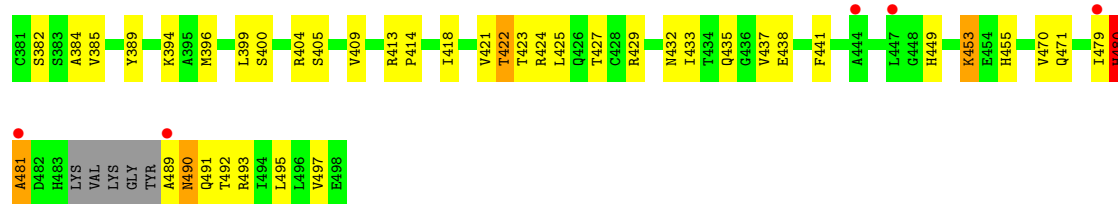


• Molecule 1: PROTEIN (PYRUVATE KINASE)

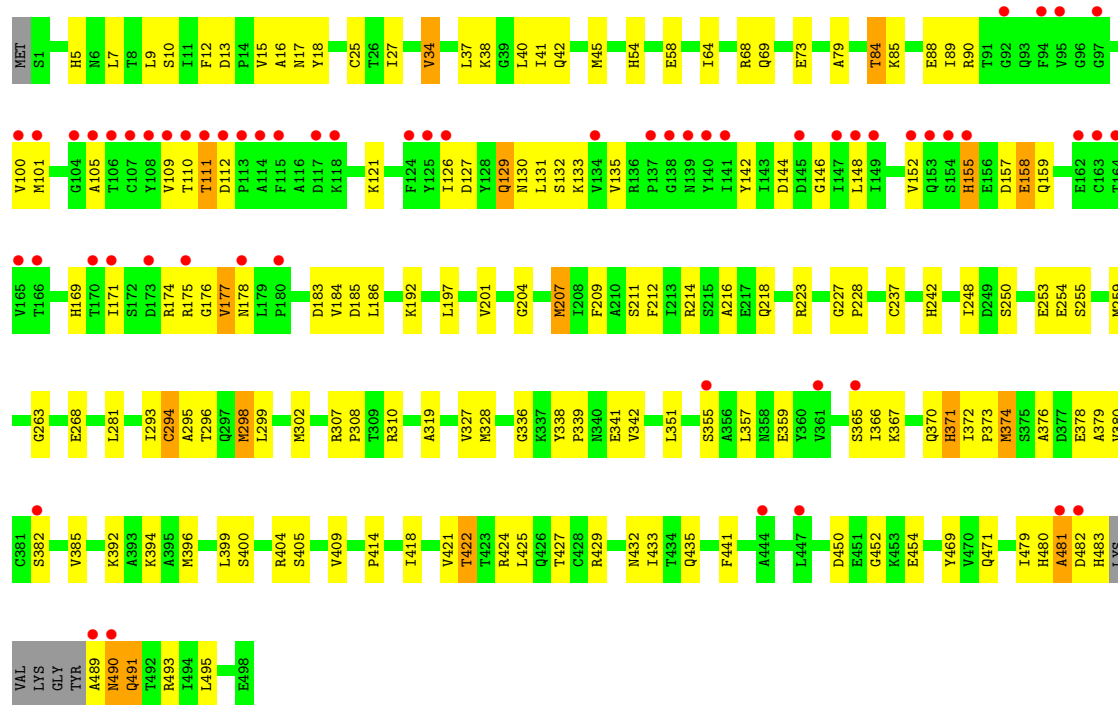


• Molecule 1: PROTEIN (PYRUVATE KINASE)

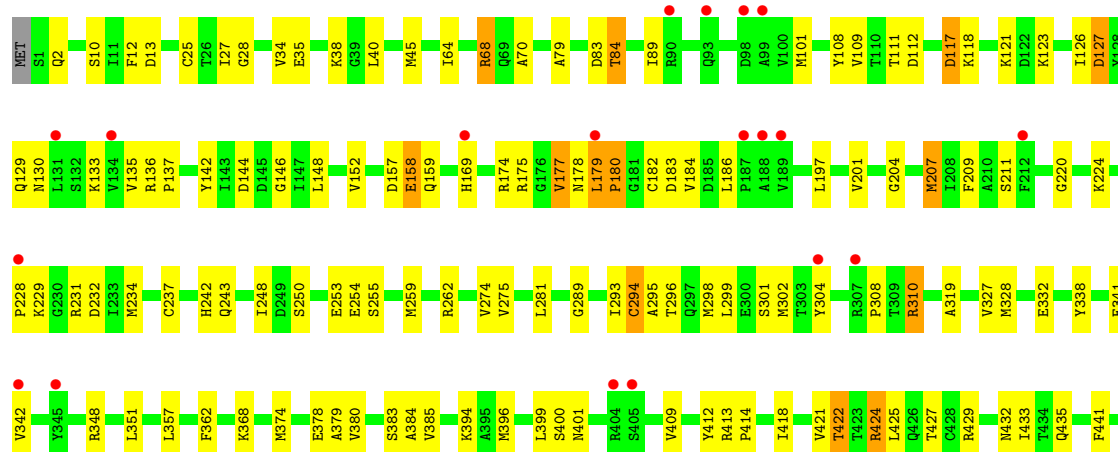




● Molecule 1: PROTEIN (PYRUVATE KINASE)

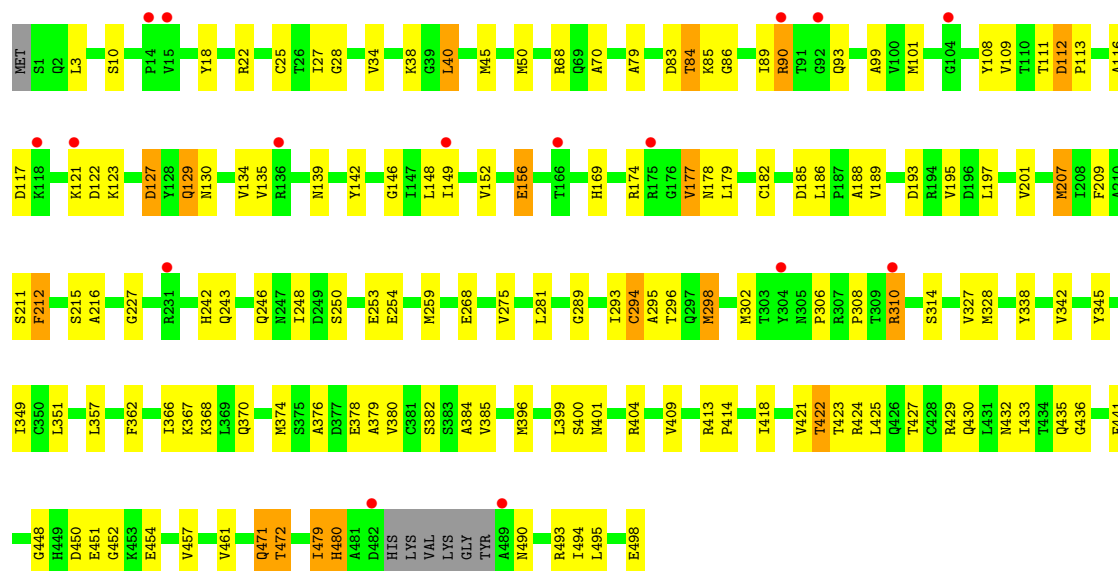


● Molecule 1: PROTEIN (PYRUVATE KINASE)

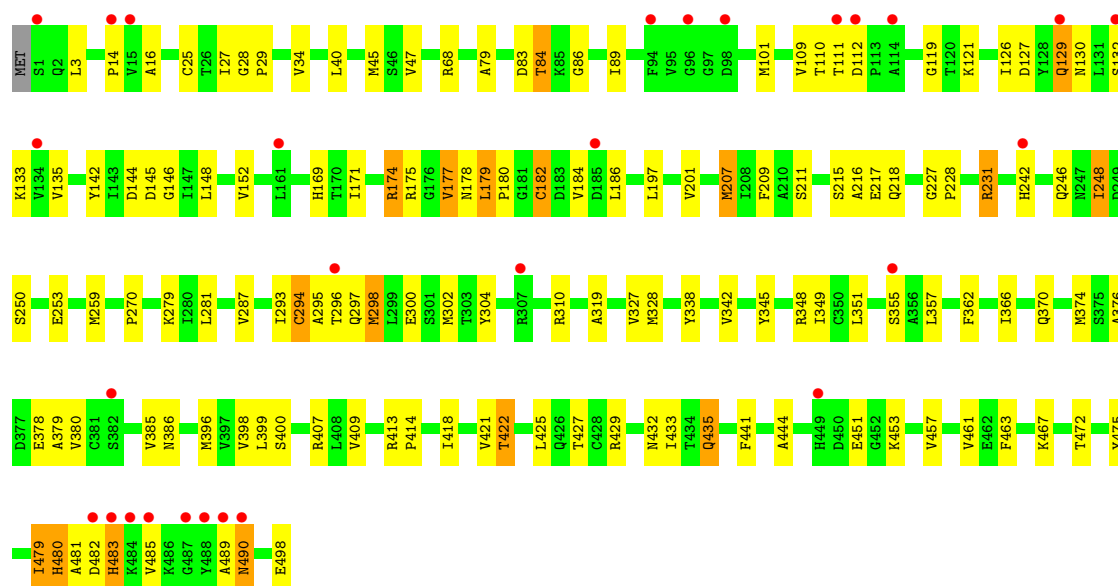




• Molecule 1: PROTEIN (PYRUVATE KINASE)



• Molecule 1: PROTEIN (PYRUVATE KINASE)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	121.65Å 132.64Å 181.00Å 90.00° 97.11° 90.00°	Depositor
Resolution (Å)	30.00 – 2.35 30.00 – 2.35	Depositor EDS
% Data completeness (in resolution range)	67.9 (30.00-2.35) 67.9 (30.00-2.35)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.209 , 0.256 0.224 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	36.9	Xtriage
Anisotropy	0.576	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 44.7	EDS
L-test for twinning ¹	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	32986	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.05 % 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 7.2506e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Theoretical 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: 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	0.69	4/3794 (0.1%)	1.08	29/5136 (0.6%)
1	B	0.54	0/3778	1.04	20/5114 (0.4%)
1	C	0.60	1/3802 (0.0%)	1.03	17/5147 (0.3%)
1	D	0.59	0/3813	1.05	23/5162 (0.4%)
1	E	0.59	0/3813	1.05	20/5162 (0.4%)
1	F	0.57	0/3794	1.05	12/5136 (0.2%)
1	G	0.58	0/3832	1.07	23/5190 (0.4%)
1	H	0.58	0/3802	1.01	17/5147 (0.3%)
All	All	0.59	5/30428 (0.0%)	1.05	161/41194 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	E	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	373	PRO	N-CD	13.84	1.67	1.47
1	A	372	ILE	CA-C	9.52	1.61	1.52
1	A	372	ILE	C-N	-7.04	1.20	1.34
1	A	234	MET	SD-CE	-5.66	1.65	1.79
1	C	16	ALA	CA-CB	-5.11	1.46	1.53

