



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:30 PM GMT

PDB ID : 1KMN  
Title : HISTIDYL-TRNA SYNTHETASE COMPLEXED WITH HISTIDINOL AND ATP  
Authors : Arnez, J.G.; Francklyn, C.S.; Moras, D.  
Deposited on : 1997-05-09  
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

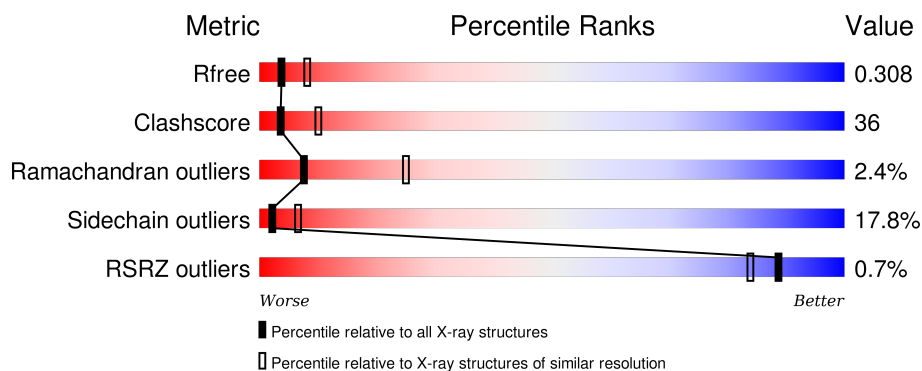
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	424	
1	B	424	
1	C	424	
1	D	424	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ATP	B	452	-	-	X	-
3	ATP	D	452	-	-	X	-

## 2 Entry composition [i](#)

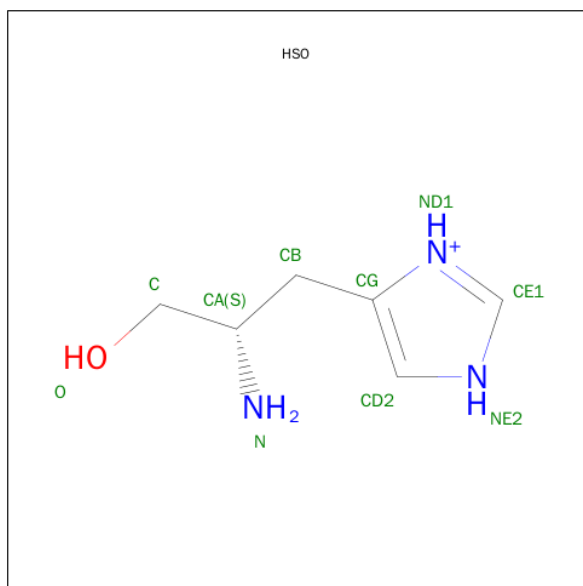
There are 4 unique types of molecules in this entry. The entry contains 14397 atoms, of which 2666 are hydrogens and 0 are deuteriums.

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 HISTIDYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	379	Total	C	H	N	O	S	0	0	0
			3612	1848	674	528	551	11			
1	B	364	Total	C	H	N	O	S	0	0	0
			3455	1768	643	505	528	11			
1	C	387	Total	C	H	N	O	S	0	0	0
			3666	1876	682	536	561	11			
1	D	364	Total	C	H	N	O	S	0	0	0
			3452	1765	643	505	528	11			

- Molecule 2 is L-HISTIDINOL (three-letter code: HSO) (formula: C<sub>6</sub>H<sub>12</sub>N<sub>3</sub>O).



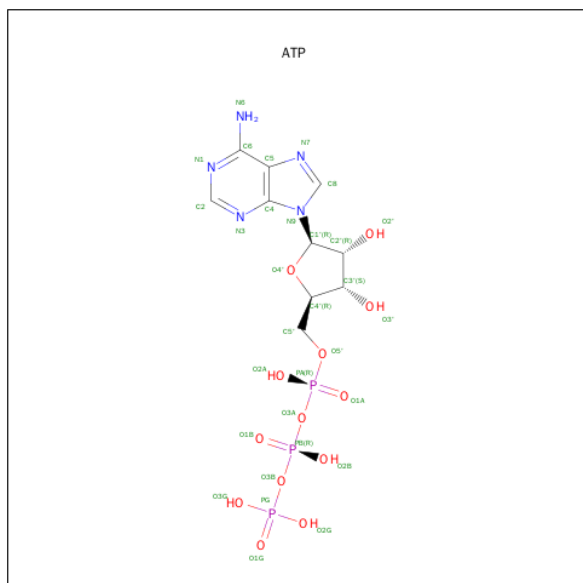
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			13	6	3	3	1		
2	B	1	Total	C	H	N	O	0	0
			13	6	3	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	H	N	O	0	0
			13	6	3	3	1		
2	D	1	Total	C	H	N	O	0	0
			13	6	3	3	1		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	2	Total	O	0	0
			2	2		

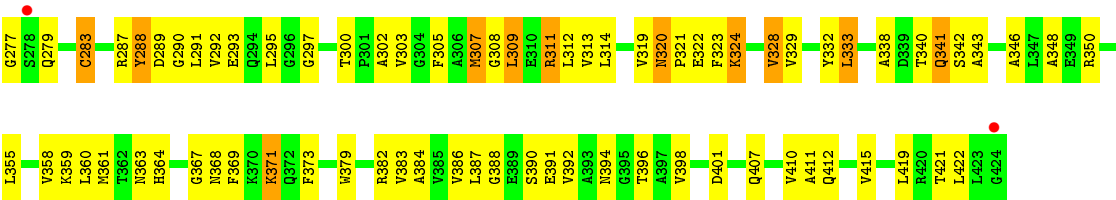


• Molecule 1: HISTIDYL-TRNA SYNTHETASE









## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.90Å 107.30Å 107.20Å 114.10° 97.40° 90.00°	Depositor
Resolution (Å)	13.00 – 2.80 13.94 – 2.60	Depositor EDS
% Data completeness (in resolution range)	64.0 (13.00-2.80) 60.5 (13.94-2.60)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.60 (at 2.61Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.249 , 0.348 0.264 , 0.308	Depositor DCC
$R_{free}$ test set	1301 reflections (2.60%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.0	Xtriage
Anisotropy	0.462	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.21 , 12.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.37$ , $\langle L^2 \rangle = 0.19$	Xtriage
Outliers	0 of 63496 reflections	Xtriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	14397	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.45% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: HSO, ATP

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	0.78	3/2991 (0.1%)	0.96	8/4046 (0.2%)
1	B	0.79	0/2863	0.92	5/3873 (0.1%)
1	C	0.74	0/3037	0.91	3/4109 (0.1%)
1	D	0.76	0/2860	0.90	2/3869 (0.1%)
All	All	0.77	3/11751 (0.0%)	0.92	18/15897 (0.1%)

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	B	0	1
1	C	0	2
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	131	GLU	CD-OE2	6.02	1.32	1.25
1	A	131	GLU	CD-OE1	-5.22	1.20	1.25
1	A	143	GLU	CB-CG	5.05	1.61	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	116	ARG	C-N-CD	-10.59	97.30	120.60
1	A	320	ASN	C-N-CD	-8.14	102.68	120.60
1	A	311	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	A	309	LEU	CA-CB-CG	-7.15	98.85	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	311	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	C	261	LEU	CA-CB-CG	6.62	130.53	115.30
1	B	360	LEU	CA-CB-CG	6.60	130.49	115.30
1	D	360	LEU	CA-CB-CG	6.25	129.68	115.30
1	A	128	LEU	N-CA-C	-5.95	94.95	111.00
1	A	155	LEU	CA-CB-CG	5.84	128.73	115.30
1	B	128	LEU	N-CA-C	-5.64	95.78	111.00
1	C	223	PRO	N-CA-CB	5.51	109.91	103.30
1	D	128	LEU	N-CA-C	-5.44	96.32	111.00
1	C	298	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	B	419	LEU	CA-CB-CG	-5.19	103.37	115.30
1	B	128	LEU	CA-CB-CG	-5.11	103.54	115.30
1	A	422	LEU	CB-CG-CD1	-5.10	102.33	111.00
1	A	90	ARG	NE-CZ-NH1	5.07	122.84	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	99	TYR	Sidechain
1	C	122	TYR	Sidechain
1	C	288	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	2938	674	2899	212	0
1	B	2812	643	2768	220	0
1	C	2984	682	2932	210	0
1	D	2809	643	2762	224	0
2	A	10	3	10	0	0
2	B	10	3	10	1	0
2	C	10	3	10	2	0
2	D	10	3	10	1	0
3	A	31	3	12	3	0
3	B	31	3	12	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	31	3	12	8	0
3	D	31	3	12	12	0
4	A	13	0	0	0	0
4	B	5	0	0	1	0
4	C	4	0	0	0	0
4	D	2	0	0	0	0
All	All	11731	2666	11449	828	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 36.

