



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 07:51 pm BST

PDB ID : 1PKL  
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](mailto: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.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

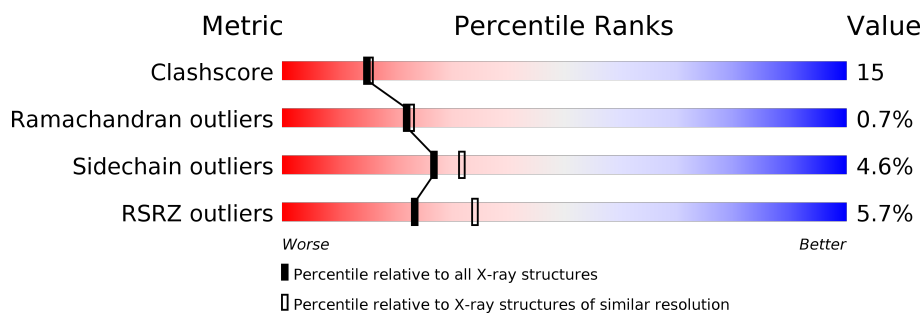
# 1 Overall quality at a glance

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	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>11%</div> <div>69%</div> <div>27%</div> <div>..</div> </div>
1	B	499	<div> <div>2%</div> <div>72%</div> <div>23%</div> <div>..</div> </div>
1	C	499	<div> <div>%</div> <div>68%</div> <div>28%</div> <div>..</div> </div>
1	D	499	<div> <div>16%</div> <div>69%</div> <div>28%</div> <div>..</div> </div>
1	E	499	<div> <div>6%</div> <div>70%</div> <div>27%</div> <div>..</div> </div>
1	F	499	<div> <div>2%</div> <div>71%</div> <div>25%</div> <div>..</div> </div>
1	G	499	<div> <div>3%</div> <div>76%</div> <div>22%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	H	499	<div><div></div><div>3%</div><div>72%</div><div>25%</div><div>..</div></div>

## 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 (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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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		

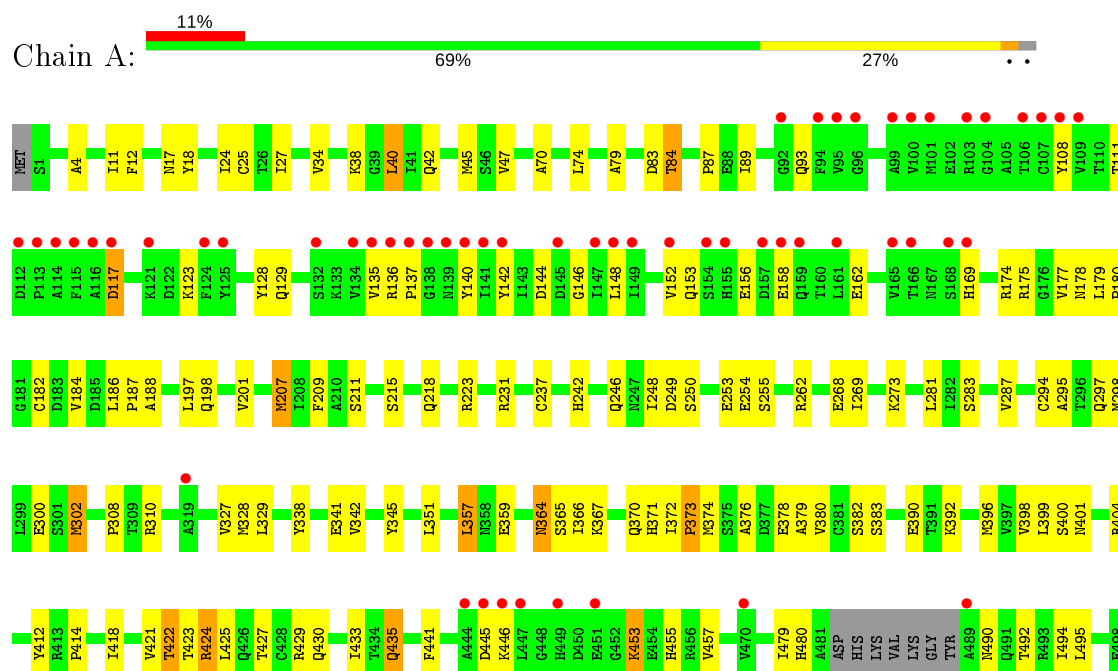
- Molecule 3 is water.

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		

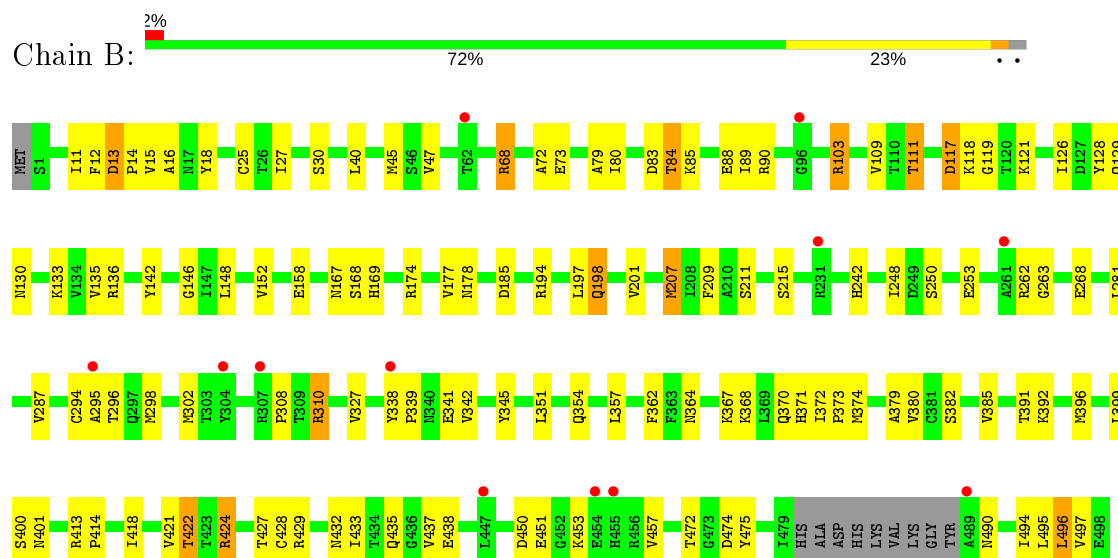
### 3 Residue-property plots [i](#)

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

#### • Molecule 1: PROTEIN (PYRUVATE KINASE)



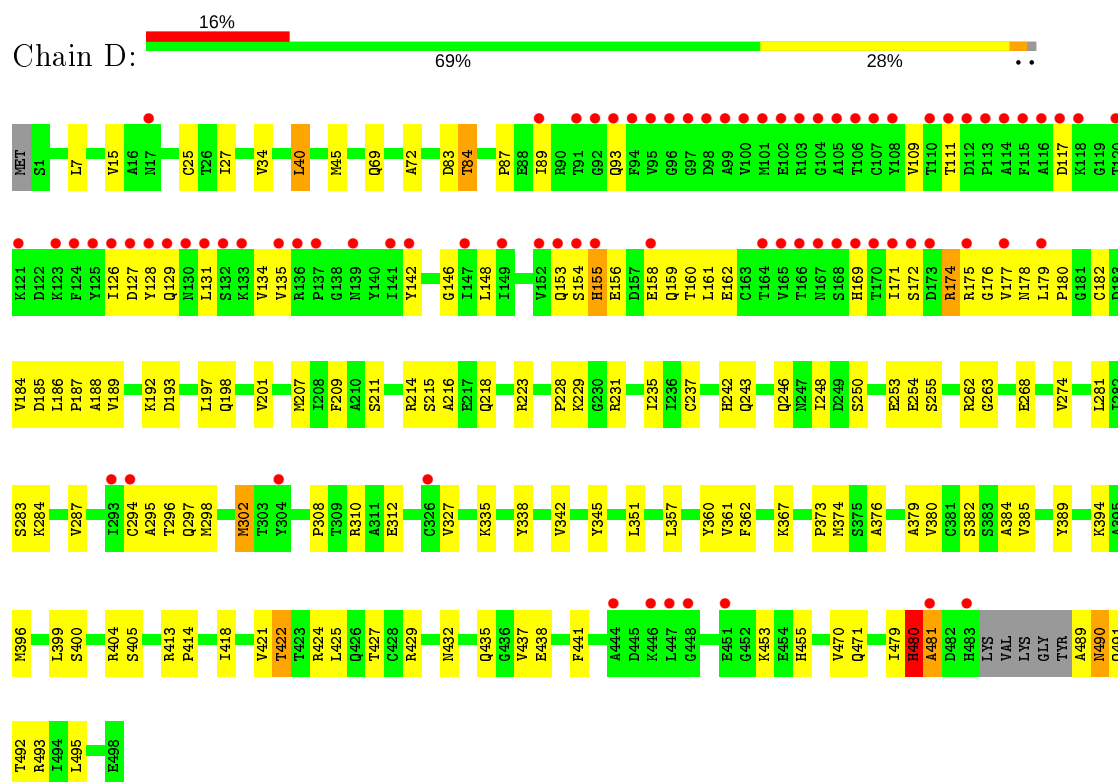
#### • Molecule 1: PROTEIN (PYRUVATE KINASE)