All (161) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	295	ALA	N-CA-C	13.99	131.17	113.55
1	D	295	ALA	N-CA-C	13.75	130.87	113.55
1	E	295	ALA	N-CA-C	13.71	130.83	113.55
1	G	295	ALA	N-CA-C	13.68	130.79	113.55
1	F	295	ALA	N-CA-C	13.34	130.36	113.55
1	B	295	ALA	N-CA-C	13.30	130.31	113.55
1	H	295	ALA	N-CA-C	13.21	130.20	113.55
1	A	295	ALA	N-CA-C	12.61	129.43	113.55
1	D	481	ALA	N-CA-C	9.78	125.94	112.93
1	A	372	ILE	O-C-N	9.58	132.25	120.66
1	G	179	LEU	CA-C-N	9.53	131.75	119.84
1	G	179	LEU	C-N-CA	9.53	131.75	119.84
1	A	373	PRO	N-CA-CB	9.11	112.62	102.60
1	B	179	LEU	CA-C-N	9.08	131.19	119.84
1	B	179	LEU	C-N-CA	9.08	131.19	119.84
1	F	179	LEU	CA-C-N	7.94	129.76	119.84
1	F	179	LEU	C-N-CA	7.94	129.76	119.84
1	F	453	LYS	N-CA-C	7.88	122.30	111.90
1	A	373	PRO	CA-N-CD	-7.86	100.49	111.50
1	H	452	GLY	N-CA-C	-7.71	105.31	114.48
1	B	119	GLY	N-CA-C	7.29	119.89	111.36
1	D	28	GLY	CA-C-N	7.13	127.45	119.32
1	D	28	GLY	C-N-CA	7.13	127.45	119.32
1	A	294	CYS	N-CA-C	-7.06	97.74	108.96
1	G	119	GLY	N-CA-C	6.91	119.44	111.36
1	G	294	CYS	N-CA-C	-6.87	98.04	108.96
1	D	480	HIS	N-CA-C	-6.77	96.76	107.93
1	C	294	CYS	N-CA-C	-6.71	98.29	108.96
1	E	452	GLY	N-CA-C	-6.64	106.78	114.69
1	H	294	CYS	N-CA-C	-6.61	98.45	108.96
1	E	110	THR	N-CA-C	6.54	120.07	109.40
1	E	294	CYS	N-CA-C	-6.53	98.58	108.96
1	D	294	CYS	N-CA-C	-6.50	98.63	108.96
1	G	182	CYS	N-CA-C	6.46	119.44	108.90
1	H	112	ASP	CA-C-N	6.45	126.14	119.56
1	H	112	ASP	C-N-CA	6.45	126.14	119.56
1	C	296	THR	N-CA-C	6.43	120.11	110.14
1	G	110	THR	N-CA-C	6.41	119.62	109.50
1	E	112	ASP	CA-C-N	6.37	126.05	119.56
1	E	112	ASP	C-N-CA	6.37	126.05	119.56
1	F	296	THR	N-CA-C	6.35	119.98	110.14
1	G	112	ASP	CA-C-N	6.34	126.03	119.56
1	G	112	ASP	C-N-CA	6.34	126.03	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	296	THR	N-CA-C	6.33	119.95	110.14
1	A	112	ASP	CA-C-N	6.30	125.99	119.56
1	A	112	ASP	C-N-CA	6.30	125.99	119.56
1	B	294	CYS	N-CA-C	-6.28	98.98	108.96
1	F	294	CYS	N-CA-C	-6.28	98.98	108.96
1	B	496	LEU	N-CA-C	-6.27	97.05	108.02
1	G	16	ALA	N-CA-C	-6.22	100.62	109.96
1	E	296	THR	N-CA-C	6.22	119.78	110.14
1	G	216	ALA	N-CA-C	-6.22	104.61	111.82
1	H	296	THR	N-CA-C	6.21	119.76	110.14
1	B	300	GLU	N-CA-C	6.19	118.53	111.11
1	B	112	ASP	CA-C-N	6.16	125.84	119.56
1	B	112	ASP	C-N-CA	6.16	125.84	119.56
1	A	296	THR	N-CA-C	6.16	119.69	110.14
1	B	296	THR	N-CA-C	6.14	119.66	110.14
1	E	319	ALA	N-CA-C	-6.08	104.73	111.36
1	A	110	THR	N-CA-C	6.04	118.75	108.90
1	G	86	GLY	CA-C-N	6.02	125.93	119.85
1	G	86	GLY	C-N-CA	6.02	125.93	119.85
1	E	129	GLN	N-CA-C	6.02	119.72	112.38
1	A	372	ILE	CA-C-O	-5.99	114.83	119.98
1	D	112	ASP	CA-C-N	5.98	125.66	119.56
1	D	112	ASP	C-N-CA	5.98	125.66	119.56
1	E	227	GLY	CA-C-N	5.95	125.50	119.19
1	E	227	GLY	C-N-CA	5.95	125.50	119.19
1	A	129	GLN	N-CA-C	5.87	119.54	112.38
1	E	450	ASP	N-CA-C	5.83	119.28	111.24
1	H	129	GLN	N-CA-C	5.79	119.82	112.87
1	A	176	GLY	N-CA-C	5.79	118.59	111.93
1	C	112	ASP	CA-C-N	5.78	125.46	119.56
1	C	112	ASP	C-N-CA	5.78	125.46	119.56
1	A	55	GLY	CA-C-O	-5.76	118.26	122.23
1	C	227	GLY	CA-C-N	5.75	125.29	119.19
1	C	227	GLY	C-N-CA	5.75	125.29	119.19
1	D	215	SER	N-CA-C	5.71	118.52	108.75
1	A	31	THR	N-CA-C	5.70	121.51	113.02
1	D	296	THR	N-CA-C	5.68	118.94	110.14
1	H	127	ASP	N-CA-C	5.67	122.88	110.80
1	F	112	ASP	CA-C-N	5.66	125.34	119.56
1	F	112	ASP	C-N-CA	5.66	125.34	119.56
1	C	129	GLN	N-CA-C	5.65	119.65	112.87
1	B	184	VAL	N-CA-C	5.55	116.10	107.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	28	GLY	CA-C-N	5.54	125.00	119.24
1	F	28	GLY	C-N-CA	5.54	125.00	119.24
1	A	90	ARG	N-CA-C	5.51	118.43	109.06
1	D	227	GLY	CA-C-N	5.43	124.94	119.19
1	D	227	GLY	C-N-CA	5.43	124.94	119.19
1	C	176	GLY	N-CA-C	5.42	117.71	111.36
1	B	129	GLN	N-CA-C	5.42	119.38	112.87
1	E	176	GLY	N-CA-C	5.42	117.70	111.36
1	C	127	ASP	N-CA-C	5.41	122.32	110.80
1	G	28	GLY	CA-C-N	5.39	124.85	119.24
1	G	28	GLY	C-N-CA	5.39	124.85	119.24
1	B	100	VAL	N-CA-C	5.39	115.02	107.37
1	D	300	GLU	N-CA-C	5.38	117.57	111.11
1	E	111	THR	N-CA-C	-5.38	106.67	113.18
1	D	89	ILE	CB-CA-C	-5.37	104.45	111.81
1	B	127	ASP	N-CA-C	5.37	122.23	110.80
1	H	28	GLY	CA-C-N	5.36	125.44	119.32
1	H	28	GLY	C-N-CA	5.36	125.44	119.32
1	A	451	GLU	N-CA-C	-5.36	102.55	110.48
1	A	227	GLY	CA-C-N	5.36	124.87	119.19
1	A	227	GLY	C-N-CA	5.36	124.87	119.19
1	D	453	LYS	N-CA-C	5.36	122.21	110.80
1	H	227	GLY	CA-C-N	5.35	124.86	119.19
1	H	227	GLY	C-N-CA	5.35	124.86	119.19
1	D	127	ASP	N-CA-C	5.34	122.18	110.80
1	B	28	GLY	CA-C-N	5.34	125.67	119.47
1	B	28	GLY	C-N-CA	5.34	125.67	119.47
1	E	127	ASP	N-CA-C	5.32	122.14	110.80
1	D	423	THR	N-CA-C	-5.31	106.48	113.17
1	D	103	ARG	N-CA-C	5.30	122.09	110.80
1	H	86	GLY	CA-C-N	5.29	125.55	119.83
1	H	86	GLY	C-N-CA	5.29	125.55	119.83
1	A	452	GLY	N-CA-C	-5.28	108.03	115.32
1	A	127	ASP	N-CA-C	5.28	122.04	110.80
1	G	227	GLY	CA-C-N	5.27	124.77	119.19
1	G	227	GLY	C-N-CA	5.27	124.77	119.19
1	A	295	ALA	CA-C-N	-5.26	113.66	122.92
1	A	295	ALA	C-N-CA	-5.26	113.66	122.92
1	A	372	ILE	CA-C-N	5.26	139.62	127.00
1	A	372	ILE	C-N-CA	5.26	139.62	127.00
1	F	127	ASP	N-CA-C	5.25	121.99	110.80
1	E	482	ASP	N-CA-C	5.23	117.02	108.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	ALA	N-CA-C	5.21	117.90	110.24
1	B	212	PHE	N-CA-C	5.20	118.57	111.39
1	A	336	GLY	N-CA-C	5.20	118.05	112.33
1	D	319	ALA	N-CA-C	-5.18	105.81	111.82
1	C	212	PHE	N-CA-C	5.18	118.53	111.39
1	C	491	GLN	N-CA-C	5.18	116.28	108.46
1	D	100	VAL	N-CA-C	5.17	114.72	107.37
1	G	127	ASP	N-CA-C	5.17	121.82	110.80
1	C	319	ALA	N-CA-C	-5.17	105.72	111.36
1	G	319	ALA	N-CA-C	-5.17	105.73	111.36
1	H	423	THR	N-CA-C	-5.16	106.67	113.17
1	E	100	VAL	N-CA-C	5.15	114.68	107.37
1	E	481	ALA	N-CA-C	-5.15	101.37	109.50
1	G	248	ILE	N-CA-C	5.15	116.49	110.62
1	A	319	ALA	N-CA-C	-5.14	105.76	111.36
1	H	454	GLU	N-CA-C	5.14	116.88	111.28
1	G	129	GLN	N-CA-C	5.13	119.03	112.87
1	D	449	HIS	N-CA-C	5.13	119.02	112.87
1	C	454	GLU	N-CA-C	5.12	116.86	111.28
1	E	212	PHE	N-CA-C	5.12	118.46	111.39
1	D	212	PHE	N-CA-C	5.11	118.44	111.39
1	B	319	ALA	N-CA-C	-5.10	105.80	111.36
1	A	262	ARG	N-CA-C	5.10	117.23	111.11
1	C	216	ALA	N-CA-C	-5.08	105.74	111.28
1	E	454	GLU	N-CA-C	5.06	116.79	111.28
1	H	212	PHE	N-CA-C	5.05	118.36	111.39
1	B	227	GLY	CA-C-N	5.05	124.54	119.19
1	B	227	GLY	C-N-CA	5.05	124.54	119.19
1	C	336	GLY	N-CA-C	5.04	117.88	112.33
1	F	319	ALA	N-CA-C	-5.04	105.86	111.36
1	C	132	SER	N-CA-C	5.03	116.84	111.36
1	G	300	GLU	N-CA-C	5.02	117.14	111.11
1	D	497	VAL	N-CA-C	5.02	116.14	109.37
1	A	100	VAL	N-CA-C	5.01	114.49	107.37

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	18	TYR	Sidechain
1	E	18	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3740	0	3743	134	0
1	B	3725	0	3731	129	0
1	C	3748	0	3747	139	0
1	D	3758	0	3754	126	0
1	E	3758	0	3754	134	0
1	F	3740	0	3743	126	0
1	G	3777	0	3761	116	0
1	H	3748	0	3747	128	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
3	A	315	0	0	32	0
3	B	366	0	0	30	0
3	C	453	0	0	37	0
3	D	244	0	0	18	0
3	E	386	0	0	38	0
3	F	399	0	0	32	0
3	G	389	0	0	24	0
3	H	400	0	0	38	0
All	All	32986	0	29980	996	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 17.