All (828) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:MET:HE3	1:C:79:THR:HG21	1.27	1.08
1:A:136:GLN:HG2	1:A:301:PRO:HG2	1.34	1.05
1:A:120:GLY:HA3	1:A:279:GLN:HG2	1.38	1.03
1:C:350:ARG:HH22	1:C:412:GLN:HG2	1.19	1.02
1:C:370:LYS:HE2	1:C:370:LYS:HA	1.43	1.00
1:B:311:ARG:NH1	3:B:452:ATP:H2'	1.76	1.00
1:B:311:ARG:CZ	3:B:452:ATP:H2'	1.93	0.98
1:A:382:ARG:HG2	1:A:403:ARG:HH21	1.30	0.96
1:C:311:ARG:NH2	3:C:452:ATP:H2'	1.78	0.96
1:C:15:LEU:HD22	1:D:97:LEU:HD11	1.45	0.95
1:C:46:VAL:HG23	1:D:8:ILE:HD12	1.51	0.92
1:D:33:LEU:HD23	1:D:147:LEU:HD11	1.53	0.91
1:D:46:VAL:HG13	1:D:80:LEU:HD12	1.53	0.90
1:C:46:VAL:HG12	1:C:80:LEU:HD12	1.53	0.90
1:D:293:GLU:HA	1:D:297:GLY:O	1.71	0.90
1:A:32:VAL:HG13	1:A:150:ARG:HD2	1.50	0.90
1:B:67:MET:HE3	1:B:79:THR:HG21	1.54	0.90
1:C:259:ARG:HH11	1:C:259:ARG:HG3	1.37	0.89
1:A:97:LEU:HD11	1:B:15:LEU:HD12	1.52	0.89
1:C:14:TYR:HB2	1:D:42:ARG:HB2	1.55	0.89
1:A:178:ARG:HG3	1:A:178:ARG:HH11	1.37	0.87
1:D:15:LEU:HD22	1:D:15:LEU:H	1.36	0.87
1:C:331:ILE:HB	1:C:360:LEU:HD12	1.57	0.86
1:C:400:LYS:HG2	1:C:407:GLN:HB3	1.55	0.86
1:B:265:ASN:ND2	1:B:266:ARG:HE	1.73	0.85
1:A:371:LYS:HE2	1:A:375:ARG:HH21	1.41	0.85
1:A:22:TRP:O	1:A:26:GLU:HG3	1.77	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:ARG:HH21	3:C:452:ATP:C2'	1.89	0.85
1:C:105:LEU:HD23	1:C:131:GLU:O	1.78	0.84
1:B:141:ASP:HB2	1:B:240:LEU:HD13	1.60	0.84
1:B:382:ARG:HG3	1:B:382:ARG:HH11	1.40	0.84
1:B:46:VAL:HG13	1:B:80:LEU:HD12	1.60	0.83
1:B:67:MET:CE	1:B:79:THR:HG21	2.09	0.83
1:D:130:CYS:SG	1:D:305:PHE:CE2	2.72	0.83
1:A:388:GLY:O	1:A:392:VAL:HG23	1.79	0.82
1:A:14:TYR:HB2	1:B:42:ARG:HB2	1.58	0.82
1:D:234:ARG:HG2	1:D:234:ARG:HH11	1.42	0.82
1:C:256:ARG:HD2	1:C:256:ARG:O	1.80	0.82
1:A:261:LEU:HD23	1:A:264:TYR:HE2	1.43	0.81
1:C:42:ARG:HB2	1:D:14:TYR:HB2	1.62	0.81
1:A:382:ARG:HG2	1:A:403:ARG:NH2	1.94	0.81
1:C:322:GLU:HG3	1:C:324:LYS:HE3	1.63	0.81
1:B:167:SER:HA	1:B:266:ARG:O	1.80	0.81
1:C:104:ARG:HG2	1:C:132:VAL:HG13	1.61	0.81
1:B:382:ARG:HG3	1:B:382:ARG:NH1	1.93	0.80
1:D:332:TYR:CE1	1:D:363:ASN:HB2	2.17	0.80
1:D:121:ARG:HH22	3:D:452:ATP:PG	2.05	0.79
1:B:278:SER:CA	1:B:311:ARG:HB3	2.12	0.79
1:A:259:ARG:HH11	1:A:259:ARG:HG3	1.49	0.78
1:C:168:ILE:HG22	1:C:265:ASN:O	1.84	0.78
1:D:412:GLN:HA	1:D:415:VAL:HG23	1.66	0.78
1:C:311:ARG:NH2	3:C:452:ATP:C2'	2.46	0.78
1:D:383:VAL:HG11	1:D:419:LEU:CD2	2.14	0.78
1:B:21:ILE:O	1:B:25:ILE:HG13	1.83	0.77
1:C:334:VAL:HG11	1:C:373:PHE:HE1	1.48	0.77
1:D:142:ALA:HA	1:D:145:ILE:HD12	1.65	0.77
1:C:350:ARG:NH2	1:C:412:GLN:HG2	1.98	0.77
1:C:287:ARG:HA	1:C:303:VAL:HG12	1.67	0.77
1:D:241:CYS:SG	1:D:251:TYR:CZ	2.76	0.77
1:C:25:ILE:HD13	1:C:316:VAL:HG21	1.66	0.76
1:A:52:PHE:CE1	1:A:82:PRO:HD2	2.20	0.76
1:A:345:MET:HG3	1:A:362:THR:HG21	1.67	0.75
1:C:169:GLY:HA3	1:C:229:LEU:CD2	2.16	0.75
1:A:310:GLU:O	1:A:314:LEU:HD13	1.86	0.75
1:D:328:VAL:HG22	1:D:329:VAL:HG23	1.69	0.75
1:A:352:ARG:HB2	1:B:150:ARG:HH12	1.49	0.75
1:C:168:ILE:HD11	1:C:258:VAL:HG22	1.70	0.74
1:C:334:VAL:HG21	1:C:373:PHE:CE1	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:LEU:HD23	1:C:271:TRP:CE2	2.22	0.74
1:C:423:LEU:HD12	1:C:424:GLY:O	1.87	0.74
1:A:9:ARG:NE	1:A:9:ARG:H	1.85	0.74
1:C:115:GLU:O	1:C:117:PRO:HD3	1.88	0.73
1:C:397:ALA:HB2	1:C:412:GLN:NE2	2.04	0.73
1:A:105:LEU:N	1:A:105:LEU:HD23	2.03	0.73
1:C:383:VAL:HG11	1:C:422:LEU:HD13	1.70	0.73
1:B:311:ARG:NH1	3:B:452:ATP:C2'	2.52	0.73
1:C:167:SER:HA	1:C:266:ARG:O	1.88	0.73
1:B:234:ARG:HH21	1:B:237:PHE:HD2	1.36	0.73
1:C:178:ARG:HA	1:C:181:LEU:HB3	1.71	0.72
1:B:38:TYR:CE1	1:B:104:ARG:HD3	2.25	0.72
1:D:141:ASP:HB2	1:D:240:LEU:HD13	1.71	0.72
1:C:136:GLN:HG3	1:C:301:PRO:HG2	1.72	0.72
1:C:254:ASN:OD1	1:C:256:ARG:HG3	1.89	0.72
1:B:24:ARG:HD3	1:B:325:ALA:HB1	1.70	0.72
1:D:265:ASN:ND2	1:D:289:ASP:H	1.88	0.72
1:C:67:MET:CE	1:C:79:THR:HG21	2.13	0.72
1:A:414:SER:O	1:A:418:HIS:HD2	1.73	0.71
1:C:169:GLY:HA3	1:C:229:LEU:HD21	1.72	0.71
1:B:255:GLN:HA	1:B:255:GLN:OE1	1.89	0.71
1:A:160:HIS:O	1:A:161:VAL:HG13	1.90	0.71
1:B:293:GLU:HA	1:B:297:GLY:O	1.91	0.71
1:D:73:ARG:HG3	1:D:73:ARG:HH11	1.56	0.71
1:B:114:HIS:CE1	1:B:123:ARG:HH21	2.08	0.71
1:C:371:LYS:HD2	1:C:375:ARG:HE	1.56	0.71
1:D:244:LEU:HD12	1:D:251:TYR:HD2	1.55	0.71
1:A:256:ARG:HD2	1:A:256:ARG:O	1.91	0.70
1:C:364:HIS:HD2	1:D:104:ARG:NH2	1.89	0.70
1:C:12:ASN:ND2	1:C:12:ASN:H	1.86	0.70
1:C:388:GLY:O	1:C:392:VAL:HG23	1.90	0.70
1:D:333:LEU:HD13	1:D:348:ALA:HB2	1.74	0.70
1:B:28:THR:O	1:B:32:VAL:HG23	1.92	0.70
1:D:28:THR:O	1:D:32:VAL:HG23	1.92	0.70
1:A:9:ARG:H	1:A:9:ARG:HE	1.40	0.70
1:C:324:LYS:HD2	1:C:324:LYS:H	1.57	0.69
1:D:264:TYR:HA	1:D:287:ARG:O	1.92	0.69
1:C:352:ARG:HB2	1:D:150:ARG:HH12	1.56	0.69
1:D:104:ARG:C	1:D:105:LEU:HG	2.11	0.69
1:A:42:ARG:HB2	1:B:14:TYR:HB2	1.72	0.69
1:C:89:VAL:HG21	1:C:291:LEU:HD22	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:GLY:HA3	1:A:98:LEU:HD11	1.74	0.69
1:D:257:LEU:HD23	1:D:268:VAL:HG12	1.73	0.69
1:B:332:TYR:CE1	1:B:363:ASN:HB2	2.28	0.68
1:A:244:LEU:HD12	1:A:249:ILE:HB	1.74	0.68
1:B:331:ILE:HD11	1:B:423:LEU:HD11	1.74	0.68
1:A:178:ARG:HG3	1:A:179:ASP:N	2.08	0.68
1:A:239:GLY:O	1:A:243:LEU:HD13	1.93	0.68
1:C:5:ILE:HD12	1:D:51:LEU:HG	1.75	0.68
1:B:264:TYR:HA	1:B:287:ARG:O	1.92	0.68
1:B:121:ARG:HH12	3:B:452:ATP:PG	2.16	0.68
1:D:308:GLY:O	1:D:311:ARG:HG2	1.92	0.68
1:D:307:MET:SD	1:D:312:LEU:HD22	2.33	0.68
1:D:257:LEU:HD11	1:D:270:GLU:OE2	1.93	0.68
1:C:52:PHE:CE2	1:C:82:PRO:HD2	2.28	0.68
1:C:234:ARG:NH1	1:C:237:PHE:HD2	1.92	0.68
1:A:60:THR:O	1:A:64:GLU:HG3	1.94	0.68
1:D:111:MET:HB2	1:D:125:PHE:CE1	2.29	0.67
1:D:235:GLU:HG2	1:D:236:HIS:N	2.09	0.67
1:C:105:LEU:O	1:C:130:CYS:HB2	1.94	0.67
1:B:52:PHE:CE1	1:B:82:PRO:HD2	2.28	0.67
1:D:167:SER:HA	1:D:266:ARG:O	1.95	0.67
1:A:332:TYR:HD2	1:A:376:ALA:HB2	1.59	0.67
1:C:111:MET:HB2	1:C:125:PHE:CE1	2.29	0.67
1:C:272:VAL:HG12	1:C:281:THR:HG22	1.76	0.66
1:B:382:ARG:CG	1:B:382:ARG:HH11	2.09	0.66
1:C:311:ARG:HH21	3:C:452:ATP:C1'	2.09	0.66
1:C:44:PRO:HA	1:D:124:GLN:HE22	1.61	0.66
1:B:388:GLY:O	1:B:392:VAL:HG23	1.96	0.65
1:D:259:ARG:HB2	1:D:264:TYR:CD2	2.31	0.65
1:B:91:ALA:O	1:B:95:HIS:HD2	1.79	0.65
1:A:171:LEU:HD13	1:A:174:ARG:HH12	1.60	0.65
1:B:383:VAL:HG11	1:B:419:LEU:HD21	1.79	0.65
1:D:121:ARG:NH2	3:D:452:ATP:PG	2.70	0.65
1:D:47:GLU:HB2	1:D:52:PHE:CE2	2.32	0.65
1:A:373:PHE:O	1:A:376:ALA:HB3	1.97	0.65
1:C:22:TRP:O	1:C:26:GLU:HG3	1.97	0.65
1:A:97:LEU:HD23	1:A:97:LEU:N	2.12	0.65
1:D:168:ILE:HG22	1:D:265:ASN:O	1.96	0.65
1:A:60:THR:HG22	1:A:62:VAL:H	1.61	0.65
1:C:160:HIS:O	1:C:161:VAL:HG13	1.97	0.64
1:B:237:PHE:O	1:B:241:CYS:SG	2.53	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:TYR:N	1:B:38:TYR:HD1	1.96	0.64
1:B:9:ARG:HE	1:B:116:ARG:HH22	1.45	0.64
1:A:309:LEU:O	1:A:313:VAL:HG23	1.97	0.64
1:B:105:LEU:O	1:B:130:CYS:HB2	1.97	0.64
1:C:347:LEU:HG	1:C:351:LEU:CD1	2.28	0.64
1:A:113:ARG:HG3	1:A:125:PHE:HE2	1.62	0.64
1:C:271:TRP:HB2	1:C:283:CYS:HB3	1.80	0.64
1:C:36:TYR:HE1	1:C:150:ARG:HD2	1.62	0.64
1:D:263:TYR:HD2	1:D:291:LEU:HD13	1.63	0.64
1:D:311:ARG:HG3	1:D:311:ARG:HH11	1.63	0.64
1:C:309:LEU:O	1:C:313:VAL:HG23	1.97	0.64
1:C:92:GLY:HA3	1:C:98:LEU:HD11	1.80	0.64
1:B:74:ASN:HB3	1:B:76:ASP:OD1	1.97	0.63
1:B:383:VAL:HG11	1:B:419:LEU:CD2	2.28	0.63
1:C:116:ARG:HH11	1:C:116:ARG:HG3	1.62	0.63
1:C:40:GLU:HB2	1:C:106:TRP:CZ2	2.34	0.63
1:A:165:LEU:HD12	1:A:166:ASN:H	1.63	0.63
1:D:135:LEU:O	1:D:287:ARG:NH2	2.32	0.63
1:A:141:ASP:HB2	1:A:240:LEU:HD13	1.80	0.63
1:B:152:TRP:CD1	1:B:161:VAL:HG21	2.34	0.63
1:B:89:VAL:HG21	1:B:291:LEU:HD21	1.80	0.63
1:A:33:LEU:HD23	1:A:147:LEU:HD11	1.80	0.62
1:B:135:LEU:HD23	1:B:140:ILE:HD13	1.81	0.62
1:D:127:GLN:NE2	3:D:452:ATP:H5'1	2.14	0.62
1:C:352:ARG:CB	1:D:150:ARG:HH12	2.11	0.62
1:C:52:PHE:HB3	1:C:56:ILE:HD12	1.80	0.62
1:A:175:ALA:O	1:A:178:ARG:HG2	1.99	0.62
1:D:15:LEU:CD2	1:D:15:LEU:H	2.11	0.62
1:B:265:ASN:ND2	1:B:266:ARG:NE	2.46	0.62
1:B:21:ILE:HD12	1:B:21:ILE:H	1.64	0.62
1:A:45:ILE:HG12	1:B:124:GLN:HE22	1.63	0.62
1:D:105:LEU:O	1:D:130:CYS:HB2	1.99	0.62
1:B:10:GLY:HA3	1:B:123:ARG:HG2	1.80	0.62
1:D:49:THR:O	1:D:53:LYS:HG3	2.00	0.62
1:A:178:ARG:HG3	1:A:179:ASP:H	1.63	0.62
1:D:259:ARG:NH2	3:D:452:ATP:O1A	2.33	0.62
1:B:343:ALA:O	1:B:346:ALA:HB3	2.00	0.62
1:A:163:LEU:HD21	1:A:165:LEU:HD22	1.81	0.62
1:A:381:ALA:O	1:A:402:LEU:HD12	1.99	0.62
1:D:72:ASP:HB2	1:D:78:LEU:CD2	2.30	0.61
1:C:259:ARG:NH2	3:C:452:ATP:O1A	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:259:ARG:HG2	1:D:268:VAL:HG13	1.82	0.61
1:D:157:ILE:HG22	1:D:319:VAL:CG1	2.30	0.61
1:B:38:TYR:N	1:B:38:TYR:CD1	2.68	0.61
1:D:412:GLN:HA	1:D:415:VAL:CG2	2.31	0.61
1:C:287:ARG:O	1:C:288:TYR:HB3	1.98	0.61
1:A:383:VAL:HG11	1:A:422:LEU:HD13	1.83	0.61
1:B:125:PHE:HE1	1:B:127:GLN:HG3	1.66	0.61
1:C:347:LEU:HG	1:C:351:LEU:HD12	1.83	0.61
1:B:68:TYR:HB2	1:B:80:LEU:HB2	1.82	0.60
1:C:29:LEU:HD11	1:C:312:LEU:CD2	2.31	0.60
1:B:141:ASP:O	1:B:145:ILE:HD12	2.01	0.60
1:B:251:TYR:HD1	1:B:251:TYR:H	1.47	0.60
1:D:45:ILE:O	1:D:81:ARG:HG2	2.01	0.60
1:B:418:HIS:O	1:B:422:LEU:HD23	2.01	0.60
1:B:168:ILE:HG13	1:B:265:ASN:O	2.02	0.60
1:A:259:ARG:HH11	1:A:259:ARG:CG	2.14	0.60