- Molecule 1: PROTEIN (PYRUVATE KINASE)



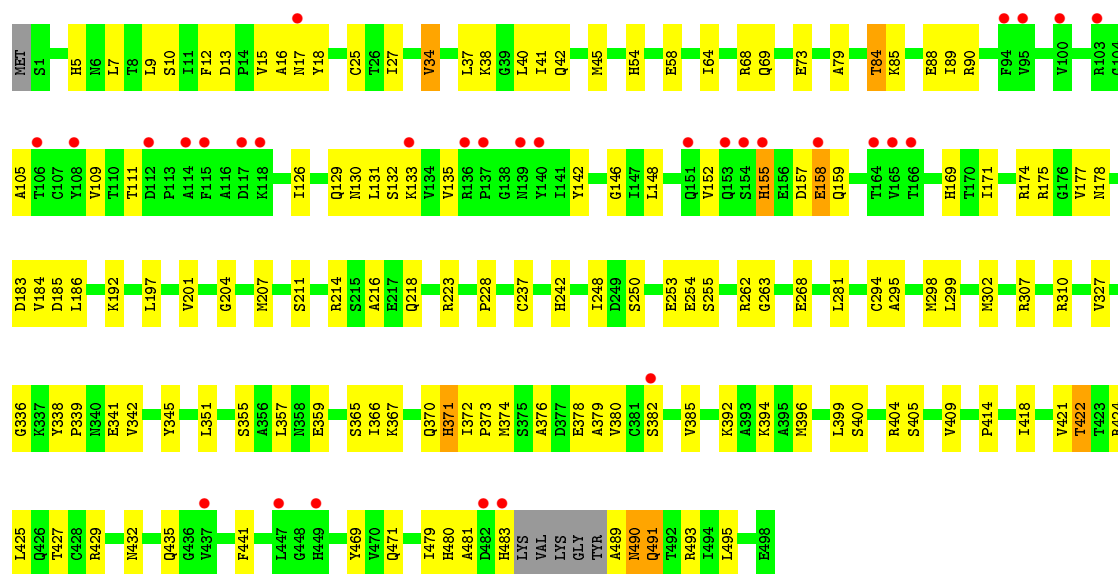
- Molecule 1: PROTEIN (PYRUVATE KINASE)



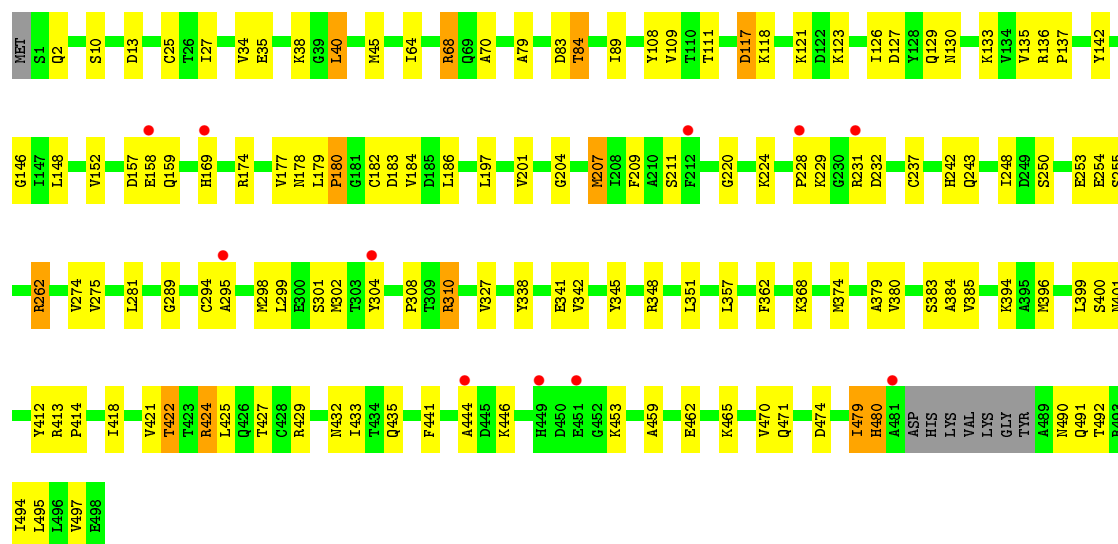
- Molecule 1: PROTEIN (PYRUVATE KINASE)



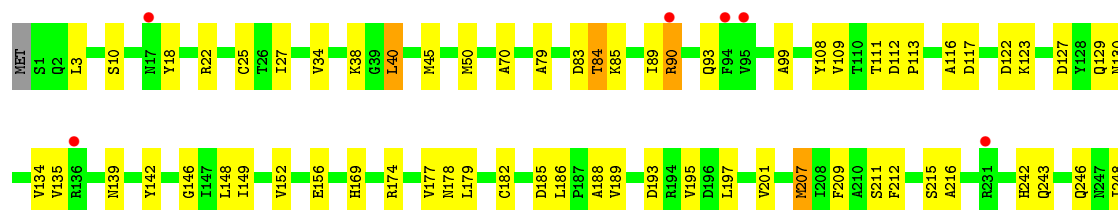
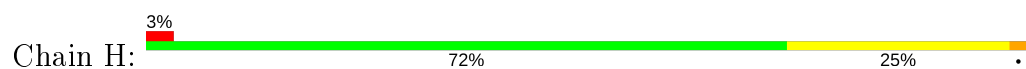


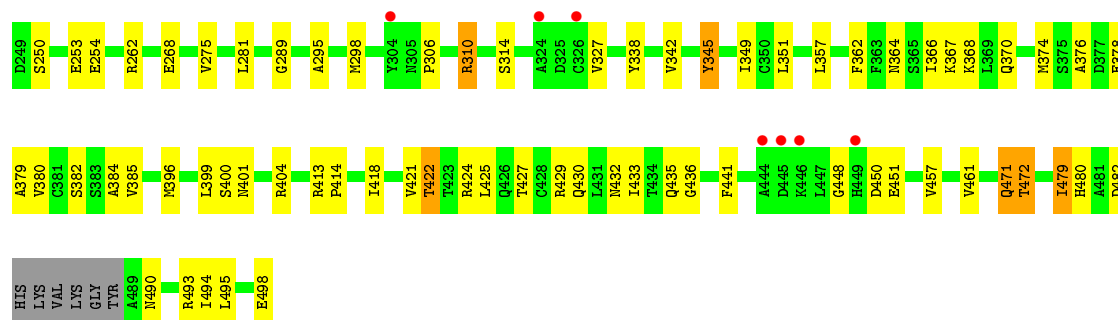


• Molecule 1: PROTEIN (PYRUVATE KINASE)