All (996) 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:C:25:CYS:HB2	1:C:45:MET:HE3	1.43	0.99
1:F:27:ILE:HD11	1:F:45:MET:HE1	1.47	0.96
1:B:424:ARG:HB3	1:B:424:ARG:HH11	1.27	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:ILE:HD11	1:D:45:MET:HE1	1.47	0.94
1:D:25:CYS:HB2	1:D:45:MET:HE3	1.49	0.94
1:H:27:ILE:HD11	1:H:45:MET:HE1	1.50	0.94
1:G:27:ILE:HD11	1:G:45:MET:HE1	1.50	0.93
1:E:25:CYS:HB2	1:E:45:MET:HE3	1.50	0.92
1:E:27:ILE:HD11	1:E:45:MET:HE1	1.51	0.92
1:E:374:MET:HE2	1:E:379:ALA:HA	1.48	0.92
1:C:374:MET:HE2	1:C:379:ALA:HA	1.48	0.91
1:G:25:CYS:HB2	1:G:45:MET:HE3	1.49	0.91
1:A:490:ASN:HD22	1:B:494:ILE:HB	1.34	0.91
1:G:380:VAL:HG12	1:G:479:ILE:HD11	1.52	0.91
1:E:310:ARG:HH11	1:G:297:GLN:HE22	0.96	0.90
1:C:27:ILE:HD11	1:C:45:MET:HE1	1.51	0.90
1:H:25:CYS:HB2	1:H:45:MET:HE3	1.54	0.90
1:A:27:ILE:HD11	1:A:45:MET:HE1	1.53	0.89
1:F:25:CYS:HB2	1:F:45:MET:HE3	1.53	0.89
1:C:472:THR:HG23	1:C:498:GLU:HA	1.52	0.89
1:B:13:ASP:HB2	1:B:14:PRO:HD2	1.55	0.89
1:B:27:ILE:HD11	1:B:45:MET:HE1	1.54	0.87
1:D:298:MET:SD	3:D:3056:HOH:O	2.30	0.87
1:H:374:MET:HE3	1:H:378:GLU:HG3	1.56	0.87
1:B:25:CYS:HB2	1:B:45:MET:HE3	1.55	0.86
1:A:374:MET:HE2	1:A:379:ALA:HA	1.58	0.86
1:A:84:THR:HG21	3:A:3163:HOH:O	1.76	0.85
1:F:495:LEU:HB2	3:F:2124:HOH:O	1.76	0.84
1:E:310:ARG:HH11	1:G:297:GLN:NE2	1.73	0.84
1:A:25:CYS:HB2	1:A:45:MET:HE3	1.57	0.84
1:B:302:MET:HE2	1:B:308:PRO:HB3	1.58	0.84
1:E:342:VAL:HB	3:E:1676:HOH:O	1.77	0.83
1:A:495:LEU:HB3	3:A:3298:HOH:O	1.76	0.83
1:E:310:ARG:NH1	1:G:297:GLN:HE22	1.75	0.82
1:A:25:CYS:HB2	1:A:45:MET:CE	2.10	0.82
1:A:207:MET:HE1	1:A:433:ILE:HG21	1.62	0.82
1:B:15:VAL:HG21	3:B:3344:HOH:O	1.80	0.81
1:A:374:MET:HE3	1:A:378:GLU:HG3	1.62	0.81
1:C:25:CYS:HB2	1:C:45:MET:CE	2.11	0.81
1:H:207:MET:HE1	1:H:433:ILE:HG21	1.63	0.80
1:C:87:PRO:HG3	1:C:214:ARG:HH22	1.47	0.80
1:D:215:SER:HA	3:D:3240:HOH:O	1.82	0.79
1:G:472:THR:HG23	1:G:498:GLU:HA	1.63	0.79
1:C:380:VAL:HG21	1:C:490:ASN:HD21	1.47	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:25:CYS:HB2	1:D:45:MET:CE	2.13	0.79
1:C:87:PRO:HG2	3:C:3430:HOH:O	1.82	0.79
1:E:400:SER:O	1:E:422:THR:HG23	1.82	0.79
1:F:135:VAL:HG11	1:F:152:VAL:HG21	1.66	0.78
1:G:207:MET:HE1	1:G:433:ILE:HG21	1.65	0.78
1:B:207:MET:HE1	1:B:433:ILE:HG21	1.65	0.78
1:E:25:CYS:HB2	1:E:45:MET:CE	2.12	0.78
1:F:374:MET:HE2	1:F:379:ALA:HA	1.65	0.78
1:B:310:ARG:HG3	1:D:297:GLN:NE2	1.99	0.78
1:G:259:MET:HE2	1:G:328:MET:HE1	1.64	0.78
1:G:130:ASN:HB3	1:G:133:LYS:HE2	1.64	0.78
1:G:374:MET:HE3	1:G:378:GLU:HG3	1.66	0.77
1:A:338:TYR:O	1:A:342:VAL:HG23	1.83	0.77
1:F:25:CYS:HB2	1:F:45:MET:CE	2.14	0.77
1:H:108:TYR:CE1	1:H:156:GLU:HG3	2.20	0.77
1:A:87:PRO:HG2	1:A:187:PRO:O	1.85	0.77
1:A:376:ALA:HB1	1:A:490:ASN:HD21	1.49	0.77
1:C:207:MET:HE1	1:C:433:ILE:HG21	1.66	0.77
1:B:374:MET:HE2	1:B:379:ALA:HA	1.67	0.76
1:C:380:VAL:HG21	1:C:490:ASN:ND2	1.99	0.76
1:G:25:CYS:HB2	1:G:45:MET:CE	2.14	0.76
1:D:493:ARG:NH1	1:D:495:LEU:HD21	2.00	0.76
1:F:302:MET:HE2	1:F:342:VAL:HA	1.68	0.76
1:F:207:MET:HE1	1:F:433:ILE:HG21	1.67	0.75
1:F:394:LYS:HB2	1:F:470:VAL:HG12	1.67	0.75
1:B:14:PRO:HD3	3:B:3362:HOH:O	1.86	0.75
1:B:25:CYS:HB2	1:B:45:MET:CE	2.16	0.75
1:H:310:ARG:HH12	1:H:314:SER:HB3	1.51	0.75
1:E:207:MET:HE1	1:E:433:ILE:HG21	1.68	0.75
1:F:374:MET:HE3	1:F:378:GLU:HG3	1.69	0.75
1:C:377:ASP:HB3	3:C:3242:HOH:O	1.87	0.75
1:A:359:GLU:HG2	3:A:3020:HOH:O	1.84	0.75
1:C:248:ILE:HG12	1:C:281:LEU:HD22	1.69	0.75
1:H:310:ARG:NH1	1:H:314:SER:HB3	2.01	0.75
1:B:101:MET:HE1	1:B:121:LYS:HA	1.68	0.75
1:G:338:TYR:O	1:G:342:VAL:HG23	1.87	0.74
1:D:187:PRO:HG3	3:D:3206:HOH:O	1.86	0.74
1:H:259:MET:HE2	1:H:328:MET:HE1	1.69	0.74
1:H:451:GLU:HA	3:H:2558:HOH:O	1.86	0.74
1:H:25:CYS:HB2	1:H:45:MET:CE	2.16	0.74
1:H:189:VAL:HG13	1:H:193:ASP:HB2	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:ILE:HG12	3:B:3014:HOH:O	1.88	0.74
1:D:374:MET:HE2	1:D:379:ALA:HA	1.68	0.74
1:E:259:MET:HE2	1:E:328:MET:HE1	1.70	0.74
1:A:400:SER:O	1:A:422:THR:HG23	1.88	0.74
1:C:374:MET:HE1	3:C:3428:HOH:O	1.88	0.74
3:E:1760:HOH:O	1:G:348:ARG:HD2	1.87	0.74
1:B:198:GLN:HB3	3:B:3085:HOH:O	1.87	0.74
1:E:374:MET:HE1	3:E:1729:HOH:O	1.88	0.74
1:C:171:ILE:HA	1:C:175:ARG:NH1	2.02	0.73
1:C:259:MET:HE2	1:C:328:MET:HE1	1.69	0.73
1:G:248:ILE:HG12	1:G:281:LEU:HD22	1.70	0.73
1:C:400:SER:O	1:C:422:THR:HG23	1.88	0.73
1:D:312:GLU:HG2	3:D:3227:HOH:O	1.87	0.73
1:A:187:PRO:HG3	3:A:3302:HOH:O	1.88	0.73
1:F:229:LYS:HB2	3:F:2153:HOH:O	1.89	0.73
1:G:355:SER:HB3	3:G:2938:HOH:O	1.89	0.73
1:B:338:TYR:O	1:B:342:VAL:HG23	1.88	0.73
1:H:374:MET:HE1	3:H:2255:HOH:O	1.89	0.72
1:A:490:ASN:ND2	1:B:494:ILE:HB	2.04	0.72
1:F:400:SER:O	1:F:422:THR:HG23	1.90	0.72
1:F:101:MET:HE1	1:F:121:LYS:HA	1.70	0.72
1:H:139:ASN:HB3	3:H:2197:HOH:O	1.89	0.72
1:D:248:ILE:HG12	1:D:281:LEU:HD22	1.72	0.72
1:A:297:GLN:HA	3:A:3296:HOH:O	1.88	0.72
1:B:400:SER:O	1:B:422:THR:HG23	1.90	0.72
1:A:430:GLN:HA	3:A:3284:HOH:O	1.89	0.71
1:B:198:GLN:HG2	3:B:3358:HOH:O	1.89	0.71
1:D:171:ILE:HA	1:D:175:ARG:HH11	1.55	0.71
1:F:35:GLU:HG2	3:F:2137:HOH:O	1.90	0.71
1:C:254:GLU:HG2	3:C:3288:HOH:O	1.90	0.71
1:D:101:MET:HE1	1:D:121:LYS:HA	1.71	0.71
1:F:248:ILE:HG12	1:F:281:LEU:HD22	1.71	0.71
1:B:259:MET:HE2	1:B:328:MET:HE1	1.73	0.71
1:C:338:TYR:O	1:C:342:VAL:HG23	1.91	0.71
1:E:101:MET:HE1	1:E:121:LYS:HA	1.72	0.71
1:E:359:GLU:HG2	3:E:1731:HOH:O	1.89	0.71
1:A:259:MET:HE2	1:A:328:MET:HE1	1.72	0.71
1:E:310:ARG:HD2	1:G:297:GLN:NE2	2.04	0.71
1:G:297:GLN:HB2	3:G:2941:HOH:O	1.90	0.71
1:C:223:ARG:HD2	3:C:3231:HOH:O	1.91	0.70
1:C:364:ASN:HB3	3:C:3415:HOH:O	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:204:GLY:HA3	3:E:1737:HOH:O	1.90	0.70
1:F:338:TYR:O	1:F:342:VAL:HG23	1.91	0.70
1:A:248:ILE:HG12	1:A:281:LEU:HD22	1.72	0.70
1:H:101:MET:HE1	1:H:121:LYS:HA	1.73	0.70
1:D:361:VAL:HA	3:D:3247:HOH:O	1.90	0.70
1:F:380:VAL:HG21	1:F:490:ASN:HD21	1.56	0.70
1:H:368:LYS:HD2	3:H:2293:HOH:O	1.90	0.70
1:H:430:GLN:HA	3:H:2539:HOH:O	1.91	0.70
1:F:259:MET:HE2	1:F:328:MET:HE1	1.73	0.70
1:G:179:LEU:HB3	1:G:182:CYS:HB2	1.74	0.70
1:D:72:ALA:HA	3:D:3225:HOH:O	1.91	0.70
1:D:207:MET:HE1	1:D:433:ILE:HG21	1.74	0.70
1:D:338:TYR:O	1:D:342:VAL:HG23	1.92	0.70
1:H:248:ILE:HG12	1:H:281:LEU:HD22	1.73	0.70
1:B:248:ILE:HG12	1:B:281:LEU:HD22	1.73	0.69
1:A:373:PRO:HG3	1:B:392:LYS:HG3	1.73	0.69
1:C:214:ARG:NH1	1:C:218:GLN:HE22	1.91	0.69
1:A:101:MET:HE1	1:A:121:LYS:HA	1.73	0.69
1:C:101:MET:HE1	1:C:121:LYS:HA	1.74	0.69
1:A:38:LYS:O	1:A:42:GLN:HG3	1.93	0.69
1:D:400:SER:O	1:D:422:THR:HG23	1.93	0.69
1:C:175:ARG:HG2	3:C:3408:HOH:O	1.92	0.69
1:D:109:VAL:HG12	1:D:131:LEU:HD21	1.75	0.69
1:E:338:TYR:O	1:E:342:VAL:HG23	1.92	0.69
1:H:374:MET:HE3	1:H:378:GLU:CG	2.22	0.69
1:G:398:VAL:HG13	1:G:479:ILE:HG22	1.73	0.69
1:B:168:SER:HB3	3:B:3114:HOH:O	1.92	0.69
1:H:338:TYR:O	1:H:342:VAL:HG23	1.92	0.69
1:D:259:MET:HE2	1:D:328:MET:HE1	1.73	0.68
1:A:300:GLU:HG2	3:A:3296:HOH:O	1.94	0.68
1:A:365:SER:HB3	1:C:3:LEU:HD23	1.76	0.68
1:C:140:TYR:CD1	1:C:149:ILE:HD11	2.28	0.68
1:E:365:SER:HB3	1:G:3:LEU:HD23	1.76	0.68
1:H:400:SER:O	1:H:422:THR:HG23	1.94	0.68
1:E:396:MET:CE	1:E:414:PRO:HG2	2.24	0.68
1:C:64:ILE:O	1:C:68:ARG:HG2	1.92	0.68
1:D:367:LYS:HE2	1:D:382:SER:HB2	1.74	0.68
1:H:382:SER:HB2	3:H:2544:HOH:O	1.94	0.68
1:G:242:HIS:O	1:G:246:GLN:HG3	1.93	0.68
1:A:382:SER:HB3	3:A:3012:HOH:O	1.92	0.67
1:F:348:ARG:HG2	3:H:1930:HOH:O	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:MET:HE2	1:A:379:ALA:CA	2.24	0.67
1:B:396:MET:HE2	1:B:414:PRO:HG2	1.76	0.67
1:G:396:MET:CE	1:G:414:PRO:HG2	2.24	0.67
1:G:101:MET:HE1	1:G:121:LYS:HA	1.75	0.67
1:E:248:ILE:HG12	1:E:281:LEU:HD22	1.76	0.67
1:F:474:ASP:O	1:F:497:VAL:HG23	1.94	0.67
1:D:216:ALA:HB1	1:D:254:GLU:HG3	1.75	0.67
1:D:396:MET:HE2	1:D:414:PRO:HG2	1.75	0.67
1:B:13:ASP:HB2	1:B:14:PRO:CD	2.25	0.67
1:E:493:ARG:NH1	1:E:495:LEU:HD21	2.10	0.67
1:D:396:MET:CE	1:D:414:PRO:HG2	2.24	0.67
1:G:400:SER:O	1:G:422:THR:HG23	1.95	0.67
1:C:497:VAL:HA	3:C:3061:HOH:O	1.95	0.66
1:E:85:LYS:HE3	3:E:1545:HOH:O	1.94	0.66
1:F:471:GLN:HB3	3:F:2155:HOH:O	1.94	0.66
1:H:396:MET:CE	1:H:414:PRO:HG2	2.24	0.66
1:B:84:THR:HG21	3:B:3068:HOH:O	1.95	0.66
1:A:396:MET:CE	1:A:414:PRO:HG2	2.26	0.66
1:B:30:SER:HB2	3:B:3356:HOH:O	1.96	0.66
1:B:396:MET:CE	1:B:414:PRO:HG2	2.25	0.66
1:B:68:ARG:HH11	1:B:80:ILE:HD12	1.61	0.65
1:H:374:MET:HE2	1:H:379:ALA:HA	1.79	0.65
1:H:396:MET:HE2	1:H:414:PRO:HG2	1.78	0.65
1:A:136:ARG:HB3	1:A:137:PRO:HD2	1.79	0.65
1:F:396:MET:CE	1:F:414:PRO:HG2	2.27	0.65
1:F:396:MET:HE2	1:F:414:PRO:HG2	1.78	0.65
1:H:494:ILE:HB	1:G:490:ASN:ND2	2.12	0.64
1:C:396:MET:CE	1:C:414:PRO:HG2	2.26	0.64
1:D:207:MET:HE3	1:D:209:PHE:HE1	1.61	0.64
1:B:474:ASP:O	1:B:497:VAL:HG23	1.97	0.64
1:C:310:ARG:HG2	3:C:3272:HOH:O	1.95	0.64
1:A:396:MET:HE2	1:A:414:PRO:HG2	1.77	0.64
1:F:302:MET:HB3	1:F:342:VAL:HG22	1.80	0.64
1:C:191:ALA:HA	3:C:3412:HOH:O	1.98	0.64
1:A:207:MET:HE1	1:A:433:ILE:CG2	2.27	0.64
1:A:207:MET:HE3	1:A:209:PHE:HE1	1.62	0.64
1:F:495:LEU:HD23	3:F:1964:HOH:O	1.97	0.64
1:H:116:ALA:HB2	3:H:2531:HOH:O	1.97	0.64
1:B:130:ASN:O	1:B:133:LYS:HG2	1.98	0.64
1:G:207:MET:HE1	1:G:433:ILE:CG2	2.28	0.64
1:C:189:VAL:HG23	1:C:193:ASP:CB	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:396:MET:HE2	1:C:414:PRO:HG2	1.80	0.63
1:E:396:MET:HE2	1:E:414:PRO:HG2	1.80	0.63
1:E:184:VAL:HG12	1:E:186:LEU:H	1.63	0.63
1:F:64:ILE:CG2	1:F:68:ARG:HH21	2.11	0.63
1:H:207:MET:HE3	1:H:209:PHE:HE1	1.64	0.63
1:C:16:ALA:HB3	3:C:3414:HOH:O	1.98	0.63
1:F:232:ASP:HB3	3:F:1940:HOH:O	1.98	0.63
1:H:185:ASP:HB3	3:H:2435:HOH:O	1.96	0.63
1:G:396:MET:HE2	1:G:414:PRO:HG2	1.80	0.63
1:F:207:MET:HE1	1:F:433:ILE:CG2	2.28	0.63
1:F:275:VAL:HG22	1:H:310:ARG:NH2	2.13	0.63
1:F:302:MET:SD	1:F:308:PRO:HD3	2.39	0.63
1:E:207:MET:HE3	1:E:209:PHE:CE1	2.34	0.63
1:F:459:ALA:O	1:F:462:GLU:HG2	1.99	0.63
1:C:38:LYS:O	1:C:42:GLN:HG3	1.99	0.62
1:H:135:VAL:HG11	1:H:152:VAL:HG21	1.80	0.62
1:F:242:HIS:CE1	3:F:2133:HOH:O	2.51	0.62
1:G:453:LYS:O	1:G:457:VAL:HG23	1.99	0.62
3:A:3044:HOH:O	1:C:3:LEU:HD13	1.99	0.62
1:E:111:THR:HG23	1:E:129:GLN:HA	1.80	0.62
1:B:424:ARG:HH11	1:B:424:ARG:CB	2.09	0.62
1:C:207:MET:HE1	1:C:433:ILE:CG2	2.28	0.62
1:D:394:LYS:HB2	1:D:470:VAL:HG12	1.82	0.62
1:E:192:LYS:HE2	3:E:1408:HOH:O	1.98	0.62
1:E:392:LYS:HG3	3:E:1756:HOH:O	1.98	0.62
1:C:29:PRO:HB2	3:C:3310:HOH:O	1.98	0.62
1:H:306:PRO:HG2	3:H:2513:HOH:O	1.99	0.62
1:C:374:MET:HE2	1:C:379:ALA:CA	2.26	0.62
1:C:453:LYS:O	1:C:457:VAL:HG23	2.00	0.62
1:E:302:MET:HE2	1:E:308:PRO:HB3	1.80	0.62
1:F:2:GLN:HG2	3:H:1822:HOH:O	2.00	0.62
1:B:118:LYS:HE3	3:B:3236:HOH:O	2.00	0.61
1:B:370:GLN:HB2	3:B:3130:HOH:O	1.99	0.61
1:H:382:SER:HB3	3:H:2255:HOH:O	2.00	0.61
1:A:242:HIS:O	1:A:246:GLN:HG3	2.00	0.61
1:B:302:MET:HE2	1:B:308:PRO:CB	2.29	0.61
1:E:207:MET:HE3	1:E:209:PHE:HE1	1.63	0.61
1:F:444:ALA:HB3	3:F:1951:HOH:O	2.01	0.61
1:G:142:TYR:HB3	1:G:146:GLY:HA2	1.81	0.61
1:E:207:MET:HE1	1:E:433:ILE:CG2	2.29	0.61
1:A:111:THR:HG23	1:A:129:GLN:HA	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:135:VAL:HG11	1:G:152:VAL:HG21	1.81	0.61
