



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 09:48 pm BST

PDB ID : 1HKX
Title : Crystal structure of calcium/calmodulin-dependent protein kinase
Authors : Hoelz, A.; Nairn, A.C.; Kuriyan, J.
Deposited on : 2003-03-12
Resolution : 2.65 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 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

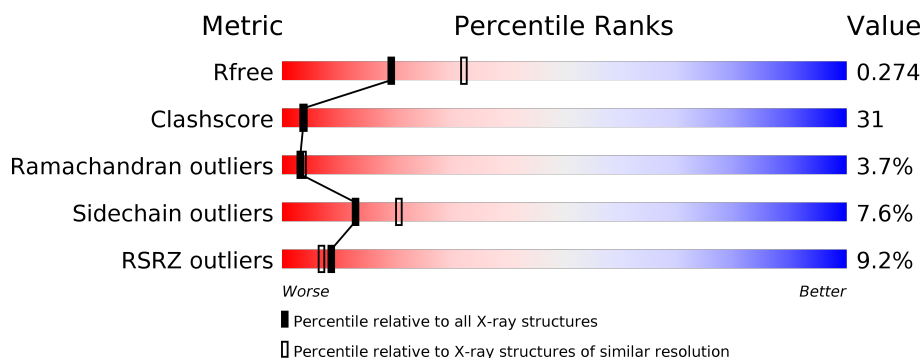
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	147	<div> <div>9%</div> <div> <div></div> <div>57%</div> <div>33%</div> <div>6%</div> <div>•</div> </div> </div>
1	B	147	<div> <div>5%</div> <div> <div></div> <div>56%</div> <div>31%</div> <div>5%</div> <div>7%</div> </div> </div>
1	C	147	<div> <div>8%</div> <div> <div></div> <div>48%</div> <div>40%</div> <div>6%</div> <div>5%</div> </div> </div>
1	D	147	<div> <div>12%</div> <div> <div></div> <div>46%</div> <div>41%</div> <div>6%</div> <div>6%</div> </div> </div>
1	E	147	<div> <div>10%</div> <div> <div></div> <div>56%</div> <div>37%</div> <div>5%</div> <div>•</div> </div> </div>
1	F	147	<div> <div>10%</div> <div> <div></div> <div>53%</div> <div>33%</div> <div>7%</div> <div>5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	147	
1	H	147	
1	I	147	
1	J	147	
1	K	147	
1	L	147	
1	M	147	
1	N	147	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DTT	A	1475	X	X	X	X
3	CL	I	1475	-	-	X	-
4	TBR	A	2000	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15690 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 CALCIUM/CALMODULIN-DEPENDENT PROTEIN KINASE TYPE II ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	0	1
			1135	713	201	215	6			
1	B	136	Total	C	N	O	S	0	0	1
			1096	689	196	206	5			
1	C	139	Total	C	N	O	S	0	0	1
			1120	704	199	212	5			
1	D	138	Total	C	N	O	S	0	0	1
			1113	700	198	210	5			
1	E	144	Total	C	N	O	S	0	0	1
			1156	726	206	218	6			
1	F	139	Total	C	N	O	S	0	0	1
			1120	704	199	212	5			
1	G	136	Total	C	N	O	S	0	0	1
			1096	689	196	206	5			
1	H	143	Total	C	N	O	S	0	0	1
			1152	724	205	217	6			
1	I	135	Total	C	N	O	S	0	0	1
			1088	685	195	203	5			
1	J	139	Total	C	N	O	S	0	0	1
			1120	704	199	212	5			
1	K	135	Total	C	N	O	S	0	0	1
			1088	685	195	203	5			
1	L	135	Total	C	N	O	S	0	0	1
			1088	685	195	203	5			
1	M	139	Total	C	N	O	S	0	0	1
			1120	704	199	212	5			
1	N	136	Total	C	N	O	S	0	0	1
			1096	689	196	206	5			

- Molecule 2 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: $C_4H_{10}O_2S_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			8	4	2	2		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

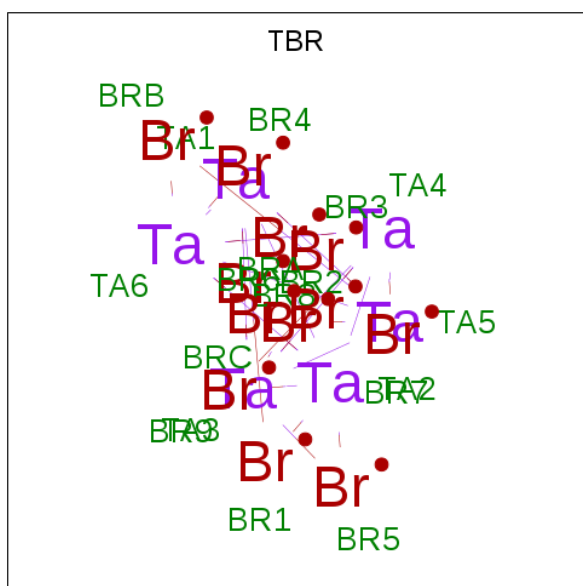
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Cl	0	0
			1	1		
3	J	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		
3	K	1	Total	Cl	0	0
			1	1		
3	E	1	Total	Cl	0	0
			1	1		
3	H	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		
3	I	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		
3	A	1	Total	Cl	0	0
			1	1		
3	N	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	1	Total	Cl	0	0
			1	1		
3	F	1	Total	Cl	0	0
			1	1		
3	M	1	Total	Cl	0	0
			1	1		

- Molecule 4 is HEXATANTALUM DODECABROMIDE (three-letter code: TBR) (formula: $\text{Br}_{12}\text{Ta}_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Br	Ta	0	0
			18	12	6		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total	O	0	0
			6	6		
5	B	4	Total	O	0	0
			4	4		
5	C	5	Total	O	0	0
			5	5		
5	D	4	Total	O	0	0
			4	4		
5	E	4	Total	O	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	4	Total 4	O 4	0	0
5	G	7	Total 7	O 7	0	0
5	H	6	Total 6	O 6	0	0
5	I	2	Total 2	O 2	0	0
5	J	3	Total 3	O 3	0	0
5	K	4	Total 4	O 4	0	0
5	L	5	Total 5	O 5	0	0
5	M	4	Total 4	O 4	0	0
5	N	4	Total 4	O 4	0	0

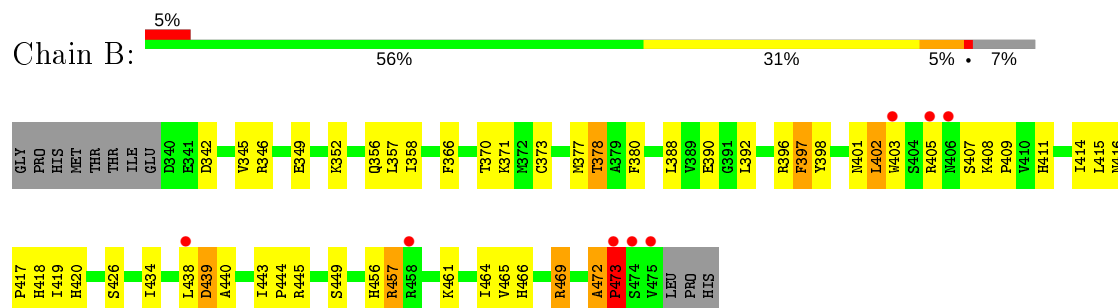
3 Residue-property plots [i](#)

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

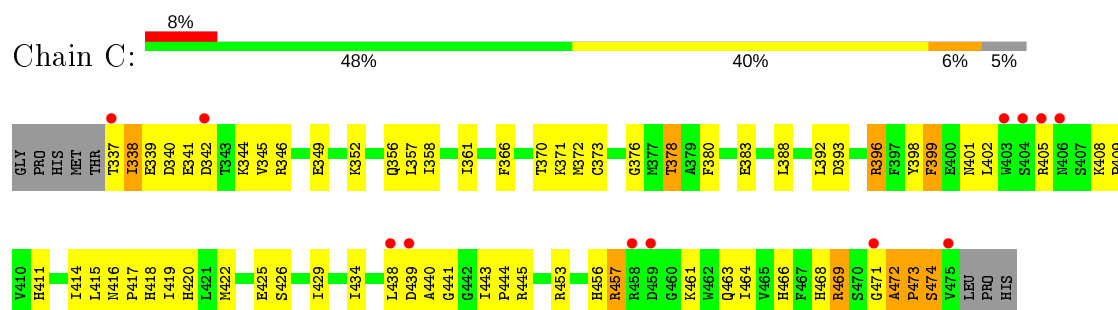
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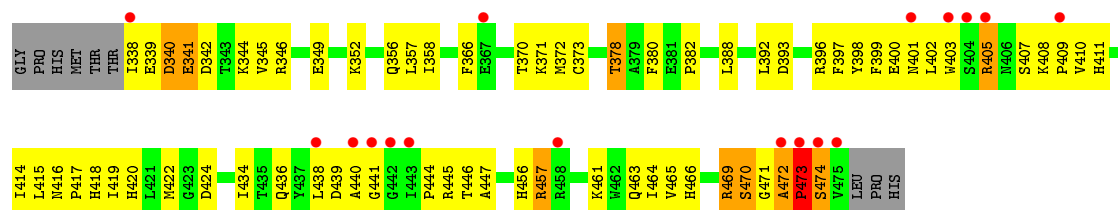
- Molecule 1: CALCIUM/CALMODULIN-DEPENDENT PROTEIN KINASE TYPE II ALPHA CHAIN



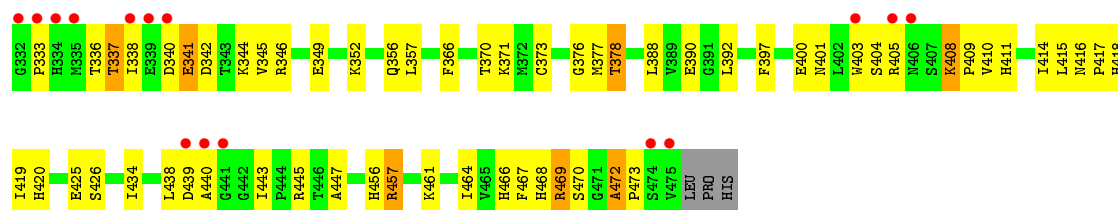
- Molecule 1: CALCIUM/CALMODULIN-DEPENDENT PROTEIN KINASE TYPE II ALPHA CHAIN



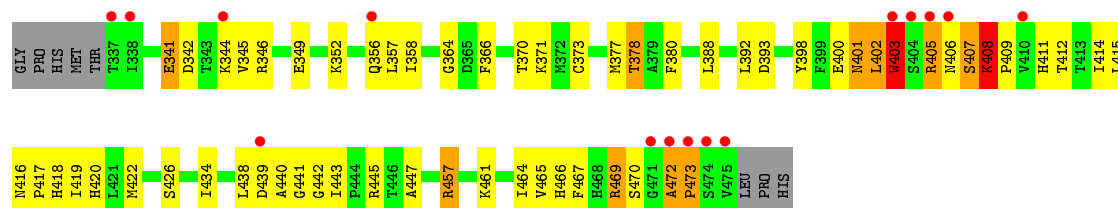
- Molecule 1: CALCIUM/CALMODULIN-DEPENDENT PROTEIN KINASE TYPE II ALPHA CHAIN



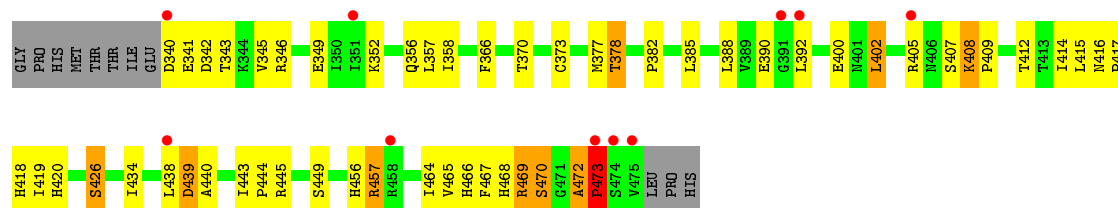
• Molecule 1: CALCIUM/CALMODULIN-DEPENDENT PROTEIN KINASE TYPE II ALPHA CHAIN



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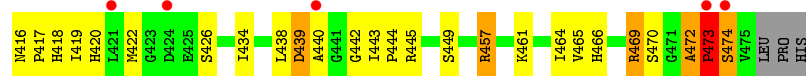


• Molecule 1: CALCIUM/CALMODULIN-DEPENDENT PROTEIN KINASE TYPE II ALPHA CHAIN



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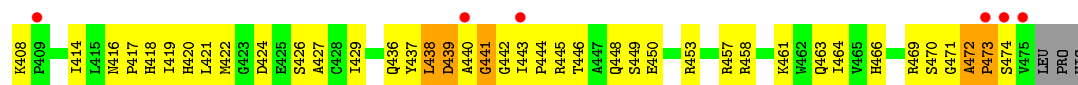




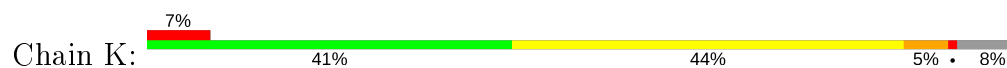
• Molecule 1: CALCIUM/CALMODULIN-DEPENDENT PROTEIN KINASE TYPE II ALPHA CHAIN



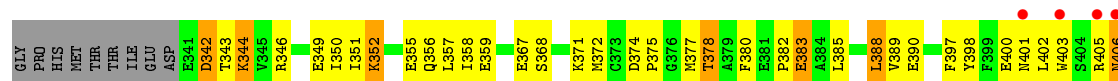
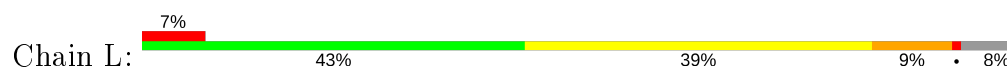
• Molecule 1: CALCIUM/CALMODULIN-DEPENDENT PROTEIN KINASE TYPE II ALPHA CHAIN

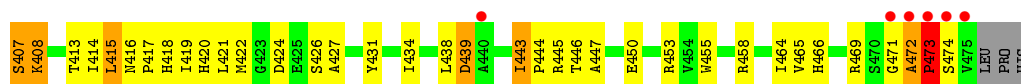


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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	147.95Å 118.04Å 157.82Å 90.00° 110.91° 90.00°	Depositor
Resolution (Å)	19.84 – 2.65 89.76 – 2.65	Depositor EDS
% Data completeness (in resolution range)	93.7 (19.84-2.65) 96.2 (89.76-2.65)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.65Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.246 , 0.279 0.243 , 0.274	Depositor DCC
R_{free} test set	6774 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	54.8	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 59.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	15690	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, TBR, DTT