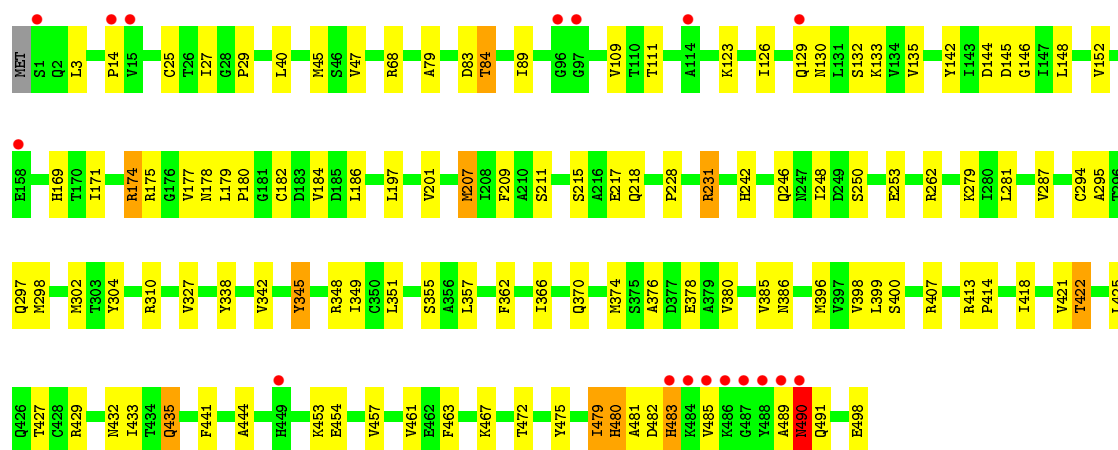
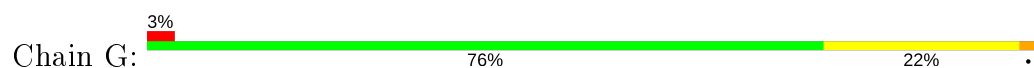


• Molecule 1: PROTEIN (PYRUVATE KINASE)





● 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, $\alpha$ , $\beta$ , $\gamma$	121.65Å 132.64Å 181.00Å 90.00° 97.11° 90.00°	Depositor
Resolution (Å)	30.00 – 2.35 29.82 – 2.35	Depositor EDS
% Data completeness (in resolution range)	67.9 (30.00-2.35) 67.9 (29.82-2.35)	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 <sup>2</sup> )	36.9	Xtriage
Anisotropy	0.576	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 45.8	EDS
L-test for twinning <sup>1</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	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 <sup>2</sup> )	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.*

<sup>1</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	0.54	2/3794 (0.1%)	0.70	4/5136 (0.1%)
1	B	0.43	0/3778	0.67	2/5114 (0.0%)
1	C	0.47	0/3802	0.68	1/5147 (0.0%)
1	D	0.45	0/3813	0.68	3/5162 (0.1%)
1	E	0.46	0/3813	0.68	1/5162 (0.0%)
1	F	0.46	0/3794	0.67	1/5136 (0.0%)
1	G	0.47	0/3832	0.68	1/5190 (0.0%)
1	H	0.45	0/3802	0.66	1/5147 (0.0%)
All	All	0.47	2/30428 (0.0%)	0.68	14/41194 (0.0%)

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 (2) 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	C-N	-7.04	1.20	1.34

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	373	PRO	CA-N-CD	-7.86	100.49	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	373	PRO	N-CA-CB	7.77	112.62	103.30
1	C	295	ALA	N-CA-C	7.47	131.17	111.00
1	D	295	ALA	N-CA-C	7.36	130.87	111.00
1	E	295	ALA	N-CA-C	7.34	130.83	111.00
1	G	295	ALA	N-CA-C	7.33	130.79	111.00
1	F	295	ALA	N-CA-C	7.17	130.36	111.00
1	B	295	ALA	N-CA-C	7.15	130.31	111.00
1	H	295	ALA	N-CA-C	7.11	130.20	111.00
1	A	295	ALA	N-CA-C	6.83	129.43	111.00
1	A	372	ILE	O-C-N	5.87	132.25	121.10
1	D	481	ALA	N-CA-C	5.53	125.94	111.00
1	D	480	HIS	N-CA-C	-5.27	96.76	111.00
1	B	496	LEU	N-CA-C	-5.17	97.05	111.00

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	121	0
1	B	3725	0	3731	110	0
1	C	3748	0	3747	132	0
1	D	3758	0	3754	115	0
1	E	3758	0	3754	126	0
1	F	3740	0	3743	113	0
1	G	3777	0	3761	106	0
1	H	3748	0	3747	116	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	30	0
3	B	366	0	0	29	0
3	C	453	0	0	38	0
3	D	244	0	0	18	0
3	E	386	0	0	38	0
3	F	399	0	0	31	0
3	G	389	0	0	24	0
3	H	400	0	0	37	0
All	All	32986	0	29980	903	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 15.