1:F:130:ASN:HB3	1:F:133:LYS:HE2	1.81	0.61
1:G:215:SER:HB2	1:G:218:GLN:HG3	1.82	0.61
1:A:357:LEU:HD13	3:A:3020:HOH:O	2.01	0.61
1:F:380:VAL:HG21	1:F:490:ASN:ND2	2.15	0.61
1:G:298:MET:HE1	1:G:327:VAL:HG12	1.83	0.61
1:B:242:HIS:HB3	3:B:3338:HOH:O	2.01	0.61
1:B:374:MET:HE3	1:B:378:GLU:HG3	1.82	0.61
1:B:119:GLY:HA3	3:B:3330:HOH:O	2.01	0.60
1:B:207:MET:HE3	1:B:209:PHE:HE1	1.66	0.60
1:B:207:MET:HE1	1:B:433:ILE:CG2	2.31	0.60
1:B:374:MET:HE2	1:B:379:ALA:CA	2.30	0.60
1:B:135:VAL:HG11	1:B:152:VAL:HG21	1.83	0.60
1:C:87:PRO:HG3	1:C:214:ARG:NH2	2.14	0.60
1:F:424:ARG:HH11	1:F:424:ARG:HB3	1.65	0.60
1:G:380:VAL:HG21	1:G:490:ASN:CG	2.26	0.60
1:C:135:VAL:HG11	1:C:152:VAL:HG21	1.82	0.60
1:C:380:VAL:HG21	1:C:490:ASN:CG	2.26	0.60
1:C:172:SER:H	1:C:175:ARG:CZ	2.14	0.60
1:H:242:HIS:O	1:H:246:GLN:HG3	2.01	0.60
1:C:132:SER:HB2	3:C:3026:HOH:O	2.02	0.60
1:A:42:GLN:HG2	3:A:3072:HOH:O	2.00	0.60
1:D:171:ILE:HA	1:D:175:ARG:NH1	2.17	0.60
1:E:374:MET:HE2	1:E:379:ALA:CA	2.28	0.59
1:H:380:VAL:HG21	1:H:490:ASN:HD21	1.66	0.59
1:A:365:SER:CB	1:C:3:LEU:HD23	2.32	0.59
1:B:310:ARG:HG3	1:D:297:GLN:HE22	1.66	0.59
1:D:109:VAL:HG11	1:D:126:ILE:HD12	1.84	0.59
1:D:207:MET:HE3	1:D:209:PHE:CE1	2.36	0.59
1:C:142:TYR:HB3	1:C:146:GLY:HA2	1.83	0.59
1:D:284:LYS:HE3	3:D:3215:HOH:O	2.01	0.59
1:B:364:ASN:ND2	1:B:368:LYS:HE2	2.18	0.59
1:A:207:MET:HE3	1:A:209:PHE:CE1	2.37	0.59
3:C:3419:HOH:O	1:D:491:GLN:HG3	2.02	0.59
1:H:310:ARG:HH12	1:H:314:SER:CB	2.16	0.59
1:A:404:ARG:HD3	3:A:3237:HOH:O	2.02	0.59
1:C:94:PHE:HB3	3:C:3446:HOH:O	2.02	0.59
1:C:157:ASP:HB2	3:C:3176:HOH:O	2.02	0.59
1:D:179:LEU:HB3	1:D:182:CYS:HB2	1.85	0.59
1:E:310:ARG:HB3	3:G:2941:HOH:O	2.02	0.59
1:D:198:GLN:HB2	3:D:3027:HOH:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:MET:HE1	3:A:3012:HOH:O	2.03	0.58
1:E:5:HIS:HE1	3:E:1608:HOH:O	1.86	0.58
1:H:134:VAL:CG1	1:H:182:CYS:HB3	2.33	0.58
1:C:189:VAL:HG23	1:C:193:ASP:HB2	1.84	0.58
1:F:254:GLU:HG2	3:F:1869:HOH:O	2.04	0.58
1:H:111:THR:CG2	1:H:129:GLN:HA	2.33	0.58
1:G:207:MET:HE3	1:G:209:PHE:HE1	1.68	0.58
1:C:179:LEU:HB3	1:C:182:CYS:HB2	1.85	0.58
1:D:142:TYR:HB3	1:D:146:GLY:HA2	1.85	0.58
1:E:365:SER:CB	1:G:3:LEU:HD23	2.34	0.58
1:E:490:ASN:O	1:E:491:GLN:HB2	2.02	0.58
1:A:283:SER:HB3	1:C:3:LEU:HD12	1.86	0.58
1:B:207:MET:HE3	1:B:209:PHE:CE1	2.39	0.58
1:F:384:ALA:HB2	1:F:479:ILE:HD11	1.85	0.58
1:A:401:ASN:HA	1:A:422:THR:HG23	1.85	0.58
1:F:465:LYS:HD2	3:F:2141:HOH:O	2.02	0.58
1:A:302:MET:HE3	1:A:342:VAL:HG13	1.86	0.58
1:D:89:ILE:HD11	1:D:186:LEU:HD11	1.86	0.58
1:F:374:MET:HE2	1:F:379:ALA:CA	2.34	0.58
1:A:89:ILE:HG12	1:A:186:LEU:HD11	1.85	0.57
1:F:380:VAL:HG21	1:F:490:ASN:OD1	2.04	0.57
1:H:189:VAL:HG13	1:H:193:ASP:CB	2.35	0.57
1:A:142:TYR:HB3	1:A:146:GLY:HA2	1.87	0.57
1:B:142:TYR:HB3	1:B:146:GLY:HA2	1.85	0.57
1:D:302:MET:CE	1:D:342:VAL:HA	2.34	0.57
1:D:422:THR:HG21	1:D:427:THR:HB	1.86	0.57
1:H:207:MET:HE1	1:H:433:ILE:CG2	2.33	0.57
1:C:187:PRO:HG2	3:C:3450:HOH:O	2.04	0.57
1:E:479:ILE:HG22	1:E:480:HIS:N	2.20	0.57
1:D:479:ILE:HG22	1:D:480:HIS:H	1.69	0.57
1:A:144:ASP:CG	1:A:175:ARG:HD3	2.30	0.57
1:F:142:TYR:HB3	1:F:146:GLY:HA2	1.87	0.57
1:F:289:GLY:HA2	3:F:2162:HOH:O	2.03	0.57
1:F:422:THR:HG21	1:F:427:THR:HB	1.86	0.57
1:A:492:THR:HG21	3:A:3280:HOH:O	2.04	0.57
1:G:109:VAL:HG11	1:G:126:ILE:HD12	1.87	0.56
1:D:156:GLU:HB2	1:D:160:THR:HB	1.87	0.56
1:E:493:ARG:HD3	3:E:1724:HOH:O	2.05	0.56
1:G:111:THR:CG2	1:G:129:GLN:HA	2.34	0.56
1:A:422:THR:HG21	1:A:427:THR:HB	1.87	0.56
1:A:455:HIS:HD2	3:A:3291:HOH:O	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:LYS:HB2	3:B:3345:HOH:O	2.04	0.56
1:C:207:MET:HE3	1:C:209:PHE:HE1	1.70	0.56
1:C:392:LYS:HD2	1:D:373:PRO:HD3	1.87	0.56
1:D:479:ILE:HG22	1:D:480:HIS:N	2.20	0.56
1:H:207:MET:HE3	1:H:209:PHE:CE1	2.39	0.56
1:E:223:ARG:HD2	3:E:1591:HOH:O	2.04	0.56
1:E:370:GLN:NE2	3:E:1651:HOH:O	2.38	0.56
1:D:229:LYS:HE2	3:D:3138:HOH:O	2.06	0.56
1:A:184:VAL:HG12	1:A:186:LEU:HG	1.88	0.56
1:E:130:ASN:O	1:E:133:LYS:HG2	2.05	0.56
1:B:371:HIS:HB3	3:B:3301:HOH:O	2.04	0.55
1:G:297:GLN:HG3	3:G:2935:HOH:O	2.06	0.55
1:A:374:MET:HE3	1:A:378:GLU:CG	2.32	0.55
1:A:424:ARG:HD2	3:A:3047:HOH:O	2.06	0.55
1:B:84:THR:HG22	1:B:211:SER:HB2	1.88	0.55
1:E:307:ARG:HG2	3:E:1738:HOH:O	2.06	0.55
1:F:180:PRO:HB3	3:F:2125:HOH:O	2.06	0.55
1:H:374:MET:HE2	1:H:379:ALA:CA	2.36	0.55
1:F:383:SER:HB2	3:F:1834:HOH:O	2.05	0.55
1:G:422:THR:HG21	1:G:427:THR:HB	1.87	0.55
1:C:207:MET:HE3	1:C:209:PHE:CE1	2.42	0.55
1:E:184:VAL:HB	1:E:214:ARG:HH12	1.72	0.55
1:D:215:SER:HB3	1:D:218:GLN:HG3	1.88	0.55
1:E:38:LYS:O	1:E:42:GLN:HG3	2.07	0.55
1:E:293:ILE:HG21	1:E:328:MET:HE3	1.87	0.55
1:H:142:TYR:HB3	1:H:146:GLY:HA2	1.89	0.55
1:A:302:MET:CE	1:A:342:VAL:HA	2.36	0.55
1:B:18:TYR:HD2	1:B:354:GLN:HE22	1.54	0.55
1:C:474:ASP:O	1:C:497:VAL:HG23	2.06	0.55
1:E:216:ALA:HB1	1:E:254:GLU:CG	2.36	0.55
1:H:422:THR:HG21	1:H:427:THR:HB	1.88	0.55
1:B:68:ARG:NH1	1:B:80:ILE:HD12	2.21	0.55
1:C:108:TYR:O	1:C:123:LYS:HA	2.07	0.55
1:D:89:ILE:CD1	1:D:186:LEU:HD11	2.37	0.55
1:D:335:LYS:HE3	3:D:3232:HOH:O	2.06	0.55
1:E:15:VAL:HG13	3:E:1754:HOH:O	2.05	0.55
1:E:171:ILE:HA	1:E:175:ARG:NH1	2.22	0.55
3:E:1614:HOH:O	1:G:3:LEU:HD13	2.07	0.55
1:C:111:THR:CG2	1:C:129:GLN:HA	2.38	0.55
1:D:298:MET:HE1	1:D:327:VAL:HG12	1.88	0.55
1:E:489:ALA:O	1:E:490:ASN:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:380:VAL:CG1	1:G:479:ILE:HD11	2.32	0.55
1:C:242:HIS:CE1	3:C:3426:HOH:O	2.59	0.54
1:H:384:ALA:HB2	1:H:479:ILE:HD11	1.89	0.54
1:B:422:THR:HG21	1:B:427:THR:HB	1.89	0.54
1:B:453:LYS:O	1:B:457:VAL:HG23	2.08	0.54
1:C:159:GLN:HG3	3:C:3387:HOH:O	2.07	0.54
1:D:302:MET:HE3	1:D:342:VAL:HA	1.88	0.54
1:E:142:TYR:HB3	1:E:146:GLY:HA2	1.88	0.54
1:G:182:CYS:HA	3:G:2913:HOH:O	2.06	0.54
1:A:137:PRO:HB3	1:A:153:GLN:O	2.08	0.54
1:B:367:LYS:CE	1:B:382:SER:HB2	2.37	0.54
1:G:171:ILE:HA	1:G:175:ARG:NH1	2.22	0.54
1:A:89:ILE:HD12	1:A:128:TYR:HB2	1.88	0.54
1:D:207:MET:HE1	1:D:433:ILE:CG2	2.37	0.54
1:D:294:CYS:O	1:D:298:MET:HE2	2.07	0.54
1:E:367:LYS:HG2	3:F:2122:HOH:O	2.07	0.54
1:H:135:VAL:CG1	1:H:152:VAL:HG21	2.38	0.54
1:B:396:MET:CE	1:B:418:ILE:HG12	2.37	0.54
1:A:215:SER:OG	1:A:218:GLN:HG3	2.08	0.54
1:G:207:MET:HE3	1:G:209:PHE:CE1	2.42	0.54
1:E:469:TYR:HE1	3:E:1748:HOH:O	1.90	0.54
1:H:142:TYR:HB2	1:H:178:ASN:HB2	1.90	0.54
1:C:446:LYS:O	1:C:447:LEU:HD23	2.07	0.54
1:F:229:LYS:HD2	3:F:2069:HOH:O	2.07	0.54
1:H:404:ARG:HG3	3:H:2537:HOH:O	2.08	0.54
1:A:398:VAL:HG13	1:A:479:ILE:HG23	1.88	0.53
1:A:401:ASN:ND2	1:A:423:THR:H	2.06	0.53
1:C:214:ARG:HH11	1:C:218:GLN:HE22	1.55	0.53
1:E:490:ASN:ND2	1:F:494:ILE:HB	2.23	0.53
1:E:310:ARG:HG2	3:G:2941:HOH:O	2.07	0.53
1:H:472:THR:HG23	1:H:498:GLU:HA	1.90	0.53
1:B:15:VAL:HG23	1:B:15:VAL:O	2.09	0.53
1:G:453:LYS:HD2	3:G:2918:HOH:O	2.07	0.53
1:B:293:ILE:HG21	1:B:328:MET:HE3	1.91	0.53
1:C:380:VAL:HG21	1:C:490:ASN:OD1	2.09	0.53
1:D:111:THR:HG22	1:D:111:THR:O	2.08	0.53
1:B:401:ASN:HA	1:B:422:THR:HG23	1.90	0.53
1:B:496:LEU:HB2	3:B:3317:HOH:O	2.09	0.53
1:E:298:MET:HE1	1:E:327:VAL:HG12	1.90	0.53
1:E:373:PRO:HB2	3:E:1410:HOH:O	2.07	0.53
1:F:207:MET:HE3	1:F:209:PHE:HE1	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:50:MET:HA	3:H:2230:HOH:O	2.08	0.53
1:D:396:MET:CE	1:D:418:ILE:HG12	2.39	0.53
1:E:424:ARG:HD2	3:E:1512:HOH:O	2.09	0.53
1:F:207:MET:HE3	1:F:209:PHE:CE1	2.44	0.53
1:H:310:ARG:C	1:H:310:ARG:HD3	2.34	0.53
1:A:38:LYS:HG2	1:A:70:ALA:HB1	1.92	0.52
1:D:87:PRO:HD3	1:D:188:ALA:O	2.09	0.52
1:D:396:MET:HE1	1:D:409:VAL:CG1	2.39	0.52
1:F:298:MET:HE1	1:F:327:VAL:HG12	1.92	0.52
1:H:380:VAL:HG21	1:H:490:ASN:ND2	2.24	0.52
1:H:34:VAL:HG23	3:H:2364:HOH:O	2.08	0.52
1:F:34:VAL:O	1:F:38:LYS:HG3	2.09	0.52
1:G:374:MET:HE2	1:G:379:ALA:HA	1.90	0.52
1:C:396:MET:HE1	1:C:409:VAL:CG1	2.38	0.52
1:H:90:ARG:HG2	1:H:127:ASP:OD2	2.09	0.52
1:C:396:MET:CE	1:C:418:ILE:HG12	2.39	0.52
1:E:132:SER:HB3	1:E:155:HIS:CE1	2.45	0.52
1:G:380:VAL:HG12	1:G:479:ILE:CD1	2.33	0.52
1:E:84:THR:HG22	1:E:211:SER:HB2	1.90	0.52
1:E:382:SER:HB3	3:E:1729:HOH:O	2.08	0.52
1:G:480:HIS:O	1:G:490:ASN:HA	2.10	0.52
1:E:135:VAL:HG11	1:E:152:VAL:HG21	1.90	0.52
1:F:396:MET:HE1	1:F:409:VAL:CG1	2.40	0.52
1:F:491:GLN:HG2	1:F:492:THR:N	2.24	0.52
1:H:396:MET:HE3	1:H:418:ILE:HG12	1.91	0.52
1:G:228:PRO:O	1:G:231:ARG:NE	2.37	0.52
1:B:263:GLY:H	1:B:296:THR:HG1	1.54	0.52
1:G:396:MET:HE1	1:G:414:PRO:HG2	1.92	0.52
1:A:302:MET:HE1	1:A:345:TYR:HB3	1.92	0.52
1:C:422:THR:HG21	1:C:427:THR:HB	1.91	0.52
1:E:69:GLN:O	1:E:73:GLU:HG3	2.10	0.52
1:F:108:TYR:O	1:F:123:LYS:HA	2.10	0.52
1:C:133:LYS:HG3	3:C:3150:HOH:O	2.08	0.52
1:E:422:THR:HG21	1:E:427:THR:HB	1.91	0.52
1:F:374:MET:HE3	1:F:378:GLU:CG	2.39	0.52
1:H:111:THR:HG23	1:H:129:GLN:HA	1.91	0.51
1:A:401:ASN:HA	1:A:422:THR:CG2	2.40	0.51
1:B:111:THR:CG2	1:B:129:GLN:HA	2.40	0.51
1:E:396:MET:CE	1:E:418:ILE:HG12	2.40	0.51
1:F:84:THR:HG22	1:F:211:SER:HB2	1.91	0.51
1:G:14:PRO:HG2	3:G:2610:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:374:MET:HE3	1:G:378:GLU:CG	2.39	0.51
1:A:422:THR:HG21	1:A:427:THR:CB	2.41	0.51
1:C:189:VAL:HG23	1:C:193:ASP:HB3	1.90	0.51
1:D:302:MET:HE3	1:D:342:VAL:HG13	1.92	0.51
1:H:396:MET:CE	1:H:418:ILE:HG12	2.40	0.51
1:B:396:MET:HE1	1:B:409:VAL:CG1	2.40	0.51
1:C:106:THR:HG23	3:C:3434:HOH:O	2.09	0.51
1:F:396:MET:CE	1:F:418:ILE:HG12	2.40	0.51
1:G:145:ASP:HB2	3:G:2700:HOH:O	2.10	0.51
1:B:424:ARG:HB3	1:B:424:ARG:NH1	2.11	0.51
1:C:310:ARG:HD3	1:C:310:ARG:C	2.36	0.51
1:D:396:MET:HE3	1:D:418:ILE:HG12	1.92	0.51
1:E:250:SER:HA	3:E:1757:HOH:O	2.11	0.51
1:A:108:TYR:O	1:A:123:LYS:HA	2.10	0.51
1:E:9:LEU:HD23	3:E:1743:HOH:O	2.10	0.51
1:H:212:PHE:HZ	3:H:2566:HOH:O	1.92	0.51
1:G:130:ASN:CB	1:G:133:LYS:HE2	2.38	0.51
1:C:14:PRO:HB2	3:C:3137:HOH:O	2.11	0.51
1:C:184:VAL:HG12	1:C:186:LEU:H	1.76	0.51
1:E:380:VAL:HG21	1:E:490:ASN:HD21	1.75	0.51
1:H:493:ARG:HH12	1:H:495:LEU:HD13	1.75	0.51
1:F:111:THR:HG21	3:F:1803:HOH:O	2.09	0.51
1:C:310:ARG:HD3	1:C:310:ARG:O	2.10	0.51
1:H:242:HIS:HD2	1:H:268:GLU:OE2	1.93	0.51
1:H:367:LYS:HE3	3:G:2636:HOH:O	2.10	0.51
1:H:376:ALA:O	1:H:380:VAL:HG23	2.11	0.51
1:A:246:GLN:HG2	1:C:12:PHE:CE2	2.46	0.51
1:C:84:THR:HG22	1:C:211:SER:HB2	1.92	0.51
1:H:298:MET:HE1	1:H:327:VAL:HG12	1.91	0.51
1:G:29:PRO:HB2	3:G:2696:HOH:O	2.11	0.51
1:C:298:MET:HE1	1:C:327:VAL:HG12	1.93	0.50
1:H:85:LYS:HE3	3:H:2561:HOH:O	2.11	0.50
1:G:413:ARG:NH1	3:G:2687:HOH:O	2.40	0.50
1:D:404:ARG:HG2	3:D:3135:HOH:O	2.10	0.50
1:F:368:LYS:HE2	3:F:2140:HOH:O	2.10	0.50
1:F:401:ASN:HA	1:F:422:THR:HG23	1.94	0.50
1:F:422:THR:HG21	1:F:427:THR:CB	2.41	0.50
1:H:382:SER:CB	3:H:2255:HOH:O	2.58	0.50
1:A:223:ARG:HG3	3:A:3300:HOH:O	2.12	0.50
1:C:364:ASN:O	1:C:368:LYS:HG3	2.12	0.50
1:H:38:LYS:HG2	1:H:70:ALA:HB1	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ALA:HB2	1:A:429:ARG:O	2.11	0.50
1:C:498:GLU:N	3:C:3061:HOH:O	2.44	0.50
1:E:132:SER:HB3	1:E:155:HIS:HE1	1.77	0.50
1:H:79:ALA:HB2	1:H:429:ARG:O	2.11	0.50
1:A:179:LEU:HB3	1:A:182:CYS:HB2	1.93	0.50
1:A:494:ILE:HD12	1:B:380:VAL:HG23	1.94	0.50
1:D:422:THR:HG21	1:D:427:THR:CB	2.41	0.50