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	0.46	0/1163	0.70	3/1575 (0.2%)
1	B	0.43	0/1124	0.64	0/1522
1	C	0.41	0/1148	0.61	0/1555
1	D	0.42	0/1141	0.62	0/1545
1	E	0.41	0/1186	0.59	0/1607
1	F	0.42	0/1148	0.62	0/1555
1	G	0.41	0/1124	0.63	0/1522
1	H	0.42	0/1182	0.67	0/1601
1	I	0.41	0/1116	0.65	0/1511
1	J	0.46	0/1148	0.69	0/1555
1	K	0.44	0/1116	0.66	0/1511
1	L	0.45	0/1116	0.69	1/1511 (0.1%)
1	M	0.44	0/1148	0.67	0/1555
1	N	0.41	0/1124	0.62	0/1522
All	All	0.43	0/15984	0.65	4/21647 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	439	ASP	CB-CG-OD2	6.51	124.16	118.30
1	A	471	GLY	N-CA-C	-5.38	99.64	113.10
1	A	439	ASP	N-CA-CB	5.31	120.16	110.60
1	L	421	LEU	CA-CB-CG	5.25	127.37	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1135	0	1089	72	0
1	B	1096	0	1049	69	0
1	C	1120	0	1073	72	0
1	D	1113	0	1066	91	0
1	E	1156	0	1106	68	0
1	F	1120	0	1073	86	0
1	G	1096	0	1049	68	0
1	H	1152	0	1104	72	0
1	I	1088	0	1045	71	0
1	J	1120	0	1073	88	0
1	K	1088	0	1045	91	0
1	L	1088	0	1045	83	0
1	M	1120	0	1073	58	0
1	N	1096	0	1049	65	0
2	A	8	0	8	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	2	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
4	A	18	0	0	4	0
5	A	6	0	0	1	0
5	B	4	0	0	0	0
5	C	5	0	0	0	0
5	D	4	0	0	0	0
5	E	4	0	0	0	0
5	F	4	0	0	0	0
5	G	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	6	0	0	1	0
5	I	2	0	0	1	0
5	J	3	0	0	0	0
5	K	4	0	0	0	0
5	L	5	0	0	0	0
5	M	4	0	0	0	0
5	N	4	0	0	0	0
All	All	15690	0	14947	955	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 31.