All (903) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:ARG:HB3	1:B:424:ARG:HH11	1.27	0.95
1:D:27:ILE:HD11	1:D:45:MET:HE1	1.51	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: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:D:298:MET:SD	3:D:3056:HOH:O	2.30	0.87
1:C:25:CYS:HB2	1:C:45:MET:HE2	1.56	0.86
1:E:27:ILE:HD11	1:E:45:MET:HE1	1.56	0.85
1:A:84:THR:HG21	3:A:3163:HOH:O	1.76	0.85
1:A:27:ILE:HD11	1:A:45:MET:HE1	1.59	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: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:B:302:MET:HE2	1:B:308:PRO:HB3	1.59	0.83
1:B:27:ILE:HD11	1:B:45:MET:HE1	1.61	0.83
1:G:27:ILE:HD11	1:G:45:MET:HE1	1.60	0.83
1:F:27:ILE:HD11	1:F:45:MET:HE1	1.61	0.82
1:E:310:ARG:NH1	1:G:297:GLN:HE22	1.75	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:CYS:HB2	1:A:45:MET:CE	2.10	0.82
1:B:15:VAL:HG21	3:B:3344:HOH:O	1.80	0.81
1:C:25:CYS:HB2	1:C:45:MET:CE	2.11	0.81
1:F:25:CYS:HB2	1:F:45:MET:HE2	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:H:27:ILE:HD11	1:H:45:MET:HE1	1.64	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
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:E:25:CYS:HB2	1:E:45:MET:CE	2.12	0.79
1:F:135:VAL:HG11	1:F:152:VAL:HG21	1.66	0.78
1:A:302:MET:HE1	1:A:342:VAL:HA	1.65	0.78
1:B:396:MET:HE1	1:B:414:PRO:HG2	1.66	0.78
1:B:310:ARG:HG3	1:D:297:GLN:NE2	1.99	0.78
1:G:130:ASN:HB3	1:G:133:LYS:HE2	1.64	0.78
1:G:25:CYS:HB2	1:G:45:MET:CE	2.14	0.78
1:A:338:TYR:O	1:A:342:VAL:HG23	1.83	0.77
1:C:396:MET:HE1	1:C:414:PRO:HG2	1.67	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:G:396:MET:HE1	1:G:414:PRO:HG2	1.67	0.77
1:A:25:CYS:HB2	1:A:45:MET:HE2	1.67	0.77
1:H:25:CYS:HB2	1:H:45:MET:HE2	1.64	0.76
1:C:380:VAL:HG21	1:C:490:ASN:ND2	1.99	0.76
1:D:493:ARG:NH1	1:D:495:LEU:HD21	2.00	0.76
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:E:396:MET:HE1	1:E:414:PRO:HG2	1.68	0.75
1:H:310:ARG:HH12	1:H:314:SER:HB3	1.51	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:A:396:MET:HE1	1:A:414:PRO:HG2	1.69	0.74
1:G:338:TYR:O	1:G:342:VAL:HG23	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:187:PRO:HG3	3:D:3206:HOH:O	1.86	0.74
1:E:374:MET:HE1	3:E:1729:HOH:O	1.86	0.74
1:H:451:GLU:HA	3:H:2558:HOH:O	1.86	0.74
1:H:189:VAL:HG13	1:H:193:ASP:HB2	1.69	0.74
1:H:25:CYS:HB2	1:H:45:MET:CE	2.16	0.74
1:B:11:ILE:HG12	3:B:3014:HOH:O	1.88	0.74
1:A:400:SER:O	1:A:422:THR:HG23	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:C:171:ILE:HA	1:C:175:ARG:NH1	2.02	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:396:MET:HE1	1:D:414:PRO:HG2	1.70	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:F:396:MET:HE1	1:F:414:PRO:HG2	1.70	0.73
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: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:G:25:CYS:HB2	1:G:45:MET:HE2	1.72	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:F:248:ILE:HG12	1:F:281:LEU:HD22	1.71	0.71
1:H:396:MET:HE1	1:H:414:PRO:HG2	1.72	0.71
1:C:338:TYR:O	1:C:342:VAL:HG23	1.91	0.71
1:E:359:GLU:HG2	3:E:1731:HOH:O	1.89	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:25:CYS:HB2	1:E:45:MET:HE3	1.72	0.70
1:A:248:ILE:HG12	1:A:281:LEU:HD22	1.72	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:G:179:LEU:HB3	1:G:182:CYS:HB2	1.74	0.70
1:D:338:TYR:O	1:D:342:VAL:HG23	1.92	0.70
1:D:72:ALA:HA	3:D:3225:HOH:O	1.91	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:E:374:MET:HE2	1:E:379:ALA: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: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: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:C:27:ILE:HD11	1:C:45:MET:HE1	1.75	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:D:25:CYS:HB2	1:D:45:MET:HE2	1.74	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:396:MET:CE	1:G:414:PRO:HG2	2.24	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:B:25:CYS:HB2	1:B:45:MET:HE2	1.78	0.66
1:A:396:MET:CE	1:A:414:PRO:HG2	2.26	0.66
1:D:25:CYS:HB2	1:D:45:MET:HE3	1.77	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: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: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: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: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:E:25:CYS:HB2	1:E:45:MET:HE2	1.78	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:B:25:CYS:HB2	1:B:45:MET:HE3	1.80	0.63
1:C:189:VAL:HG23	1:C:193:ASP:CB	2.28	0.63
1:E:184:VAL:HG12	1:E:186:LEU:H	1.63	0.63
1:C:374:MET:HE2	1:C:379:ALA:HA	1.81	0.63
1:F:64:ILE:CG2	1:F:68:ARG:HH21	2.11	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:F:275:VAL:HG22	1:H:310:ARG:NH2	2.13	0.63
1:A:25:CYS:HB2	1:A:45:MET:HE3	1.80	0.63
1:F:302:MET:SD	1:F:308:PRO:HD3	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CB	1:B:424:ARG:HH11	2.09	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:453:LYS:O	1:C:457:VAL:HG23	2.00	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: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:A:111:THR:HG23	1:A:129:GLN:HA	1.83	0.61
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:B:242:HIS:HB3	3:B:3338:HOH:O	2.01	0.61
1:B:119:GLY:HA3	3:B:3330:HOH:O	2.01	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:HB3	1:F:424:ARG:HH11	1.65	0.60
1:C:135:VAL:HG11	1:C:152:VAL:HG21	1.82	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:G:25:CYS:HB2	1:G:45:MET:HE3	1.82	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:ASN:ND2	1:B:368:LYS:HE2	2.18	0.59
1:F:302:MET:HE2	1:F:342:VAL:HA	1.83	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:157:ASP:HB2	3:C:3176:HOH:O	2.02	0.59
1:C:94:PHE:HB3	3:C:3446: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
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: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:374:MET:CE	1:E:379:ALA:HA	2.33	0.58
1:E:490:ASN:O	1:E:491:GLN:HB2	2.02	0.58
1:E:365:SER:CB	1:G:3:LEU:HD23	2.34	0.58
1:A:283:SER:HB3	1:C:3:LEU:HD12	1.86	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:D:89:ILE:HD11	1:D:186:LEU:HD11	1.86	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:G:298:MET:HE1	1:G:327:VAL:HG12	1.86	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:392:LYS:HD2	1:D:373:PRO:HD3	1.87	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
1:B:121:LYS:HB2	3:B:3345:HOH:O	2.04	0.56
1:D:302:MET:HE1	1:D:342:VAL:HA	1.86	0.56
1:D:479:ILE:HG22	1:D:480:HIS:N	2.20	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:C:380:VAL:HG21	1:C:490:ASN:CG	2.26	0.55
1:G:380:VAL:HG21	1:G:490:ASN:CG	2.26	0.55
1:G:297:GLN:HG3	3:G:2935:HOH:O	2.06	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: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: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:H:142:TYR:HB3	1:H:146:GLY:HA2	1.89	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:335:LYS:HE3	3:D:3232:HOH:O	2.06	0.55
1:D:89:ILE:CD1	1:D:186:LEU:HD11	2.37	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: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:C:374:MET:CE	1:C:379:ALA:HA	2.38	0.54
1:H:384:ALA:HB2	1:H:479:ILE:HD11	1.89	0.54
1:A:302:MET:CE	1:A:342:VAL:HA	2.36	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: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:E:367:LYS:HG2	3:F:2122:HOH:O	2.07	0.54