1:A:259:ARG:NH2	3:A:452:ATP:O1A	2.34	0.60
1:B:106:TRP:HA	1:B:130:CYS:HA	1.82	0.60
1:C:259:ARG:CG	1:C:259:ARG:HH11	2.11	0.60
1:C:334:VAL:HG11	1:C:373:PHE:CE1	2.32	0.60
1:A:251:TYR:H	1:A:251:TYR:HD1	1.50	0.60
1:C:340:THR:HG23	1:C:387:LEU:HD13	1.83	0.60
1:C:277:GLY:O	1:C:311:ARG:HG2	2.02	0.60
1:A:165:LEU:HD13	1:A:269:PHE:HB3	1.83	0.60
1:A:298:ARG:HH11	1:A:298:ARG:HG3	1.66	0.59
1:C:38:TYR:CE2	1:C:104:ARG:HB3	2.37	0.59
1:D:279:GLN:H	1:D:311:ARG:NH2	1.99	0.59
1:A:29:LEU:HD13	1:A:128:LEU:HD23	1.83	0.59
1:C:293:GLU:HA	1:C:297:GLY:O	2.03	0.59
1:D:141:ASP:HB2	1:D:240:LEU:CD1	2.32	0.59
1:C:226:GLY:O	1:C:229:LEU:HB2	2.02	0.59
1:B:333:LEU:HD13	1:B:385:VAL:O	2.03	0.59
1:C:368:ASN:OD1	1:C:370:LYS:HB2	2.03	0.59
1:B:12:ASN:H	1:B:12:ASN:ND2	1.99	0.59
1:B:15:LEU:O	1:B:19:THR:HG23	2.02	0.59
1:C:72:ASP:HB2	1:C:78:LEU:HD22	1.84	0.59
1:C:72:ASP:HB2	1:C:78:LEU:CD2	2.32	0.59
1:A:165:LEU:HD23	1:A:251:TYR:HD2	1.68	0.59
1:C:345:MET:HG3	1:C:362:THR:HG21	1.84	0.59
1:D:136:GLN:HE22	1:D:266:ARG:HH12	1.50	0.59
1:A:83:GLU:HG3	1:A:84:GLY:N	2.13	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:GLN:HA	1:B:118:GLN:NE2	2.17	0.59
1:A:22:TRP:HH2	1:A:310:GLU:HG3	1.68	0.59
1:C:105:LEU:N	1:C:105:LEU:CD2	2.66	0.59
1:D:157:ILE:HG22	1:D:319:VAL:HG11	1.84	0.59
1:D:67:MET:CE	1:D:79:THR:HG21	2.33	0.59
1:D:67:MET:HE2	1:D:79:THR:HG21	1.85	0.59
1:B:58:GLU:CD	1:B:58:GLU:H	2.06	0.59
1:A:293:GLU:HA	1:A:297:GLY:O	2.02	0.59
1:D:141:ASP:O	1:D:145:ILE:HG13	2.02	0.58
1:A:355:LEU:O	1:A:358:VAL:HG22	2.03	0.58
1:D:99:TYR:O	1:D:101:GLN:HG2	2.02	0.58
1:C:104:ARG:HG2	1:C:132:VAL:CG1	2.33	0.58
1:A:163:LEU:HD23	1:A:251:TYR:HB3	1.85	0.58
1:D:332:TYR:CZ	1:D:363:ASN:HB2	2.38	0.58
1:D:21:ILE:O	1:D:25:ILE:HG13	2.03	0.58
1:C:313:VAL:HG12	1:C:317:GLN:NE2	2.17	0.58
1:A:167:SER:HA	1:A:266:ARG:O	2.02	0.58
1:B:21:ILE:N	1:B:21:ILE:HD12	2.19	0.58
1:C:291:LEU:HD21	1:C:295:LEU:HD22	1.84	0.58
1:D:30:LYS:HB2	1:D:30:LYS:HZ3	1.68	0.58
1:B:234:ARG:NH2	1:B:237:PHE:HD2	2.01	0.58
1:A:254:ASN:OD1	1:A:256:ARG:HG3	2.03	0.58
1:B:331:ILE:HD12	1:B:331:ILE:N	2.19	0.58
1:A:147:LEU:O	1:A:147:LEU:HD23	2.04	0.58
1:A:173:ALA:O	1:A:177:TYR:HB2	2.04	0.58
1:D:38:TYR:N	1:D:38:TYR:CD1	2.72	0.58
1:D:234:ARG:CG	1:D:234:ARG:HH11	2.14	0.58
1:B:112:PHE:HA	1:B:123:ARG:O	2.04	0.58
1:A:307:MET:SD	1:A:312:LEU:HD22	2.43	0.58
1:C:259:ARG:NH1	1:C:259:ARG:HG3	2.15	0.57
1:D:106:TRP:HA	1:D:130:CYS:HA	1.85	0.57
1:C:311:ARG:NH2	3:C:452:ATP:C4	2.72	0.57
2:C:451:HSO:H	3:C:452:ATP:O1A	2.04	0.57
1:D:38:TYR:HD1	1:D:38:TYR:N	2.01	0.57
1:C:382:ARG:HB2	1:C:382:ARG:HH11	1.69	0.57
1:C:22:TRP:CE2	1:C:313:VAL:HG21	2.40	0.57
1:D:52:PHE:HB2	1:D:67:MET:HE1	1.86	0.57
1:B:130:CYS:SG	1:B:305:PHE:CE1	2.96	0.57
1:B:43:LEU:HD11	1:B:88:CYS:HA	1.86	0.57
1:D:265:ASN:HD21	1:D:289:ASP:H	1.50	0.57
1:C:174:ARG:HH11	1:C:174:ARG:HG3	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:LEU:N	1:C:105:LEU:HD23	2.20	0.57
1:C:254:ASN:HD21	1:C:256:ARG:NE	2.02	0.57
1:C:81:ARG:HE	1:C:111:MET:HE2	1.69	0.57
1:C:381:ALA:O	1:C:402:LEU:HD12	2.03	0.57
1:C:257:LEU:HD11	1:C:270:GLU:HG2	1.87	0.57
1:B:46:VAL:CG1	1:B:80:LEU:HD12	2.32	0.57
1:C:181:LEU:HG	1:C:182:VAL:N	2.19	0.57
1:B:47:GLU:HB2	1:B:52:PHE:HE2	1.70	0.56
1:A:331:ILE:O	1:A:360:LEU:HA	2.05	0.56
1:A:72:ASP:HB2	1:A:78:LEU:HD22	1.86	0.56
1:C:47:GLU:OE2	1:C:90:ARG:HD3	2.05	0.56
1:A:384:ALA:HB2	1:A:402:LEU:HD21	1.85	0.56
1:B:265:ASN:HD21	1:B:266:ARG:HE	1.52	0.56
1:C:182:VAL:HA	1:C:185:LEU:HB2	1.86	0.56
1:C:234:ARG:HH12	1:C:237:PHE:HD2	1.53	0.56
1:B:311:ARG:CZ	3:B:452:ATP:C2'	2.77	0.56
1:B:283:CYS:SG	1:B:305:PHE:HD2	2.29	0.56
1:B:72:ASP:HB2	1:B:78:LEU:HD11	1.87	0.56
1:A:264:TYR:HA	1:A:287:ARG:O	2.06	0.56
1:D:311:ARG:HD3	3:D:452:ATP:N3	2.20	0.56
1:B:259:ARG:HG2	1:B:268:VAL:HG13	1.88	0.56
1:B:137:GLY:O	1:B:140:ILE:HG22	2.06	0.56
1:A:178:ARG:CG	1:A:178:ARG:HH11	2.15	0.56
1:B:141:ASP:HB2	1:B:240:LEU:CD1	2.32	0.56
1:D:164:GLU:HB2	1:D:270:GLU:HG3	1.87	0.56
1:B:89:VAL:HG21	1:B:291:LEU:CD2	2.36	0.56
1:A:163:LEU:HD23	1:A:251:TYR:CB	2.35	0.56
1:A:254:ASN:HD21	1:A:256:ARG:NH2	2.04	0.56
1:C:147:LEU:O	1:C:147:LEU:HD23	2.06	0.56
1:B:261:LEU:HD12	1:B:263:TYR:CZ	2.42	0.55
1:B:287:ARG:O	1:B:288:TYR:HB3	2.06	0.55
1:D:72:ASP:HB2	1:D:78:LEU:HD22	1.88	0.55
1:C:147:LEU:HD23	1:C:147:LEU:C	2.26	0.55
1:B:14:TYR:HE2	1:B:126:HIS:HE1	1.54	0.55
1:C:113:ARG:HD2	1:C:125:PHE:CE1	2.41	0.55
1:A:394:ASN:O	1:A:396:THR:HG23	2.07	0.55
1:A:8:ILE:CD1	1:A:8:ILE:H	2.19	0.55
1:C:81:ARG:HD2	1:C:111:MET:SD	2.45	0.55
1:C:313:VAL:HG12	1:C:317:GLN:HE21	1.72	0.55
1:C:166:ASN:HB3	1:C:268:VAL:HG23	1.87	0.55
1:A:382:ARG:HG3	1:A:403:ARG:HE	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:121:ARG:NH2	3:D:452:ATP:O2G	2.40	0.55
1:C:355:LEU:O	1:C:358:VAL:HG22	2.06	0.55
1:D:103:GLN:HG3	1:D:105:LEU:HD21	1.88	0.55
1:B:283:CYS:SG	1:B:305:PHE:CD2	3.00	0.55
1:C:345:MET:SD	1:C:364:HIS:HE1	2.29	0.55
1:A:273:THR:OG1	1:A:275:SER:HB3	2.07	0.55
1:C:99:TYR:O	1:C:101:GLN:HG3	2.07	0.55
1:A:95:HIS:HB2	1:A:97:LEU:HD21	1.89	0.54
1:A:361:MET:SD	1:B:104:ARG:NH1	2.80	0.54
1:D:368:ASN:ND2	1:D:371:LYS:HE3	2.22	0.54
1:B:47:GLU:HB2	1:B:52:PHE:CE2	2.42	0.54
1:B:274:ASN:N	1:B:274:ASN:OD1	2.40	0.54
1:A:171:LEU:HD22	1:A:171:LEU:H	1.72	0.54
1:D:383:VAL:HG12	1:D:384:ALA:N	2.22	0.54
1:A:292:VAL:HG21	1:A:300:THR:HG22	1.89	0.54
1:D:147:LEU:HD23	1:D:147:LEU:O	2.07	0.54
1:D:49:THR:HG23	1:D:79:THR:OG1	2.08	0.54
1:A:178:ARG:HG3	1:A:178:ARG:NH1	2.09	0.54
1:C:225:LEU:O	1:C:229:LEU:HG	2.08	0.54
1:C:33:LEU:HD23	1:C:147:LEU:HD11	1.89	0.54
1:B:278:SER:C	1:B:280:GLY:H	2.10	0.54
1:D:166:ASN:HD22	1:D:168:ILE:HD13	1.73	0.53
1:D:133:PHE:HE1	1:D:288:TYR:OH	1.91	0.53
1:B:69:THR:HA	1:B:78:LEU:O	2.07	0.53
1:D:136:GLN:HE22	1:D:266:ARG:NH1	2.05	0.53
1:D:148:THR:O	1:D:151:TRP:HB2	2.08	0.53
1:A:382:ARG:CG	1:A:403:ARG:HE	2.21	0.53
1:C:46:VAL:HG23	1:D:8:ILE:CD1	2.32	0.53
1:A:105:LEU:N	1:A:105:LEU:CD2	2.72	0.53
1:B:320:ASN:C	1:B:322:GLU:H	2.11	0.53
1:D:141:ASP:CB	1:D:240:LEU:HD13	2.39	0.53
1:D:319:VAL:C	1:D:321:PRO:HD3	2.28	0.53
1:D:321:PRO:O	1:D:324:LYS:NZ	2.42	0.53
1:C:169:GLY:HA3	1:C:229:LEU:HD22	1.89	0.53
1:D:125:PHE:CD2	3:D:452:ATP:C6	2.96	0.53
1:B:288:TYR:O	1:B:288:TYR:CD1	2.62	0.53
1:D:311:ARG:HG3	1:D:311:ARG:NH1	2.24	0.53
1:C:234:ARG:NH1	1:C:237:PHE:CD2	2.76	0.53
1:C:335:ALA:HB1	1:C:340:THR:HG21	1.90	0.53
3:B:452:ATP:H8	3:B:452:ATP:O2B	1.92	0.53
1:A:174:ARG:HH11	1:A:174:ARG:HB2	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:168:ILE:HD11	1:D:258:VAL:HG12	1.89	0.52
1:A:105:LEU:H	1:A:105:LEU:HD23	1.74	0.52
1:A:89:VAL:O	1:A:93:ILE:HG13	2.09	0.52
1:A:45:ILE:HD13	1:A:81:ARG:NH2	2.24	0.52
1:C:328:VAL:HG21	1:C:379:TRP:HE3	1.74	0.52
1:B:278:SER:CA	1:B:311:ARG:HD3	2.40	0.52
1:A:382:ARG:NH2	1:A:423:LEU:HD22	2.24	0.52
1:B:312:LEU:HD23	1:B:313:VAL:N	2.24	0.52
1:C:22:TRP:NE1	1:C:313:VAL:HG11	2.24	0.52
1:C:370:LYS:CE	1:C:370:LYS:HA	2.27	0.52
1:C:106:TRP:HA	1:C:130:CYS:HA	1.92	0.52
1:B:74:ASN:O	1:B:74:ASN:ND2	2.42	0.52
1:A:375:ARG:O	1:A:379:TRP:CD1	2.62	0.52
1:D:119:LYS:HG3	1:D:122:TYR:OH	2.10	0.52
1:B:259:ARG:CG	1:B:268:VAL:HG13	2.39	0.52
1:D:21:ILE:HD12	1:D:21:ILE:H	1.74	0.52
1:A:45:ILE:H	1:B:124:GLN:HE22	1.58	0.52
1:A:174:ARG:HH21	1:A:265:ASN:HA	1.75	0.52
1:D:328:VAL:O	1:D:359:LYS:HD3	2.09	0.52
1:A:298:ARG:NH1	1:A:298:ARG:HG3	2.25	0.52
1:C:412:GLN:HA	1:C:415:VAL:HG23	1.91	0.52
1:D:139:ASP:O	1:D:142:ALA:HB3	2.09	0.52
1:B:412:GLN:HA	1:B:415:VAL:HG23	1.92	0.52
1:A:261:LEU:HD23	1:A:264:TYR:CE2	2.32	0.52
1:A:345:MET:CE	1:B:146:MET:SD	2.98	0.52
1:C:283:CYS:SG	1:C:305:PHE:CD1	3.02	0.52
1:B:354:GLU:OE1	1:B:416:ALA:HB2	2.09	0.52
1:D:91:ALA:O	1:D:95:HIS:HD2	1.92	0.52
1:C:331:ILE:O	1:C:360:LEU:HA	2.10	0.52
1:D:73:ARG:HH11	1:D:73:ARG:CG	2.22	0.52
1:B:415:VAL:HG12	1:B:419:LEU:HD12	1.91	0.52
1:D:130:CYS:SG	1:D:305:PHE:HE2	2.32	0.51
1:A:345:MET:HE3	1:B:146:MET:SD	2.50	0.51
1:A:410:VAL:HG12	1:A:411:ALA:N	2.24	0.51
1:A:422:LEU:O	1:A:422:LEU:HD23	2.10	0.51
1:A:273:THR:C	1:A:275:SER:H	2.13	0.51
1:B:111:MET:HB2	1:B:125:PHE:CE1	2.44	0.51
1:D:133:PHE:HE1	1:D:288:TYR:HH	1.57	0.51
1:B:332:TYR:CZ	1:B:363:ASN:HB2	2.45	0.51
1:A:5:ILE:HD12	1:B:54:ARG:NH2	2.25	0.51
1:A:136:GLN:HG2	1:A:301:PRO:CG	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:ILE:HG12	1:D:297:GLY:HA3	1.92	0.51
1:A:352:ARG:CB	1:B:150:ARG:HH12	2.22	0.51
1:A:332:TYR:CD2	1:A:376:ALA:HB2	2.43	0.51
1:B:89:VAL:HG12	1:B:292:VAL:HG12	1.93	0.51
1:A:11:MET:HG2	1:A:124:GLN:HB2	1.93	0.51
1:B:410:VAL:HG12	1:B:411:ALA:N	2.24	0.51
1:B:240:LEU:O	1:B:244:LEU:HD23	2.10	0.51
1:B:133:PHE:HE1	1:B:288:TYR:OH	1.92	0.51
1:B:370:LYS:CD	1:B:370:LYS:H	2.24	0.51
1:B:371:LYS:O	1:B:375:ARG:HG3	2.11	0.51
1:B:132:VAL:HG21	1:B:140:ILE:HD11	1.93	0.51
1:B:311:ARG:HD2	3:B:452:ATP:O2'	2.10	0.51
1:A:28:THR:O	1:A:32:VAL:HG23	2.11	0.51
1:D:311:ARG:NH1	3:D:452:ATP:O2'	2.43	0.51
1:B:369:PHE:HB2	1:B:370:LYS:HZ1	1.76	0.51
1:D:136:GLN:NE2	1:D:266:ARG:HH12	2.08	0.51
1:A:241:CYS:O	1:A:245:GLU:HG3	2.11	0.51
1:B:244:LEU:HD12	1:B:249:ILE:HB	1.92	0.50
1:D:259:ARG:CB	1:D:264:TYR:CE2	2.94	0.50
1:B:287:ARG:HA	1:B:303:VAL:HG13	1.92	0.50