All (955) 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:E:378:THR:HG22	1:E:466:HIS:ND1	1.63	1.12
1:B:378:THR:HG22	1:B:466:HIS:ND1	1.65	1.11
1:N:378:THR:HG22	1:N:466:HIS:ND1	1.65	1.09
1:C:409:PRO:HD2	1:C:438:LEU:HD12	1.31	1.07
1:M:458:ARG:HB2	1:M:458:ARG:HH11	1.14	1.07
1:D:378:THR:HG22	1:D:466:HIS:ND1	1.68	1.06
1:D:447:ALA:HB1	1:D:473:PRO:HG3	1.36	1.05
1:C:378:THR:HG22	1:C:466:HIS:ND1	1.71	1.03
1:G:378:THR:HG22	1:G:466:HIS:ND1	1.71	1.03
1:G:449:SER:HB3	1:G:473:PRO:HD2	1.39	1.03
1:K:437:TYR:HE2	1:K:445:ARG:HB2	1.21	1.03
1:F:378:THR:HG22	1:F:466:HIS:ND1	1.76	1.01
1:K:447:ALA:HB1	1:K:473:PRO:HG3	1.40	1.00
1:A:378:THR:HG22	1:A:466:HIS:ND1	1.76	1.00
1:I:378:THR:HG22	1:I:466:HIS:ND1	1.77	0.99
1:N:449:SER:HB3	1:N:473:PRO:HD2	1.44	0.98
1:A:337:THR:HG23	1:A:338:ILE:HD12	1.45	0.98
1:B:402:LEU:HB3	1:B:405:ARG:HH12	1.29	0.97
1:B:449:SER:HB3	1:B:473:PRO:HD2	1.45	0.97
1:F:402:LEU:HB3	1:F:405:ARG:HH11	1.27	0.97
1:D:403:TRP:HA	1:D:405:ARG:HH11	1.25	0.96
1:M:458:ARG:HB2	1:M:458:ARG:NH1	1.77	0.96
1:D:403:TRP:HA	1:D:405:ARG:NH1	1.80	0.96
1:H:378:THR:HG22	1:H:466:HIS:ND1	1.80	0.96
1:J:408:LYS:HD3	1:J:438:LEU:HB2	1.48	0.95
1:D:382:PRO:HG2	1:D:472:ALA:HA	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:340:ASP:CG	1:G:341:GLU:H	1.73	0.91
1:K:370:THR:HG22	1:K:392:LEU:HD23	1.53	0.90
1:C:472:ALA:H	1:C:473:PRO:HD3	1.36	0.89
1:J:472:ALA:H	1:J:473:PRO:HD3	1.38	0.88
1:K:378:THR:HG22	1:K:466:HIS:ND1	1.88	0.88
1:C:337:THR:HG22	1:C:339:GLU:HG2	1.55	0.88
1:M:449:SER:HB3	1:M:473:PRO:HD2	1.55	0.87
1:I:469:ARG:HH11	1:I:469:ARG:HG3	1.41	0.86
1:C:371:LYS:HD3	1:C:461:LYS:HE2	1.57	0.86
1:G:469:ARG:HH11	1:G:469:ARG:HG3	1.43	0.84
1:H:449:SER:HB3	1:H:473:PRO:HD2	1.59	0.83
1:I:472:ALA:H	1:I:473:PRO:CD	1.91	0.83
1:B:469:ARG:HH11	1:B:469:ARG:HG3	1.44	0.83
1:H:357:LEU:HD22	1:H:464:ILE:HD11	1.60	0.83
1:L:378:THR:HG22	1:L:466:HIS:ND1	1.93	0.83
1:J:337:THR:HG21	1:J:341:GLU:HG3	1.60	0.83
1:D:378:THR:HG23	1:D:388:LEU:HD21	1.61	0.83
1:K:401:ASN:HD22	1:M:438:LEU:HD21	1.42	0.83
1:H:469:ARG:HH11	1:H:469:ARG:HG3	1.44	0.82
1:I:409:PRO:HG2	1:I:438:LEU:HD12	1.62	0.82
1:A:357:LEU:HD22	1:A:464:ILE:HD11	1.61	0.82
1:B:438:LEU:HD21	1:D:401:ASN:HB3	1.60	0.82
1:C:357:LEU:HD22	1:C:464:ILE:HD11	1.58	0.82
1:C:378:THR:HG23	1:C:388:LEU:HD21	1.59	0.82
1:E:378:THR:HG23	1:E:388:LEU:HD21	1.60	0.82
1:K:437:TYR:CE2	1:K:445:ARG:HB2	2.12	0.82
1:M:414:ILE:HG22	1:M:417:PRO:HG3	1.60	0.82
1:F:469:ARG:HG3	1:F:469:ARG:HH11	1.45	0.81
1:A:469:ARG:HH11	1:A:469:ARG:HG3	1.43	0.81
1:E:469:ARG:HH11	1:E:469:ARG:HG3	1.46	0.81
1:B:378:THR:HG23	1:B:388:LEU:HD21	1.63	0.81
1:B:444:PRO:HB3	1:D:397:PHE:CE2	2.16	0.81
1:D:407:SER:O	1:D:408:LYS:HG3	1.79	0.81
1:N:469:ARG:HG3	1:N:469:ARG:HH11	1.47	0.80
1:G:408:LYS:H	1:G:408:LYS:HD3	1.47	0.80
1:E:403:TRP:C	1:E:405:ARG:H	1.85	0.80
1:K:357:LEU:HD22	1:K:464:ILE:HD11	1.63	0.80
1:A:378:THR:HG23	1:A:388:LEU:HD21	1.64	0.79
1:L:472:ALA:H	1:L:473:PRO:HD2	1.48	0.79
1:L:443:ILE:HD12	1:L:443:ILE:H	1.45	0.79
1:N:378:THR:HG23	1:N:388:LEU:HD21	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:357:LEU:HD22	1:E:464:ILE:HD11	1.65	0.78
1:A:339:GLU:HG2	2:A:1475:DTT:S1	2.22	0.78
1:B:438:LEU:HD11	1:D:401:ASN:HD22	1.49	0.78
1:F:378:THR:HG23	1:F:388:LEU:HD21	1.66	0.78
1:F:357:LEU:HD22	1:F:464:ILE:HD11	1.64	0.78
1:G:378:THR:HG23	1:G:388:LEU:HD21	1.65	0.78
1:H:378:THR:HG23	1:H:388:LEU:HD21	1.65	0.78
1:J:469:ARG:HG3	1:J:469:ARG:HH11	1.49	0.78
1:G:357:LEU:HD22	1:G:464:ILE:HD11	1.66	0.78
1:I:357:LEU:HD22	1:I:464:ILE:HD11	1.66	0.77
1:F:447:ALA:HB1	1:F:473:PRO:HB3	1.66	0.77
1:C:469:ARG:HG3	1:C:469:ARG:HH11	1.50	0.77
1:J:439:ASP:C	1:J:441:GLY:H	1.85	0.77
1:A:401:ASN:ND2	1:C:438:LEU:HD11	1.99	0.76
1:D:357:LEU:HD22	1:D:464:ILE:HD11	1.66	0.76
1:J:340:ASP:OD1	1:J:341:GLU:HG2	1.86	0.76
1:D:469:ARG:HH11	1:D:469:ARG:HG3	1.51	0.76
1:A:338:ILE:HD12	1:A:338:ILE:H	1.51	0.75
1:H:438:LEU:HD11	1:J:401:ASN:HB3	1.69	0.75
1:J:450:GLU:HG2	1:J:470:SER:HB2	1.68	0.74
1:A:405:ARG:HA	1:A:408:LYS:HB3	1.69	0.74
1:B:357:LEU:HD22	1:B:464:ILE:HD11	1.70	0.74
1:D:447:ALA:HB1	1:D:473:PRO:CG	2.17	0.73
1:K:346:ARG:HH11	1:K:346:ARG:HB2	1.53	0.73
1:J:378:THR:HG23	1:J:466:HIS:ND1	2.03	0.72
1:M:405:ARG:HA	1:M:408:LYS:HB3	1.70	0.72
1:K:357:LEU:CD2	1:K:464:ILE:HD11	2.20	0.72
1:D:358:ILE:HD12	1:D:414:ILE:HD11	1.72	0.72
1:L:401:ASN:C	1:L:402:LEU:HD22	2.09	0.72
1:K:441:GLY:C	1:K:443:ILE:H	1.92	0.71
1:C:371:LYS:CD	1:C:461:LYS:HE2	2.20	0.71
1:A:402:LEU:HB3	1:A:405:ARG:NE	2.05	0.71
1:A:401:ASN:HD22	1:C:438:LEU:HD11	1.55	0.71
1:M:396:ARG:HD3	1:M:400:GLU:OE1	1.90	0.71
1:D:411:HIS:NE2	1:F:393:ASP:OD2	2.23	0.71
1:C:366:PHE:CZ	1:C:396:ARG:HB3	2.26	0.70
1:E:472:ALA:H	1:E:473:PRO:CD	2.04	0.70
1:E:409:PRO:HD2	1:E:438:LEU:HD12	1.72	0.70
1:G:340:ASP:CG	1:G:341:GLU:N	2.43	0.70
1:N:449:SER:HB3	1:N:473:PRO:CD	2.21	0.70
1:C:409:PRO:CD	1:C:438:LEU:HD12	2.18	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:400:GLU:HA	1:K:403:TRP:HE1	1.55	0.70
1:K:346:ARG:NH1	1:K:346:ARG:HB2	2.07	0.70
1:I:403:TRP:CE3	1:I:403:TRP:HA	2.26	0.70
1:C:358:ILE:HD12	1:C:414:ILE:HD11	1.74	0.70
1:C:472:ALA:N	1:C:473:PRO:HD3	2.07	0.69
1:N:357:LEU:HD22	1:N:464:ILE:HD11	1.73	0.69
1:J:471:GLY:O	1:J:472:ALA:HB2	1.90	0.69
3:I:1475:CL:CL	5:I:2002:HOH:O	2.46	0.69
1:K:382:PRO:HG2	1:K:472:ALA:HA	1.73	0.69
1:F:358:ILE:HD12	1:F:414:ILE:HD11	1.75	0.69
1:M:422:MET:HB2	1:M:426:SER:OG	1.93	0.69
2:A:1475:DTT:H42	4:A:2000:TBR:BR5	2.47	0.69
1:I:378:THR:HG23	1:I:388:LEU:HD21	1.72	0.69
1:K:443:ILE:HD12	1:K:445:ARG:HH12	1.57	0.69
1:E:378:THR:CG2	1:E:466:HIS:ND1	2.52	0.68
1:C:420:HIS:NE2	1:D:378:THR:HB	2.08	0.68
1:I:439:ASP:CG	1:I:440:ALA:H	1.95	0.68
1:I:403:TRP:HE3	1:I:403:TRP:HA	1.57	0.68
1:C:473:PRO:O	1:C:474:SER:HB2	1.94	0.68
1:I:443:ILE:HB	1:I:445:ARG:HH12	1.59	0.67
1:K:378:THR:HG23	1:K:388:LEU:HD11	1.76	0.67
1:L:342:ASP:HB2	1:L:346:ARG:HH12	1.58	0.67
1:E:397:PHE:O	1:E:400:GLU:HG2	1.94	0.67
1:C:378:THR:HB	1:D:420:HIS:NE2	2.09	0.67
1:D:399:PHE:O	1:D:403:TRP:HB3	1.94	0.67
1:B:378:THR:CG2	1:B:466:HIS:ND1	2.51	0.67
1:I:469:ARG:CG	1:I:469:ARG:HH11	2.08	0.67
1:H:439:ASP:CG	1:H:440:ALA:H	1.98	0.66
1:C:352:LYS:HG2	1:C:356:GLN:NE2	2.11	0.66
1:J:373:CYS:HB2	1:J:392:LEU:HD21	1.76	0.66
1:J:378:THR:CG2	1:J:466:HIS:ND1	2.58	0.66
1:I:352:LYS:HG2	1:I:356:GLN:NE2	2.11	0.66
1:N:402:LEU:HD23	1:N:405:ARG:HH21	1.59	0.66
1:D:371:LYS:HD3	1:D:461:LYS:HE2	1.77	0.66
1:J:457:ARG:HG3	1:J:461:LYS:O	1.95	0.66
1:I:397:PHE:CE2	1:K:444:PRO:HB3	2.31	0.66
1:J:352:LYS:O	1:J:356:GLN:HG3	1.95	0.66
1:J:404:SER:O	1:J:408:LYS:HB3	1.95	0.65
1:M:472:ALA:HB3	1:M:473:PRO:HD3	1.77	0.65
1:N:472:ALA:H	1:N:473:PRO:CD	2.09	0.65
1:D:398:TYR:O	1:D:402:LEU:HB3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:469:ARG:HH11	1:G:469:ARG:CG	2.09	0.65
1:N:443:ILE:HB	1:N:445:ARG:NH1	2.11	0.65
1:N:472:ALA:H	1:N:473:PRO:HD2	1.62	0.65
1:I:408:LYS:O	1:I:410:VAL:HG23	1.97	0.65
1:I:426:SER:HB2	1:J:422:MET:HB3	1.79	0.65
1:K:441:GLY:O	1:K:443:ILE:HG13	1.95	0.65
1:A:469:ARG:CG	1:A:469:ARG:HH11	2.10	0.65
1:G:414:ILE:HG22	1:G:417:PRO:HG3	1.79	0.65
1:H:469:ARG:HH11	1:H:469:ARG:CG	2.09	0.65
1:J:403:TRP:CE3	1:J:406:ASN:HB2	2.31	0.65
1:J:439:ASP:C	1:J:441:GLY:N	2.50	0.65
1:K:472:ALA:H	1:K:473:PRO:HD2	1.61	0.65
1:A:471:GLY:C	1:A:473:PRO:HD2	2.17	0.65
1:K:447:ALA:HB1	1:K:473:PRO:CG	2.22	0.65
1:K:420:HIS:NE2	1:L:378:THR:HB	2.12	0.65
1:N:402:LEU:HD23	1:N:405:ARG:NH2	2.11	0.65
1:E:352:LYS:HG2	1:E:356:GLN:NE2	2.12	0.64
1:F:400:GLU:C	1:F:401:ASN:HD22	1.99	0.64
1:E:468:HIS:NE2	1:F:470:SER:HB2	2.11	0.64
1:H:408:LYS:HD3	1:H:408:LYS:H	1.62	0.64
1:L:446:THR:O	1:N:385:LEU:HD11	1.96	0.64
1:F:469:ARG:CG	1:F:469:ARG:HH11	2.10	0.64
1:M:367:GLU:H	1:M:367:GLU:CD	2.00	0.64
1:A:393:ASP:OD2	1:C:411:HIS:NE2	2.30	0.64
1:F:352:LYS:HG2	1:F:356:GLN:NE2	2.13	0.64
1:L:383:GLU:N	1:L:383:GLU:OE1	2.30	0.64
1:D:352:LYS:HG2	1:D:356:GLN:NE2	2.13	0.64
1:L:378:THR:HG23	1:L:388:LEU:HD21	1.80	0.64
2:A:1475:DTT:H12	4:A:2000:TBR:BR8	2.53	0.64
1:H:439:ASP:HA	1:H:442:GLY:H	1.63	0.64
1:C:414:ILE:HG22	1:C:417:PRO:HG3	1.79	0.64
1:G:352:LYS:HG2	1:G:356:GLN:NE2	2.13	0.64
1:H:352:LYS:HG2	1:H:356:GLN:NE2	2.12	0.64
1:N:352:LYS:HG2	1:N:356:GLN:NE2	2.13	0.64
1:M:456:HIS:HD2	1:N:422:MET:HB3	1.63	0.64
1:I:443:ILE:HB	1:I:445:ARG:NH1	2.14	0.63
1:N:414:ILE:HG22	1:N:417:PRO:HG3	1.80	0.63
1:D:378:THR:CG2	1:D:466:HIS:ND1	2.55	0.63
1:L:398:TYR:O	1:L:402:LEU:HD23	1.98	0.63
1:J:408:LYS:HD3	1:J:438:LEU:CB	2.26	0.63
1:D:338:ILE:HD11	1:E:333:PRO:HG2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:420:HIS:NE2	1:H:378:THR:HB	2.14	0.63
1:I:414:ILE:HG22	1:I:417:PRO:HG3	1.79	0.63
1:L:443:ILE:O	1:L:445:ARG:HG2	1.98	0.63
1:A:414:ILE:HG22	1:A:417:PRO:HG3	1.80	0.63
1:B:402:LEU:HB3	1:B:405:ARG:NH1	2.10	0.63
1:D:473:PRO:O	1:D:474:SER:HB2	1.97	0.63
1:I:346:ARG:O	1:I:349:GLU:HB3	1.98	0.63
1:D:414:ILE:HG22	1:D:417:PRO:HG3	1.79	0.63
1:G:405:ARG:HA	1:G:408:LYS:HE2	1.79	0.63
1:I:380:PHE:CE1	1:J:450:GLU:HB2	2.32	0.63
1:N:469:ARG:CG	1:N:469:ARG:HH11	2.12	0.63
1:E:414:ILE:HG22	1:E:417:PRO:HG3	1.79	0.63
1:B:409:PRO:HD2	1:B:438:LEU:HD12	1.80	0.62
1:H:414:ILE:HG22	1:H:417:PRO:HG3	1.80	0.62
1:E:469:ARG:CG	1:E:469:ARG:HH11	2.12	0.62
1:I:472:ALA:H	1:I:473:PRO:HD3	1.64	0.62
1:N:346:ARG:O	1:N:349:GLU:HB3	1.99	0.62
1:B:346:ARG:O	1:B:349:GLU:HB3	1.99	0.62
1:B:469:ARG:CG	1:B:469:ARG:HH11	2.10	0.62
1:F:414:ILE:HG22	1:F:417:PRO:HG3	1.82	0.62
1:C:441:GLY:O	1:C:443:ILE:HG13	1.99	0.62
1:E:371:LYS:HD3	1:E:461:LYS:HE2	1.80	0.62
1:J:350:ILE:HD13	1:J:427:ALA:HB1	1.82	0.62
1:M:420:HIS:NE2	1:N:378:THR:HB	2.13	0.62
1:D:396:ARG:O	1:D:400:GLU:HG2	1.99	0.62
1:E:378:THR:HB	1:F:420:HIS:NE2	2.13	0.62
1:F:472:ALA:N	1:F:473:PRO:CD	2.63	0.62
1:K:356:GLN:O	1:K:359:GLU:HB3	1.99	0.62
1:G:416:ASN:N	1:G:417:PRO:HD3	2.14	0.62
1:I:396:ARG:HG2	1:I:396:ARG:HH11	1.63	0.62
1:M:341:GLU:HG2	1:M:341:GLU:O	1.99	0.62
1:E:443:ILE:HB	1:E:445:ARG:NH1	2.14	0.62
1:F:402:LEU:HB3	1:F:405:ARG:NH1	2.08	0.62
1:G:346:ARG:O	1:G:349:GLU:HB3	2.00	0.62
1:L:350:ILE:HD13	1:L:427:ALA:HB1	1.81	0.62
1:F:401:ASN:HD22	1:F:401:ASN:N	1.97	0.62
1:L:443:ILE:HD12	1:L:443:ILE:N	2.15	0.61
1:D:403:TRP:C	1:D:405:ARG:HD2	2.21	0.61
1:K:404:SER:O	1:K:408:LYS:HG2	2.00	0.61
1:I:401:ASN:HD22	1:K:438:LEU:HD11	1.66	0.61
1:M:342:ASP:C	1:M:344:LYS:H	2.03	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:ILE:HG22	1:B:417:PRO:HG3	1.82	0.61
1:N:378:THR:CG2	1:N:466:HIS:ND1	2.52	0.61
1:A:337:THR:HG23	1:A:338:ILE:H	1.65	0.61
1:D:346:ARG:O	1:D:349:GLU:HB3	2.00	0.61
1:F:346:ARG:O	1:F:349:GLU:HB3	2.00	0.61
1:E:420:HIS:NE2	1:F:378:THR:HB	2.15	0.61
1:F:406:ASN:C	1:F:408:LYS:H	2.02	0.61
1:B:352:LYS:HG2	1:B:356:GLN:NE2	2.16	0.61
1:L:351:ILE:HG22	1:L:355:GLU:OE2	2.01	0.61
1:D:444:PRO:HG2	1:F:401:ASN:O	2.01	0.61
1:H:449:SER:HB3	1:H:473:PRO:CD	2.31	0.61
1:B:438:LEU:HD11	1:D:401:ASN:ND2	2.14	0.61
1:I:380:PHE:CZ	1:J:450:GLU:HB2	2.36	0.60
1:J:469:ARG:HD3	1:J:473:PRO:HD2	1.82	0.60
1:F:405:ARG:O	1:F:408:LYS:HD3	2.00	0.60
1:C:352:LYS:HG2	1:C:356:GLN:HE21	1.66	0.60
1:A:352:LYS:HG2	1:A:356:GLN:NE2	2.16	0.60
1:F:352:LYS:HG2	1:F:356:GLN:HE21	1.66	0.60
1:L:352:LYS:HG3	1:L:356:GLN:HE21	1.66	0.60
1:M:352:LYS:HG3	1:M:356:GLN:HE21	1.67	0.60
1:N:443:ILE:HB	1:N:445:ARG:HH12	1.64	0.60
1:C:346:ARG:O	1:C:349:GLU:HB3	2.00	0.60
1:G:440:ALA:HB3	1:G:445:ARG:NH1	2.16	0.60
1:D:469:ARG:HH11	1:D:469:ARG:CG	2.15	0.60
1:I:352:LYS:HG2	1:I:356:GLN:HE21	1.65	0.60
1:K:402:LEU:HD12	1:M:444:PRO:HG2	1.84	0.60
1:F:341:GLU:O	1:F:344:LYS:HB3	2.02	0.60
1:F:364:GLY:HA3	1:F:405:ARG:NH2	2.17	0.60
1:H:444:PRO:HG2	1:J:402:LEU:HG	1.83	0.60
1:L:472:ALA:H	1:L:473:PRO:CD	2.12	0.60
1:B:416:ASN:N	1:B:417:PRO:HD3	2.17	0.60
1:K:386:GLY:HA2	1:L:450:GLU:OE1	2.01	0.60
1:F:472:ALA:H	1:F:473:PRO:CD	2.13	0.60
1:K:469:ARG:HH11	1:K:469:ARG:HB2	1.67	0.60
1:E:408:LYS:N	1:E:408:LYS:HD3	2.17	0.60
1:D:416:ASN:N	1:D:417:PRO:HD3	2.17	0.59
1:G:465:VAL:HG22	1:H:420:HIS:ND1	2.17	0.59
1:K:469:ARG:NH1	1:K:469:ARG:HB2	2.17	0.59
1:K:448:GLN:O	1:K:473:PRO:HG2	2.02	0.59
1:G:456:HIS:HD2	1:H:422:MET:HB3	1.68	0.59
1:N:416:ASN:N	1:N:417:PRO:HD3	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:352:LYS:HG2	1:D:356:GLN:HE21	1.68	0.59
1:K:382:PRO:HB2	1:K:383:GLU:OE2	2.03	0.59
1:C:469:ARG:CG	1:C:469:ARG:HH11	2.15	0.59
1:L:346:ARG:O	1:L:349:GLU:HB3	2.02	0.59
1:M:461:LYS:HD3	1:M:461:LYS:H	1.68	0.59
1:J:469:ARG:CD	1:J:473:PRO:HD2	2.33	0.59
1:E:346:ARG:O	1:E:349:GLU:HB3	2.03	0.59
1:M:370:THR:HG23	1:M:392:LEU:HD22	1.85	0.59
1:H:403:TRP:HA	1:H:403:TRP:CE3	2.37	0.59
1:H:403:TRP:HA	1:H:403:TRP:HE3	1.68	0.59
1:J:373:CYS:SG	1:J:464:ILE:HD11	2.42	0.59
1:K:381:GLU:OE2	1:K:469:ARG:NH2	2.36	0.59
1:A:403:TRP:HA	1:A:403:TRP:CE3	2.38	0.59
1:E:425:GLU:HA	1:E:457:ARG:HB3	1.85	0.59
1:F:411:HIS:NE2	1:H:393:ASP:OD2	2.36	0.59
1:F:416:ASN:N	1:F:417:PRO:HD3	2.18	0.59
1:L:342:ASP:HB2	1:L:346:ARG:NH1	2.18	0.58
1:A:342:ASP:HA	1:A:345:VAL:HG22	1.85	0.58
1:H:339:GLU:O	1:H:342:ASP:OD1	2.20	0.58
1:H:416:ASN:N	1:H:417:PRO:HD3	2.18	0.58
1:F:472:ALA:H	1:F:473:PRO:HD2	1.69	0.58
1:A:403:TRP:HA	1:A:403:TRP:HE3	1.68	0.58
1:B:403:TRP:C	1:B:405:ARG:H	2.06	0.58
1:J:424:ASP:O	1:J:457:ARG:NH2	2.37	0.58
1:K:441:GLY:O	1:K:443:ILE:N	2.36	0.58
1:I:342:ASP:HA	1:I:345:VAL:HG22	1.85	0.58
1:J:414:ILE:HG22	1:J:417:PRO:HG3	1.85	0.58
1:C:468:HIS:NE2	1:D:470:SER:HB2	2.18	0.58
1:E:472:ALA:N	1:E:473:PRO:CD	2.66	0.58
1:N:440:ALA:HB3	1:N:445:ARG:NH1	2.17	0.58
1:B:438:LEU:CD1	1:D:401:ASN:HD22	2.15	0.58
1:F:358:ILE:HG21	1:F:412:THR:HG21	1.84	0.58
1:K:422:MET:O	1:K:426:SER:HB3	2.03	0.58
1:B:358:ILE:HD12	1:B:414:ILE:HD11	1.86	0.58
1:F:403:TRP:HA	1:F:403:TRP:CE3	2.39	0.58
1:H:398:TYR:O	1:H:402:LEU:HD12	2.04	0.58
1:C:416:ASN:N	1:C:417:PRO:HD3	2.18	0.58
1:F:409:PRO:HD2	1:F:438:LEU:HD12	1.85	0.58
1:H:370:THR:HA	1:H:392:LEU:CD2	2.34	0.58
1:D:408:LYS:CD	1:D:439:ASP:HB2	2.34	0.57
1:M:345:VAL:HA	1:M:348:GLN:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:GLY:O	1:A:473:PRO:HD2	2.04	0.57
1:B:396:ARG:O	1:B:397:PHE:HB2	2.04	0.57
1:C:378:THR:CG2	1:C:466:HIS:ND1	2.60	0.57
1:E:403:TRP:C	1:E:405:ARG:N	2.56	0.57
1:A:378:THR:HB	1:B:420:HIS:NE2	2.18	0.57
1:A:416:ASN:N	1:A:417:PRO:HD3	2.19	0.57
1:E:352:LYS:HG2	1:E:356:GLN:HE21	1.69	0.57
1:F:378:THR:CG2	1:F:466:HIS:ND1	2.62	0.57