1:G:123:LYS:NZ	3:G:2732:HOH:O	2.40	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:D:294:CYS:O	1:D:298:MET:HE2	2.08	0.54
1:A:215:SER:OG	1:A:218:GLN:HG3	2.08	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:C:374:MET:HE1	3:C:3428:HOH:O	2.08	0.54
1:A:401:ASN:ND2	1:A:423:THR:H	2.06	0.53
1:A:398:VAL:HG13	1:A:479:ILE:HG23	1.88	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:C:380:VAL:HG21	1:C:490:ASN:OD1	2.09	0.53
1:D:111:THR:O	1:D:111:THR:HG22	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:373:PRO:HB2	3:E:1410:HOH:O	2.07	0.53
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:424:ARG:HD2	3:E:1512:HOH:O	2.09	0.53
1:F:491:GLN:HG2	1:F:492:THR:N	2.24	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:H:380:VAL:HG21	1:H:490:ASN:ND2	2.24	0.52
1:D:298:MET:HE1	1:D:327:VAL:HG12	1.91	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:A:144:ASP:CG	1:A:175:ARG:HD3	2.30	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:298:MET:HE1	1:F:327:VAL:HG12	1.92	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: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:F:27:ILE:HD11	1:F:45:MET:CE	2.38	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:H:111:THR:HG23	1:H:129:GLN:HA	1.91	0.51
1:A:374:MET:HE2	1:A:379:ALA:N	2.26	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
1:A:374:MET:HE2	1:A:378:GLU:C	2.31	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:E:299:LEU:HD13	1:E:302:MET:HE3	1.91	0.51
1:F:374:MET:HE1	1:F:379:ALA:HA	1.92	0.51
1:H:396:MET:CE	1:H:418:ILE:HG12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:145:ASP:HB2	3:G:2700:HOH:O	2.10	0.51
1:B:424:ARG:NH1	1:B:424:ARG:HB3	2.11	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:G:130:ASN:CB	1:G:133:LYS:HE2	2.38	0.51
1:H:212:PHE:HZ	3:H:2566:HOH:O	1.92	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:O	1:C:310:ARG:HD3	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:G:29:PRO:HB2	3:G:2696:HOH:O	2.11	0.51
1:G:413:ARG:NH1	3:G:2687:HOH:O	2.40	0.50
1:H:85:LYS:HE3	3:H:2561:HOH:O	2.11	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:B:374:MET:HE1	1:B:379:ALA:HA	1.93	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:374:MET:HE3	1:H:378:GLU:HG3	1.94	0.50
1:H:38:LYS:HG2	1:H:70:ALA:HB1	1.92	0.50
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:25:CYS:HB2	1:F:45:MET:HE3	1.91	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:G:396:MET:CE	1:G:418:ILE:HG12	2.42	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:H:374:MET:CE	1:H:378:GLU:HG3	2.41	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: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: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:E:109:VAL:HG11	1:E:126:ILE:HD12	1.95	0.49
1:E:299:LEU:HB3	1:E:302:MET:HE2	1.95	0.49
1:F:302:MET:HE2	1:F:342:VAL:HG22	1.94	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
1:F:294:CYS:O	1:F:298:MET:HE2	2.13	0.49
1:H:25:CYS:HB2	1:H:45:MET:HE3	1.94	0.49
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: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: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:B:391:THR:HB	1:B:475:TYR:CD2	2.48	0.48
1:F:243:GLN:HG2	3:F:2133:HOH:O	2.12	0.48
1:E:310:ARG:HD2	1:G:297:GLN:HE21	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:64:ILE:O	1:E:68:ARG:HG3	2.13	0.48
1:B:12:PHE:CE2	1:D:246:GLN:HG3	2.49	0.48
1:D:302:MET:HE3	1:D:342:VAL:HG13	1.94	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:B:298:MET:HE1	1:B:327:VAL:HG12	1.96	0.48
1:C:310:ARG:NH1	1:C:314:SER:HB3	2.28	0.48
1:H:22:ARG:CZ	3:H:2501:HOH:O	2.61	0.48
1:A:374:MET:HE3	1:A:378:GLU:HG3	1.95	0.48
1:B:401:ASN:HA	1:B:422:THR:CG2	2.44	0.48
1:H:111:THR:O	1:H:111:THR:HG22	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:C:27:ILE:HD11	1:C:45:MET:CE	2.42	0.48
1:C:298:MET:HE1	1:C:327:VAL:HG12	1.95	0.48
1:E:216:ALA:HB1	1:E:254:GLU:HG3	1.95	0.48
1:G:174:ARG:HD3	3:G:2802:HOH:O	2.14	0.48
1:G:481:ALA:O	1:G:482:ASP:HB2	2.14	0.48
1:H:89:ILE:HG13	1:H:186:LEU:HD11	1.96	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:H:310:ARG:HD3	1:H:310:ARG:C	2.34	0.48
1:A:140:TYR:O	1:A:180:PRO:HD2	2.14	0.48
1:F:399:LEU:HD22	1:F:421:VAL:HB	1.96	0.48
1:F:380:VAL:CG2	1:F:490:ASN:HD21	2.25	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:GLN:HG3	3:A:3046:HOH:O	2.14	0.47
1:C:25:CYS:HB2	1:C:45:MET:HE3	1.92	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:G:250:SER:O	1:G:253:GLU:HB3	2.14	0.47
1:E:184:VAL:HG12	1:E:185:ASP:N	2.29	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: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:C:310:ARG:C	1:C:310:ARG:HD3	2.36	0.47
1:D:111:THR:N	1:D:159:GLN:O	2.47	0.47
1:B:294:CYS:O	1:B:298:MET:HE2	2.14	0.47
1:E:12:PHE:CE1	1:G:242:HIS:HB2	2.50	0.47
1:H:27:ILE:HD11	1:H:45:MET:CE	2.41	0.47
1:A:197:LEU:O	1:A:201:VAL:HG23	2.13	0.46
1:B:135:VAL:HG12	1:B:136:ARG:N	2.30	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:G:111:THR:HG23	1:G:129:GLN:HA	1.97	0.46
1:H:93:GLN:HG2	3:H:2356:HOH:O	2.14	0.46
3:A:3083:HOH:O	1:C:310:ARG:HD2	2.14	0.46
1:B:135:VAL:CG1	1:B:152:VAL:HG21	2.44	0.46
1:E:298:MET:HE3	1:E:327:VAL:HB	1.96	0.46
1:F:242:HIS:HB3	3:F:1791:HOH:O	2.14	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:27:ILE:HD11	1:G:45:MET:CE	2.40	0.46
1:G:385:VAL:HG22	1:G:414:PRO:HG3	1.96	0.46
1:G:83:ASP:HA	1:G:209:PHE:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:364:ASN:O	1:B:368:LYS:HG2	2.16	0.46
1:B:79:ALA:HB2	1:B:429:ARG:O	2.15	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: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: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: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:489:ALA:O	1:D:490:ASN:HB2	2.16	0.46
1:E:298:MET:HE1	1:E:327:VAL:HG12	1.97	0.46
1:G:362:PHE:HB3	1:G:413:ARG:HG3	1.97	0.46
1:D:34:VAL:HG23	3:D:3090:HOH:O	2.16	0.45
1:F:40:LEU:HD23	1:F:45:MET:HE3	1.97	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:298:MET:HE1	1:H:327:VAL:HG12	1.98	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:G:142:TYR:HB2	1:G:178:ASN:HB2	1.98	0.45
1:G:47:VAL:HG22	1:G:79:ALA:HB3	1.98	0.45
1:H:83:ASP:HA	1:H:209:PHE:HB2	1.98	0.45
1:D:491:GLN:HG2	1:D:492:THR:N	2.30	0.45
1:G:345:TYR:O	1:G:349:ILE:HG13	2.17	0.45
1:D:142:TYR:HB2	1:D:178:ASN:HB2	1.98	0.45
3:C:3418:HOH:O	1:D:480:HIS:CE1	2.68	0.45
1:E:374:MET:HE3	1:E:378:GLU:C	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:THR:HG22	1:A:211:SER:HB2	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:F:380:VAL:HG21	1:F:490:ASN:CG	2.37	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: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:A:135:VAL:HG11	1:A:152:VAL:HG21	1.99	0.45
1:A:34:VAL:O	1:A:38:LYS:HG3	2.17	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:F:135:VAL:HG12	1:F:136:ARG:N	2.32	0.45
1:G:444:ALA:HB3	3:G:2947:HOH:O	2.17	0.45
1:G:380:VAL:HG21	1:G:490:ASN:OD1	2.16	0.45
1:H:242:HIS:CD2	3:H:2175:HOH:O	2.69	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:E:294:CYS:O	1:E:298:MET:HE2	2.17	0.44
1:G:479:ILE:HG23	1:G:480:HIS:N	2.33	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:109:VAL:HG12	1:C:124:PHE:CZ	2.52	0.44
1:A:366:ILE:HD12	1:C:3:LEU:HD21	1.99	0.44