1:A:232:GLU:HB2	1:A:266:ARG:NH2	2.26	0.50
1:C:259:ARG:NH1	1:C:264:TYR:CZ	2.79	0.50
1:D:93:ILE:HD11	1:D:292:VAL:O	2.11	0.50
1:D:288:TYR:CE1	1:D:302:ALA:HB1	2.46	0.50
1:C:165:LEU:O	1:C:253:VAL:HA	2.12	0.50
1:B:375:ARG:HA	1:B:378:LYS:HG3	1.92	0.50
1:D:130:CYS:SG	1:D:305:PHE:CZ	3.01	0.50
1:A:178:ARG:CG	1:A:178:ARG:NH1	2.72	0.50
1:D:263:TYR:HB3	1:D:291:LEU:HD12	1.93	0.50
1:A:136:GLN:CG	1:A:301:PRO:HG2	2.24	0.50
1:A:386:VAL:HB	1:A:398:VAL:HB	1.94	0.50
1:A:135:LEU:HD12	1:A:140:ILE:HG12	1.94	0.50
1:D:388:GLY:O	1:D:392:VAL:HG23	2.12	0.50
1:A:287:ARG:HG2	1:A:288:TYR:H	1.76	0.50
1:A:127:GLN:HE21	3:A:452:ATP:H5'1	1.76	0.50
1:C:152:TRP:HB3	1:C:158:SER:HA	1.92	0.50
1:A:383:VAL:HG22	1:A:422:LEU:HD22	1.94	0.50
1:C:332:TYR:CZ	1:C:363:ASN:HB2	2.46	0.50
1:A:74:ASN:HA	1:D:73:ARG:O	2.12	0.50
1:A:384:ALA:CB	1:A:402:LEU:HD21	2.42	0.50
1:D:146:MET:HG3	1:D:249:ILE:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:GLY:H	1:B:229:LEU:HD11	1.77	0.50
1:D:383:VAL:HG11	1:D:419:LEU:HD21	1.94	0.50
1:C:89:VAL:HG21	1:C:291:LEU:CD2	2.38	0.50
1:A:347:LEU:HD13	1:A:412:GLN:HG2	1.93	0.50
1:A:343:ALA:O	1:A:346:ALA:HB3	2.12	0.50
1:B:381:ALA:O	1:B:402:LEU:HD12	2.10	0.50
1:B:369:PHE:HB2	1:B:370:LYS:NZ	2.27	0.50
1:A:40:GLU:HB2	1:A:106:TRP:CZ2	2.46	0.50
1:B:125:PHE:CE1	1:B:127:GLN:HG3	2.47	0.49
1:A:171:LEU:HA	1:A:174:ARG:HH12	1.77	0.49
1:D:265:ASN:OD1	1:D:266:ARG:N	2.45	0.49
1:A:332:TYR:CZ	1:A:363:ASN:HB2	2.47	0.49
1:B:151:TRP:CZ3	1:B:307:MET:HE2	2.47	0.49
1:B:390:SER:HB2	1:B:391:GLU:OE1	2.12	0.49
1:A:157:ILE:O	1:A:157:ILE:HD12	2.12	0.49
1:D:85:THR:O	1:D:89:VAL:HG23	2.12	0.49
1:A:165:LEU:HD12	1:A:166:ASN:N	2.27	0.49
1:B:320:ASN:O	1:B:322:GLU:N	2.45	0.49
1:B:278:SER:C	1:B:280:GLY:N	2.64	0.49
1:D:244:LEU:HD12	1:D:251:TYR:CD2	2.43	0.49
1:C:315:LEU:HD12	1:C:315:LEU:O	2.12	0.49
1:D:369:PHE:O	1:D:373:PHE:CD2	2.65	0.49
1:C:350:ARG:HH22	1:C:412:GLN:CG	2.08	0.49
1:C:371:LYS:HD2	1:C:375:ARG:NE	2.27	0.49
1:B:121:ARG:NH1	1:B:311:ARG:HH22	2.10	0.49
1:D:259:ARG:NH1	1:D:264:TYR:OH	2.45	0.49
1:C:287:ARG:HA	1:C:303:VAL:CG1	2.41	0.49
1:B:85:THR:OG1	2:B:451:HSO:N	2.45	0.49
1:B:254:ASN:HB3	1:B:257:LEU:HB2	1.95	0.49
1:A:367:GLY:O	1:A:372:GLN:NE2	2.45	0.49
1:C:259:ARG:CG	1:C:259:ARG:NH1	2.72	0.49
1:D:52:PHE:O	1:D:56:ILE:HB	2.11	0.49
1:C:410:VAL:HG12	1:C:411:ALA:N	2.27	0.49
1:A:241:CYS:SG	1:A:251:TYR:HE2	2.36	0.49
1:C:343:ALA:O	1:C:346:ALA:HB3	2.12	0.49
1:A:146:MET:CE	1:B:345:MET:SD	3.00	0.49
1:B:15:LEU:N	1:B:15:LEU:HD22	2.28	0.49
1:D:135:LEU:CD1	1:D:140:ILE:HG12	2.42	0.49
1:D:288:TYR:CE1	1:D:302:ALA:CB	2.96	0.49
1:A:287:ARG:NH1	1:A:303:VAL:CG2	2.75	0.49
1:A:8:ILE:H	1:A:8:ILE:HD13	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:152:TRP:HB3	1:D:158:SER:HA	1.95	0.49
1:D:74:ASN:HB3	1:D:76:ASP:OD1	2.13	0.49
1:A:279:GLN:HB2	1:A:311:ARG:NH1	2.29	0.48
1:D:265:ASN:OD1	1:D:266:ARG:HD3	2.13	0.48
1:B:261:LEU:HD12	1:B:263:TYR:CE2	2.48	0.48
1:D:138:PRO:HB2	1:D:240:LEU:HB2	1.95	0.48
1:A:8:ILE:CD1	1:A:8:ILE:N	2.75	0.48
1:A:43:LEU:HB3	1:A:44:PRO:HD2	1.95	0.48
1:B:69:THR:HG23	1:B:78:LEU:O	2.14	0.48
1:C:104:ARG:HH22	1:D:364:HIS:HD2	1.60	0.48
1:D:136:GLN:NE2	1:D:266:ARG:NH1	2.62	0.48
1:C:182:VAL:O	1:C:185:LEU:N	2.46	0.48
1:C:335:ALA:HB1	1:C:340:THR:CG2	2.43	0.48
1:A:232:GLU:HB2	1:A:266:ARG:HH21	1.78	0.48
3:B:452:ATP:C8	3:B:452:ATP:O2B	2.67	0.48
1:C:36:TYR:HB3	1:C:38:TYR:CE1	2.47	0.48
1:D:291:LEU:HD21	1:D:295:LEU:CD1	2.43	0.48
1:B:9:ARG:HG2	1:B:9:ARG:HH11	1.77	0.48
1:A:5:ILE:HG22	1:A:6:GLN:N	2.29	0.48
1:D:115:GLU:O	1:D:117:PRO:HD3	2.12	0.48
1:D:126:HIS:ND1	1:D:126:HIS:N	2.61	0.48
1:B:99:TYR:O	1:B:100:ASN:ND2	2.47	0.48
1:B:67:MET:HE2	1:B:79:THR:HG21	1.91	0.48
1:D:383:VAL:HG22	1:D:422:LEU:HD13	1.95	0.48
1:C:110:PRO:O	1:C:111:MET:HE2	2.13	0.48
1:C:239:GLY:O	1:C:243:LEU:HG	2.13	0.48
1:D:106:TRP:HB3	1:D:130:CYS:HB3	1.95	0.48
1:C:152:TRP:CD1	1:C:161:VAL:HG21	2.49	0.48
1:A:89:VAL:HG13	1:A:292:VAL:HG12	1.96	0.48
1:A:41:ILE:HG22	1:A:106:TRP:O	2.13	0.48
1:C:47:GLU:HB2	1:C:52:PHE:CE1	2.49	0.48
1:B:369:PHE:N	1:B:370:LYS:HZ2	2.12	0.48
1:D:93:ILE:HG23	1:D:99:TYR:OH	2.14	0.48
1:D:259:ARG:HH11	1:D:259:ARG:HG3	1.79	0.48
1:C:316:VAL:O	1:C:320:ASN:HB2	2.13	0.48
1:B:368:ASN:OD1	1:B:370:LYS:HD2	2.14	0.48
1:D:410:VAL:HG12	1:D:411:ALA:N	2.29	0.48
1:D:386:VAL:HG12	1:D:387:LEU:N	2.29	0.48
1:A:171:LEU:HA	1:A:174:ARG:NH1	2.29	0.47
1:D:251:TYR:C	1:D:251:TYR:HD1	2.18	0.47
1:A:72:ASP:HB2	1:A:78:LEU:CD2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:CYS:SG	1:B:307:MET:HG3	2.54	0.47
1:D:69:THR:HA	1:D:78:LEU:O	2.14	0.47
1:D:136:GLN:O	1:D:287:ARG:NH2	2.47	0.47
1:D:379:TRP:CE3	1:D:379:TRP:HA	2.47	0.47
1:C:111:MET:HB2	1:C:125:PHE:CZ	2.49	0.47
1:A:72:ASP:C	1:A:74:ASN:H	2.17	0.47
1:A:45:ILE:HD13	1:A:81:ARG:CZ	2.44	0.47
1:B:21:ILE:CD1	1:B:21:ILE:H	2.26	0.47
1:D:263:TYR:CD2	1:D:291:LEU:HD13	2.46	0.47
1:C:364:HIS:HD2	1:D:104:ARG:HH22	1.58	0.47
1:D:51:LEU:HD21	1:D:295:LEU:HD13	1.96	0.47
1:A:116:ARG:O	1:A:118:GLN:HG3	2.15	0.47
1:D:259:ARG:HG2	1:D:268:VAL:CG1	2.45	0.47
1:D:73:ARG:NH1	1:D:73:ARG:CG	2.78	0.47
1:C:234:ARG:HA	1:C:234:ARG:HD3	1.74	0.47
1:A:111:MET:HB2	1:A:125:PHE:CZ	2.49	0.47
1:D:367:GLY:HA2	1:D:371:LYS:HD2	1.95	0.47
1:A:32:VAL:CG1	1:A:150:ARG:HD2	2.36	0.47
1:D:383:VAL:CG2	1:D:422:LEU:HD13	2.44	0.47
1:C:334:VAL:HG21	1:C:373:PHE:HE1	1.75	0.47
1:D:361:MET:HE2	1:D:379:TRP:HE1	1.80	0.47
1:A:414:SER:O	1:A:418:HIS:CD2	2.60	0.47
1:B:148:THR:HB	1:B:152:TRP:CZ2	2.49	0.47
1:A:411:ALA:O	1:A:415:VAL:HG13	2.14	0.47
1:D:51:LEU:HD22	1:D:86:ALA:HB1	1.97	0.47
1:C:44:PRO:O	1:C:81:ARG:NH1	2.48	0.47
1:B:367:GLY:HA2	1:B:371:LYS:HD2	1.96	0.47
1:C:179:ASP:O	1:C:183:ALA:HB2	2.15	0.47
1:A:333:LEU:HD23	1:A:334:VAL:O	2.15	0.47
1:B:231:GLU:O	1:B:235:GLU:HG3	2.15	0.47
1:C:311:ARG:NH2	3:C:452:ATP:N3	2.62	0.47
1:C:369:PHE:HA	1:C:372:GLN:HG3	1.97	0.47
1:B:89:VAL:HG11	1:B:291:LEU:CD2	2.45	0.47
1:D:251:TYR:C	1:D:251:TYR:CD1	2.88	0.47
1:B:241:CYS:HB2	1:B:242:LYS:HE2	1.97	0.47
1:B:112:PHE:N	1:B:112:PHE:CD1	2.82	0.46
1:D:72:ASP:HB2	1:D:78:LEU:HD21	1.97	0.46
1:C:46:VAL:HG22	1:D:11:MET:SD	2.55	0.46
1:A:171:LEU:O	1:A:175:ALA:N	2.47	0.46
1:C:60:THR:O	1:C:64:GLU:HG3	2.15	0.46
1:C:36:TYR:HB3	1:C:38:TYR:CD1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:451:HSO:H	3:D:452:ATP:PA	2.55	0.46
1:A:272:VAL:HG12	1:A:281:THR:HA	1.96	0.46
1:D:81:ARG:HA	1:D:82:PRO:HD2	1.75	0.46
1:C:139:ASP:HA	1:C:243:LEU:CD1	2.45	0.46
1:C:385:VAL:HG12	1:C:385:VAL:O	2.15	0.46
1:D:135:LEU:HD13	1:D:140:ILE:HG12	1.97	0.46
1:C:185:LEU:HA	1:C:185:LEU:HD23	1.75	0.46
1:A:351:LEU:HD21	1:A:415:VAL:CG2	2.45	0.46
1:A:146:MET:HE1	1:B:345:MET:SD	2.56	0.46
1:D:33:LEU:HD13	1:D:106:TRP:CG	2.51	0.46
1:C:169:GLY:CA	1:C:229:LEU:HD21	2.43	0.46
1:B:113:ARG:O	1:B:123:ARG:HA	2.15	0.46
1:D:235:GLU:CG	1:D:236:HIS:N	2.79	0.46
1:A:46:VAL:HG23	1:B:8:ILE:HD12	1.98	0.46
1:B:341:GLN:NE2	1:B:364:HIS:ND1	2.64	0.46
1:A:47:GLU:OE2	1:A:90:ARG:HD3	2.15	0.46
1:B:121:ARG:NH1	3:B:452:ATP:O2G	2.48	0.46
1:C:345:MET:SD	1:C:364:HIS:CE1	3.09	0.46
1:D:291:LEU:HD21	1:D:295:LEU:HD11	1.98	0.46
1:B:121:ARG:NH1	3:B:452:ATP:O1G	2.45	0.46
1:D:122:TYR:H	3:D:452:ATP:HN62	1.64	0.46
1:B:157:ILE:HG22	1:B:319:VAL:CG1	2.46	0.46
1:C:85:THR:OG1	2:C:451:HSO:CD2	2.64	0.46
1:A:22:TRP:CH2	1:A:310:GLU:HG3	2.49	0.46
1:B:138:PRO:HB3	1:B:240:LEU:HB2	1.96	0.46
1:B:287:ARG:NH2	1:B:303:VAL:HG21	2.31	0.46
1:D:152:TRP:HB3	1:D:157:ILE:HD12	1.98	0.46
1:B:89:VAL:HG11	1:B:291:LEU:HD23	1.97	0.46
1:B:160:HIS:ND1	1:B:319:VAL:HG21	2.31	0.46
1:C:397:ALA:HB2	1:C:412:GLN:HE21	1.80	0.46
1:A:382:ARG:HH21	1:A:423:LEU:HD22	1.81	0.46
1:A:150:ARG:HG3	1:A:150:ARG:HH11	1.81	0.46
1:B:25:ILE:HG21	1:B:312:LEU:HD21	1.98	0.46
1:C:332:TYR:OH	1:C:363:ASN:HB2	2.16	0.46
1:A:391:GLU:HA	1:A:396:THR:OG1	2.16	0.45
1:B:54:ARG:O	1:B:294:GLN:NE2	2.49	0.45
1:A:135:LEU:CD1	1:A:140:ILE:HG12	2.46	0.45
1:A:99:TYR:O	1:A:101:GLN:HG3	2.15	0.45
1:B:67:MET:HB3	1:B:79:THR:HG21	1.98	0.45
1:A:287:ARG:NH1	1:A:303:VAL:HG21	2.31	0.45
1:A:46:VAL:HG12	1:A:80:LEU:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:343:ALA:O	1:D:346:ALA:HB3	2.17	0.45
1:A:165:LEU:CD1	1:A:269:PHE:HB3	2.47	0.45
1:B:157:ILE:HD13	1:B:315:LEU:HD23	1.99	0.45
1:A:259:ARG:CG	1:A:259:ARG:NH1	2.77	0.45
1:B:288:TYR:CE1	1:B:302:ALA:CB	2.99	0.45
1:A:48:GLN:HB3	1:A:50:PRO:HD2	1.97	0.45
1:B:361:MET:HE1	1:B:379:TRP:CE2	2.51	0.45
1:A:59:VAL:HG22	1:A:59:VAL:O	2.17	0.45
1:A:261:LEU:N	1:A:261:LEU:HD22	2.31	0.45
1:D:259:ARG:HB2	1:D:264:TYR:HD2	1.80	0.45
1:B:291:LEU:HD23	1:B:291:LEU:C	2.37	0.45
1:A:412:GLN:HA	1:A:415:VAL:HG13	1.99	0.45
1:C:17:GLY:O	1:C:21:ILE:HD12	2.17	0.45
1:D:127:GLN:HE22	3:D:452:ATP:H5'1	1.81	0.45
1:D:152:TRP:CE3	1:D:157:ILE:HD11	2.52	0.45
1:A:60:THR:HG22	1:A:62:VAL:HG23	1.99	0.45
1:B:89:VAL:O	1:B:93:ILE:HG13	2.17	0.45
1:A:5:ILE:CG2	1:A:6:GLN:N	2.79	0.45
1:D:160:HIS:O	1:D:161:VAL:HG13	2.16	0.45
1:C:368:ASN:ND2	1:C:371:LYS:HB2	2.32	0.45
1:C:32:VAL:HG13	1:C:150:ARG:CD	2.47	0.45
1:C:334:VAL:HG12	1:C:369:PHE:HE1	1.81	0.45
1:B:14:TYR:HE2	1:B:126:HIS:CE1	2.32	0.45
1:B:331:ILE:HD13	1:B:358:VAL:CG1	2.47	0.45