1:E:396:MET:HE1	1:E:414:PRO:HG2	1.92	0.50
1:F:453:LYS:HE2	1:F:480:HIS:CE1	2.46	0.50
1:B:341:GLU:HG2	3:B:3099:HOH:O	2.12	0.50
1:C:145:ASP:HB2	3:C:3135:HOH:O	2.11	0.50
1:D:34:VAL:HG21	1:D:69:GLN:OE1	2.12	0.50
1:E:7:LEU:HD11	1:G:287:VAL:HG21	1.94	0.50
1:G:293:ILE:HG21	1:G:328:MET:HE3	1.94	0.50
1:C:399:LEU:HD22	1:C:421:VAL:HB	1.94	0.50
1:F:301:SER:HA	1:F:304:TYR:CE1	2.47	0.50
1:F:380:VAL:HG21	1:F:490:ASN:CG	2.37	0.50
1:G:279:LYS:HG3	3:G:2587:HOH:O	2.12	0.50
1:F:262:ARG:HB3	3:H:2519:HOH:O	2.12	0.49
1:H:374:MET:HE2	1:H:379:ALA:N	2.26	0.49
1:G:396:MET:CE	1:G:418:ILE:HG12	2.42	0.49
1:B:123:LYS:NZ	3:B:3017:HOH:O	2.45	0.49
1:C:93:GLN:HB2	1:C:117:ASP:HA	1.92	0.49
1:D:455:HIS:HE1	3:D:3218:HOH:O	1.95	0.49
1:B:197:LEU:O	1:B:201:VAL:HG23	2.12	0.49
1:B:310:ARG:HH22	1:D:274:VAL:HG21	1.76	0.49
1:D:134:VAL:HG12	1:D:182:CYS:HB3	1.95	0.49
1:E:223:ARG:HD3	3:E:1534:HOH:O	2.12	0.49
1:H:396:MET:HE1	1:H:414:PRO:HG2	1.94	0.49
1:H:404:ARG:HA	3:H:2537:HOH:O	2.11	0.49
1:H:493:ARG:NH1	1:H:495:LEU:HD13	2.28	0.49
1:B:396:MET:HE3	1:B:418:ILE:HG12	1.94	0.49
1:E:130:ASN:HA	1:E:133:LYS:HE3	1.95	0.49
1:E:339:PRO:HD2	3:E:1418:HOH:O	2.13	0.49
1:F:242:HIS:CD2	3:F:1791:HOH:O	2.65	0.49
1:C:396:MET:HE3	1:C:418:ILE:HG12	1.94	0.49
1:F:294:CYS:O	1:F:298:MET:HE2	2.13	0.49
1:E:109:VAL:HG11	1:E:126:ILE:HD12	1.95	0.49
1:H:367:LYS:HG3	3:G:2636:HOH:O	2.12	0.49
1:B:472:THR:HA	1:B:497:VAL:O	2.12	0.49
1:D:455:HIS:CE1	3:D:3218:HOH:O	2.65	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:LYS:O	1:A:457:VAL:HG23	2.13	0.49
1:D:405:SER:OG	1:D:481:ALA:HB3	2.13	0.49
1:G:84:THR:HG22	1:G:211:SER:HB2	1.93	0.49
1:A:298:MET:HE1	1:A:327:VAL:HG12	1.95	0.49
1:B:298:MET:HE1	1:B:327:VAL:HG12	1.95	0.49
1:C:87:PRO:HB2	1:C:186:LEU:HD13	1.93	0.49
1:E:242:HIS:HD2	1:E:268:GLU:OE2	1.94	0.49
1:F:228:PRO:O	1:F:231:ARG:HG3	2.12	0.49
1:G:197:LEU:O	1:G:201:VAL:HG23	2.13	0.49
1:A:396:MET:HE1	1:A:409:VAL:CG1	2.43	0.48
1:D:156:GLU:OE2	1:D:162:GLU:HB2	2.13	0.48
1:G:355:SER:HA	3:G:2937:HOH:O	2.11	0.48
1:C:111:THR:HG23	1:C:129:GLN:HA	1.94	0.48
1:H:302:MET:HE1	1:H:345:TYR:HB3	1.94	0.48
1:B:391:THR:HB	1:B:475:TYR:CD2	2.48	0.48
1:E:302:MET:HE3	1:E:342:VAL:HG13	1.95	0.48
1:F:243:GLN:HG2	3:F:2133:HOH:O	2.12	0.48
1:A:374:MET:HE2	1:A:379:ALA:N	2.28	0.48
1:E:64:ILE:O	1:E:68:ARG:HG3	2.13	0.48
1:E:310:ARG:HD2	1:G:297:GLN:HE21	1.78	0.48
1:B:12:PHE:CE2	1:D:246:GLN:HG3	2.49	0.48
1:A:396:MET:CE	1:A:418:ILE:HG12	2.44	0.48
1:B:103:ARG:HG3	1:B:167:ASN:HA	1.96	0.48
1:C:144:ASP:CG	1:C:175:ARG:HD3	2.39	0.48
1:C:310:ARG:NH1	1:C:314:SER:HB3	2.28	0.48
1:E:374:MET:CE	1:E:379:ALA:HA	2.33	0.48
1:H:22:ARG:CZ	3:H:2501:HOH:O	2.61	0.48
1:B:401:ASN:HA	1:B:422:THR:CG2	2.44	0.48
1:H:111:THR:HG22	1:H:111:THR:O	2.13	0.48
1:H:179:LEU:HB3	1:H:182:CYS:HB2	1.95	0.48
1:H:422:THR:HG21	1:H:427:THR:CB	2.44	0.48
1:E:216:ALA:HB1	1:E:254:GLU:HG3	1.95	0.48
1:H:89:ILE:HG13	1:H:186:LEU:HD11	1.96	0.48
1:G:174:ARG:HD3	3:G:2802:HOH:O	2.14	0.48
1:A:367:LYS:HE3	1:A:382:SER:HB2	1.95	0.48
1:D:223:ARG:NH1	1:D:235:ILE:HG13	2.29	0.48
1:F:109:VAL:CG1	1:F:126:ILE:HD12	2.44	0.48
1:G:481:ALA:O	1:G:482:ASP:HB2	2.14	0.48
1:A:140:TYR:O	1:A:180:PRO:HD2	2.14	0.48
1:E:396:MET:HE1	1:E:409:VAL:CG1	2.43	0.48
1:F:380:VAL:CG2	1:F:490:ASN:HD21	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:399:LEU:HD22	1:F:421:VAL:HB	1.96	0.48
1:E:142:TYR:HB2	1:E:178:ASN:HB2	1.95	0.47
1:F:38:LYS:HG2	1:F:70:ALA:HB1	1.96	0.47
1:E:228:PRO:HB3	3:E:1762:HOH:O	2.14	0.47
1:B:136:ARG:NE	3:B:3113:HOH:O	2.45	0.47
1:D:362:PHE:HB3	1:D:413:ARG:HG3	1.96	0.47
1:E:17:ASN:HB3	3:E:1514:HOH:O	2.14	0.47
1:E:157:ASP:C	1:E:159:GLN:H	2.22	0.47
1:F:179:LEU:HB3	1:F:182:CYS:HB2	1.97	0.47
1:A:11:ILE:HG12	3:A:3220:HOH:O	2.14	0.47
1:D:367:LYS:CE	1:D:382:SER:HB2	2.41	0.47
1:D:385:VAL:HG22	1:D:414:PRO:HG3	1.96	0.47
1:F:374:MET:HE1	3:F:1798:HOH:O	2.14	0.47
1:H:243:GLN:HG3	3:H:2175:HOH:O	2.15	0.47
1:H:448:GLY:HA2	3:H:2493:HOH:O	2.14	0.47
1:B:142:TYR:HB2	1:B:178:ASN:HB2	1.96	0.47
1:C:136:ARG:HB3	1:C:137:PRO:HD2	1.96	0.47
1:C:149:ILE:HG23	1:C:167:ASN:OD1	2.15	0.47
1:A:435:GLN:HG3	3:A:3046:HOH:O	2.14	0.47
1:C:234:MET:HE2	1:C:430:GLN:HG2	1.96	0.47
1:E:79:ALA:HB2	1:E:429:ARG:O	2.14	0.47
1:E:481:ALA:HB3	3:E:1744:HOH:O	2.13	0.47
1:F:111:THR:HG22	1:F:159:GLN:O	2.15	0.47
1:F:220:GLY:O	1:F:224:LYS:HG3	2.15	0.47
1:G:399:LEU:HD22	1:G:421:VAL:HB	1.96	0.47
1:C:140:TYR:CE1	1:C:149:ILE:HD11	2.49	0.47
1:C:366:ILE:HD11	3:C:3224:HOH:O	2.13	0.47
1:C:418:ILE:CD1	3:C:3425:HOH:O	2.63	0.47
1:D:293:ILE:HG21	1:D:328:MET:HE3	1.97	0.47
1:E:184:VAL:HG12	1:E:185:ASP:N	2.29	0.47
1:H:293:ILE:HG21	1:H:328:MET:HE3	1.97	0.47
1:G:144:ASP:CG	1:G:175:ARG:HD3	2.40	0.47
1:G:250:SER:O	1:G:253:GLU:HB3	2.14	0.47
1:G:429:ARG:O	1:G:432:ASN:HB2	2.14	0.47
1:A:89:ILE:HD11	1:A:186:LEU:HD21	1.95	0.47
1:B:399:LEU:HD22	1:B:421:VAL:HB	1.97	0.47
1:B:422:THR:HG21	1:B:427:THR:CB	2.45	0.47
1:D:93:GLN:CD	1:D:174:ARG:HH21	2.23	0.47
1:D:184:VAL:HG12	1:D:185:ASP:N	2.29	0.47
1:B:109:VAL:CG1	1:B:126:ILE:HD12	2.45	0.47
1:B:374:MET:HE3	1:B:378:GLU:CG	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:THR:N	1:D:159:GLN:O	2.47	0.47
1:E:12:PHE:CE1	1:G:242:HIS:HB2	2.50	0.47
1:A:25:CYS:HB2	1:A:45:MET:HE2	1.91	0.46
1:A:197:LEU:O	1:A:201:VAL:HG23	2.13	0.46
1:A:302:MET:HE1	1:A:342:VAL:HA	1.97	0.46
1:B:135:VAL:HG12	1:B:136:ARG:N	2.30	0.46
1:C:293:ILE:HG21	1:C:328:MET:HE3	1.97	0.46
1:C:394:LYS:HB2	1:C:470:VAL:HG12	1.97	0.46
1:D:214:ARG:HD2	1:D:243:GLN:NE2	2.29	0.46
1:E:422:THR:HG21	1:E:427:THR:CB	2.45	0.46
1:F:362:PHE:HB3	1:F:413:ARG:HG3	1.97	0.46
1:H:93:GLN:HG2	3:H:2356:HOH:O	2.14	0.46
1:G:111:THR:HG23	1:G:129:GLN:HA	1.97	0.46
3:A:3083:HOH:O	1:C:310:ARG:HD2	2.14	0.46
1:B:294:CYS:O	1:B:298:MET:HE2	2.13	0.46
1:B:135:VAL:CG1	1:B:152:VAL:HG21	2.44	0.46
1:F:242:HIS:HB3	3:F:1791:HOH:O	2.14	0.46
1:G:259:MET:CE	1:G:328:MET:HE1	2.40	0.46
1:A:142:TYR:HB2	1:A:178:ASN:HB2	1.97	0.46
1:E:197:LEU:O	1:E:201:VAL:HG23	2.15	0.46
1:E:228:PRO:HD3	3:E:1762:HOH:O	2.14	0.46
1:G:83:ASP:HA	1:G:209:PHE:HB2	1.98	0.46
1:G:385:VAL:HG22	1:G:414:PRO:HG3	1.96	0.46
1:A:186:LEU:HB3	1:A:187:PRO:HD2	1.97	0.46
1:D:84:THR:HG22	1:D:211:SER:HB2	1.97	0.46
1:E:396:MET:HE3	1:E:418:ILE:HG12	1.97	0.46
1:H:396:MET:HE1	1:H:409:VAL:CG1	2.45	0.46
1:B:79:ALA:HB2	1:B:429:ARG:O	2.15	0.46
1:B:364:ASN:O	1:B:368:LYS:HG2	2.16	0.46
1:C:497:VAL:HG12	1:C:498:GLU:N	2.31	0.46
1:E:371:HIS:CE1	3:E:1518:HOH:O	2.68	0.46
1:F:183:ASP:CG	3:F:2133:HOH:O	2.58	0.46
1:B:367:LYS:HE3	1:B:382:SER:HB2	1.96	0.46
1:D:250:SER:O	1:D:253:GLU:HB3	2.15	0.46
1:D:263:GLY:H	1:D:296:THR:HG1	1.58	0.46
1:D:374:MET:HE3	1:D:378:GLU:HG3	1.97	0.46
1:D:429:ARG:O	1:D:432:ASN:HB2	2.16	0.46
1:D:480:HIS:CE1	1:D:490:ASN:H	2.33	0.46
1:A:287:VAL:HG21	1:C:7:LEU:HD11	1.97	0.46
1:D:185:ASP:HA	1:D:214:ARG:NH2	2.30	0.46
1:E:294:CYS:O	1:E:298:MET:HE2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:380:VAL:HG23	1:F:494:ILE:HD12	1.97	0.46
1:E:392:LYS:HE3	3:E:1756:HOH:O	2.15	0.46
1:H:450:ASP:N	3:H:2382:HOH:O	2.49	0.46
1:E:263:GLY:HA2	3:E:1740:HOH:O	2.16	0.46
1:H:122:ASP:HB2	3:H:2245:HOH:O	2.16	0.46
1:A:12:PHE:HB3	3:A:3310:HOH:O	2.16	0.46
1:A:376:ALA:HB1	1:A:490:ASN:ND2	2.25	0.46
1:D:396:MET:HE1	1:D:414:PRO:HG2	1.97	0.46
1:D:489:ALA:O	1:D:490:ASN:HB2	2.16	0.46
1:H:302:MET:HE1	1:H:345:TYR:CB	2.46	0.46
1:G:362:PHE:HB3	1:G:413:ARG:HG3	1.97	0.46
1:G:396:MET:HE1	1:G:409:VAL:CG1	2.45	0.46
1:D:34:VAL:HG23	3:D:3090:HOH:O	2.16	0.45
1:B:250:SER:O	1:B:253:GLU:HB3	2.16	0.45
1:F:109:VAL:HG11	1:F:126:ILE:HD12	1.98	0.45
1:F:129:GLN:HG2	3:F:1892:HOH:O	2.15	0.45
1:H:471:GLN:NE2	3:H:2459:HOH:O	2.47	0.45
1:A:283:SER:O	1:A:287:VAL:HG23	2.15	0.45
1:B:111:THR:HB	3:B:3035:HOH:O	2.16	0.45
1:E:374:MET:HE3	1:E:378:GLU:HG3	1.99	0.45
1:A:396:MET:HE3	1:A:418:ILE:HG12	1.98	0.45
1:H:83:ASP:HA	1:H:209:PHE:HB2	1.98	0.45
1:G:47:VAL:HG22	1:G:79:ALA:HB3	1.98	0.45
1:G:142:TYR:HB2	1:G:178:ASN:HB2	1.98	0.45
1:B:259:MET:CE	1:B:328:MET:HE1	2.43	0.45
1:B:374:MET:HE2	1:B:379:ALA:N	2.32	0.45
1:G:345:TYR:O	1:G:349:ILE:HG13	2.17	0.45
3:C:3418:HOH:O	1:D:480:HIS:CE1	2.68	0.45
1:D:142:TYR:HB2	1:D:178:ASN:HB2	1.98	0.45
1:F:169:HIS:CE1	3:F:2154:HOH:O	2.68	0.45
1:H:250:SER:O	1:H:253:GLU:HB3	2.16	0.45
1:A:84:THR:HG22	1:A:211:SER:HB2	1.98	0.45
1:A:293:ILE:HG21	1:A:328:MET:HE3	1.98	0.45
1:B:385:VAL:HG22	1:B:414:PRO:HG3	1.98	0.45
1:C:14:PRO:HB3	3:C:3357:HOH:O	2.17	0.45
1:E:372:ILE:HG23	1:E:373:PRO:HA	1.98	0.45
1:G:396:MET:HE3	1:G:418:ILE:HG12	1.98	0.45
1:B:194:ARG:HD3	3:B:3098:HOH:O	2.16	0.45
1:C:125:TYR:HB3	3:C:3451:HOH:O	2.16	0.45
1:C:148:LEU:HB2	1:C:169:HIS:HD2	1.81	0.45
1:D:491:GLN:HG2	1:D:492:THR:N	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:396:MET:HE3	1:F:418:ILE:HG12	1.99	0.45
1:H:84:THR:HG22	1:H:211:SER:HB2	1.97	0.45
1:H:289:GLY:HA3	3:H:2460:HOH:O	2.15	0.45
1:H:345:TYR:O	1:H:349:ILE:HG13	2.17	0.45
1:C:130:ASN:OD1	1:C:133:LYS:HD2	2.16	0.45
1:E:16:ALA:HA	3:E:1558:HOH:O	2.17	0.45
1:E:394:LYS:HD3	3:E:1770:HOH:O	2.17	0.45
1:F:299:LEU:HB3	1:F:302:MET:HG3	1.99	0.45
1:H:18:TYR:OH	1:H:436:GLY:HA2	2.15	0.45
1:G:374:MET:HE1	3:G:2940:HOH:O	2.15	0.45
1:A:34:VAL:O	1:A:38:LYS:HG3	2.17	0.45
1:A:135:VAL:HG11	1:A:152:VAL:HG21	1.99	0.45
1:A:392:LYS:HG3	1:B:373:PRO:HB3	1.99	0.45
1:B:136:ARG:HD2	3:B:3243:HOH:O	2.16	0.45
1:B:364:ASN:HD21	1:B:368:LYS:HE2	1.80	0.45
1:C:172:SER:HB2	3:C:3133:HOH:O	2.16	0.45
1:C:457:VAL:O	1:C:461:VAL:HG23	2.17	0.45
1:D:399:LEU:HD22	1:D:421:VAL:HB	1.99	0.45
1:H:242:HIS:CD2	3:H:2175:HOH:O	2.69	0.45
1:G:380:VAL:HG21	1:G:490:ASN:OD1	2.16	0.45
1:G:444:ALA:HB3	3:G:2947:HOH:O	2.17	0.45
1:C:142:TYR:HB2	1:C:178:ASN:HB2	1.99	0.44
1:C:306:PRO:HG2	1:C:307:ARG:HG2	1.97	0.44
1:G:489:ALA:HB1	1:G:490:ASN:H	1.58	0.44
1:B:354:GLN:HG3	3:B:3359:HOH:O	2.15	0.44
1:A:366:ILE:HG22	1:A:412:TYR:CE1	2.52	0.44
1:A:399:LEU:CD1	1:A:453:LYS:HB3	2.48	0.44
1:C:294:CYS:O	1:C:298:MET:HE2	2.18	0.44
1:H:148:LEU:HB2	1:H:169:HIS:HD2	1.82	0.44
1:H:178:ASN:HA	3:H:2204:HOH:O	2.17	0.44
1:H:385:VAL:HG22	1:H:414:PRO:HG3	1.98	0.44
1:G:294:CYS:O	1:G:298:MET:HE2	2.18	0.44
1:G:479:ILE:HG23	1:G:480:HIS:N	2.33	0.44
1:A:396:MET:HE1	1:A:414:PRO:HG2	1.97	0.44
1:A:425:LEU:HD13	1:A:441:PHE:CG	2.52	0.44
1:B:362:PHE:HB3	1:B:413:ARG:HG3	1.99	0.44
1:C:197:LEU:O	1:C:201:VAL:HG23	2.17	0.44
1:D:111:THR:HG23	1:D:129:GLN:HA	2.00	0.44
1:F:135:VAL:HG12	1:F:136:ARG:N	2.32	0.44
1:A:366:ILE:HD12	1:C:3:LEU:HD21	1.99	0.44
1:C:109:VAL:HG12	1:C:124:PHE:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:VAL:HG23	1:D:193:ASP:CB	2.48	0.44
1:G:184:VAL:HG12	1:G:186:LEU:H	1.81	0.44
1:B:103:ARG:C	1:B:105:ALA:H	2.26	0.44
1:B:109:VAL:HG11	1:B:126:ILE:HD12	1.99	0.44
1:H:215:SER:HB3	3:H:2469:HOH:O	2.18	0.44
1:G:302:MET:HB3	1:G:342:VAL:HG22	2.00	0.44
1:G:422:THR:HG21	1:G:427:THR:CB	2.47	0.44
1:A:237:CYS:SG	1:A:255:SER:HB3	2.57	0.44
1:A:399:LEU:HD22	1:A:421:VAL:HB	1.99	0.44
1:B:130:ASN:HA	1:B:133:LYS:HE3	2.00	0.44
1:B:135:VAL:CG1	1:B:136:ARG:N	2.80	0.44
1:C:396:MET:HE1	1:C:414:PRO:HG2	1.96	0.44
1:H:149:ILE:HD13	3:H:2551:HOH:O	2.16	0.44