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:H:396:MET:HE2	1:H:414:PRO:HG2	2.00	0.44
1:B:109:VAL:HG11	1:B:126:ILE:HD12	1.99	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:H:215:SER:HB3	3:H:2469:HOH:O	2.18	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: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:263:GLY:H	1:D:296:THR:HG1	1.61	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: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:H:10:SER:N	3:H:2563:HOH:O	2.41	0.44
1:H:396:MET:HE3	1:H:418:ILE:HG12	2.00	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:207:MET:CE	1:C:433:ILE:HG21	2.48	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:F:207:MET:CE	1:F:433:ILE:HG21	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:G:294:CYS:O	1:G:298:MET:HE2	2.18	0.43
1:A:250:SER:O	1:A:253:GLU:HB3	2.18	0.43
1:A:298:MET:HE1	1:A:327:VAL:HG12	1.99	0.43
1:E:425:LEU:HD13	1:E:441:PHE:CG	2.53	0.43
1:E:54:HIS:HD2	3:E:1733:HOH:O	2.01	0.43
1:F:429:ARG:O	1:F:432:ASN:HB2	2.17	0.43
1:B:16:ALA:O	1:B:18:TYR:N	2.46	0.43
1:C:144:ASP:CG	1:C:175:ARG:HD3	2.39	0.43
1:C:294:CYS:O	1:C:298:MET:HE2	2.19	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:207:MET:CE	1:A:433:ILE:HG21	2.48	0.43
1:A:374:MET:HE1	1:A:379:ALA:HA	2.00	0.43
1:A:396:MET:HE1	1:A:414:PRO:CG	2.45	0.43
1:A:4:ALA:HB1	3:A:3212:HOH:O	2.18	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:G:207:MET:CE	1:G:433:ILE:HG21	2.49	0.43
1:H:134:VAL:HG12	1:H:182:CYS:HB3	2.01	0.43
1:H:298:MET:HE3	1:H:327:VAL:HB	2.01	0.43
1:A:83:ASP:HA	1:A:209:PHE:HB2	2.00	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:HG3	1:F:446:LYS:O	2.19	0.43
1:H:108:TYR:O	1:H:123:LYS:HA	2.19	0.43
1:B:373:PRO:HB2	3:B:3309:HOH:O	2.18	0.43
1:B:73:GLU:HG3	3:B:3150:HOH:O	2.19	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:479:ILE:HG22	1:E:480:HIS:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:54:HIS:CD2	3:E:1733:HOH:O	2.71	0.43
1:B:83:ASP:HA	1:B:209:PHE:HB2	2.00	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:G:304:TYR:HB3	3:G:2833:HOH:O	2.19	0.43
1:F:310:ARG:HH22	1:H:275:VAL:CG2	2.31	0.43
1:H:429:ARG:O	1:H:432:ASN:HB2	2.19	0.43
1:B:372:ILE:HB	3:B:3167:HOH:O	2.19	0.43
1:B:367:LYS:HE2	1:B:382:SER:HB2	2.01	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:E:157:ASP:C	1:E:159:GLN:H	2.22	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:G:178:ASN:O	1:G:180:PRO:HD3	2.18	0.43
1:H:494:ILE:O	1:G:490:ASN:ND2	2.51	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:HA	1:H:40:LEU:HD12	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:197:LEU:O	1:F:201:VAL:HG23	2.20	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:B:207:MET:CE	1:B:433:ILE:HG21	2.48	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
1:D:93:GLN:CD	1:D:174:ARG:HH21	2.23	0.42
1:E:399:LEU:HD22	1:E:421:VAL:HB	2.00	0.42
1:G:144:ASP:CG	1:G:175:ARG:HD3	2.40	0.42
1:G:374:MET:CE	1:G:378:GLU:HG3	2.49	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:F:479:ILE:CG2	1:F:480:HIS:N	2.82	0.42
1:E:385:VAL:HG22	1:E:414:PRO:HG3	2.02	0.42
1:E:89:ILE:CG2	1:E:177:VAL:HG22	2.50	0.42
3:F:1773:HOH:O	1:H:3:LEU:HD12	2.19	0.42
1:B:380:VAL:HG21	1:B:490:ASN:ND2	2.35	0.42
1:C:273:LYS:NZ	3:C:3248:HOH:O	2.51	0.42
1:G:374:MET:HE2	1:G:378:GLU:HG3	2.02	0.42
1:H:362:PHE:HB3	1:H:413:ARG:HG3	2.01	0.42
1:H:374:MET:HE1	1:H:379:ALA:HA	2.01	0.42
1:A:148:LEU:HB2	1:A:169:HIS:HD2	1.84	0.42
1:A:142:TYR:O	1:A:177:VAL:HA	2.20	0.42
1:C:153:GLN:NE2	1:C:164:THR:OG1	2.52	0.42
1:C:83:ASP:HA	1:C:209:PHE:HB2	2.02	0.42
1:C:298:MET:HE3	1:C:327:VAL:HB	2.02	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:437:VAL:HG12	1:B:438:GLU:N	2.34	0.41
1:B:310:ARG:NH2	1:D:274:VAL:HG11	2.35	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:242:HIS:HB3	3:A:3286:HOH:O	2.19	0.41
1:A:294:CYS:O	1:A:298:MET:HE2	2.21	0.41
1:A:40:LEU:HD23	1:A:45:MET:HE3	2.02	0.41
1:A:38:LYS:HD2	1:A:74:LEU:HG	2.01	0.41
1:C:283:SER:O	1:C:287:VAL:HG23	2.20	0.41
1:F:183:ASP:CG	3:F:2133:HOH:O	2.58	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: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: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:H:90:ARG:HD2	3:H:2203:HOH:O	2.20	0.41
1:B:148:LEU:HB2	1:B:169:HIS:HD2	1.85	0.41
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: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:H:99:ALA:HA	3:H:2529:HOH:O	2.19	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:298:MET:HE3	1:A:327:VAL:HB	2.01	0.41
1:A:494:ILE:HD12	1:B:380:VAL:CG2	2.51	0.41
1:C:396:MET:HE1	1:C:414:PRO:CG	2.45	0.41
1:D:111:THR:OG1	1:D:131:LEU:HB3	2.21	0.41
1:D:374:MET:HE1	1:D:379:ALA:HA	2.03	0.41
1:E:302:MET:HB3	1:E:342:VAL:HG22	2.03	0.41
1:E:89:ILE:HG21	1:E:177:VAL:HG22	2.01	0.41
1:F:274:VAL:HB	3:F:1776:HOH:O	2.19	0.41
1:A:376:ALA:O	1:A:380:VAL:HG23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:380:VAL:HG21	1:E:490:ASN:ND2	2.35	0.41
1:E:34:VAL:O	1:E:38:LYS:HG3	2.21	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:399:LEU:HD22	1:H:421:VAL:HB	2.03	0.41
1:A:374:MET:CE	1:A:379:ALA:HA	2.51	0.41
1:B:475:TYR:HA	1:B:495:LEU:O	2.21	0.41
1:B:47:VAL:HG22	1:B:79:ALA:HB3	2.03	0.41
1:C:362:PHE:HB3	1:C:413:ARG:HG3	2.02	0.41
1:F:158:GLU:HB2	3:F:2046:HOH:O	2.21	0.41
1:G:79:ALA:HB2	1:G:429:ARG:O	2.20	0.41
1:H:197:LEU:O	1:H:201:VAL:HG23	2.20	0.41
1:C:104:GLY:N	1:C:165:VAL:O	2.53	0.41
1:C:386:ASN:ND2	3:C:3093:HOH:O	2.53	0.41
1:D:142:TYR:O	1:D:177:VAL:HA	2.21	0.41
1:F:83:ASP:HA	1:F:209:PHE:HB2	2.03	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: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:E:374:MET:HE3	1:E:379:ALA:N	2.36	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:123:LYS:NZ	3:C:3307:HOH:O	2.53	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:D:298:MET:HE3	1:D:327:VAL:HB	2.02	0.40
1:F:135:VAL:CG1	1:F:136:ARG:N	2.84	0.40
1:G:142:TYR:O	1:G:177:VAL:HA	2.21	0.40
1:H:112:ASP:HA	1:H:113:PRO:HD3	1.93	0.40
1:H:207:MET:HE2	1:H:209:PHE:CE1	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:207:MET:CE	1:H:433:ILE:HG21	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:E:396:MET:HE1	1:E:414:PRO:CG	2.46	0.40
1:G:407:ARG:HD3	3:G:2570:HOH:O	2.20	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:24:ILE:HG12	1:A:47:VAL:HB	2.04	0.40
1:A:370:GLN:NE2	3:A:3161:HOH:O	2.42	0.40
1:D:437:VAL:HG12	1:D:438:GLU:N	2.36	0.40
1:F:425:LEU:HD13	1:F:441:PHE:CG	2.57	0.40
1:F:89:ILE:HG21	1:F:177:VAL:HG22	2.03	0.40
1:G:111:THR:HG21	1:G:129:GLN:HA	2.04	0.40
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: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:HA	1:D:40:LEU:HD12	1.88	0.40
1:D:396:MET:HE3	1:D:418:ILE:HG12	2.04	0.40
1:F:142:TYR:O	1:F:177:VAL:HA	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	487/499 (98%)	458 (94%)	26 (5%)	3 (1%)	25	27
1	B	485/499 (97%)	457 (94%)	26 (5%)	2 (0%)	34	38
1	C	488/499 (98%)	463 (95%)	23 (5%)	2 (0%)	34	38
1	D	489/499 (98%)	455 (93%)	30 (6%)	4 (1%)	19	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	489/499 (98%)	460 (94%)	23 (5%)	6 (1%)	13	11
1	F	487/499 (98%)	462 (95%)	23 (5%)	2 (0%)	34	38
1	G	496/499 (99%)	466 (94%)	26 (5%)	4 (1%)	19	20
1	H	488/499 (98%)	466 (96%)	19 (4%)	3 (1%)	25	27
All	All	3909/3992 (98%)	3687 (94%)	196 (5%)	26 (1%)	22	23