1:C:45:ILE:HG12	1:D:124:GLN:OE1	2.17	0.45
1:C:4:ASN:HD21	1:D:93:ILE:HG21	1.82	0.45
1:D:241:CYS:SG	1:D:251:TYR:OH	2.54	0.45
1:B:419:LEU:HA	1:B:419:LEU:HD23	1.67	0.45
1:A:151:TRP:O	1:A:155:LEU:HD22	2.17	0.45
1:A:254:ASN:HD21	1:A:256:ARG:CZ	2.29	0.44
1:D:25:ILE:HD12	1:D:313:VAL:HG22	1.99	0.44
1:B:125:PHE:CD2	3:B:452:ATP:C6	3.05	0.44
1:A:127:GLN:NE2	3:A:452:ATP:H5'1	2.32	0.44
1:B:350:ARG:NH1	1:B:412:GLN:HB3	2.31	0.44
1:A:309:LEU:HD23	1:A:309:LEU:HA	1.66	0.44
1:B:341:GLN:NE2	1:B:364:HIS:HA	2.33	0.44
1:A:57:GLY:O	1:A:63:VAL:HG21	2.16	0.44
1:A:120:GLY:C	1:A:311:ARG:HH21	2.21	0.44
1:C:163:LEU:HD12	1:C:165:LEU:HD12	1.99	0.44
1:B:244:LEU:HA	1:B:244:LEU:HD13	1.84	0.44
1:B:20:ALA:HB3	1:B:21:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:PHE:HZ	1:D:45:ILE:HG13	1.83	0.44
1:A:49:THR:HG23	1:A:79:THR:OG1	2.17	0.44
1:D:290:GLY:O	1:D:293:GLU:HG2	2.17	0.44
1:B:15:LEU:H	1:B:15:LEU:HD22	1.82	0.44
1:D:98:LEU:CD2	1:D:133:PHE:HD2	2.30	0.44
1:D:312:LEU:O	1:D:313:VAL:C	2.55	0.44
1:C:116:ARG:NH1	1:C:116:ARG:HG3	2.28	0.44
1:D:163:LEU:HD23	1:D:251:TYR:HB3	1.98	0.44
1:D:151:TRP:CZ3	1:D:307:MET:HE2	2.52	0.44
1:C:174:ARG:HA	1:C:177:TYR:HB3	1.99	0.44
1:A:274:ASN:N	1:A:274:ASN:HD22	2.15	0.44
1:A:97:LEU:CD2	1:A:97:LEU:N	2.81	0.44
1:D:234:ARG:NH1	1:D:234:ARG:CG	2.77	0.44
1:D:148:THR:HG22	1:D:152:TRP:CZ2	2.53	0.44
1:B:291:LEU:O	1:B:295:LEU:HG	2.18	0.44
1:D:369:PHE:HB3	1:D:373:PHE:HE2	1.83	0.44
1:C:40:GLU:HG2	1:D:19:THR:HB	2.00	0.44
1:D:332:TYR:OH	1:D:363:ASN:OD1	2.33	0.44
1:C:45:ILE:O	1:C:81:ARG:HG2	2.18	0.44
1:D:253:VAL:O	1:D:253:VAL:HG13	2.18	0.44
1:B:73:ARG:HG3	4:B:512:HOH:O	2.18	0.44
1:C:386:VAL:HB	1:C:398:VAL:HB	1.99	0.44
1:C:52:PHE:CD2	1:C:82:PRO:HD2	2.52	0.44
1:C:326:ASP:HB2	1:C:359:LYS:NZ	2.33	0.44
1:C:38:TYR:CD2	1:C:104:ARG:HB3	2.53	0.43
1:C:12:ASN:H	1:C:12:ASN:HD22	1.62	0.43
1:C:5:ILE:HD12	1:D:51:LEU:CG	2.45	0.43
1:A:16:PRO:HG3	1:B:105:LEU:CD2	2.48	0.43
1:B:148:THR:O	1:B:151:TRP:HB2	2.18	0.43
1:C:166:ASN:O	1:C:268:VAL:HG22	2.18	0.43
1:C:274:ASN:OD1	1:C:275:SER:N	2.50	0.43
1:D:288:TYR:CD1	1:D:288:TYR:O	2.70	0.43
1:A:233:SER:OG	1:A:266:ARG:HG2	2.19	0.43
1:A:257:LEU:HD13	1:A:268:VAL:HG12	2.00	0.43
1:B:333:LEU:HB3	1:B:362:THR:HA	2.01	0.43
1:B:336:SER:O	1:B:340:THR:HG21	2.18	0.43
1:A:291:LEU:O	1:A:291:LEU:HD12	2.17	0.43
1:C:43:LEU:HA	1:C:44:PRO:HD3	1.86	0.43
1:B:85:THR:O	1:B:89:VAL:CG2	2.66	0.43
1:A:27:GLY:O	1:A:28:THR:C	2.57	0.43
1:D:383:VAL:HG11	1:D:419:LEU:HD23	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:ILE:HG13	1:D:145:ILE:H	1.50	0.43
1:D:320:ASN:N	1:D:321:PRO:HD3	2.33	0.43
1:D:47:GLU:HB2	1:D:52:PHE:CZ	2.53	0.43
1:C:331:ILE:HD12	1:C:331:ILE:N	2.33	0.43
1:B:288:TYR:O	1:B:288:TYR:HD1	2.01	0.43
1:D:49:THR:N	1:D:50:PRO:HD2	2.32	0.43
1:A:45:ILE:HG12	1:B:124:GLN:NE2	2.31	0.43
1:B:391:GLU:OE1	1:B:391:GLU:N	2.51	0.43
1:A:90:ARG:NH2	1:B:13:ASP:OD2	2.49	0.43
1:C:251:TYR:H	1:C:251:TYR:HD1	1.66	0.43
1:C:141:ASP:OD1	1:C:287:ARG:NH2	2.51	0.43
1:A:15:LEU:O	1:A:16:PRO:C	2.57	0.43
1:A:147:LEU:C	1:A:147:LEU:HD23	2.38	0.43
1:C:312:LEU:HD12	1:C:312:LEU:HA	1.77	0.43
1:C:40:GLU:O	1:D:19:THR:HG21	2.19	0.43
1:D:383:VAL:CG1	1:D:384:ALA:N	2.81	0.43
1:D:329:VAL:HB	1:D:379:TRP:HB3	2.01	0.43
1:B:98:LEU:HD22	1:B:133:PHE:CD2	2.52	0.43
1:B:161:VAL:HG23	1:B:271:TRP:CE3	2.54	0.43
1:A:167:SER:HB2	1:A:237:PHE:CD1	2.54	0.43
1:D:340:THR:O	1:D:343:ALA:N	2.51	0.43
1:A:169:GLY:HA3	1:A:229:LEU:CD2	2.48	0.43
1:D:133:PHE:CE1	1:D:288:TYR:OH	2.71	0.43
1:C:163:LEU:HD23	1:C:271:TRP:NE1	2.33	0.43
1:A:386:VAL:HG12	1:A:387:LEU:N	2.34	0.43
1:D:128:LEU:HB3	1:D:309:LEU:HD11	2.00	0.43
1:C:164:GLU:HA	1:C:252:THR:O	2.19	0.43
1:B:41:ILE:O	1:B:41:ILE:HG23	2.19	0.43
1:B:108:ILE:HB	1:B:128:LEU:HD12	1.99	0.43
1:B:314:LEU:HA	1:B:317:GLN:OE1	2.19	0.43
1:D:292:VAL:HG21	1:D:300:THR:HG22	2.01	0.43
1:D:166:ASN:ND2	1:D:168:ILE:HD13	2.34	0.43
1:D:287:ARG:O	1:D:288:TYR:HB3	2.19	0.43
1:D:324:LYS:HD2	1:D:324:LYS:N	2.34	0.43
1:B:81:ARG:HA	1:B:82:PRO:HD2	1.98	0.43
1:C:19:THR:O	1:C:22:TRP:N	2.52	0.43
1:D:386:VAL:HB	1:D:398:VAL:HB	2.01	0.43
1:A:49:THR:N	1:A:50:PRO:CD	2.81	0.43
1:A:152:TRP:HB3	1:A:158:SER:HA	2.01	0.43
1:B:30:LYS:O	1:B:33:LEU:HB2	2.19	0.42
1:D:314:LEU:HD23	1:D:314:LEU:HA	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:ALA:HA	1:A:94:GLU:HB3	2.01	0.42
1:C:331:ILE:HD12	1:C:331:ILE:H	1.84	0.42
1:C:47:GLU:HB2	1:C:52:PHE:HE1	1.84	0.42
1:A:278:SER:CA	1:A:311:ARG:HD3	2.49	0.42
1:D:40:GLU:HG3	1:D:106:TRP:CH2	2.55	0.42
1:B:232:GLU:OE1	1:B:266:ARG:NH1	2.51	0.42
1:D:168:ILE:HG23	1:D:168:ILE:O	2.20	0.42
1:C:334:VAL:CG1	1:C:373:PHE:HE1	2.26	0.42
1:C:181:LEU:O	1:C:184:PHE:HB3	2.19	0.42
1:B:83:GLU:OE2	1:B:85:THR:HB	2.19	0.42
1:B:370:LYS:H	1:B:370:LYS:CE	2.31	0.42
1:B:5:ILE:N	1:B:5:ILE:HD12	2.33	0.42
1:A:319:VAL:HG12	1:A:320:ASN:HD22	1.82	0.42
1:C:347:LEU:HG	1:C:351:LEU:HD11	2.00	0.42
1:D:68:TYR:OH	1:D:123:ARG:NE	2.52	0.42
1:C:63:VAL:HA	1:C:67:MET:SD	2.60	0.42
1:B:242:LYS:O	1:B:243:LEU:C	2.56	0.42
1:A:139:ASP:HA	1:A:243:LEU:HD23	2.01	0.42
1:B:288:TYR:CE1	1:B:302:ALA:HB1	2.55	0.42
1:B:72:ASP:HB2	1:B:78:LEU:CD1	2.48	0.42
1:D:46:VAL:CG1	1:D:80:LEU:HD12	2.35	0.42
1:A:165:LEU:HD13	1:A:269:PHE:CB	2.49	0.42
1:A:166:ASN:O	1:A:268:VAL:N	2.50	0.42
1:D:125:PHE:CE1	1:D:127:GLN:HG3	2.55	0.42
1:B:259:ARG:HB2	1:B:264:TYR:CD2	2.55	0.42
1:C:347:LEU:HD12	1:C:347:LEU:HA	1.80	0.42
1:B:157:ILE:HG22	1:B:319:VAL:HG11	2.01	0.42
1:D:259:ARG:CG	1:D:268:VAL:HG13	2.48	0.42
1:C:163:LEU:CD1	1:C:165:LEU:HD12	2.50	0.42
1:B:361:MET:CE	1:B:379:TRP:NE1	2.83	0.42
1:A:184:PHE:C	1:A:184:PHE:CD1	2.93	0.42
1:C:256:ARG:HD2	1:C:256:ARG:C	2.39	0.42
1:A:287:ARG:NH1	1:A:303:VAL:HG22	2.35	0.42
1:D:235:GLU:HG2	1:D:236:HIS:H	1.81	0.42
1:C:45:ILE:CD1	1:C:81:ARG:NH2	2.83	0.42
1:A:10:GLY:O	1:A:123:ARG:N	2.51	0.42
1:D:361:MET:HE2	1:D:379:TRP:NE1	2.35	0.41
1:A:112:PHE:CD1	1:A:112:PHE:N	2.88	0.41
1:A:80:LEU:HD23	1:A:112:PHE:CD2	2.55	0.41
1:B:8:ILE:O	1:B:9:ARG:C	2.58	0.41
1:C:307:MET:SD	1:C:312:LEU:HD22	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:MET:HE2	1:B:379:TRP:NE1	2.35	0.41
1:A:34:GLY:O	1:A:36:TYR:N	2.52	0.41
1:C:334:VAL:HG21	1:C:373:PHE:CD1	2.53	0.41
1:B:161:VAL:HA	1:B:272:VAL:O	2.20	0.41
1:A:410:VAL:HG12	1:A:411:ALA:O	2.20	0.41
1:A:383:VAL:HG11	1:A:422:LEU:CD1	2.49	0.41
1:A:231:GLU:HA	1:A:231:GLU:OE1	2.21	0.41
1:B:139:ASP:HA	1:B:243:LEU:HD13	2.02	0.41
1:A:68:TYR:HB2	1:A:80:LEU:HB2	2.03	0.41
1:A:44:PRO:HA	1:B:124:GLN:OE1	2.19	0.41
1:D:391:GLU:HG2	1:D:398:VAL:HG23	2.02	0.41
1:B:33:LEU:HD11	1:B:128:LEU:HD21	2.00	0.41
1:D:394:ASN:O	1:D:396:THR:HG23	2.20	0.41
1:D:257:LEU:HD21	1:D:270:GLU:HG2	2.03	0.41
1:A:105:LEU:O	1:A:130:CYS:HB2	2.20	0.41
1:B:9:ARG:HE	1:B:116:ARG:NH2	2.15	0.41
1:A:230:ASP:OD2	1:A:233:SER:HB2	2.21	0.41
1:D:265:ASN:HD22	1:D:288:TYR:HA	1.85	0.41
1:B:312:LEU:HD23	1:B:312:LEU:C	2.41	0.41
1:D:89:VAL:HG21	1:D:291:LEU:HD22	2.03	0.41
1:D:283:CYS:SG	1:D:307:MET:HB2	2.60	0.41
1:B:102:GLU:OE2	1:B:135:LEU:HD21	2.20	0.41
1:A:90:ARG:NH2	1:B:7:ALA:HB2	2.36	0.41
1:D:103:GLN:HA	1:D:103:GLN:OE1	2.21	0.41
1:B:265:ASN:HD22	1:B:266:ARG:NE	2.15	0.41
1:C:106:TRP:HB3	1:C:130:CYS:HB3	2.03	0.41
1:B:244:LEU:HD12	1:B:249:ILE:CG2	2.51	0.41
1:A:8:ILE:O	1:A:9:ARG:C	2.58	0.41
1:A:383:VAL:CG2	1:A:422:LEU:HD22	2.51	0.41
1:C:105:LEU:H	1:C:105:LEU:HD23	1.84	0.41
1:D:415:VAL:HG12	1:D:419:LEU:CD1	2.51	0.41
1:B:287:ARG:HG3	1:B:302:ALA:O	2.21	0.41
1:D:322:GLU:HA	1:D:324:LYS:NZ	2.36	0.41
1:C:44:PRO:HA	1:D:124:GLN:NE2	2.32	0.41
1:B:130:CYS:SG	1:B:305:PHE:HE1	2.44	0.41
1:A:410:VAL:CG1	1:A:411:ALA:N	2.84	0.41
1:C:102:GLU:OE1	1:C:135:LEU:HD21	2.21	0.41
1:C:171:LEU:HD13	1:C:171:LEU:N	2.36	0.41
1:D:263:TYR:HB3	1:D:291:LEU:CD1	2.51	0.40
1:C:56:ILE:HG23	1:C:261:LEU:HD13	2.03	0.40
1:B:91:ALA:O	1:B:95:HIS:CD2	2.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ASN:N	1:B:54:ARG:HH22	2.18	0.40
1:B:235:GLU:H	1:B:235:GLU:HG3	1.75	0.40
1:B:341:GLN:HE22	1:B:364:HIS:HA	1.84	0.40
1:D:128:LEU:CB	1:D:309:LEU:HD11	2.51	0.40
1:D:259:ARG:NH1	1:D:264:TYR:CZ	2.89	0.40
1:C:254:ASN:HD21	1:C:256:ARG:CZ	2.35	0.40
1:D:311:ARG:HD3	3:D:452:ATP:C2	2.56	0.40
1:C:5:ILE:HG21	1:D:48:GLN:HB2	2.04	0.40
1:B:397:ALA:HB3	1:B:415:VAL:HG21	2.03	0.40
1:C:174:ARG:O	1:C:177:TYR:N	2.54	0.40
1:D:368:ASN:HD21	1:D:371:LYS:HE3	1.84	0.40
1:D:273:THR:CG2	1:D:277:GLY:H	2.35	0.40
1:C:73:ARG:HA	1:C:73:ARG:HD3	1.65	0.40
1:B:368:ASN:CG	1:B:370:LYS:HD2	2.41	0.40
1:D:355:LEU:HB3	1:D:358:VAL:HG21	2.03	0.40
1:D:133:PHE:CE1	1:D:302:ALA:HB1	2.57	0.40
1:C:56:ILE:HG12	1:C:261:LEU:HD12	2.04	0.40
1:B:47:GLU:OE2	1:B:90:ARG:HD3	2.21	0.40
1:B:163:LEU:HD23	1:B:251:TYR:HB3	2.03	0.40
1:A:41:ILE:HG23	1:A:41:ILE:O	2.21	0.40
1:B:374:ALA:O	1:B:377:ASP:HB2	2.21	0.40
1:A:121:ARG:HG2	1:A:121:ARG:H	1.59	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	375/424 (88%)	326 (87%)	38 (10%)	11 (3%)	6	19
1	B	360/424 (85%)	317 (88%)	35 (10%)	8 (2%)	8	28
1	C	383/424 (90%)	331 (86%)	41 (11%)	11 (3%)	6	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	360/424 (85%)	317 (88%)	38 (11%)	5 (1%)	14	42
All	All	1478/1696 (87%)	1291 (87%)	152 (10%)	35 (2%)	7	25