1:K:383:GLU:HB3	1:K:398:TYR:OH	2.03	0.57
1:N:352:LYS:HG2	1:N:356:GLN:HE21	1.69	0.57
1:A:448:GLN:O	1:A:473:PRO:HG2	2.04	0.57
1:G:443:ILE:HB	1:G:445:ARG:NH1	2.19	0.57
1:G:390:GLU:OE2	1:H:418:HIS:HE1	1.87	0.57
1:K:472:ALA:N	1:K:473:PRO:CD	2.67	0.57
1:A:420:HIS:ND1	1:B:465:VAL:HG22	2.18	0.57
1:E:416:ASN:N	1:E:417:PRO:HD3	2.19	0.57
1:G:352:LYS:HG2	1:G:356:GLN:HE21	1.70	0.57
1:I:406:ASN:C	1:I:408:LYS:H	2.07	0.57
1:F:441:GLY:O	1:F:443:ILE:HG13	2.04	0.57
1:H:346:ARG:O	1:H:349:GLU:HB3	2.05	0.57
1:A:443:ILE:HB	1:A:445:ARG:HH12	1.68	0.57
1:D:370:THR:HA	1:D:392:LEU:CD2	2.34	0.57
1:E:371:LYS:NZ	1:E:461:LYS:HE2	2.19	0.57
1:E:401:ASN:HD21	1:G:409:PRO:HG2	1.69	0.57
1:M:401:ASN:O	1:M:402:LEU:HG	2.04	0.57
1:I:370:THR:HA	1:I:392:LEU:CD2	2.35	0.57
1:L:355:GLU:O	1:L:359:GLU:HG3	2.05	0.57
1:L:407:SER:O	1:L:408:LYS:HB2	2.04	0.57
1:L:438:LEU:HD21	1:L:444:PRO:HG3	1.86	0.57
1:G:443:ILE:HB	1:G:445:ARG:HH12	1.69	0.57
1:H:352:LYS:HG2	1:H:356:GLN:HE21	1.69	0.57
1:M:407:SER:C	1:M:409:PRO:HD3	2.25	0.57
1:C:472:ALA:H	1:C:473:PRO:CD	2.15	0.56
1:C:469:ARG:HD3	1:C:473:PRO:HG2	1.87	0.56
1:G:370:THR:HA	1:G:392:LEU:CD2	2.35	0.56
1:H:337:THR:O	1:H:338:ILE:HG13	2.04	0.56
1:J:448:GLN:HG2	1:J:449:SER:N	2.21	0.56
1:C:357:LEU:HD22	1:C:464:ILE:CD1	2.33	0.56
1:F:440:ALA:O	1:F:445:ARG:NH1	2.36	0.56
1:J:443:ILE:O	1:J:445:ARG:HG3	2.05	0.56
1:J:469:ARG:HH11	1:J:469:ARG:CG	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:340:ASP:C	1:G:342:ASP:H	2.08	0.56
1:H:342:ASP:HA	1:H:345:VAL:HG22	1.87	0.56
1:M:449:SER:HB2	1:M:470:SER:O	2.05	0.56
1:A:346:ARG:O	1:A:349:GLU:HB3	2.05	0.56
1:G:342:ASP:HA	1:G:345:VAL:HG22	1.87	0.56
1:G:378:THR:CG2	1:G:466:HIS:ND1	2.58	0.56
1:H:439:ASP:O	1:H:440:ALA:HB3	2.04	0.56
1:D:408:LYS:HB2	1:D:408:LYS:HZ2	1.71	0.56
1:E:370:THR:HA	1:E:392:LEU:CD2	2.36	0.56
1:C:342:ASP:HA	1:C:345:VAL:HG22	1.88	0.56
1:J:429:ILE:CG2	1:J:453:ARG:HB2	2.35	0.56
1:A:420:HIS:NE2	1:B:378:THR:HB	2.21	0.56
1:D:408:LYS:HD3	1:D:439:ASP:HB2	1.88	0.56
1:I:402:LEU:HD12	1:I:405:ARG:NH1	2.20	0.56
1:K:472:ALA:N	1:K:473:PRO:HD2	2.21	0.56
1:J:471:GLY:O	1:J:472:ALA:CB	2.54	0.56
1:L:443:ILE:HB	1:L:445:ARG:NE	2.20	0.56
1:C:370:THR:HA	1:C:392:LEU:CD2	2.35	0.55
1:H:357:LEU:CD2	1:H:464:ILE:HD11	2.35	0.55
1:M:408:LYS:N	1:M:409:PRO:HD3	2.21	0.55
1:G:408:LYS:H	1:G:408:LYS:CD	2.19	0.55
1:A:370:THR:HA	1:A:392:LEU:CD2	2.36	0.55
1:B:370:THR:HA	1:B:392:LEU:CD2	2.36	0.55
1:B:371:LYS:HD3	1:B:461:LYS:HE2	1.88	0.55
1:F:370:THR:HA	1:F:392:LEU:CD2	2.36	0.55
1:F:411:HIS:CE1	1:H:393:ASP:OD2	2.59	0.55
1:K:439:ASP:C	1:K:442:GLY:H	2.08	0.55
1:L:401:ASN:O	1:L:402:LEU:HD13	2.06	0.55
1:M:383:GLU:N	1:M:383:GLU:OE2	2.30	0.55
1:M:406:ASN:C	1:M:408:LYS:H	2.10	0.55
1:A:422:MET:HB3	1:B:456:HIS:HD2	1.72	0.55
1:L:469:ARG:HH11	1:L:469:ARG:HG3	1.72	0.55
1:N:370:THR:HA	1:N:392:LEU:CD2	2.36	0.55
1:C:371:LYS:NZ	1:C:461:LYS:HE2	2.22	0.55
1:D:472:ALA:HB3	1:D:473:PRO:HD3	1.89	0.55
1:L:458:ARG:NH1	1:L:458:ARG:HB2	2.22	0.55
1:B:403:TRP:HA	1:B:405:ARG:NH2	2.22	0.55
1:D:444:PRO:HG3	1:F:401:ASN:HB3	1.87	0.55
1:I:416:ASN:N	1:I:417:PRO:HD3	2.21	0.55
1:I:472:ALA:N	1:I:473:PRO:CD	2.63	0.55
1:L:416:ASN:O	1:L:418:HIS:HD2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:441:GLY:C	1:K:443:ILE:N	2.60	0.55
1:M:403:TRP:CE3	1:M:403:TRP:HA	2.42	0.55
1:I:378:THR:CG2	1:I:466:HIS:ND1	2.63	0.55
1:L:472:ALA:N	1:L:473:PRO:CD	2.68	0.55
1:K:401:ASN:ND2	1:M:438:LEU:HD21	2.15	0.55
1:A:337:THR:HG23	1:A:338:ILE:CD1	2.30	0.54
1:F:407:SER:O	1:F:408:LYS:HB3	2.05	0.54
1:K:358:ILE:HD12	1:K:414:ILE:HD11	1.89	0.54
1:N:443:ILE:HD12	1:N:445:ARG:HH22	1.71	0.54
1:D:342:ASP:HA	1:D:345:VAL:HG22	1.88	0.54
1:H:472:ALA:HB3	1:H:473:PRO:HD3	1.89	0.54
1:A:402:LEU:HB3	1:A:405:ARG:CD	2.37	0.54
1:I:409:PRO:CG	1:I:438:LEU:HD12	2.36	0.54
1:M:403:TRP:HE3	1:M:403:TRP:HA	1.73	0.54
1:I:465:VAL:HG22	1:J:420:HIS:ND1	2.23	0.54
1:A:418:HIS:HE1	1:B:390:GLU:OE2	1.91	0.54
1:D:438:LEU:HD21	1:F:401:ASN:OD1	2.08	0.54
1:E:373:CYS:HB2	1:E:392:LEU:HD21	1.90	0.54
1:K:473:PRO:O	1:K:475:VAL:N	2.41	0.54
1:F:400:GLU:HG2	1:F:403:TRP:CZ2	2.43	0.54
1:I:472:ALA:N	1:I:473:PRO:HD3	2.23	0.54
1:K:377:MET:HE3	1:K:464:ILE:HB	1.89	0.54
1:M:468:HIS:NE2	1:N:470:SER:HB2	2.22	0.54
1:M:444:PRO:O	1:M:445:ARG:HD3	2.06	0.54
1:B:352:LYS:HG2	1:B:356:GLN:HE21	1.73	0.54
1:K:471:GLY:O	1:K:472:ALA:HB2	2.08	0.54
1:L:438:LEU:HD23	1:L:444:PRO:HA	1.89	0.54
1:B:411:HIS:NE2	1:D:393:ASP:OD2	2.38	0.54
1:K:439:ASP:C	1:K:441:GLY:N	2.60	0.54
1:L:443:ILE:HD13	1:L:445:ARG:HH21	1.73	0.53
1:I:396:ARG:HD3	1:I:396:ARG:O	2.07	0.53
1:M:458:ARG:CB	1:M:458:ARG:HH11	2.04	0.53
1:I:472:ALA:H	1:I:473:PRO:HD2	1.72	0.53
1:L:413:THR:HG22	1:L:415:LEU:HD23	1.90	0.53
1:L:453:ARG:HD2	1:L:464:ILE:CD1	2.39	0.53
1:N:440:ALA:HB3	1:N:445:ARG:HH12	1.73	0.53
1:N:469:ARG:NH2	1:N:474:SER:HA	2.24	0.53
1:C:361:ILE:HA	1:C:399:PHE:CZ	2.44	0.53
1:D:440:ALA:HB3	1:D:445:ARG:NH1	2.23	0.53
1:I:469:ARG:CG	1:I:469:ARG:NH1	2.70	0.53
1:L:378:THR:CG2	1:L:466:HIS:ND1	2.68	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:342:ASP:HA	1:N:345:VAL:HG22	1.91	0.53
1:I:439:ASP:HB3	1:I:443:ILE:H	1.73	0.53
1:K:383:GLU:OE2	1:K:383:GLU:N	2.42	0.53
1:G:358:ILE:HG21	1:G:412:THR:HG21	1.91	0.53
1:B:401:ASN:HD22	1:N:438:LEU:HD11	1.73	0.53
1:J:378:THR:HG22	1:J:466:HIS:HB2	1.91	0.53
1:M:451:GLU:OE2	1:M:469:ARG:HD3	2.09	0.53
1:B:444:PRO:HB3	1:D:397:PHE:HE2	1.70	0.52
1:G:456:HIS:CD2	1:H:422:MET:HB3	2.43	0.52
1:J:403:TRP:HB3	1:J:406:ASN:HB3	1.91	0.52
1:C:471:GLY:O	1:C:472:ALA:HB2	2.10	0.52
1:G:402:LEU:O	1:G:405:ARG:HG3	2.09	0.52
1:I:439:ASP:OD2	1:I:443:ILE:HD12	2.10	0.52
1:J:381:GLU:OE2	1:J:383:GLU:HB2	2.10	0.52
1:B:396:ARG:HG3	1:B:396:ARG:HH11	1.75	0.52
1:C:373:CYS:HB2	1:C:392:LEU:HD21	1.92	0.52
1:F:403:TRP:HA	1:F:403:TRP:HE3	1.73	0.52
1:G:472:ALA:H	1:G:473:PRO:HD2	1.74	0.52
1:H:371:LYS:HD3	1:H:461:LYS:HE2	1.91	0.52
1:A:471:GLY:C	1:A:473:PRO:CD	2.77	0.52
1:K:465:VAL:HG22	1:L:420:HIS:ND1	2.25	0.52
1:A:469:ARG:NH1	1:A:469:ARG:CG	2.73	0.52
1:J:340:ASP:C	1:J:342:ASP:H	2.11	0.52
1:J:403:TRP:CE3	1:J:403:TRP:HA	2.45	0.52
1:L:343:THR:HG22	1:L:346:ARG:NH2	2.25	0.52
1:E:357:LEU:HD22	1:E:464:ILE:CD1	2.35	0.52
1:H:398:TYR:O	1:H:402:LEU:HB2	2.10	0.52
1:A:402:LEU:HB3	1:A:405:ARG:CZ	2.39	0.52
1:C:338:ILE:C	1:C:340:ASP:H	2.13	0.52
1:B:398:TYR:O	1:B:402:LEU:HB2	2.09	0.52
1:E:341:GLU:O	1:E:344:LYS:HB3	2.10	0.52
1:A:422:MET:HB3	1:B:456:HIS:CD2	2.46	0.51
1:D:408:LYS:NZ	1:D:408:LYS:HB2	2.25	0.51
1:H:373:CYS:HB2	1:H:392:LEU:HD21	1.92	0.51
1:K:366:PHE:CZ	1:K:396:ARG:HG2	2.45	0.51
1:L:443:ILE:HB	1:L:445:ARG:HE	1.75	0.51
1:E:371:LYS:CD	1:E:461:LYS:HE2	2.40	0.51
1:F:441:GLY:O	1:F:443:ILE:N	2.43	0.51
1:H:336:THR:HG23	1:H:340:ASP:HB2	1.92	0.51
1:I:394:PHE:HE2	1:K:434:ILE:HG21	1.75	0.51
1:L:377:MET:HA	1:L:465:VAL:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:422:MET:HB3	1:N:426:SER:HB2	1.92	0.51
1:D:446:THR:OG1	1:F:398:TYR:OH	2.22	0.51
1:I:373:CYS:HB2	1:I:392:LEU:HD21	1.93	0.51
1:K:409:PRO:HG2	1:K:438:LEU:CD1	2.40	0.51
1:M:419:ILE:N	1:M:419:ILE:HD12	2.25	0.51
1:A:352:LYS:HG2	1:A:356:GLN:HE21	1.74	0.51
1:D:403:TRP:O	1:D:405:ARG:HD2	2.11	0.51
1:I:357:LEU:HD22	1:I:464:ILE:CD1	2.39	0.51
1:J:347:LYS:HG2	1:J:421:LEU:HD21	1.92	0.51
1:L:350:ILE:CD1	1:L:427:ALA:HB1	2.41	0.51
1:J:446:THR:HG22	1:L:385:LEU:HD11	1.93	0.51
1:L:415:LEU:HD12	1:N:387:ASN:HB3	1.93	0.51
1:C:396:ARG:HH11	1:C:396:ARG:HG2	1.75	0.51
1:E:400:GLU:HG3	1:E:401:ASN:OD1	2.11	0.51
1:J:440:ALA:HB3	1:J:445:ARG:HD2	1.92	0.51
1:L:416:ASN:N	1:L:417:PRO:HD3	2.24	0.51
1:A:423:GLY:N	4:A:2000:TBR:BRC	2.96	0.51
1:G:402:LEU:O	1:G:405:ARG:NH1	2.44	0.51
1:K:378:THR:HB	1:L:420:HIS:NE2	2.26	0.51
1:D:472:ALA:N	1:D:473:PRO:HD2	2.25	0.51
1:J:450:GLU:CG	1:J:470:SER:HB2	2.38	0.51
1:C:425:GLU:HA	1:C:457:ARG:HB3	1.93	0.51
1:I:404:SER:HB3	1:I:407:SER:OG	2.10	0.51
1:J:472:ALA:N	1:J:473:PRO:HD3	2.17	0.51
1:A:357:LEU:CD2	1:A:464:ILE:HD11	2.37	0.51
1:F:373:CYS:HB2	1:F:392:LEU:HD21	1.93	0.51
1:J:457:ARG:HG3	1:J:461:LYS:C	2.31	0.51
1:N:340:ASP:O	1:N:342:ASP:N	2.44	0.51
1:C:392:LEU:N	1:C:392:LEU:HD12	2.26	0.50
1:A:358:ILE:HG21	1:A:412:THR:HG21	1.92	0.50
1:D:457:ARG:NH1	1:D:457:ARG:HG2	2.26	0.50
1:E:342:ASP:HA	1:E:345:VAL:HG22	1.93	0.50
1:N:373:CYS:HB2	1:N:392:LEU:HD21	1.92	0.50
1:A:339:GLU:CG	2:A:1475:DTT:S1	2.99	0.50
1:B:443:ILE:HG23	1:B:444:PRO:HD2	1.92	0.50
1:C:357:LEU:CD2	1:C:464:ILE:HD11	2.35	0.50
1:L:419:ILE:HD12	1:L:419:ILE:N	2.26	0.50
1:L:414:ILE:HG23	1:L:431:TYR:CD1	2.46	0.50
1:M:339:GLU:O	1:M:340:ASP:C	2.49	0.50
1:F:342:ASP:HA	1:F:345:VAL:HG22	1.94	0.50
1:F:364:GLY:HA3	1:F:405:ARG:CZ	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:LEU:HD12	1:A:392:LEU:N	2.27	0.50
1:D:357:LEU:HD22	1:D:464:ILE:CD1	2.41	0.50
1:H:392:LEU:HD12	1:H:392:LEU:N	2.27	0.50
1:F:443:ILE:HB	1:F:445:ARG:NH1	2.26	0.50
1:D:472:ALA:H	1:D:473:PRO:HD2	1.76	0.50
1:K:367:GLU:CD	1:K:367:GLU:H	2.15	0.50
1:A:373:CYS:HB2	1:A:392:LEU:HD21	1.93	0.50
1:A:378:THR:CG2	1:A:466:HIS:ND1	2.62	0.50
1:J:347:LYS:HB3	1:J:419:ILE:HD12	1.93	0.50
1:L:350:ILE:HD12	1:L:419:ILE:HG21	1.94	0.50
1:E:403:TRP:O	1:E:405:ARG:N	2.44	0.50
1:F:469:ARG:NH1	1:F:469:ARG:CG	2.73	0.50
1:L:367:GLU:HA	1:L:367:GLU:OE1	2.12	0.50
1:A:457:ARG:HG2	5:A:2006:HOH:O	2.10	0.49
1:D:371:LYS:CD	1:D:461:LYS:HE2	2.42	0.49
1:G:373:CYS:HB2	1:G:392:LEU:HD21	1.94	0.49
1:E:456:HIS:CD2	1:F:422:MET:HB3	2.47	0.49
1:L:406:ASN:C	1:L:408:LYS:H	2.15	0.49
1:M:341:GLU:CG	1:M:341:GLU:O	2.59	0.49
1:N:469:ARG:CG	1:N:469:ARG:NH1	2.74	0.49
1:F:406:ASN:O	1:F:408:LYS:N	2.43	0.49
1:F:457:ARG:HG2	1:F:457:ARG:NH1	2.26	0.49
1:G:340:ASP:OD1	1:G:343:THR:HG23	2.12	0.49
1:G:468:HIS:NE2	1:H:470:SER:HB3	2.27	0.49
1:H:472:ALA:HB3	1:H:473:PRO:CD	2.42	0.49
1:N:392:LEU:N	1:N:392:LEU:HD12	2.27	0.49
1:B:373:CYS:HB2	1:B:392:LEU:HD21	1.94	0.49
1:M:349:GLU:O	1:M:352:LYS:HB3	2.12	0.49
1:C:456:HIS:CD2	1:D:422:MET:HB3	2.47	0.49
1:A:371:LYS:HD3	1:A:461:LYS:HE2	1.94	0.49
1:D:471:GLY:O	1:D:472:ALA:HB2	2.11	0.49
1:M:415:LEU:HB2	1:M:432:ILE:HB	1.95	0.49
1:C:372:MET:O	1:C:463:GLN:HA	2.12	0.49
1:D:346:ARG:NH2	1:D:424:ASP:OD1	2.46	0.49
1:E:401:ASN:C	1:E:403:TRP:H	2.14	0.49
1:I:425:GLU:HB3	1:I:457:ARG:HB3	1.94	0.49
1:B:416:ASN:O	1:B:418:HIS:HD2	1.95	0.49
1:N:357:LEU:HD22	1:N:464:ILE:CD1	2.43	0.49
1:N:433:ARG:HH12	1:N:475:VAL:N	2.11	0.49
1:A:393:ASP:OD2	1:C:411:HIS:CE1	2.66	0.49
1:B:457:ARG:HG2	1:B:457:ARG:NH1	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:373:CYS:HB2	1:D:392:LEU:HD21	1.94	0.49
1:G:385:LEU:HD11	1:I:446:THR:HG22	1.95	0.49
1:H:341:GLU:HG3	5:H:2001:HOH:O	2.13	0.49
1:I:390:GLU:OE2	1:J:418:HIS:HE1	1.96	0.49
1:K:418:HIS:HE1	1:L:390:GLU:OE2	1.96	0.49
1:B:398:TYR:CE1	1:N:436:GLN:NE2	2.81	0.49
1:F:403:TRP:HE3	1:F:405:ARG:HH22	1.61	0.48
1:J:337:THR:OG1	1:J:338:ILE:N	2.46	0.48
1:J:350:ILE:HA	1:J:353:VAL:HG22	1.95	0.48
1:J:354:THR:O	1:J:358:ILE:HG12	2.13	0.48
1:M:378:THR:HA	1:M:389:VAL:O	2.13	0.48
1:M:370:THR:HA	1:M:392:LEU:HD21	1.94	0.48
1:B:472:ALA:HB3	1:B:473:PRO:HD3	1.95	0.48
1:C:398:TYR:O	1:C:402:LEU:HB3	2.13	0.48
1:G:469:ARG:CG	1:G:469:ARG:NH1	2.71	0.48
1:H:352:LYS:CG	1:H:356:GLN:HE21	2.26	0.48
1:M:378:THR:HB	1:M:388:LEU:HD11	1.95	0.48
1:E:447:ALA:HB1	1:E:473:PRO:HG2	1.95	0.48
1:F:415:LEU:HD11	1:F:434:ILE:HD12	1.94	0.48
1:J:429:ILE:HG22	1:J:453:ARG:HB2	1.95	0.48
1:K:402:LEU:O	1:K:405:ARG:CZ	2.60	0.48
1:K:439:ASP:O	1:K:441:GLY:N	2.46	0.48
1:L:344:LYS:O	1:L:344:LYS:HD2	2.13	0.48
1:L:368:SER:HB3	1:L:372:MET:HE2	1.96	0.48
1:K:420:HIS:CG	1:L:465:VAL:HG22	2.49	0.48
1:D:396:ARG:HG3	1:D:396:ARG:HH11	1.79	0.48
1:L:357:LEU:HD22	1:L:464:ILE:CD1	2.44	0.48
1:N:341:GLU:OE1	1:N:341:GLU:HA	2.12	0.48
1:A:443:ILE:HB	1:A:445:ARG:NH1	2.27	0.48
1:B:405:ARG:C	1:B:407:SER:H	2.16	0.48
1:E:418:HIS:CD2	1:F:388:LEU:HD13	2.48	0.48
1:I:392:LEU:N	1:I:392:LEU:HD12	2.28	0.48
1:I:371:LYS:HD3	1:I:461:LYS:HE2	1.95	0.48
1:M:416:ASN:N	1:M:417:PRO:HD3	2.29	0.48
1:L:446:THR:HG22	1:N:385:LEU:CD1	2.43	0.48
1:E:397:PHE:HE2	1:G:444:PRO:HB3	1.79	0.48
1:K:350:ILE:HB	1:K:419:ILE:HD13	1.95	0.48
1:K:393:ASP:OD2	1:K:396:ARG:NH1	2.47	0.48
1:K:420:HIS:HB2	1:K:428:CYS:HB3	1.96	0.48
1:K:443:ILE:O	1:K:445:ARG:HG3	2.14	0.48
1:L:400:GLU:HA	1:L:403:TRP:CZ2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:415:LEU:HD11	1:C:434:ILE:HD12	1.95	0.48
1:F:392:LEU:HD12	1:F:392:LEU:N	2.29	0.48
1:I:439:ASP:CG	1:I:440:ALA:N	2.66	0.48
1:M:459:ASP:OD2	1:M:461:LYS:HE3	2.13	0.48
1:F:371:LYS:HD3	1:F:461:LYS:HE2	1.96	0.48
1:K:420:HIS:ND1	1:L:465:VAL:CG2	2.77	0.48
1:G:402:LEU:HB3	1:G:405:ARG:CZ	2.44	0.48
1:M:450:GLU:HB3	1:N:380:PHE:CE1	2.49	0.48
1:N:439:ASP:O	1:N:440:ALA:HB3	2.14	0.48
1:C:457:ARG:NH1	1:C:457:ARG:HG2	2.29	0.47
1:D:392:LEU:HD12	1:D:392:LEU:N	2.28	0.47
1:H:473:PRO:O	1:H:474:SER:HB3	2.14	0.47
1:J:368:SER:O	1:J:372:MET:HG3	2.13	0.47
1:N:415:LEU:HD11	1:N:434:ILE:HD12	1.96	0.47
1:A:457:ARG:NH1	1:A:457:ARG:HG2	2.29	0.47
1:D:439:ASP:CG	1:D:440:ALA:H	2.17	0.47
1:F:357:LEU:HD22	1:F:464:ILE:CD1	2.40	0.47
1:B:440:ALA:O	1:B:445:ARG:NH1	2.48	0.47
1:C:371:LYS:NZ	1:C:461:LYS:CE	2.77	0.47
1:H:472:ALA:O	1:H:473:PRO:O	2.32	0.47
1:H:472:ALA:H	1:H:473:PRO:HD2	1.79	0.47
1:M:353:VAL:HG23	1:M:455:TRP:CZ2	2.48	0.47
1:B:392:LEU:HD12	1:B:392:LEU:N	2.29	0.47
1:F:408:LYS:HG3	1:F:439:ASP:OD2	2.14	0.47
1:I:433:ARG:NH1	1:I:474:SER:O	2.47	0.47
1:A:343:THR:HG21	4:A:2000:TBR:BR7	2.70	0.47
1:E:416:ASN:O	1:E:418:HIS:HD2	1.98	0.47
1:I:415:LEU:HD11	1:I:434:ILE:HD12	1.96	0.47
1:K:450:GLU:HB2	1:K:470:SER:HB3	1.95	0.47
1:L:469:ARG:NE	1:L:474:SER:O	2.46	0.47
1:B:469:ARG:NH1	1:B:469:ARG:CG	2.72	0.47
1:F:441:GLY:C	1:F:443:ILE:H	2.17	0.47
1:I:406:ASN:C	1:I:408:LYS:N	2.68	0.47
1:B:401:ASN:ND2	1:N:438:LEU:HD11	2.28	0.47
1:C:416:ASN:O	1:C:418:HIS:HD2	1.97	0.47
1:E:366:PHE:O	1:E:370:THR:HG23	2.15	0.47
1:M:352:LYS:O	1:M:356:GLN:HG3	2.15	0.47
1:E:457:ARG:HG2	1:E:457:ARG:NH1	2.29	0.47
1:G:378:THR:HB	1:H:420:HIS:NE2	2.30	0.47
1:I:416:ASN:O	1:I:418:HIS:HD2	1.97	0.47
1:J:408:LYS:C	1:J:408:LYS:HD2	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:419:ILE:N	1:F:419:ILE:HD12	2.30	0.47
1:G:416:ASN:O	1:G:418:HIS:HD2	1.97	0.47
1:H:416:ASN:O	1:H:418:HIS:HD2	1.98	0.47
1:L:469:ARG:HH11	1:L:469:ARG:CG	2.27	0.47
1:M:353:VAL:HG23	1:M:354:THR:N	2.30	0.47