1:A:269:ILE:HG22	1:A:273:LYS:HB2	2.00	0.44
1:B:89:ILE:HG23	1:B:128:TYR:HB2	1.99	0.44
1:D:471:GLN:HG3	3:D:3234:HOH:O	2.17	0.44
1:E:299:LEU:HD13	1:E:302:MET:CE	2.48	0.44
1:E:376:ALA:O	1:E:380:VAL:HG23	2.18	0.44
1:F:338:TYR:HB3	1:F:341:GLU:HB2	2.00	0.44
1:H:10:SER:N	3:H:2563:HOH:O	2.41	0.44
1:G:376:ALA:O	1:G:380:VAL:HG23	2.17	0.44
1:G:463:PHE:CZ	1:G:467:LYS:HE3	2.52	0.44
1:A:479:ILE:HG12	1:A:480:HIS:N	2.33	0.44
1:C:11:ILE:HA	3:C:3191:HOH:O	2.17	0.44
1:C:422:THR:HG21	1:C:427:THR:CB	2.48	0.44
1:C:429:ARG:O	1:C:432:ASN:HB2	2.16	0.44
1:D:376:ALA:O	1:D:380:VAL:HG23	2.18	0.44
1:F:142:TYR:HB2	1:F:178:ASN:HB2	2.00	0.44
1:G:297:GLN:CG	3:G:2935:HOH:O	2.65	0.44
1:G:480:HIS:HE1	1:G:483:HIS:HA	1.83	0.44
1:B:85:LYS:HE2	1:B:88:GLU:OE2	2.18	0.43
1:C:493:ARG:NH2	3:C:3418:HOH:O	2.51	0.43
1:D:180:PRO:HA	1:D:268:GLU:HB3	1.99	0.43
1:D:189:VAL:HG23	1:D:193:ASP:HB2	1.99	0.43
1:E:355:SER:HB3	3:E:1443:HOH:O	2.17	0.43
1:F:148:LEU:HB2	1:F:169:HIS:HD2	1.83	0.43
1:B:11:ILE:HA	3:B:3036:HOH:O	2.18	0.43
1:C:47:VAL:HG22	1:C:79:ALA:HB3	2.00	0.43
1:D:148:LEU:HB2	1:D:169:HIS:HD2	1.83	0.43
1:D:422:THR:HG22	1:D:424:ARG:H	1.83	0.43
1:E:10:SER:HB3	1:E:13:ASP:OD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:404:ARG:HD3	3:E:1541:HOH:O	2.17	0.43
1:G:109:VAL:CG1	1:G:126:ILE:HD12	2.48	0.43
1:A:250:SER:O	1:A:253:GLU:HB3	2.18	0.43
1:D:223:ARG:HH21	1:D:231:ARG:C	2.26	0.43
1:E:54:HIS:HD2	3:E:1733:HOH:O	2.01	0.43
1:E:425:LEU:HD13	1:E:441:PHE:CG	2.53	0.43
1:F:429:ARG:O	1:F:432:ASN:HB2	2.17	0.43
1:G:302:MET:HE1	1:G:345:TYR:HB3	1.99	0.43
1:B:16:ALA:O	1:B:18:TYR:N	2.46	0.43
1:E:89:ILE:HG13	1:E:186:LEU:HD11	1.99	0.43
1:G:215:SER:HB3	1:G:217:GLU:OE1	2.18	0.43
1:A:4:ALA:HB1	3:A:3212:HOH:O	2.18	0.43
1:B:178:ASN:CG	1:B:267:VAL:HG11	2.43	0.43
1:C:384:ALA:HB1	1:C:479:ILE:HD11	2.01	0.43
1:E:336:GLY:HA3	3:E:1382:HOH:O	2.18	0.43
1:F:310:ARG:HH22	1:H:275:VAL:HG22	1.82	0.43
1:H:134:VAL:HG12	1:H:182:CYS:HB3	2.01	0.43
1:A:83:ASP:HA	1:A:209:PHE:HB2	2.00	0.43
1:A:234:MET:HE1	1:A:433:ILE:HD11	2.01	0.43
1:C:471:GLN:O	1:C:497:VAL:HB	2.18	0.43
1:D:109:VAL:CG1	1:D:126:ILE:HD12	2.47	0.43
1:E:429:ARG:O	1:E:432:ASN:HB2	2.19	0.43
1:F:446:LYS:O	1:F:446:LYS:HG3	2.19	0.43
1:H:108:TYR:O	1:H:123:LYS:HA	2.19	0.43
1:B:73:GLU:HG3	3:B:3150:HOH:O	2.19	0.43
1:B:373:PRO:HB2	3:B:3309:HOH:O	2.18	0.43
1:C:425:LEU:HD13	1:C:441:PHE:CG	2.54	0.43
1:E:37:LEU:O	1:E:41:ILE:HG13	2.18	0.43
1:E:54:HIS:CD2	3:E:1733:HOH:O	2.71	0.43
1:E:479:ILE:HG22	1:E:480:HIS:H	1.83	0.43
1:B:83:ASP:HA	1:B:209:PHE:HB2	2.00	0.43
1:C:273:LYS:NZ	3:C:3248:HOH:O	2.51	0.43
1:C:302:MET:HG2	1:C:305:ASN:O	2.18	0.43
1:D:153:GLN:O	1:D:154:SER:HB3	2.18	0.43
1:G:89:ILE:HG13	1:G:186:LEU:HD11	2.00	0.43
1:G:457:VAL:O	1:G:461:VAL:HG23	2.19	0.43
1:A:390:GLU:HG2	3:A:3023:HOH:O	2.18	0.43
1:A:424:ARG:NH1	3:A:3104:HOH:O	2.51	0.43
1:F:10:SER:HB3	1:F:13:ASP:OD2	2.19	0.43
1:F:250:SER:O	1:F:253:GLU:HB3	2.19	0.43
1:F:310:ARG:HH22	1:H:275:VAL:CG2	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:429:ARG:O	1:H:432:ASN:HB2	2.19	0.43
1:G:304:TYR:HB3	3:G:2833:HOH:O	2.19	0.43
1:B:367:LYS:HE2	1:B:382:SER:HB2	2.01	0.43
1:B:372:ILE:HB	3:B:3167:HOH:O	2.19	0.43
1:C:142:TYR:O	1:C:177:VAL:HA	2.19	0.43
1:C:385:VAL:HG22	1:C:414:PRO:HG3	2.01	0.43
1:D:83:ASP:HA	1:D:209:PHE:HB2	2.01	0.43
1:D:214:ARG:HD2	1:D:243:GLN:CD	2.44	0.43
1:E:237:CYS:SG	1:E:255:SER:HB3	2.59	0.43
1:F:79:ALA:HB2	1:F:429:ARG:O	2.18	0.43
1:F:293:ILE:HG21	1:F:328:MET:HE3	2.01	0.43
1:H:494:ILE:O	1:G:490:ASN:ND2	2.51	0.43
1:G:178:ASN:O	1:G:180:PRO:HD3	2.18	0.43
1:A:383:SER:CB	3:B:3003:HOH:O	2.67	0.42
1:E:250:SER:O	1:E:253:GLU:HB3	2.19	0.42
1:F:117:ASP:OD1	1:F:118:LYS:HG3	2.19	0.42
1:H:40:LEU:HD12	1:H:40:LEU:HA	1.89	0.42
1:B:117:ASP:OD1	1:B:118:LYS:HG3	2.19	0.42
1:D:192:LYS:HE2	3:D:3214:HOH:O	2.19	0.42
1:H:457:VAL:O	1:H:461:VAL:HG23	2.19	0.42
1:A:93:GLN:HB2	1:A:117:ASP:HA	2.01	0.42
1:A:310:ARG:HG3	1:C:297:GLN:NE2	2.34	0.42
1:D:89:ILE:HD12	1:D:128:TYR:HB2	2.02	0.42
1:D:197:LEU:O	1:D:201:VAL:HG23	2.18	0.42
1:F:135:VAL:CG1	1:F:152:VAL:HG21	2.44	0.42
1:F:401:ASN:HA	1:F:422:THR:CG2	2.48	0.42
1:H:380:VAL:CG2	1:H:490:ASN:HD21	2.33	0.42
1:A:294:CYS:O	1:A:298:MET:HE2	2.19	0.42
1:C:472:THR:HG23	1:C:498:GLU:CA	2.36	0.42
1:D:135:VAL:HG11	1:D:161:LEU:HD13	2.01	0.42
1:A:302:MET:HG3	1:A:308:PRO:HB3	2.01	0.42
1:D:373:PRO:HG2	3:D:3238:HOH:O	2.19	0.42
1:F:197:LEU:O	1:F:201:VAL:HG23	2.20	0.42
1:H:480:HIS:ND1	1:H:480:HIS:C	2.78	0.42
1:G:148:LEU:HB2	1:G:169:HIS:HD2	1.85	0.42
1:G:366:ILE:O	1:G:370:GLN:HG2	2.19	0.42
1:G:425:LEU:HD13	1:G:441:PHE:CG	2.55	0.42
1:B:339:PRO:HG2	3:B:3356:HOH:O	2.19	0.42
1:C:250:SER:O	1:C:253:GLU:HB3	2.19	0.42
1:D:155:HIS:N	1:D:155:HIS:CD2	2.87	0.42
1:D:283:SER:O	1:D:287:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:399:LEU:HD22	1:E:421:VAL:HB	2.00	0.42
1:H:195:VAL:HG13	3:H:2526:HOH:O	2.20	0.42
1:B:428:CYS:HB3	3:B:3162:HOH:O	2.19	0.42
1:C:376:ALA:O	1:C:380:VAL:HG23	2.19	0.42
1:F:368:LYS:HG3	3:F:2140:HOH:O	2.20	0.42
1:E:89:ILE:CG2	1:E:177:VAL:HG22	2.50	0.42
1:E:385:VAL:HG22	1:E:414:PRO:HG3	2.02	0.42
3:F:1773:HOH:O	1:H:3:LEU:HD12	2.19	0.42
1:A:234:MET:HE2	3:A:3284:HOH:O	2.19	0.42
1:B:380:VAL:HG21	1:B:490:ASN:ND2	2.35	0.42
1:H:362:PHE:HB3	1:H:413:ARG:HG3	2.01	0.42
1:A:142:TYR:O	1:A:177:VAL:HA	2.20	0.42
1:A:148:LEU:HB2	1:A:169:HIS:HD2	1.84	0.42
1:C:83:ASP:HA	1:C:209:PHE:HB2	2.02	0.42
1:C:153:GLN:NE2	1:C:164:THR:OG1	2.52	0.42
1:C:345:TYR:O	1:C:349:ILE:HG13	2.20	0.42
1:E:338:TYR:HB3	1:E:341:GLU:HB2	2.01	0.42
1:B:310:ARG:NH2	1:D:274:VAL:HG11	2.35	0.41
1:B:437:VAL:HG12	1:B:438:GLU:N	2.34	0.41
1:C:259:MET:CE	1:C:328:MET:HE1	2.45	0.41
1:D:425:LEU:HD13	1:D:441:PHE:CG	2.55	0.41
1:E:68:ARG:HG2	1:E:68:ARG:HH11	1.84	0.41
1:F:136:ARG:HB3	1:F:137:PRO:HD2	2.02	0.41
1:F:479:ILE:CG2	1:F:480:HIS:N	2.82	0.41
3:H:2674:HOH:O	1:G:475:TYR:HE2	2.03	0.41
1:G:479:ILE:HD13	1:G:480:HIS:H	1.85	0.41
1:B:287:VAL:HG21	1:D:7:LEU:HD11	2.02	0.41
1:E:148:LEU:HB2	1:E:169:HIS:HD2	1.85	0.41
1:F:121:LYS:HG2	3:F:1807:HOH:O	2.19	0.41
1:A:38:LYS:HD2	1:A:74:LEU:HG	2.01	0.41
1:A:242:HIS:HB3	3:A:3286:HOH:O	2.19	0.41
1:C:283:SER:O	1:C:287:VAL:HG23	2.20	0.41
1:F:341:GLU:HG2	3:F:1891:HOH:O	2.20	0.41
1:H:109:VAL:O	1:H:109:VAL:HG23	2.20	0.41
1:A:302:MET:HE1	1:A:345:TYR:CB	2.50	0.41
1:D:302:MET:HG3	1:D:308:PRO:HB3	2.01	0.41
1:E:58:GLU:HG3	3:E:1601:HOH:O	2.19	0.41
1:H:90:ARG:HD2	3:H:2203:HOH:O	2.20	0.41
1:G:386:ASN:ND2	3:G:2604:HOH:O	2.53	0.41
1:G:398:VAL:HG13	1:G:479:ILE:CG2	2.45	0.41
1:B:148:LEU:HB2	1:B:169:HIS:HD2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:VAL:HG23	3:C:3169:HOH:O	2.19	0.41
1:D:89:ILE:O	1:D:176:GLY:HA2	2.20	0.41
1:H:99:ALA:HA	3:H:2529:HOH:O	2.19	0.41
1:H:111:THR:HG22	3:H:2178:HOH:O	2.19	0.41
1:H:366:ILE:O	1:H:370:GLN:HG2	2.20	0.41
1:A:364:ASN:HD22	1:A:364:ASN:HA	1.66	0.41
1:B:142:TYR:O	1:B:177:VAL:HA	2.20	0.41
1:D:15:VAL:O	1:D:15:VAL:HG23	2.20	0.41
1:D:237:CYS:SG	1:D:255:SER:HB3	2.59	0.41
1:D:360:TYR:HD1	1:D:389:TYR:CE1	2.38	0.41
1:E:405:SER:O	1:E:409:VAL:HG23	2.20	0.41
1:F:130:ASN:ND2	3:F:1887:HOH:O	2.53	0.41
1:F:385:VAL:HG21	1:F:412:TYR:HB2	2.01	0.41
1:A:494:ILE:HD12	1:B:380:VAL:CG2	2.51	0.41
1:B:452:GLY:C	1:B:453:LYS:HD2	2.46	0.41
1:D:111:THR:OG1	1:D:131:LEU:HB3	2.21	0.41
1:E:89:ILE:HG21	1:E:177:VAL:HG22	2.01	0.41
1:E:302:MET:HB3	1:E:342:VAL:HG22	2.03	0.41
1:F:274:VAL:HB	3:F:1776:HOH:O	2.19	0.41
1:H:294:CYS:O	1:H:298:MET:HE2	2.20	0.41
1:A:376:ALA:O	1:A:380:VAL:HG23	2.21	0.41
1:B:302:MET:HE2	1:B:308:PRO:CG	2.51	0.41
1:D:374:MET:HE2	1:D:379:ALA:CA	2.45	0.41
1:E:34:VAL:O	1:E:38:LYS:HG3	2.21	0.41
1:E:216:ALA:HB1	1:E:254:GLU:HG2	2.01	0.41
1:E:242:HIS:CD2	1:E:268:GLU:OE2	2.73	0.41
1:E:310:ARG:CG	3:G:2941:HOH:O	2.65	0.41
1:E:380:VAL:HG21	1:E:490:ASN:ND2	2.35	0.41
1:F:184:VAL:HG12	1:F:186:LEU:H	1.85	0.41
1:F:204:GLY:HA2	3:F:1926:HOH:O	2.20	0.41
1:F:237:CYS:SG	1:F:255:SER:HB3	2.61	0.41
1:H:374:MET:HE2	1:H:378:GLU:C	2.46	0.41
1:H:399:LEU:HD22	1:H:421:VAL:HB	2.03	0.41
1:B:47:VAL:HG22	1:B:79:ALA:HB3	2.03	0.41
1:B:475:TYR:HA	1:B:495:LEU:O	2.21	0.41
1:C:104:GLY:N	1:C:165:VAL:O	2.53	0.41
1:C:362:PHE:HB3	1:C:413:ARG:HG3	2.02	0.41
1:C:386:ASN:ND2	3:C:3093:HOH:O	2.53	0.41
1:C:396:MET:HE1	1:C:409:VAL:HG12	2.03	0.41
1:D:142:TYR:O	1:D:177:VAL:HA	2.21	0.41
1:E:144:ASP:CG	1:E:175:ARG:HD3	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:83:ASP:HA	1:F:209:PHE:HB2	2.03	0.41
1:F:158:GLU:HB2	3:F:2046:HOH:O	2.21	0.41
1:F:234:MET:HE1	1:F:433:ILE:HD11	2.01	0.41
1:F:396:MET:HE1	1:F:414:PRO:HG2	1.99	0.41
1:H:197:LEU:O	1:H:201:VAL:HG23	2.20	0.41
1:H:216:ALA:HB1	1:H:254:GLU:HG3	2.03	0.41
1:H:422:THR:HG22	1:H:424:ARG:H	1.85	0.41
1:G:79:ALA:HB2	1:G:429:ARG:O	2.20	0.41
1:A:328:MET:HG2	1:A:329:LEU:N	2.36	0.41
1:C:385:VAL:HG21	1:C:412:TYR:HB2	2.03	0.41
1:E:214:ARG:HD2	1:E:218:GLN:HE22	1.86	0.41
1:F:332:GLU:CD	1:F:332:GLU:H	2.29	0.41
1:H:142:TYR:O	1:H:177:VAL:HA	2.21	0.41
1:H:401:ASN:HA	1:H:422:THR:HG23	2.03	0.41
1:A:198:GLN:HB3	3:A:3176:HOH:O	2.21	0.40
1:A:249:ASP:HA	3:A:3186:HOH:O	2.21	0.40
1:A:338:TYR:HB3	1:A:341:GLU:HB2	2.02	0.40
1:C:178:ASN:ND2	3:C:3069:HOH:O	2.54	0.40
1:D:242:HIS:CD2	3:D:3199:HOH:O	2.74	0.40
1:F:135:VAL:CG1	1:F:136:ARG:N	2.84	0.40
1:H:112:ASP:HA	1:H:113:PRO:HD3	1.93	0.40
1:G:142:TYR:O	1:G:177:VAL:HA	2.21	0.40
1:A:446:LYS:HG3	3:A:3276:HOH:O	2.21	0.40
1:A:455:HIS:CD2	3:A:3291:HOH:O	2.69	0.40
1:B:72:ALA:HA	3:B:3031:HOH:O	2.21	0.40
1:D:172:SER:H	1:D:175:ARG:HD2	1.84	0.40
1:D:384:ALA:CB	1:D:479:ILE:HD11	2.51	0.40
1:H:425:LEU:HD13	1:H:441:PHE:CG	2.56	0.40
1:A:445:ASP:HB2	3:A:3276:HOH:O	2.21	0.40
1:D:228:PRO:HB2	1:D:231:ARG:HH21	1.86	0.40
1:F:144:ASP:CG	1:F:175:ARG:HD3	2.45	0.40
1:G:407:ARG:HD3	3:G:2570:HOH:O	2.20	0.40
1:A:24:ILE:HG12	1:A:47:VAL:HB	2.04	0.40
1:A:135:VAL:CG1	1:A:152:VAL:HG21	2.50	0.40
1:A:156:GLU:OE2	1:A:162:GLU:HB2	2.21	0.40
1:A:370:GLN:NE2	3:A:3161:HOH:O	2.42	0.40
1:B:396:MET:HE1	1:B:409:VAL:HG12	2.03	0.40
1:D:437:VAL:HG12	1:D:438:GLU:N	2.36	0.40
1:F:89:ILE:HG21	1:F:177:VAL:HG22	2.03	0.40
1:F:425:LEU:HD13	1:F:441:PHE:CG	2.57	0.40
1:G:111:THR:HG21	1:G:129:GLN:HA	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:130:ASN:O	1:G:133:LYS:HG2	2.21	0.40
1:G:435:GLN:NE2	3:G:2644:HOH:O	2.54	0.40
1:A:471:GLN:O	1:A:472:THR:C	2.65	0.40
1:B:429:ARG:O	1:B:432:ASN:HB2	2.21	0.40
1:C:56:SER:N	3:C:3113:HOH:O	2.35	0.40
1:D:40:LEU:HD12	1:D:40:LEU:HA	1.88	0.40
1:F:10:SER:C	1:F:12:PHE:H	2.30	0.40
1:F:142:TYR:O	1:F:177:VAL:HA	2.21	0.40
1:H:302:MET:HE2	1:H:308:PRO:HD3	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	A	487/499 (98%)	458 (94%)	26 (5%)	3 (1%)	21	24
1	B	485/499 (97%)	457 (94%)	26 (5%)	2 (0%)	30	34
1	C	488/499 (98%)	463 (95%)	23 (5%)	2 (0%)	30	34
1	D	489/499 (98%)	455 (93%)	30 (6%)	4 (1%)	16	17
1	E	489/499 (98%)	460 (94%)	23 (5%)	6 (1%)	10	9
1	F	487/499 (98%)	462 (95%)	23 (5%)	2 (0%)	30	34
1	G	496/499 (99%)	466 (94%)	26 (5%)	4 (1%)	16	17
1	H	488/499 (98%)	466 (96%)	19 (4%)	3 (1%)	21	24
All	All	3909/3992 (98%)	3687 (94%)	196 (5%)	26 (1%)	18	20