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	288	TYR
1	A	338	ALA
1	B	64	GLU
1	B	288	TYR
1	B	338	ALA
1	C	137	GLY
1	C	276	LEU
1	C	278	SER
1	C	288	TYR
1	C	338	ALA
1	D	288	TYR
1	A	8	ILE
1	A	73	ARG
1	A	137	GLY
1	A	321	PRO
1	B	117	PRO
1	B	137	GLY
1	C	136	GLN
1	C	341	GLN
1	C	366	GLY
1	D	137	GLY
1	D	338	ALA
1	A	341	GLN
1	A	366	GLY
1	B	276	LEU
1	D	64	GLU
1	D	341	GLN
1	A	16	PRO
1	B	321	PRO
1	C	16	PRO
1	C	340	THR
1	B	341	GLN
1	A	82	PRO
1	A	365	GLY
1	C	365	GLY

### 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	299/342 (87%)	251 (84%)	48 (16%)	3	9
1	B	286/342 (84%)	235 (82%)	51 (18%)	2	6
1	C	301/342 (88%)	247 (82%)	54 (18%)	2	6
1	D	285/342 (83%)	229 (80%)	56 (20%)	1	5
All	All	1171/1368 (86%)	962 (82%)	209 (18%)	2	6

All (209) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ILE
1	A	9	ARG
1	A	15	LEU
1	A	16	PRO
1	A	18	GLU
1	A	19	THR
1	A	35	SER
1	A	39	SER
1	A	48	GLN
1	A	65	LYS
1	A	67	MET
1	A	78	LEU
1	A	97	LEU
1	A	105	LEU
1	A	116	ARG
1	A	121	ARG
1	A	128	LEU
1	A	139	ASP
1	A	140	ILE
1	A	161	VAL
1	A	174	ARG
1	A	235	GLU
1	A	246	SER
1	A	251	TYR