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	483	HIS
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%)	391 (95%)	19 (5%)	27	32
1	B	409/417 (98%)	386 (94%)	23 (6%)	21	23
1	C	411/417 (99%)	390 (95%)	21 (5%)	24	27
1	D	412/417 (99%)	397 (96%)	15 (4%)	35	43
1	E	412/417 (99%)	393 (95%)	19 (5%)	27	32
1	F	410/417 (98%)	393 (96%)	17 (4%)	30	37
1	G	411/417 (99%)	393 (96%)	18 (4%)	28	34
1	H	411/417 (99%)	393 (96%)	18 (4%)	28	34
All	All	3286/3336 (98%)	3136 (95%)	150 (5%)	27	32

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

Mol	Chain	Res	Type
1	A	17	ASN
1	A	40	LEU
1	A	84	THR
1	A	117	ASP
1	A	158	GLU
1	A	207	MET
1	A	231	ARG
1	A	254	GLU
1	A	262	ARG
1	A	268	GLU
1	A	302	MET
1	A	345	TYR
1	A	351	LEU
1	A	357	LEU
1	A	364	ASN
1	A	371	HIS
1	A	422	THR
1	A	424	ARG
1	A	435	GLN
1	B	13	ASP
1	B	40	LEU
1	B	68	ARG
1	B	84	THR

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Mol	Chain	Res	Type
1	B	90	ARG
1	B	103	ARG
1	B	111	THR
1	B	117	ASP
1	B	158	GLU
1	B	185	ASP
1	B	198	GLN
1	B	207	MET
1	B	215	SER
1	B	262	ARG
1	B	268	GLU
1	B	310	ARG
1	B	345	TYR
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	117	ASP
1	C	132	SER
1	C	149	ILE
1	C	153	GLN
1	C	207	MET
1	C	215	SER
1	C	231	ARG
1	C	262	ARG
1	C	307	ARG
1	C	310	ARG
1	C	345	TYR
1	C	351	LEU
1	C	357	LEU
1	C	364	ASN
1	C	374	MET
1	C	377	ASP
1	C	422	THR
1	C	435	GLN
1	D	40	LEU
1	D	84	THR

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Mol	Chain	Res	Type
1	D	117	ASP
1	D	155	HIS
1	D	158	GLU
1	D	207	MET
1	D	262	ARG
1	D	302	MET
1	D	310	ARG
1	D	345	TYR
1	D	351	LEU
1	D	357	LEU
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	183	ASP
1	E	207	MET
1	E	262	ARG
1	E	345	TYR
1	E	351	LEU
1	E	357	LEU
1	E	366	ILE
1	E	371	HIS
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	180	PRO
1	F	207	MET
1	F	262	ARG
1	F	310	ARG
1	F	345	TYR

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Mol	Chain	Res	Type
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	F	480	HIS
1	H	40	LEU
1	H	84	THR
1	H	90	ARG
1	H	117	ASP
1	H	130	ASN
1	H	207	MET
1	H	262	ARG
1	H	310	ARG
1	H	345	TYR
1	H	351	LEU
1	H	357	LEU
1	H	364	ASN
1	H	422	THR
1	H	435	GLN
1	H	471	GLN
1	H	479	ILE
1	H	480	HIS
1	H	482	ASP
1	G	40	LEU
1	G	68	ARG
1	G	84	THR
1	G	132	SER
1	G	207	MET
1	G	231	ARG
1	G	262	ARG
1	G	310	ARG
1	G	345	TYR
1	G	351	LEU
1	G	357	LEU
1	G	422	THR
1	G	435	GLN
1	G	454	GLU
1	G	479	ILE
1	G	480	HIS
1	G	490	ASN

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Mol	Chain	Res	Type
1	G	491	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	ASN
1	A	151	GLN
1	A	155	HIS
1	A	242	HIS
1	A	286	ASN
1	A	364	ASN
1	A	386	ASN
1	A	401	ASN
1	A	471	GLN
1	A	490	ASN
1	B	139	ASN
1	B	153	GLN
1	B	305	ASN
1	B	364	ASN
1	B	401	ASN
1	B	471	GLN
1	B	491	GLN
1	C	139	ASN
1	C	218	GLN
1	C	242	HIS
1	C	297	GLN
1	C	305	ASN
1	C	386	ASN
1	C	401	ASN
1	C	491	GLN
1	D	139	ASN
1	D	155	HIS
1	D	243	GLN
1	D	286	ASN
1	D	297	GLN
1	D	401	ASN
1	D	491	GLN
1	E	139	ASN
1	E	151	GLN
1	E	198	GLN
1	E	242	HIS
1	E	246	GLN

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Mol	Chain	Res	Type
1	E	286	ASN
1	E	305	ASN
1	E	364	ASN
1	E	401	ASN
1	E	483	HIS
1	F	139	ASN
1	F	242	HIS
1	F	278	GLN
1	F	286	ASN
1	F	322	ASN
1	F	401	ASN
1	H	69	GLN
1	H	139	ASN
1	H	151	GLN
1	H	155	HIS
1	H	242	HIS
1	H	246	GLN
1	H	278	GLN
1	H	305	ASN
1	H	322	ASN
1	H	364	ASN
1	H	401	ASN
1	H	491	GLN
1	G	139	ASN
1	G	151	GLN
1	G	153	GLN
1	G	297	GLN
1	G	401	ASN
1	G	480	HIS
1	G	490	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	H	3006	-	4,4,4	0.26	0	6,6,6	0.31	0
2	SO4	A	3000	-	4,4,4	0.26	0	6,6,6	0.20	0
2	SO4	E	3004	-	4,4,4	0.40	0	6,6,6	0.23	0
2	SO4	F	3005	-	4,4,4	0.29	0	6,6,6	0.22	0
2	SO4	B	3001	-	4,4,4	0.23	0	6,6,6	0.11	0
2	SO4	C	3002	-	4,4,4	0.31	0	6,6,6	0.20	0
2	SO4	D	3003	-	4,4,4	0.33	0	6,6,6	0.24	0
2	SO4	G	3007	-	4,4,4	0.21	0	6,6,6	0.13	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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	491/499 (98%)	0.30	56 (11%) 5 7	15, 39, 100, 100	0
1	B	489/499 (97%)	0.04	12 (2%) 57 67	21, 48, 86, 100	0
1	C	492/499 (98%)	-0.13	6 (1%) 79 86	14, 38, 77, 100	0
1	D	493/499 (98%)	0.68	79 (16%) 1 3	19, 48, 100, 100	0
1	E	493/499 (98%)	0.11	31 (6%) 20 29	15, 36, 100, 100	0
1	F	491/499 (98%)	0.00	11 (2%) 62 72	19, 45, 87, 100	0
1	G	498/499 (99%)	-0.09	17 (3%) 45 57	12, 40, 91, 100	0
1	H	492/499 (98%)	-0.05	13 (2%) 56 65	16, 40, 81, 100	0
All	All	3939/3992 (98%)	0.11	225 (5%) 23 34	12, 42, 100, 100	0

All (225) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	96	GLY	12.4
1	D	137	PRO	11.8
1	D	95	VAL	10.5
1	G	488	TYR	9.0
1	D	94	PHE	7.6
1	D	100	VAL	7.6
1	A	99	ALA	7.5
1	E	95	VAL	7.4
1	D	114	ALA	7.0
1	D	105	ALA	6.9
1	A	116	ALA	6.2
1	D	124	PHE	5.9
1	A	95	VAL	5.8
1	D	136	ARG	5.8
1	D	116	ALA	5.8
1	D	128	TYR	5.7