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	483	HIS

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Mol	Chain	Res	Type
1	G	485	VAL
1	G	490	ASN
1	A	174	ARG
1	C	174	ARG
1	D	174	ARG
1	E	131	LEU
1	E	158	GLU
1	H	472	THR
1	B	174	ARG
1	C	17	ASN
1	D	490	ASN
1	E	491	GLN
1	G	174	ARG
1	E	105	ALA
1	E	490	ASN
1	F	127	ASP
1	F	174	ARG
1	A	188	ALA
1	A	453	LYS
1	B	450	ASP
1	D	127	ASP
1	D	453	LYS
1	E	174	ARG
1	H	188	ALA
1	H	174	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	410/417 (98%)	389 (95%)	21 (5%)	21	26
1	B	409/417 (98%)	390 (95%)	19 (5%)	24	31
1	C	411/417 (99%)	389 (95%)	22 (5%)	20	24
1	D	412/417 (99%)	396 (96%)	16 (4%)	28	39
1	E	412/417 (99%)	392 (95%)	20 (5%)	22	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	410/417 (98%)	394 (96%)	16 (4%)	28	39
1	G	411/417 (99%)	393 (96%)	18 (4%)	25	33
1	H	411/417 (99%)	393 (96%)	18 (4%)	25	33
All	All	3286/3336 (98%)	3136 (95%)	150 (5%)	24	31

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	34	VAL
1	A	40	LEU
1	A	84	THR
1	A	117	ASP
1	A	136	ARG
1	A	158	GLU
1	A	177	VAL
1	A	207	MET
1	A	231	ARG
1	A	254	GLU
1	A	298	MET
1	A	302	MET
1	A	351	LEU
1	A	357	LEU
1	A	364	ASN
1	A	366	ILE
1	A	371	HIS
1	A	422	THR
1	A	424	ARG
1	A	435	GLN
1	B	40	LEU
1	B	68	ARG
1	B	84	THR
1	B	103	ARG
1	B	111	THR
1	B	117	ASP
1	B	139	ASN
1	B	177	VAL
1	B	185	ASP
1	B	198	GLN
1	B	207	MET
1	B	268	GLU

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Mol	Chain	Res	Type
1	B	310	ARG
1	B	351	LEU
1	B	357	LEU
1	B	422	THR
1	B	424	ARG
1	B	435	GLN
1	B	451	GLU
1	C	34	VAL
1	C	40	LEU
1	C	84	THR
1	C	132	SER
1	C	139	ASN
1	C	149	ILE
1	C	153	GLN
1	C	177	VAL
1	C	189	VAL
1	C	207	MET
1	C	215	SER
1	C	231	ARG
1	C	298	MET
1	C	307	ARG
1	C	351	LEU
1	C	357	LEU
1	C	364	ASN
1	C	374	MET
1	C	377	ASP
1	C	399	LEU
1	C	422	THR
1	C	435	GLN
1	D	40	LEU
1	D	84	THR
1	D	117	ASP
1	D	155	HIS
1	D	158	GLU
1	D	177	VAL
1	D	207	MET
1	D	298	MET
1	D	302	MET
1	D	310	ARG
1	D	351	LEU
1	D	357	LEU
1	D	364	ASN

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Mol	Chain	Res	Type
1	D	422	THR
1	D	435	GLN
1	D	480	HIS
1	E	34	VAL
1	E	40	LEU
1	E	84	THR
1	E	88	GLU
1	E	90	ARG
1	E	155	HIS
1	E	158	GLU
1	E	177	VAL
1	E	183	ASP
1	E	207	MET
1	E	298	MET
1	E	351	LEU
1	E	357	LEU
1	E	366	ILE
1	E	371	HIS
1	E	374	MET
1	E	422	THR
1	E	435	GLN
1	E	471	GLN
1	E	483	HIS
1	F	40	LEU
1	F	68	ARG
1	F	84	THR
1	F	117	ASP
1	F	157	ASP
1	F	158	GLU
1	F	177	VAL
1	F	180	PRO
1	F	207	MET
1	F	310	ARG
1	F	351	LEU
1	F	357	LEU
1	F	422	THR
1	F	424	ARG
1	F	435	GLN
1	F	479	ILE
1	H	40	LEU
1	H	68	ARG
1	H	84	THR