1:C:472:ALA:N	1:C:473:PRO:CD	2.74	0.47
1:E:336:THR:O	1:E:337:THR:HB	2.15	0.47
1:E:401:ASN:C	1:E:403:TRP:N	2.69	0.47
1:H:377:MET:HE2	1:H:464:ILE:HG21	1.97	0.47
1:J:422:MET:HB2	1:J:426:SER:OG	2.15	0.47
1:J:439:ASP:C	1:J:442:GLY:H	2.18	0.47
1:K:429:ILE:CG2	1:K:453:ARG:HB2	2.45	0.47
1:B:402:LEU:O	1:B:405:ARG:NH1	2.48	0.47
1:B:415:LEU:HD11	1:B:434:ILE:HD12	1.97	0.47
1:A:357:LEU:HD22	1:A:464:ILE:CD1	2.41	0.46
1:A:471:GLY:O	1:A:473:PRO:CD	2.63	0.46
1:C:357:LEU:CD2	1:C:464:ILE:CD1	2.93	0.46
1:H:443:ILE:HB	1:H:445:ARG:HH12	1.80	0.46
1:H:457:ARG:HG2	1:H:457:ARG:NH1	2.30	0.46
1:I:419:ILE:N	1:I:419:ILE:HD12	2.30	0.46
1:M:342:ASP:C	1:M:344:LYS:N	2.67	0.46
1:F:402:LEU:CB	1:F:405:ARG:HH11	2.13	0.46
1:J:405:ARG:HG3	1:J:405:ARG:HH11	1.80	0.46
1:A:416:ASN:O	1:A:418:HIS:HD2	1.98	0.46
1:D:469:ARG:NH1	1:D:469:ARG:CG	2.77	0.46
1:G:405:ARG:HA	1:G:408:LYS:CE	2.43	0.46
1:I:449:SER:HB3	1:I:473:PRO:HD2	1.97	0.46
1:J:370:THR:HA	1:J:392:LEU:CD2	2.46	0.46
1:E:425:GLU:HA	1:E:457:ARG:CB	2.45	0.46
1:K:368:SER:O	1:K:372:MET:HG3	2.16	0.46
1:K:443:ILE:HB	1:K:445:ARG:HH11	1.80	0.46
1:G:440:ALA:CB	1:G:445:ARG:NH1	2.79	0.46
1:G:449:SER:HB2	1:G:470:SER:O	2.15	0.46
1:B:357:LEU:CD2	1:B:464:ILE:HD11	2.43	0.46
1:N:457:ARG:NH1	1:N:457:ARG:HG2	2.31	0.46
1:D:415:LEU:HD11	1:D:434:ILE:HD12	1.98	0.46
1:D:444:PRO:HG3	1:F:401:ASN:CB	2.45	0.46
1:G:409:PRO:HD2	1:G:438:LEU:HD12	1.98	0.46
1:H:378:THR:CG2	1:H:466:HIS:ND1	2.66	0.46
1:I:366:PHE:O	1:I:370:THR:HG23	2.16	0.46
1:L:414:ILE:HG22	1:L:417:PRO:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:403:TRP:HE3	1:N:406:ASN:HD21	1.56	0.46
1:A:405:ARG:HA	1:A:408:LYS:CB	2.42	0.46
1:D:419:ILE:HD12	1:D:419:ILE:N	2.31	0.46
1:D:440:ALA:O	1:D:445:ARG:NH1	2.49	0.46
1:H:415:LEU:HD11	1:H:434:ILE:HD12	1.97	0.46
1:H:419:ILE:N	1:H:419:ILE:HD12	2.31	0.46
1:J:458:ARG:HD3	1:J:463:GLN:OE1	2.15	0.46
1:K:352:LYS:O	1:K:356:GLN:HG3	2.16	0.46
1:F:352:LYS:CG	1:F:356:GLN:HE21	2.27	0.45
1:D:436:GLN:NE2	1:F:398:TYR:CE1	2.84	0.45
1:H:439:ASP:O	1:H:440:ALA:CB	2.64	0.45
1:H:473:PRO:O	1:H:474:SER:CB	2.65	0.45
1:A:419:ILE:N	1:A:419:ILE:HD12	2.31	0.45
1:B:396:ARG:HG3	1:B:396:ARG:NH1	2.31	0.45
1:E:341:GLU:HG3	1:E:344:LYS:HB2	1.99	0.45
1:G:366:PHE:O	1:G:370:THR:HG23	2.16	0.45
1:L:389:VAL:HG12	1:L:390:GLU:N	2.30	0.45
1:L:453:ARG:HD2	1:L:464:ILE:HD13	1.99	0.45
1:C:371:LYS:CE	1:C:461:LYS:HE2	2.46	0.45
1:I:471:GLY:O	1:I:472:ALA:HB2	2.16	0.45
1:J:377:MET:HB2	1:J:377:MET:HE3	1.69	0.45
1:N:472:ALA:N	1:N:473:PRO:CD	2.74	0.45
1:B:419:ILE:HD12	1:B:419:ILE:N	2.31	0.45
1:J:448:GLN:O	1:J:449:SER:HB3	2.16	0.45
1:L:398:TYR:HA	1:L:402:LEU:HD23	1.99	0.45
1:L:447:ALA:HB1	1:L:473:PRO:HG3	1.97	0.45
1:G:402:LEU:HB3	1:G:405:ARG:NH2	2.30	0.45
1:I:475:VAL:N	3:I:1475:CL:CL	2.87	0.45
1:I:439:ASP:HB2	1:I:443:ILE:O	2.15	0.45
1:I:457:ARG:NH1	1:I:457:ARG:HG2	2.29	0.45
1:K:439:ASP:HA	1:K:442:GLY:HA2	1.97	0.45
1:K:469:ARG:CB	1:K:469:ARG:NH1	2.80	0.45
1:N:419:ILE:HD12	1:N:419:ILE:N	2.31	0.45
1:B:396:ARG:O	1:B:397:PHE:CB	2.64	0.45
1:F:416:ASN:O	1:F:418:HIS:HD2	1.99	0.45
1:G:419:ILE:N	1:G:419:ILE:HD12	2.32	0.45
1:G:457:ARG:NH1	1:G:457:ARG:HG2	2.32	0.45
1:J:342:ASP:O	1:J:345:VAL:N	2.42	0.45
1:A:366:PHE:O	1:A:370:THR:HG23	2.17	0.45
1:C:352:LYS:CG	1:C:356:GLN:HE21	2.27	0.45
1:D:457:ARG:HG2	1:D:457:ARG:HH11	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:392:LEU:HD12	1:E:392:LEU:N	2.31	0.45
1:L:402:LEU:O	1:L:405:ARG:CZ	2.65	0.45
1:L:357:LEU:HD22	1:L:464:ILE:HD12	1.99	0.45
1:B:366:PHE:O	1:B:370:THR:HG23	2.16	0.45
1:D:440:ALA:HB3	1:D:445:ARG:HH11	1.82	0.45
1:F:457:ARG:HG2	1:F:457:ARG:HH11	1.82	0.45
1:G:415:LEU:HD11	1:G:434:ILE:HD12	1.98	0.45
1:J:439:ASP:HA	1:J:442:GLY:CA	2.47	0.45
1:G:408:LYS:HB2	1:G:438:LEU:HB2	1.99	0.45
1:C:405:ARG:HA	1:C:408:LYS:HB3	1.99	0.45
1:G:392:LEU:HD12	1:G:392:LEU:N	2.31	0.45
1:J:416:ASN:N	1:J:417:PRO:HD3	2.32	0.45
1:B:378:THR:O	1:B:466:HIS:HA	2.17	0.44
1:E:419:ILE:N	1:E:419:ILE:HD12	2.32	0.44
1:E:469:ARG:CG	1:E:469:ARG:NH1	2.74	0.44
1:F:457:ARG:CG	1:F:457:ARG:HH11	2.30	0.44
1:J:408:LYS:NZ	1:J:439:ASP:H	2.16	0.44
1:D:402:LEU:O	1:D:405:ARG:CZ	2.65	0.44
1:I:362:SER:O	1:I:405:ARG:HD2	2.17	0.44
1:J:416:ASN:O	1:J:418:HIS:HD2	2.01	0.44
1:J:437:TYR:CE1	1:J:445:ARG:HB2	2.53	0.44
1:K:396:ARG:HH11	1:K:396:ARG:HG3	1.82	0.44
1:N:352:LYS:CG	1:N:356:GLN:HE21	2.30	0.44
1:E:352:LYS:CG	1:E:356:GLN:HE21	2.28	0.44
1:G:370:THR:HG22	1:G:392:LEU:HD22	2.00	0.44
1:I:352:LYS:CG	1:I:356:GLN:HE21	2.27	0.44
1:K:383:GLU:CD	1:K:383:GLU:H	2.20	0.44
1:C:366:PHE:O	1:C:370:THR:HG23	2.18	0.44
1:E:410:VAL:HG13	1:E:410:VAL:O	2.17	0.44
1:G:378:THR:O	1:G:466:HIS:HA	2.17	0.44
1:J:403:TRP:HA	1:J:403:TRP:HE3	1.81	0.44
1:N:416:ASN:O	1:N:418:HIS:HD2	2.01	0.44
1:A:377:MET:HE2	1:A:464:ILE:HG21	2.00	0.44
1:N:370:THR:HG22	1:N:392:LEU:HD22	1.99	0.44
1:D:416:ASN:O	1:D:418:HIS:HD2	2.00	0.44
1:K:351:ILE:O	1:K:355:GLU:HG3	2.18	0.44
1:D:411:HIS:CE1	1:F:393:ASP:OD2	2.70	0.44
1:F:357:LEU:CD2	1:F:464:ILE:HD11	2.41	0.44
1:C:440:ALA:HB3	1:C:445:ARG:NH1	2.32	0.44
1:D:457:ARG:HH11	1:D:457:ARG:CG	2.31	0.44
1:F:366:PHE:O	1:F:370:THR:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:409:PRO:HD2	1:F:438:LEU:CD1	2.48	0.44
1:G:352:LYS:CG	1:G:356:GLN:HE21	2.29	0.44
1:J:374:ASP:OD1	1:J:374:ASP:C	2.56	0.44
1:N:402:LEU:O	1:N:405:ARG:HD2	2.18	0.44
1:A:339:GLU:HA	1:A:342:ASP:OD1	2.17	0.44
1:B:352:LYS:CG	1:B:356:GLN:HE21	2.31	0.44
1:E:472:ALA:N	1:E:473:PRO:HD3	2.33	0.44
1:N:377:MET:HE2	1:N:467:PHE:HD2	1.83	0.44
1:B:377:MET:HE2	1:B:464:ILE:HG21	1.99	0.43
1:C:341:GLU:O	1:C:344:LYS:HB3	2.17	0.43
1:D:352:LYS:CG	1:D:356:GLN:HE21	2.29	0.43
1:A:402:LEU:HB3	1:A:405:ARG:HD3	2.00	0.43
1:B:457:ARG:HG2	1:B:457:ARG:HH11	1.83	0.43
1:C:422:MET:HB3	1:D:456:HIS:CD2	2.53	0.43
1:J:389:VAL:HG11	1:J:394:PHE:HB3	2.01	0.43
1:K:456:HIS:HD2	1:L:422:MET:HB3	1.83	0.43
1:L:367:GLU:O	1:L:371:LYS:HG3	2.17	0.43
1:A:383:GLU:HB3	1:A:398:TYR:OH	2.19	0.43
1:A:471:GLY:O	1:A:473:PRO:N	2.52	0.43
1:C:473:PRO:O	1:C:474:SER:CB	2.66	0.43
1:E:415:LEU:HD11	1:E:434:ILE:HD12	1.99	0.43
1:I:408:LYS:NZ	1:I:408:LYS:HB3	2.32	0.43
1:L:401:ASN:O	1:L:402:LEU:HD22	2.17	0.43
1:E:390:GLU:OE2	1:F:418:HIS:HE1	2.02	0.43
1:G:340:ASP:C	1:G:342:ASP:N	2.71	0.43
1:J:337:THR:HG23	1:J:338:ILE:N	2.33	0.43
1:K:397:PHE:O	1:K:401:ASN:HB2	2.19	0.43
1:K:448:GLN:C	1:K:473:PRO:HG2	2.39	0.43
1:F:401:ASN:ND2	1:F:401:ASN:N	2.65	0.43
1:H:404:SER:C	1:H:406:ASN:H	2.21	0.43
1:H:439:ASP:HA	1:H:442:GLY:N	2.32	0.43
1:I:397:PHE:CE2	1:K:436:GLN:HB3	2.54	0.43
1:L:434:ILE:HD11	1:N:387:ASN:ND2	2.33	0.43
1:L:455:TRP:CZ3	1:L:464:ILE:HG13	2.53	0.43
1:M:371:LYS:HB3	1:M:371:LYS:HE2	1.81	0.43
1:A:352:LYS:CG	1:A:356:GLN:HE21	2.32	0.43
1:F:406:ASN:C	1:F:408:LYS:N	2.70	0.43
1:M:412:THR:HG22	1:M:413:THR:N	2.34	0.43
1:D:339:GLU:O	1:D:340:ASP:HB3	2.18	0.43
1:D:357:LEU:CD2	1:D:464:ILE:HD11	2.43	0.43
1:K:400:GLU:O	1:K:403:TRP:HD1	2.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:376:GLY:O	1:D:420:HIS:HE1	2.02	0.43
1:C:383:GLU:OE2	1:C:474:SER:HA	2.18	0.43
1:C:419:ILE:HD12	1:C:419:ILE:N	2.33	0.43
1:F:441:GLY:C	1:F:443:ILE:N	2.71	0.43
1:H:370:THR:HG22	1:H:392:LEU:CD2	2.49	0.43
1:K:370:THR:CG2	1:K:392:LEU:HD23	2.38	0.43
1:N:408:LYS:HE2	1:N:439:ASP:OD2	2.19	0.43
1:D:371:LYS:NZ	1:D:461:LYS:HE2	2.34	0.43
1:J:444:PRO:HB3	1:L:397:PHE:CE2	2.54	0.43
1:J:448:GLN:HG2	1:J:449:SER:H	1.81	0.43
1:C:457:ARG:HH11	1:C:457:ARG:CG	2.32	0.42
1:D:408:LYS:HA	1:D:409:PRO:HD3	1.76	0.42
1:G:402:LEU:HD12	1:G:402:LEU:HA	1.82	0.42
1:J:383:GLU:OE1	1:J:383:GLU:N	2.40	0.42
1:H:336:THR:CG2	1:H:340:ASP:HB2	2.49	0.42
1:H:366:PHE:O	1:H:370:THR:HG23	2.19	0.42
1:G:385:LEU:CD1	1:I:446:THR:HG22	2.49	0.42
1:K:415:LEU:CD1	1:K:434:ILE:HD12	2.48	0.42
1:L:382:PRO:HB2	1:L:383:GLU:OE1	2.20	0.42
1:M:448:GLN:HG2	1:M:449:SER:N	2.34	0.42
1:B:370:THR:HG22	1:B:392:LEU:CD2	2.49	0.42
1:B:457:ARG:CG	1:B:457:ARG:HH11	2.32	0.42
1:C:393:ASP:OD2	1:E:411:HIS:NE2	2.52	0.42
1:C:457:ARG:HG2	1:C:457:ARG:HH11	1.84	0.42
1:G:370:THR:HA	1:G:392:LEU:HD21	2.02	0.42
1:H:370:THR:HG22	1:H:392:LEU:HD22	2.01	0.42
1:K:349:GLU:O	1:K:352:LYS:HB3	2.19	0.42
1:L:471:GLY:O	1:L:472:ALA:HB2	2.19	0.42
1:B:342:ASP:HA	1:B:345:VAL:HG22	2.01	0.42
1:B:370:THR:HG22	1:B:392:LEU:HD22	2.01	0.42
1:D:370:THR:HG22	1:D:392:LEU:HD22	2.02	0.42
1:E:447:ALA:HB1	1:E:473:PRO:CG	2.49	0.42
1:F:377:MET:HE2	1:F:467:PHE:HD2	1.84	0.42
1:J:340:ASP:O	1:J:341:GLU:HB2	2.19	0.42
1:K:401:ASN:O	1:K:402:LEU:HB2	2.19	0.42
1:K:439:ASP:C	1:K:441:GLY:H	2.22	0.42
1:G:377:MET:HE2	1:G:467:PHE:HD2	1.84	0.42
1:K:443:ILE:HB	1:K:445:ARG:NH1	2.35	0.42
1:L:382:PRO:HG2	1:L:472:ALA:HA	2.02	0.42
1:E:457:ARG:CG	1:E:457:ARG:HH11	2.33	0.42
1:H:358:ILE:HG21	1:H:412:THR:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:446:THR:HG22	1:N:385:LEU:HD11	2.02	0.42
1:B:403:TRP:C	1:B:405:ARG:N	2.71	0.42
1:D:370:THR:HG22	1:D:392:LEU:CD2	2.49	0.42
1:I:406:ASN:HD22	1:I:406:ASN:HA	1.58	0.42
1:M:348:GLN:HA	1:M:348:GLN:NE2	2.35	0.42
1:M:437:TYR:HD1	1:M:439:ASP:OD1	2.03	0.42
1:B:438:LEU:CG	1:D:401:ASN:HD22	2.33	0.42
1:E:456:HIS:HD2	1:F:422:MET:HB3	1.83	0.42
1:E:457:ARG:HG2	1:E:457:ARG:HH11	1.85	0.42
1:J:439:ASP:HA	1:J:442:GLY:N	2.35	0.42
1:L:422:MET:HB2	1:L:426:SER:OG	2.20	0.42
1:A:457:ARG:HH11	1:A:457:ARG:CG	2.33	0.42
1:D:439:ASP:C	1:D:441:GLY:N	2.73	0.42
1:G:405:ARG:O	1:G:407:SER:N	2.46	0.42
1:H:438:LEU:HB3	1:H:439:ASP:H	1.43	0.42
1:H:382:PRO:HD3	1:H:469:ARG:O	2.20	0.42
1:J:353:VAL:HG23	1:J:354:THR:N	2.35	0.42
1:L:455:TRP:CH2	1:L:464:ILE:HG13	2.55	0.42
1:M:434:ILE:HD13	1:M:448:GLN:HG3	2.02	0.42
1:N:370:THR:HG22	1:N:392:LEU:CD2	2.50	0.42
1:F:402:LEU:O	1:F:403:TRP:C	2.59	0.42
1:F:403:TRP:HA	1:F:405:ARG:NH2	2.35	0.42
1:G:357:LEU:HD22	1:G:464:ILE:CD1	2.41	0.42
1:J:436:GLN:NE2	1:L:398:TYR:CE1	2.88	0.42
1:D:472:ALA:O	1:D:473:PRO:O	2.37	0.41
1:F:402:LEU:HB3	1:F:405:ARG:CD	2.50	0.41
1:E:376:GLY:O	1:F:420:HIS:HE1	2.03	0.41
1:L:358:ILE:HD12	1:L:414:ILE:HD11	2.02	0.41
1:B:342:ASP:O	1:B:345:VAL:HG22	2.20	0.41
1:J:365:ASP:OD1	1:J:368:SER:OG	2.34	0.41
1:J:439:ASP:HA	1:J:442:GLY:H	1.84	0.41
1:K:372:MET:O	1:K:463:GLN:HA	2.20	0.41
1:K:451:GLU:OE2	1:K:453:ARG:NH2	2.51	0.41
1:L:443:ILE:H	1:L:443:ILE:CD1	2.23	0.41
1:N:358:ILE:HG21	1:N:412:THR:HG21	2.00	0.41
1:B:408:LYS:HB3	1:B:439:ASP:OD2	2.21	0.41
1:D:366:PHE:O	1:D:370:THR:HG23	2.19	0.41
1:D:372:MET:O	1:D:463:GLN:HA	2.20	0.41
1:E:371:LYS:NZ	1:E:461:LYS:CE	2.83	0.41
1:E:377:MET:HE2	1:E:467:PHE:HD2	1.85	0.41
1:J:347:LYS:CG	1:J:421:LEU:HD21	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:436:GLN:NE2	1:L:398:TYR:HE1	2.19	0.41
1:E:338:ILE:C	1:E:340:ASP:H	2.22	0.41
1:F:402:LEU:O	1:F:405:ARG:HD3	2.20	0.41
1:G:370:THR:HG22	1:G:392:LEU:CD2	2.50	0.41
1:K:383:GLU:O	1:K:394:PHE:HZ	2.03	0.41
1:K:415:LEU:HD11	1:K:434:ILE:HD12	2.02	0.41
1:M:365:ASP:C	1:M:365:ASP:OD2	2.58	0.41
1:D:472:ALA:N	1:D:473:PRO:CD	2.83	0.41
1:E:472:ALA:H	1:E:473:PRO:HD2	1.84	0.41
1:H:358:ILE:HD12	1:H:414:ILE:HD11	2.02	0.41
1:I:378:THR:HB	1:J:420:HIS:NE2	2.35	0.41
1:N:403:TRP:CE3	1:N:403:TRP:HA	2.56	0.41
1:A:421:LEU:C	1:A:422:MET:HG3	2.41	0.41
1:F:370:THR:HG22	1:F:392:LEU:CD2	2.51	0.41
1:F:370:THR:HG22	1:F:392:LEU:HD22	2.02	0.41
1:H:370:THR:HA	1:H:392:LEU:HD21	2.02	0.41
1:H:469:ARG:NH1	1:H:469:ARG:CG	2.72	0.41
1:J:473:PRO:HB2	1:J:474:SER:H	1.64	0.41
1:M:406:ASN:C	1:M:408:LYS:N	2.74	0.41
1:D:405:ARG:HD2	1:D:405:ARG:H	1.86	0.41
1:H:357:LEU:HD22	1:H:464:ILE:CD1	2.41	0.41
1:J:338:ILE:HG22	1:J:339:GLU:N	2.36	0.41
1:K:437:TYR:HE2	1:K:445:ARG:CB	2.10	0.41
1:N:366:PHE:O	1:N:370:THR:HG23	2.20	0.41
1:A:370:THR:HG22	1:A:392:LEU:CD2	2.51	0.41
1:F:443:ILE:HB	1:F:445:ARG:HH12	1.85	0.41
1:I:418:HIS:CD2	1:J:388:LEU:HD23	2.56	0.41
1:K:408:LYS:HA	1:K:409:PRO:HD3	1.90	0.41
1:M:350:ILE:O	1:M:353:VAL:HG22	2.21	0.41
1:N:443:ILE:HA	1:N:444:PRO:HD3	1.93	0.41
1:K:346:ARG:O	1:K:349:GLU:HB2	2.21	0.41
1:G:357:LEU:CD2	1:G:464:ILE:HD11	2.45	0.41
1:H:439:ASP:CG	1:H:440:ALA:N	2.69	0.41
1:H:457:ARG:CG	1:H:457:ARG:HH11	2.34	0.41
1:I:402:LEU:HD12	1:I:405:ARG:HH11	1.84	0.41
1:J:346:ARG:NH1	1:J:424:ASP:OD1	2.54	0.41
1:J:439:ASP:O	1:J:441:GLY:N	2.54	0.41
1:K:402:LEU:O	1:K:405:ARG:NH2	2.54	0.41
1:C:370:THR:HG22	1:C:392:LEU:HD22	2.02	0.41
1:D:341:GLU:O	1:D:344:LYS:HB3	2.21	0.41
1:D:342:ASP:O	1:D:345:VAL:HG22	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:408:LYS:N	1:E:408:LYS:CD	2.84	0.41
1:G:426:SER:HB2	1:H:422:MET:HB3	2.03	0.41
1:A:415:LEU:HD11	1:A:434:ILE:HD12	2.02	0.40
1:A:457:ARG:HH11	1:A:457:ARG:HG2	1.85	0.40
1:C:370:THR:HG22	1:C:392:LEU:CD2	2.51	0.40
1:E:357:LEU:CD2	1:E:464:ILE:CD1	2.98	0.40
1:G:457:ARG:CG	1:G:457:ARG:HH11	2.34	0.40
1:K:439:ASP:O	1:K:440:ALA:C	2.59	0.40
1:N:364:GLY:HA3	1:N:403:TRP:HZ3	1.87	0.40
1:B:472:ALA:O	1:B:473:PRO:C	2.59	0.40
1:L:374:ASP:OD2	1:L:375:PRO:HD2	2.21	0.40
1:N:407:SER:O	1:N:408:LYS:HB2	2.21	0.40
1:A:370:THR:HA	1:A:392:LEU:HD21	2.03	0.40
1:C:401:ASN:HD22	1:E:438:LEU:HD11	1.87	0.40
1:M:450:GLU:HB3	1:N:380:PHE:CZ	2.57	0.40
1:A:357:LEU:CD2	1:A:464:ILE:CD1	3.00	0.40
1:A:402:LEU:O	1:A:405:ARG:NE	2.54	0.40
1:C:438:LEU:HB3	1:C:439:ASP:H	1.60	0.40
1:A:397:PHE:CE2	1:C:444:PRO:HB3	2.56	0.40
1:C:429:ILE:CG2	1:C:453:ARG:HB2	2.52	0.40
1:J:472:ALA:H	1:J:473:PRO:CD	2.21	0.40
1:B:443:ILE:HA	1:B:444:PRO:HD3	1.90	0.40
1:G:382:PRO:HD3	1:G:469:ARG:O	2.21	0.40
1:I:457:ARG:HH11	1:I:457:ARG:CG	2.33	0.40
1:I:397:PHE:CZ	1:K:444:PRO:HB3	2.57	0.40
1:K:465:VAL:HG22	1:L:420:HIS:CG	2.57	0.40
1:L:400:GLU:HA	1:L:403:TRP:CE2	2.56	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	139/147 (95%)	129 (93%)	7 (5%)	3 (2%)	6	9
1	B	134/147 (91%)	121 (90%)	10 (8%)	3 (2%)	6	9
1	C	137/147 (93%)	124 (90%)	9 (7%)	4 (3%)	4	6
1	D	136/147 (92%)	122 (90%)	10 (7%)	4 (3%)	4	6
1	E	142/147 (97%)	123 (87%)	14 (10%)	5 (4%)	3	4
1	F	137/147 (93%)	122 (89%)	8 (6%)	7 (5%)	2	2
1	G	134/147 (91%)	121 (90%)	8 (6%)	5 (4%)	3	4
1	H	141/147 (96%)	128 (91%)	6 (4%)	7 (5%)	2	2
1	I	133/147 (90%)	116 (87%)	14 (10%)	3 (2%)	6	8
1	J	137/147 (93%)	120 (88%)	11 (8%)	6 (4%)	2	2
1	K	133/147 (90%)	111 (84%)	16 (12%)	6 (4%)	2	2
1	L	133/147 (90%)	119 (90%)	9 (7%)	5 (4%)	3	3
1	M	137/147 (93%)	118 (86%)	12 (9%)	7 (5%)	2	2
1	N	134/147 (91%)	123 (92%)	6 (4%)	5 (4%)	3	4
All	All	1907/2058 (93%)	1697 (89%)	140 (7%)	70 (4%)	3	4