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Mol	Chain	Res	Type	RSRZ
1	D	170	THR	5.6
1	D	147	ILE	5.4
1	F	449	HIS	5.4
1	A	115	PHE	5.3
1	D	102	GLU	5.3
1	E	154	SER	5.3
1	D	164	THR	5.2
1	A	444	ALA	5.1
1	A	124	PHE	5.0
1	B	304	TYR	5.0
1	B	447	LEU	5.0
1	D	101	MET	5.0
1	A	94	PHE	4.8
1	D	121	LYS	4.6
1	G	483	HIS	4.6
1	E	115	PHE	4.6
1	A	103	ARG	4.5
1	A	155	HIS	4.5
1	D	167	ASN	4.4
1	D	92	GLY	4.4
1	D	152	VAL	4.4
1	D	304	TYR	4.4
1	A	106	THR	4.3
1	D	179	LEU	4.3
1	A	154	SER	4.3
1	A	101	MET	4.3
1	E	155	HIS	4.2
1	G	485	VAL	4.2
1	F	304	TYR	4.1
1	A	114	ALA	4.1
1	A	125	TYR	4.1
1	D	130	ASN	4.1
1	D	139	ASN	4.1
1	D	126	ILE	4.1
1	D	113	PRO	4.0
1	D	97	GLY	4.0
1	D	129	GLN	4.0
1	D	158	GLU	4.0
1	D	118	LYS	3.9
1	A	161	LEU	3.9
1	D	447	LEU	3.9
1	D	93	GLN	3.9

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Mol	Chain	Res	Type	RSRZ
1	E	137	PRO	3.9
1	D	155	HIS	3.9
1	D	115	PHE	3.9
1	D	175	ARG	3.9
1	D	99	ALA	3.8
1	A	140	TYR	3.8
1	G	484	LYS	3.8
1	A	166	THR	3.8
1	E	118	LYS	3.8
1	D	98	ASP	3.7
1	D	106	THR	3.7
1	D	171	ILE	3.6
1	E	133	LYS	3.6
1	A	152	VAL	3.6
1	G	487	GLY	3.5
1	A	446	LYS	3.5
1	A	157	ASP	3.4
1	H	17	ASN	3.4
1	D	103	ARG	3.4
1	D	149	ILE	3.4
1	A	100	VAL	3.4
1	E	140	TYR	3.3
1	D	154	SER	3.3
1	A	107	CYS	3.3
1	D	125	TYR	3.3
1	D	117	ASP	3.3
1	E	483	HIS	3.3
1	A	139	ASN	3.2
1	E	164	THR	3.2
1	A	112	ASP	3.2
1	E	153	GLN	3.2
1	A	92	GLY	3.2
1	A	108	TYR	3.2
1	E	106	THR	3.2
1	A	447	LEU	3.2
1	E	17	ASN	3.1
1	D	153	GLN	3.1
1	A	149	ILE	3.1
1	D	112	ASP	3.1
1	B	489	ALA	3.1
1	H	324	ALA	3.1
1	D	104	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	129	GLN	3.0
1	G	449	HIS	3.0
1	E	166	THR	3.0
1	D	483	HIS	3.0
1	A	147	ILE	3.0
1	A	148	LEU	2.9
1	F	444	ALA	2.9
1	D	177	VAL	2.9
1	H	231	ARG	2.9
1	G	1	SER	2.9
1	A	158	GLU	2.9
1	D	91	THR	2.9
1	D	111	THR	2.9
1	D	110	THR	2.8
1	D	108	TYR	2.8
1	D	444	ALA	2.8
1	A	159	GLN	2.8
1	E	151	GLN	2.8
1	D	168	SER	2.8
1	E	158	GLU	2.8
1	D	135	VAL	2.8
1	F	169	HIS	2.8
1	F	228	PRO	2.8
1	H	446	LYS	2.8
1	G	490	ASN	2.7
1	H	304	TYR	2.7
1	B	62	THR	2.7
1	G	14	PRO	2.7
1	D	107	CYS	2.7
1	F	451	GLU	2.7
1	D	131	LEU	2.7
1	E	447	LEU	2.7
1	H	445	ASP	2.7
1	A	449	HIS	2.7
1	B	454	GLU	2.7
1	D	294	CYS	2.7
1	F	231	ARG	2.6
1	A	319	ALA	2.6
1	G	489	ALA	2.6
1	A	136	ARG	2.6
1	D	166	THR	2.6
1	G	97	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	142	TYR	2.6
1	G	158	GLU	2.6
1	C	53	SER	2.6
1	A	165	VAL	2.6
1	D	89	ILE	2.6
1	E	103	ARG	2.5
1	E	139	ASN	2.5
1	E	382	SER	2.5
1	D	165	VAL	2.5
1	E	112	ASP	2.5
1	H	449	HIS	2.5
1	A	96	GLY	2.5
1	D	481	ALA	2.5
1	D	173	ASP	2.5
1	F	481	ALA	2.4
1	H	95	VAL	2.4
1	A	138	GLY	2.4
1	E	482	ASP	2.4
1	A	113	PRO	2.4
1	A	137	PRO	2.4
1	A	168	SER	2.4
1	A	109	VAL	2.4
1	D	127	ASP	2.4
1	E	108	TYR	2.4
1	D	448	GLY	2.4
1	G	486	LYS	2.4
1	B	338	TYR	2.4
1	H	90	ARG	2.4
1	G	96	GLY	2.4
1	E	165	VAL	2.3
1	E	136	ARG	2.3
1	D	169	HIS	2.3
1	B	307	ARG	2.3
1	F	212	PHE	2.3
1	D	141	ILE	2.3
1	A	445	ASP	2.3
1	D	120	THR	2.3
1	F	158	GLU	2.3
1	C	100	VAL	2.3
1	A	117	ASP	2.3
1	A	141	ILE	2.2
1	C	158	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	135	VAL	2.2
1	B	295	ALA	2.2
1	C	168	SER	2.2
1	E	437	VAL	2.2
1	H	136	ARG	2.2
1	A	121	LYS	2.2
1	C	489	ALA	2.2
1	A	451	GLU	2.2
1	B	231	ARG	2.1
1	B	455	HIS	2.1
1	E	449	HIS	2.1
1	E	114	ALA	2.1
1	G	114	ALA	2.1
1	D	293	ILE	2.1
1	H	326	CYS	2.1
1	A	104	GLY	2.1
1	A	145	ASP	2.1
1	E	117	ASP	2.1
1	C	382	SER	2.1
1	B	96	GLY	2.1
1	D	172	SER	2.1
1	A	489	ALA	2.1
1	D	17	ASN	2.1
1	A	470	VAL	2.1
1	E	94	PHE	2.1
1	F	295	ALA	2.1
1	D	326	CYS	2.1
1	E	100	VAL	2.1
1	G	15	VAL	2.1
1	A	142	TYR	2.1
1	H	444	ALA	2.0
1	A	132	SER	2.0
1	H	94	PHE	2.0
1	D	123	LYS	2.0
1	D	451	GLU	2.0
1	D	132	SER	2.0
1	A	134	VAL	2.0
1	D	446	LYS	2.0
1	A	169	HIS	2.0
1	B	261	ALA	2.0
1	D	133	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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	A	3000	5/5	0.98	0.08	36,36,36,36	0
2	SO4	E	3004	5/5	0.98	0.08	39,39,39,39	0
2	SO4	D	3003	5/5	0.98	0.08	44,44,44,44	0
2	SO4	F	3005	5/5	0.99	0.08	42,42,42,42	0
2	SO4	B	3001	5/5	0.99	0.07	45,45,45,45	0
2	SO4	C	3002	5/5	0.99	0.07	36,36,36,36	0
2	SO4	H	3006	5/5	0.99	0.07	41,41,41,41	0
2	SO4	G	3007	5/5	0.99	0.06	33,33,33,33	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.