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Mol	Chain	Res	Type
1	H	90	ARG
1	H	117	ASP
1	H	130	ASN
1	H	156	GLU
1	H	177	VAL
1	H	207	MET
1	H	298	MET
1	H	310	ARG
1	H	351	LEU
1	H	357	LEU
1	H	422	THR
1	H	435	GLN
1	H	471	GLN
1	H	479	ILE
1	H	480	HIS
1	G	34	VAL
1	G	40	LEU
1	G	68	ARG
1	G	84	THR
1	G	132	SER
1	G	177	VAL
1	G	207	MET
1	G	231	ARG
1	G	270	PRO
1	G	298	MET
1	G	310	ARG
1	G	351	LEU
1	G	357	LEU
1	G	422	THR
1	G	435	GLN
1	G	451	GLU
1	G	479	ILE
1	G	480	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	139	ASN
1	A	155	HIS
1	A	169	HIS
1	A	242	HIS

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Mol	Chain	Res	Type
1	A	286	ASN
1	A	318	ASN
1	A	340	ASN
1	A	364	ASN
1	A	401	ASN
1	A	471	GLN
1	A	490	ASN
1	B	60	HIS
1	B	77	ASN
1	B	139	ASN
1	B	153	GLN
1	B	155	HIS
1	B	242	HIS
1	B	305	ASN
1	B	318	ASN
1	B	364	ASN
1	B	370	GLN
1	B	371	HIS
1	B	401	ASN
1	B	471	GLN
1	B	491	GLN
1	C	54	HIS
1	C	139	ASN
1	C	169	HIS
1	C	218	GLN
1	C	242	HIS
1	C	246	GLN
1	C	297	GLN
1	C	305	ASN
1	C	370	GLN
1	C	386	ASN
1	C	401	ASN
1	C	480	HIS
1	C	491	GLN
1	D	54	HIS
1	D	139	ASN
1	D	155	HIS
1	D	243	GLN
1	D	286	ASN
1	D	297	GLN
1	D	318	ASN
1	D	386	ASN

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Mol	Chain	Res	Type
1	D	401	ASN
1	D	491	GLN
1	E	5	HIS
1	E	17	ASN
1	E	54	HIS
1	E	77	ASN
1	E	139	ASN
1	E	151	GLN
1	E	242	HIS
1	E	243	GLN
1	E	246	GLN
1	E	305	ASN
1	E	318	ASN
1	E	370	GLN
1	E	401	ASN
1	E	471	GLN
1	E	483	HIS
1	E	491	GLN
1	F	54	HIS
1	F	139	ASN
1	F	242	HIS
1	F	278	GLN
1	F	286	ASN
1	F	318	ASN
1	F	322	ASN
1	F	371	HIS
1	F	401	ASN
1	H	69	GLN
1	H	130	ASN
1	H	139	ASN
1	H	155	HIS
1	H	159	GLN
1	H	286	ASN
1	H	305	ASN
1	H	364	ASN
1	H	371	HIS
1	H	401	ASN
1	H	491	GLN
1	G	17	ASN
1	G	139	ASN
1	G	151	GLN
1	G	153	GLN

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Mol	Chain	Res	Type
1	G	297	GLN
1	G	340	ASN
1	G	370	GLN
1	G	401	ASN
1	G	426	GLN
1	G	480	HIS

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 ⓘ

8 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	E	3004	-	4,4,4	0.50	0	6,6,6	0.24	0
2	SO4	F	3005	-	4,4,4	0.40	0	6,6,6	0.25	0
2	SO4	C	3002	-	4,4,4	0.41	0	6,6,6	0.22	0
2	SO4	B	3001	-	4,4,4	0.34	0	6,6,6	0.09	0
2	SO4	A	3000	-	4,4,4	0.37	0	6,6,6	0.20	0
2	SO4	G	3007	-	4,4,4	0.31	0	6,6,6	0.13	0
2	SO4	D	3003	-	4,4,4	0.43	0	6,6,6	0.28	0
2	SO4	H	3006	-	4,4,4	0.36	0	6,6,6	0.33	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.

No monomer is involved in short contacts.

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	491/499 (98%)	0.55	63 (12%) 7 9	15, 39, 100, 100	0
1	B	489/499 (97%)	0.52	28 (5%) 29 34	21, 48, 86, 100	0
1	C	492/499 (98%)	0.21	17 (3%) 47 53	14, 38, 77, 100	0
1	D	493/499 (98%)	0.83	82 (16%) 4 5	19, 48, 100, 100	0
1	E	493/499 (98%)	0.46	58 (11%) 9 10	15, 36, 100, 100	0
1	F	491/499 (98%)	0.43	24 (4%) 35 41	19, 45, 87, 100	0
1	G	498/499 (99%)	0.29	28 (5%) 30 35	12, 40, 91, 100	0
1	H	492/499 (98%)	0.25	16 (3%) 49 56	16, 40, 81, 100	0
All	All	3939/3992 (98%)	0.44	316 (8%) 18 21	12, 42, 100, 100	0

All (316) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	488	TYR	9.1
1	A	116	ALA	6.7
1	D	92	GLY	5.7
1	D	137	PRO	5.7
1	E	361	VAL	5.7
1	F	481	ALA	5.7
1	A	99	ALA	5.4
1	D	124	PHE	5.4
1	D	125	TYR	5.2
1	A	106	THR	5.2
1	A	109	VAL	5.1
1	D	93	GLN	5.1
1	D	95	VAL	5.1
1	A	124	PHE	5.0
1	E	134	VAL	5.0
1	D	99	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
1	D	100	VAL	4.8
1	G	490	ASN	4.8
1	D	152	VAL	4.8
1	E	108	TYR	4.7
1	A	105	ALA	4.7
1	D	96	GLY	4.7
1	D	177	VAL	4.6
1	E	162	GLU	4.6
1	A	108	TYR	4.5
1	D	481	ALA	4.4
1	A	165	VAL	4.4
1	F	188	ALA	4.4
1	D	115	PHE	4.3
1	A	104	GLY	4.3
1	D	141	ILE	4.3
1	D	105	ALA	4.2
1	D	126	ILE	4.2
1	D	107	CYS	4.2
1	G	484	LYS	4.2
1	A	107	CYS	4.1
1	E	111	THR	4.1
1	A	113	PRO	4.1
1	C	382	SER	4.1
1	D	164	THR	4.0
1	D	134	VAL	4.0
1	A	152	VAL	4.0
1	D	116	ALA	4.0
1	E	141	ILE	4.0
1	A	125	TYR	3.9
1	A	101	MET	3.9
1	E	100	VAL	3.9
1	F	212	PHE	3.9
1	D	109	VAL	3.8
1	A	166	THR	3.8
1	D	2	GLN	3.8
1	G	483	HIS	3.8
1	D	117	ASP	3.7
1	D	113	PRO	3.7
1	A	115	PHE	3.7
1	E	107	CYS	3.7
1	E	155	HIS	3.7
1	D	128	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	97	GLY	3.7
1	D	165	VAL	3.7
1	D	91	THR	3.7
1	H	304	TYR	3.7
1	E	115	PHE	3.6
1	A	93	GLN	3.6
1	E	148	LEU	3.6
1	A	100	VAL	3.6
1	D	143	ILE	3.6
1	D	166	THR	3.6
1	A	198	GLN	3.6
1	E	165	VAL	3.6
1	D	132	SER	3.5
1	D	111	THR	3.5
1	E	105	ALA	3.5
1	G	489	ALA	3.5
1	A	171	ILE	3.5
1	A	162	GLU	3.5
1	E	95	VAL	3.5
1	A	372	ILE	3.5
1	G	485	VAL	3.4
1	D	154	SER	3.4
1	E	106	THR	3.4
1	F	189	VAL	3.4
1	G	132	SER	3.4
1	E	164	THR	3.3
1	C	53	SER	3.3
1	G	112	ASP	3.3
1	A	94	PHE	3.3
1	E	382	SER	3.3
1	D	444	ALA	3.3
1	D	89	ILE	3.3
1	D	155	HIS	3.3
1	D	114	ALA	3.3
1	D	171	ILE	3.3
1	D	101	MET	3.2
1	D	176	GLY	3.2
1	B	371	HIS	3.2
1	D	127	ASP	3.2
1	D	140	TYR	3.2
1	D	121	LYS	3.2
1	E	124	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	102	GLU	3.2
1	D	15	VAL	3.2
1	G	134	VAL	3.2
1	C	449	HIS	3.1
1	C	482	ASP	3.1
1	F	99	ALA	3.1
1	A	177	VAL	3.1
1	A	154	SER	3.1
1	C	212	PHE	3.1
1	A	167	ASN	3.1
1	D	104	GLY	3.1
1	E	138	GLY	3.1
1	D	131	LEU	3.1
1	E	140	TYR	3.0
1	D	110	THR	3.0
1	C	98	ASP	3.0
1	E	114	ALA	3.0
1	E	152	VAL	3.0
1	A	110	THR	3.0
1	D	94	PHE	3.0
1	A	149	ILE	3.0
1	D	147	ILE	3.0
1	D	139	ASN	3.0
1	E	481	ALA	2.9
1	A	148	LEU	2.9
1	A	143	ILE	2.9
1	E	154	SER	2.9
1	C	452	GLY	2.9
1	E	113	PRO	2.9
1	B	16	ALA	2.9
1	A	147	ILE	2.9
1	D	167	ASN	2.9
1	G	482	ASP	2.9
1	G	487	GLY	2.9
1	A	444	ALA	2.9
1	D	179	LEU	2.9
1	G	15	VAL	2.9
1	H	166	THR	2.9
1	B	185	ASP	2.9
1	A	121	LYS	2.8
1	A	155	HIS	2.8
1	A	95	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	449	HIS	2.8
1	A	228	PRO	2.8
1	D	173	ASP	2.8
1	E	92	GLY	2.8
1	F	169	HIS	2.8
1	F	187	PRO	2.8
1	B	447	LEU	2.8
1	D	150	LEU	2.8
1	C	489	ALA	2.8
1	D	187	PRO	2.8
1	D	168	SER	2.7
1	B	14	PRO	2.7
1	A	179	LEU	2.7
1	E	117	ASP	2.7
1	F	304	TYR	2.7
1	A	134	VAL	2.7
1	E	170	THR	2.7
1	G	296	THR	2.7
1	D	97	GLY	2.7
1	A	1	SER	2.7
1	A	490	ASN	2.7
1	D	182	CYS	2.7
1	D	489	ALA	2.6
1	A	92	GLY	2.6
1	A	180	PRO	2.6
1	E	365	SER	2.6
1	B	99	ALA	2.6
1	E	175	ARG	2.6
1	H	231	ARG	2.6
1	B	189	VAL	2.6
1	D	106	THR	2.6
1	H	149	ILE	2.6
1	G	129	GLN	2.6
1	H	90	ARG	2.6
1	A	164	THR	2.6
1	D	361	VAL	2.6
1	E	355	SER	2.6
1	A	163	CYS	2.6
1	B	70	ALA	2.6
1	B	55	GLY	2.6
1	A	126	ILE	2.6
1	G	1	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	226	LEU	2.5
1	B	307	ARG	2.5
1	B	489	ALA	2.5
1	D	112	ASP	2.5
1	F	98	ASP	2.5
1	A	118	LYS	2.5
1	C	361	VAL	2.5
1	A	157	ASP	2.5
1	A	91	THR	2.5
1	A	170	THR	2.5
1	F	404	ARG	2.5
1	A	161	LEU	2.5
1	E	101	MET	2.5
1	E	109	VAL	2.5
1	H	15	VAL	2.5
1	H	310	ARG	2.5
1	A	481	ALA	2.5
1	F	228	PRO	2.5
1	A	382	SER	2.4
1	F	179	LEU	2.4
1	C	103	ARG	2.4
1	E	180	PRO	2.4
1	F	90	ARG	2.4
1	A	141	ILE	2.4
1	A	150	LEU	2.4
1	E	166	THR	2.4
1	H	118	LYS	2.4
1	D	135	VAL	2.4
1	B	254	GLU	2.4
1	E	482	ASP	2.4
1	D	180	PRO	2.4
1	A	96	GLY	2.4
1	E	104	GLY	2.4
1	A	160	THR	2.4
1	D	224	LYS	2.4
1	G	355	SER	2.4
1	B	134	VAL	2.4
1	D	149	ILE	2.4
1	E	171	ILE	2.4
1	E	447	LEU	2.4
1	F	131	LEU	2.4
1	D	158	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	157	ASP	2.3
1	F	345	TYR	2.3
1	D	181	GLY	2.3
1	H	104	GLY	2.3
1	G	114	ALA	2.3
1	E	147	ILE	2.3
1	G	307	ARG	2.3
1	E	444	ALA	2.3
1	H	136	ARG	2.3
1	B	212	PHE	2.3
1	C	134	VAL	2.3
1	D	142	TYR	2.3
1	D	266	GLY	2.3
1	E	125	TYR	2.3
1	A	120	THR	2.3
1	G	449	HIS	2.3
1	D	447	LEU	2.3
1	G	185	ASP	2.3
1	C	383	SER	2.3
1	B	148	LEU	2.2
1	G	94	PHE	2.2
1	A	117	ASP	2.2
1	E	163	CYS	2.2
1	H	482	ASP	2.2
1	B	188	ALA	2.2
1	E	139	ASN	2.2
1	E	173	ASP	2.2
1	E	153	GLN	2.2
1	A	114	ALA	2.2
1	F	489	ALA	2.2
1	H	489	ALA	2.2
1	G	111	THR	2.2
1	D	161	LEU	2.2
1	D	310	ARG	2.2
1	E	112	ASP	2.2
1	F	490	ASN	2.2
1	F	444	ALA	2.2
1	B	304	TYR	2.2
1	D	479	ILE	2.2
1	G	161	LEU	2.2
1	F	342	VAL	2.2
1	E	94	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	14	PRO	2.2
1	C	129	GLN	2.2
1	E	97	GLY	2.2
1	B	179	LEU	2.1
1	B	135	VAL	2.1
1	E	178	ASN	2.1
1	A	359	GLU	2.1
1	C	217	GLU	2.1
1	H	121	LYS	2.1
1	F	93	GLN	2.1
1	D	138	GLY	2.1
1	G	96	GLY	2.1
1	G	382	SER	2.1
1	F	307	ARG	2.1
1	G	98	ASP	2.1
1	A	135	VAL	2.1
1	G	242	HIS	2.1
1	H	92	GLY	2.1
1	B	62	THR	2.1
1	B	111	THR	2.1
1	D	136	ARG	2.1
1	D	170	THR	2.1
1	E	110	THR	2.1
1	D	108	TYR	2.1
1	B	169	HIS	2.1
1	D	153	GLN	2.1
1	E	137	PRO	2.1
1	F	134	VAL	2.1
1	C	97	GLY	2.1
1	D	119	GLY	2.1
1	A	188	ALA	2.1
1	B	295	ALA	2.1
1	E	489	ALA	2.1
1	E	490	ASN	2.1
1	H	175	ARG	2.1
1	B	271	ALA	2.0
1	E	145	ASP	2.0
1	C	479	ILE	2.0
1	E	126	ILE	2.0
1	E	149	ILE	2.0
1	H	14	PRO	2.0
1	B	184	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	217	GLU	2.0
1	F	405	SER	2.0
1	B	495	LEU	2.0
1	D	178	ASN	2.0
1	C	14	PRO	2.0
1	E	118	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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
2	SO4	D	3003	5/5	0.95	0.09	44,44,44,44	0
2	SO4	A	3000	5/5	0.97	0.07	36,36,36,36	0
2	SO4	E	3004	5/5	0.97	0.07	39,39,39,39	0
2	SO4	F	3005	5/5	0.97	0.07	42,42,42,42	0
2	SO4	H	3006	5/5	0.97	0.07	41,41,41,41	0
2	SO4	B	3001	5/5	0.98	0.05	45,45,45,45	0
2	SO4	C	3002	5/5	0.98	0.07	36,36,36,36	0
2	SO4	G	3007	5/5	0.99	0.07	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.