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	472	ALA
1	B	397	PHE
1	C	472	ALA
1	C	473	PRO
1	C	474	SER
1	D	340	ASP
1	D	472	ALA
1	D	473	PRO
1	D	474	SER
1	E	439	ASP
1	E	472	ALA
1	F	402	LEU
1	F	403	TRP
1	F	472	ALA
1	G	473	PRO
1	H	335	MET
1	H	338	ILE
1	H	473	PRO
1	H	474	SER

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Mol	Chain	Res	Type
1	I	472	ALA
1	I	473	PRO
1	J	439	ASP
1	J	472	ALA
1	K	472	ALA
1	L	472	ALA
1	L	473	PRO
1	M	439	ASP
1	M	473	PRO
1	N	341	GLU
1	N	472	ALA
1	N	473	PRO
1	A	340	ASP
1	A	439	ASP
1	B	473	PRO
1	F	407	SER
1	H	472	ALA
1	J	407	SER
1	J	473	PRO
1	K	402	LEU
1	K	442	GLY
1	K	473	PRO
1	K	474	SER
1	L	439	ASP
1	M	340	ASP
1	M	406	ASN
1	E	404	SER
1	E	440	ALA
1	F	442	GLY
1	H	336	THR
1	J	340	ASP
1	K	439	ASP
1	M	404	SER
1	B	472	ALA
1	E	337	THR
1	G	400	GLU
1	G	402	LEU
1	H	439	ASP
1	I	406	ASN
1	M	472	ALA
1	C	338	ILE
1	F	408	LYS