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Mol	Chain	Res	Type
1	A	255	GLN
1	A	256	ARG
1	A	257	LEU
1	A	259	ARG
1	A	261	LEU
1	A	263	TYR
1	A	276	LEU
1	A	281	THR
1	A	295	LEU
1	A	307	MET
1	A	311	ARG
1	A	322	GLU
1	A	324	LYS
1	A	327	PRO
1	A	328	VAL
1	A	339	ASP
1	A	342	SER
1	A	354	GLU
1	A	362	THR
1	A	382	ARG
1	A	383	VAL
1	A	403	ARG
1	A	414	SER
1	A	421	THR
1	B	12	ASN
1	B	16	PRO
1	B	24	ARG
1	B	30	LYS
1	B	46	VAL
1	B	54	ARG
1	B	58	GLU
1	B	59	VAL
1	B	67	MET
1	B	71	GLU
1	B	77	SER
1	B	79	THR
1	B	89	VAL
1	B	90	ARG
1	B	105	LEU
1	B	108	ILE
1	B	116	ARG
1	B	118	GLN

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Mol	Chain	Res	Type
1	B	121	ARG
1	B	128	LEU
1	B	131	GLU
1	B	132	VAL
1	B	139	ASP
1	B	141	ASP
1	B	232	GLU
1	B	235	GLU
1	B	251	TYR
1	B	252	THR
1	B	256	ARG
1	B	257	LEU
1	B	259	ARG
1	B	261	LEU
1	B	263	TYR
1	B	266	ARG
1	B	274	ASN
1	B	293	GLU
1	B	298	ARG
1	B	303	VAL
1	B	307	MET
1	B	322	GLU
1	B	323	PHE
1	B	333	LEU
1	B	339	ASP
1	B	340	THR
1	B	342	SER
1	B	370	LYS
1	B	382	ARG
1	B	404	SER
1	B	407	GLN
1	B	408	THR
1	B	414	SER
1	C	12	ASN
1	C	16	PRO
1	C	24	ARG
1	C	35	SER
1	C	39	SER
1	C	40	GLU
1	C	48	GLN
1	C	73	ARG
1	C	74	ASN