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Mol	Chain	Res	Type
1	G	439	ASP
1	G	472	ALA
1	L	407	SER
1	L	408	LYS
1	M	343	THR
1	N	400	GLU
1	J	441	GLY
1	F	473	PRO
1	N	408	LYS

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	123/129 (95%)	113 (92%)	10 (8%)	11	17
1	B	118/129 (92%)	110 (93%)	8 (7%)	16	24
1	C	121/129 (94%)	114 (94%)	7 (6%)	20	31
1	D	120/129 (93%)	110 (92%)	10 (8%)	11	16
1	E	125/129 (97%)	118 (94%)	7 (6%)	21	33
1	F	121/129 (94%)	110 (91%)	11 (9%)	9	13
1	G	118/129 (92%)	110 (93%)	8 (7%)	16	24
1	H	125/129 (97%)	115 (92%)	10 (8%)	12	18
1	I	117/129 (91%)	107 (92%)	10 (8%)	10	15
1	J	121/129 (94%)	114 (94%)	7 (6%)	20	31
1	K	117/129 (91%)	109 (93%)	8 (7%)	16	24
1	L	117/129 (91%)	104 (89%)	13 (11%)	6	8
1	M	121/129 (94%)	110 (91%)	11 (9%)	9	13
1	N	118/129 (92%)	111 (94%)	7 (6%)	19	30
All	All	1682/1806 (93%)	1555 (92%)	127 (8%)	13	21