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Mol	Chain	Res	Type
1	C	78	LEU
1	C	80	LEU
1	C	81	ARG
1	C	83	GLU
1	C	105	LEU
1	C	108	ILE
1	C	116	ARG
1	C	117	PRO
1	C	119	LYS
1	C	153	ARG
1	C	161	VAL
1	C	165	LEU
1	C	168	ILE
1	C	171	LEU
1	C	184	PHE
1	C	234	ARG
1	C	240	LEU
1	C	251	TYR
1	C	255	GLN
1	C	256	ARG
1	C	257	LEU
1	C	261	LEU
1	C	263	TYR
1	C	270	GLU
1	C	274	ASN
1	C	276	LEU
1	C	287	ARG
1	C	303	VAL
1	C	320	ASN
1	C	322	GLU
1	C	324	LYS
1	C	327	PRO
1	C	331	ILE
1	C	339	ASP
1	C	342	SER
1	C	360	LEU
1	C	372	GLN
1	C	382	ARG
1	C	383	VAL
1	C	387	LEU
1	C	389	GLU
1	C	406	GLU

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Mol	Chain	Res	Type
1	C	412	GLN
1	C	421	THR
1	C	423	LEU
1	D	4	ASN
1	D	12	ASN
1	D	13	ASP
1	D	15	LEU
1	D	16	PRO
1	D	24	ARG
1	D	31	ASN
1	D	46	VAL
1	D	51	LEU
1	D	59	VAL
1	D	61	ASP
1	D	64	GLU
1	D	67	MET
1	D	76	ASP
1	D	78	LEU
1	D	100	ASN
1	D	101	GLN
1	D	105	LEU
1	D	115	GLU
1	D	118	GLN
1	D	121	ARG
1	D	126	HIS
1	D	131	GLU
1	D	140	ILE
1	D	141	ASP
1	D	148	THR
1	D	153	ARG
1	D	158	SER
1	D	161	VAL
1	D	168	ILE
1	D	232	GLU
1	D	234	ARG
1	D	251	TYR
1	D	257	LEU
1	D	263	TYR
1	D	266	ARG
1	D	274	ASN
1	D	283	CYS
1	D	303	VAL

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Mol	Chain	Res	Type
1	D	307	MET
1	D	309	LEU
1	D	311	ARG
1	D	320	ASN
1	D	323	PHE
1	D	324	LYS
1	D	328	VAL
1	D	333	LEU
1	D	341	GLN
1	D	342	SER
1	D	350	ARG
1	D	371	LYS
1	D	382	ARG
1	D	390	SER
1	D	401	ASP
1	D	407	GLN
1	D	421	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	255	GLN
1	A	274	ASN
1	A	317	GLN
1	A	320	ASN
1	A	363	ASN
1	A	372	GLN
1	A	418	HIS
1	B	12	ASN
1	B	95	HIS
1	B	114	HIS
1	B	118	GLN
1	B	124	GLN
1	B	166	ASN
1	B	341	GLN
1	C	4	ASN
1	C	12	ASN
1	C	100	ASN
1	C	118	GLN
1	C	255	GLN
1	C	294	GLN

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Mol	Chain	Res	Type
1	C	317	GLN
1	C	320	ASN
1	C	363	ASN
1	C	364	HIS
1	C	412	GLN
1	C	418	HIS
1	D	12	ASN
1	D	48	GLN
1	D	136	GLN
1	D	166	ASN
1	D	320	ASN
1	D	364	HIS
1	D	407	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no 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	HSO	A	451	-	5,10,10	1.96	1 (20%)	2,12,12	2.37	1 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ATP	A	452	-	24,33,33	0.76	0	31,52,52	0.89	1 (3%)
2	HSO	B	451	-	5,10,10	1.78	1 (20%)	2,12,12	2.24	1 (50%)
3	ATP	B	452	-	24,33,33	0.76	0	31,52,52	0.73	0
2	HSO	C	451	-	5,10,10	1.90	1 (20%)	2,12,12	2.41	1 (50%)
3	ATP	C	452	-	24,33,33	0.78	0	31,52,52	0.85	0
2	HSO	D	451	-	5,10,10	1.84	1 (20%)	2,12,12	2.58	1 (50%)
3	ATP	D	452	-	24,33,33	0.74	0	31,52,52	0.85	1 (3%)

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	HSO	A	451	-	-	0/5/6/6	0/1/1/1
3	ATP	A	452	-	-	0/18/38/38	0/3/3/3
2	HSO	B	451	-	-	0/5/6/6	0/1/1/1
3	ATP	B	452	-	-	0/18/38/38	0/3/3/3
2	HSO	C	451	-	-	0/5/6/6	0/1/1/1
3	ATP	C	452	-	-	0/18/38/38	0/3/3/3
2	HSO	D	451	-	-	0/5/6/6	0/1/1/1
3	ATP	D	452	-	-	0/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	451	HSO	O-C	-4.32	1.23	1.42
2	C	451	HSO	O-C	-4.09	1.24	1.42
2	D	451	HSO	O-C	-4.04	1.24	1.42
2	B	451	HSO	O-C	-3.85	1.25	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	452	ATP	O3G-PG-O2G	2.08	115.31	107.38
3	A	452	ATP	C2'-C1'-N9	2.18	117.63	114.29
2	B	451	HSO	O-C-CA	3.16	120.11	111.84
2	A	451	HSO	O-C-CA	3.25	120.36	111.84
2	C	451	HSO	O-C-CA	3.40	120.74	111.84
2	D	451	HSO	O-C-CA	3.62	121.33	111.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	452	ATP	3	0
2	B	451	HSO	1	0
3	B	452	ATP	11	0
2	C	451	HSO	2	0
3	C	452	ATP	8	0
2	D	451	HSO	1	0
3	D	452	ATP	12	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	379/424 (89%)	-0.45	1 (0%) 94 92	13, 41, 69, 81	0
1	B	364/424 (85%)	-0.38	5 (1%) 78 69	16, 44, 75, 96	0
1	C	387/424 (91%)	-0.45	0 100 100	14, 43, 69, 77	0
1	D	364/424 (85%)	-0.40	5 (1%) 78 69	16, 44, 76, 99	0
All	All	1494/1696 (88%)	-0.42	11 (0%) 89 84	13, 43, 72, 99	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	278	SER	4.4
1	B	424	GLY	3.0
1	D	424	GLY	2.8
1	B	257	LEU	2.8
1	B	59	VAL	2.6
1	D	276	LEU	2.2
1	D	242	LYS	2.2
1	D	59	VAL	2.1
1	B	60	THR	2.1
1	A	374	ALA	2.1
1	B	277	GLY	2.1

### 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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	HSO	C	451	10/10	0.91	0.18	1.83	0,31,35,41	0
2	HSO	A	451	10/10	0.92	0.18	1.77	0,28,34,37	0
2	HSO	D	451	10/10	0.93	0.16	0.45	0,35,38,40	0
2	HSO	B	451	10/10	0.94	0.15	0.32	0,26,32,32	0
3	ATP	D	452	31/31	0.91	0.17	0.15	0,57,69,70	0
3	ATP	B	452	31/31	0.91	0.15	-0.09	0,45,78,79	0
3	ATP	A	452	31/31	0.94	0.13	-0.44	0,35,47,52	0
3	ATP	C	452	31/31	0.94	0.13	-0.52	0,35,55,58	0

## 6.5 Other polymers

There are no such residues in this entry.