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	337	THR
1	A	340	ASP
1	A	378	THR
1	A	380	PHE
1	A	403	TRP
1	A	426	SER
1	A	457	ARG
1	A	465	VAL
1	A	469	ARG
1	A	473	PRO
1	B	378	THR
1	B	380	PHE
1	B	402	LEU
1	B	426	SER
1	B	439	ASP
1	B	457	ARG
1	B	469	ARG
1	B	473	PRO
1	C	378	THR
1	C	380	PHE
1	C	396	ARG
1	C	399	PHE
1	C	426	SER
1	C	457	ARG
1	C	469	ARG
1	D	341	GLU
1	D	378	THR
1	D	380	PHE
1	D	405	ARG
1	D	410	VAL
1	D	457	ARG
1	D	465	VAL
1	D	469	ARG
1	D	470	SER
1	D	473	PRO
1	E	341	GLU
1	E	378	THR
1	E	408	LYS
1	E	426	SER
1	E	457	ARG
1	E	469	ARG
1	E	470	SER
1	F	341	GLU

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Mol	Chain	Res	Type
1	F	378	THR
1	F	380	PHE
1	F	401	ASN
1	F	403	TRP
1	F	405	ARG
1	F	408	LYS
1	F	426	SER
1	F	457	ARG
1	F	465	VAL
1	F	469	ARG
1	G	378	THR
1	G	408	LYS
1	G	426	SER
1	G	439	ASP
1	G	457	ARG
1	G	469	ARG
1	G	470	SER
1	G	473	PRO
1	H	378	THR
1	H	380	PHE
1	H	403	TRP
1	H	408	LYS
1	H	410	VAL
1	H	426	SER
1	H	457	ARG
1	H	465	VAL
1	H	469	ARG
1	H	473	PRO
1	I	378	THR
1	I	380	PHE
1	I	396	ARG
1	I	402	LEU
1	I	403	TRP
1	I	406	ASN
1	I	426	SER
1	I	457	ARG
1	I	465	VAL
1	I	469	ARG
1	J	367	GLU
1	J	377	MET
1	J	378	THR
1	J	396	ARG

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Mol	Chain	Res	Type
1	J	402	LEU
1	J	403	TRP
1	J	438	LEU
1	K	349	GLU
1	K	378	THR
1	K	380	PHE
1	K	383	GLU
1	K	392	LEU
1	K	437	TYR
1	K	439	ASP
1	K	473	PRO
1	L	342	ASP
1	L	344	LYS
1	L	352	LYS
1	L	378	THR
1	L	380	PHE
1	L	383	GLU
1	L	388	LEU
1	L	406	ASN
1	L	415	LEU
1	L	424	ASP
1	L	439	ASP
1	L	443	ILE
1	L	473	PRO
1	M	339	GLU
1	M	341	GLU
1	M	355	GLU
1	M	367	GLU
1	M	393	ASP
1	M	403	TRP
1	M	415	LEU
1	M	416	ASN
1	M	435	THR
1	M	461	LYS
1	M	465	VAL
1	N	378	THR
1	N	380	PHE
1	N	426	SER
1	N	457	ARG
1	N	465	VAL
1	N	469	ARG
1	N	470	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	348	GLN
1	A	356	GLN
1	A	401	ASN
1	A	411	HIS
1	A	418	HIS
1	A	436	GLN
1	A	456	HIS
1	B	348	GLN
1	B	356	GLN
1	B	401	ASN
1	B	418	HIS
1	C	348	GLN
1	C	356	GLN
1	C	387	ASN
1	C	395	HIS
1	C	401	ASN
1	C	418	HIS
1	C	456	HIS
1	D	348	GLN
1	D	356	GLN
1	D	395	HIS
1	D	401	ASN
1	D	406	ASN
1	D	418	HIS
1	D	456	HIS
1	E	348	GLN
1	E	356	GLN
1	E	395	HIS
1	E	401	ASN
1	E	418	HIS
1	E	456	HIS
1	F	348	GLN
1	F	356	GLN
1	F	387	ASN
1	F	401	ASN
1	F	418	HIS
1	F	456	HIS
1	G	348	GLN
1	G	356	GLN
1	G	406	ASN
1	G	418	HIS

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Mol	Chain	Res	Type
1	G	456	HIS
1	H	348	GLN
1	H	356	GLN
1	H	387	ASN
1	H	411	HIS
1	H	418	HIS
1	H	436	GLN
1	H	456	HIS
1	I	348	GLN
1	I	356	GLN
1	I	387	ASN
1	I	401	ASN
1	I	406	ASN
1	I	411	HIS
1	I	418	HIS
1	I	436	GLN
1	J	411	HIS
1	J	418	HIS
1	J	436	GLN
1	K	356	GLN
1	K	387	ASN
1	K	395	HIS
1	K	401	ASN
1	K	418	HIS
1	L	348	GLN
1	L	356	GLN
1	L	363	ASN
1	L	387	ASN
1	L	401	ASN
1	L	406	ASN
1	M	348	GLN
1	M	356	GLN
1	M	411	HIS
1	M	416	ASN
1	M	418	HIS
1	M	456	HIS
1	N	348	GLN
1	N	356	GLN
1	N	395	HIS
1	N	411	HIS
1	N	418	HIS
1	N	436	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 14 are monoatomic - leaving 2 for Mogul analysis.

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	DTT	A	1475	-	7,7,7	6.33	4 (57%)	4,8,8	4.71	4 (100%)
4	TBR	A	2000	-	0,36,36	0.00	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DTT	A	1475	-	2/2/2/2	2/8/8/8	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1475	DTT	O2-C2	-15.43	1.10	1.43
2	A	1475	DTT	C4-S4	-4.53	1.72	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1475	DTT	O3-C3	-3.14	1.36	1.43
2	A	1475	DTT	C4-C3	-2.77	1.43	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1475	DTT	C3-C4-S4	-6.80	94.70	114.47
2	A	1475	DTT	C2-C1-S1	-4.52	101.31	114.47
2	A	1475	DTT	O2-C2-C3	4.08	118.10	109.72
2	A	1475	DTT	O3-C3-C2	-2.30	105.01	109.72

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1475	DTT	C2
2	A	1475	DTT	C3

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1475	DTT	O2-C2-C3-C4
2	A	1475	DTT	C1-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1475	DTT	4	0
4	A	2000	TBR	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	141/147 (95%)	0.78	13 (9%) 9 7	31, 56, 105, 116	0
1	B	136/147 (92%)	0.60	8 (5%) 22 19	30, 56, 102, 124	0
1	C	139/147 (94%)	0.78	12 (8%) 10 8	32, 58, 110, 126	0
1	D	138/147 (93%)	0.92	17 (12%) 4 2	31, 59, 114, 122	0
1	E	144/147 (97%)	0.87	15 (10%) 6 4	31, 58, 122, 159	0
1	F	139/147 (94%)	0.88	15 (10%) 5 4	30, 56, 107, 127	0
1	G	136/147 (92%)	0.66	10 (7%) 14 12	32, 55, 101, 117	0
1	H	143/147 (97%)	0.78	20 (13%) 2 2	33, 57, 110, 117	0
1	I	135/147 (91%)	0.60	11 (8%) 12 9	32, 57, 100, 119	0
1	J	139/147 (94%)	0.55	13 (9%) 8 6	28, 53, 113, 142	0
1	K	135/147 (91%)	0.63	11 (8%) 12 9	32, 57, 99, 120	0
1	L	135/147 (91%)	0.44	10 (7%) 14 12	26, 54, 92, 113	0
1	M	139/147 (94%)	0.45	11 (7%) 12 10	26, 48, 105, 130	0
1	N	136/147 (92%)	0.78	12 (8%) 10 8	31, 56, 102, 116	0
All	All	1935/2058 (94%)	0.70	178 (9%) 9 7	26, 56, 109, 159	0

All (178) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	332	GLY	15.3
1	F	475	VAL	11.3
1	D	473	PRO	11.2
1	L	475	VAL	10.9
1	K	473	PRO	10.3
1	K	475	VAL	10.1
1	N	405	ARG	10.0
1	N	475	VAL	9.7

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Mol	Chain	Res	Type	RSRZ
1	D	472	ALA	8.8
1	F	337	THR	8.7
1	N	474	SER	7.8
1	F	472	ALA	7.5
1	E	333	PRO	7.3
1	N	473	PRO	7.3
1	L	472	ALA	7.0
1	K	405	ARG	7.0
1	K	472	ALA	6.9
1	K	474	SER	6.7
1	J	405	ARG	6.6
1	L	474	SER	6.6
1	J	475	VAL	6.5
1	A	339	GLU	6.4
1	E	475	VAL	6.3
1	F	473	PRO	6.3
1	J	404	SER	6.1
1	I	405	ARG	6.0
1	E	334	HIS	5.9
1	D	338	ILE	5.7
1	C	475	VAL	5.7
1	K	406	ASN	5.7
1	J	337	THR	5.5
1	E	403	TRP	5.4
1	D	443	ILE	5.3
1	D	474	SER	5.3
1	H	405	ARG	5.2
1	B	474	SER	5.2
1	G	458	ARG	5.2
1	M	475	VAL	5.2
1	L	473	PRO	5.0
1	B	473	PRO	4.9
1	I	461	LYS	4.8
1	M	472	ALA	4.7
1	A	472	ALA	4.7
1	H	421	LEU	4.6
1	G	405	ARG	4.6
1	I	474	SER	4.5
1	G	475	VAL	4.5
1	E	405	ARG	4.5
1	L	406	ASN	4.4
1	I	403	TRP	4.4

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Mol	Chain	Res	Type	RSRZ
1	M	340	ASP	4.2
1	I	473	PRO	4.2
1	E	335	MET	4.1
1	N	404	SER	4.1
1	D	403	TRP	4.1
1	C	403	TRP	4.1
1	B	406	ASN	4.0
1	H	339	GLU	3.9
1	C	406	ASN	3.9
1	N	408	LYS	3.8
1	B	438	LEU	3.8
1	A	403	TRP	3.8
1	H	440	ALA	3.7
1	C	337	THR	3.6
1	H	340	ASP	3.6
1	M	403	TRP	3.6
1	A	400	GLU	3.6
1	B	405	ARG	3.6
1	B	458	ARG	3.6
1	D	409	PRO	3.5
1	F	474	SER	3.5
1	A	406	ASN	3.5
1	A	441	GLY	3.4
1	D	401	ASN	3.4
1	A	424	ASP	3.4
1	C	438	LEU	3.4
1	J	403	TRP	3.3
1	D	405	ARG	3.3
1	D	440	ALA	3.3
1	I	475	VAL	3.3
1	B	403	TRP	3.3
1	H	334	HIS	3.3
1	H	473	PRO	3.3
1	N	458	ARG	3.2
1	K	409	PRO	3.2
1	I	442	GLY	3.1
1	N	471	GLY	3.1
1	C	342	ASP	3.1
1	N	367	GLU	3.0
1	C	404	SER	3.0
1	N	406	ASN	3.0
1	G	473	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	338	ILE	3.0
1	F	338	ILE	3.0
1	A	344	LYS	2.9
1	F	403	TRP	2.9
1	D	458	ARG	2.9
1	L	440	ALA	2.9
1	F	406	ASN	2.9
1	A	338	ILE	2.9
1	J	401	ASN	2.8
1	H	403	TRP	2.8
1	C	405	ARG	2.8
1	M	339	GLU	2.7
1	C	439	ASP	2.7
1	A	475	VAL	2.7
1	K	437	TYR	2.7
1	F	356	GLN	2.7
1	J	409	PRO	2.7
1	D	441	GLY	2.6
1	L	405	ARG	2.6
1	H	342	ASP	2.6
1	B	475	VAL	2.6
1	E	339	GLU	2.6
1	K	344	LYS	2.6
1	D	367	GLU	2.6
1	J	473	PRO	2.6
1	K	401	ASN	2.6
1	A	407	SER	2.6
1	N	403	TRP	2.6
1	N	461	LYS	2.6
1	H	424	ASP	2.5
1	C	471	GLY	2.5
1	G	340	ASP	2.5
1	H	346	ARG	2.5
1	F	405	ARG	2.5
1	K	444	PRO	2.5
1	F	344	LYS	2.5
1	D	438	LEU	2.5
1	H	333	PRO	2.4
1	H	361	ILE	2.4
1	G	474	SER	2.4
1	C	458	ARG	2.4
1	I	406	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	423	GLY	2.4
1	E	440	ALA	2.4
1	L	471	GLY	2.4
1	I	367	GLU	2.4
1	D	475	VAL	2.4
1	F	404	SER	2.4
1	M	407	SER	2.4
1	L	403	TRP	2.4
1	C	459	ASP	2.3
1	G	391	GLY	2.3
1	J	440	ALA	2.3
1	H	338	ILE	2.3
1	D	404	SER	2.3
1	E	441	GLY	2.3
1	G	392	LEU	2.3
1	M	474	SER	2.3
1	H	341	GLU	2.3
1	D	442	GLY	2.3
1	F	439	ASP	2.3
1	M	338	ILE	2.3
1	J	407	SER	2.2
1	G	438	LEU	2.2
1	L	401	ASN	2.2
1	H	335	MET	2.2
1	M	345	VAL	2.2
1	A	335	MET	2.2
1	J	338	ILE	2.1
1	E	340	ASP	2.1
1	F	410	VAL	2.1
1	E	406	ASN	2.1
1	E	474	SER	2.1
1	J	474	SER	2.1
1	E	439	ASP	2.1
1	I	371	LYS	2.1
1	M	444	PRO	2.1
1	H	336	THR	2.1
1	G	351	ILE	2.1
1	J	443	ILE	2.1
1	F	471	GLY	2.1
1	H	474	SER	2.1
1	H	404	SER	2.0
1	M	439	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	I	460	GLY	2.0
1	H	337	THR	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, 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(\AA^2)	Q<0.9
3	CL	D	1475	1/1	0.68	0.19	68,68,68,68	0
2	DTT	A	1475	8/8	0.77	0.49	72,75,77,79	0
3	CL	H	1475	1/1	0.83	0.16	66,66,66,66	0
3	CL	E	1475	1/1	0.84	0.19	68,68,68,68	0
3	CL	K	1475	1/1	0.86	0.17	62,62,62,62	0
3	CL	L	1475	1/1	0.86	0.10	60,60,60,60	0
3	CL	F	1475	1/1	0.90	0.23	53,53,53,53	0
3	CL	N	1475	1/1	0.92	0.21	55,55,55,55	0
3	CL	C	1475	1/1	0.92	0.18	65,65,65,65	0
3	CL	G	1475	1/1	0.94	0.18	56,56,56,56	0
3	CL	I	1475	1/1	0.94	0.15	58,58,58,58	0
3	CL	A	1476	1/1	0.94	0.11	54,54,54,54	0
3	CL	J	1475	1/1	0.94	0.12	52,52,52,52	0
3	CL	B	1475	1/1	0.95	0.18	58,58,58,58	0
3	CL	M	1475	1/1	0.95	0.13	55,55,55,55	0
4	TBR	A	2000	18/18	0.95	0.08	50,53,66,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.