



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:07 AM GMT

PDB ID : 3DC1  
Title : Crystal structure of kynurenine aminotransferase II complex with alpha-ketoglutarate  
Authors : Han, Q.; Cai, T.; Tagle, D.A.; Robinson, H.; Li, J.  
Deposited on : 2008-06-03  
Resolution : 2.50 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

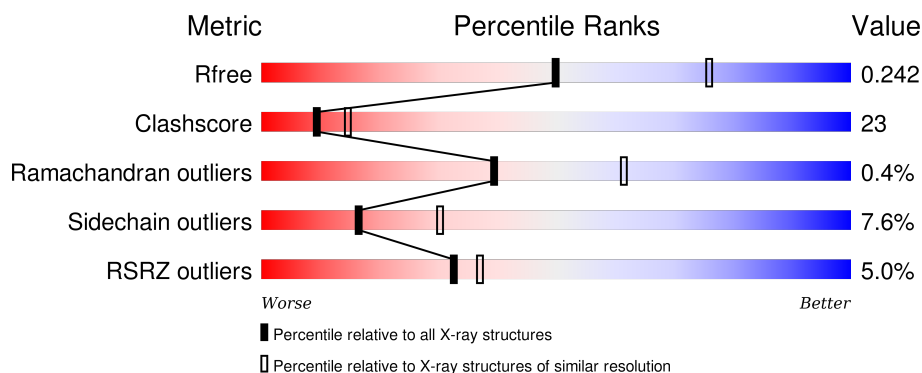
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	425	<div> <div>4%</div> <div>58% 35% 5%</div> </div>
1	B	425	<div> <div>5%</div> <div>59% 32% 6%</div> </div>
1	C	425	<div> <div>6%</div> <div>61% 34% 5%</div> </div>
1	D	425	<div> <div>4%</div> <div>60% 32% 6%</div> </div>

## 2 Entry composition [i](#)

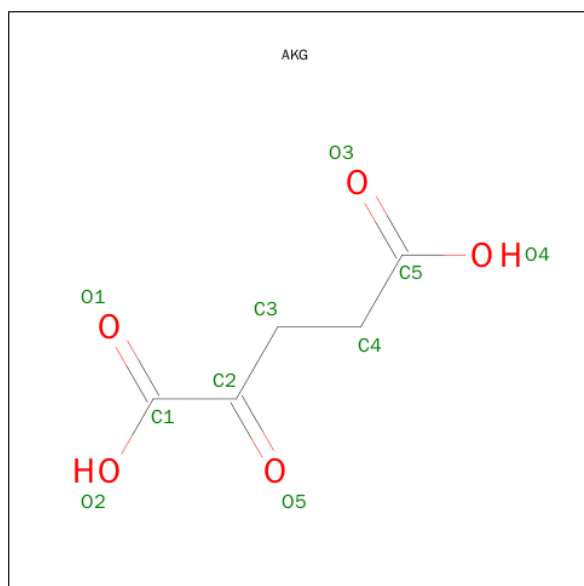
There are 4 unique types of molecules in this entry. The entry contains 14067 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Kynurenine/alpha-aminoadipate aminotransferase mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	415	Total	C	N	O	P	S	0	0	0
			3265	2097	544	606	1	17			
1	B	417	Total	C	N	O	P	S	0	0	0
			3285	2109	549	609	1	17			
1	C	425	Total	C	N	O	P	S	0	0	0
			3347	2147	560	621	1	18			
1	D	418	Total	C	N	O	P	S	0	0	0
			3296	2115	553	610	1	17			

- Molecule 2 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: C<sub>5</sub>H<sub>6</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	5	5		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

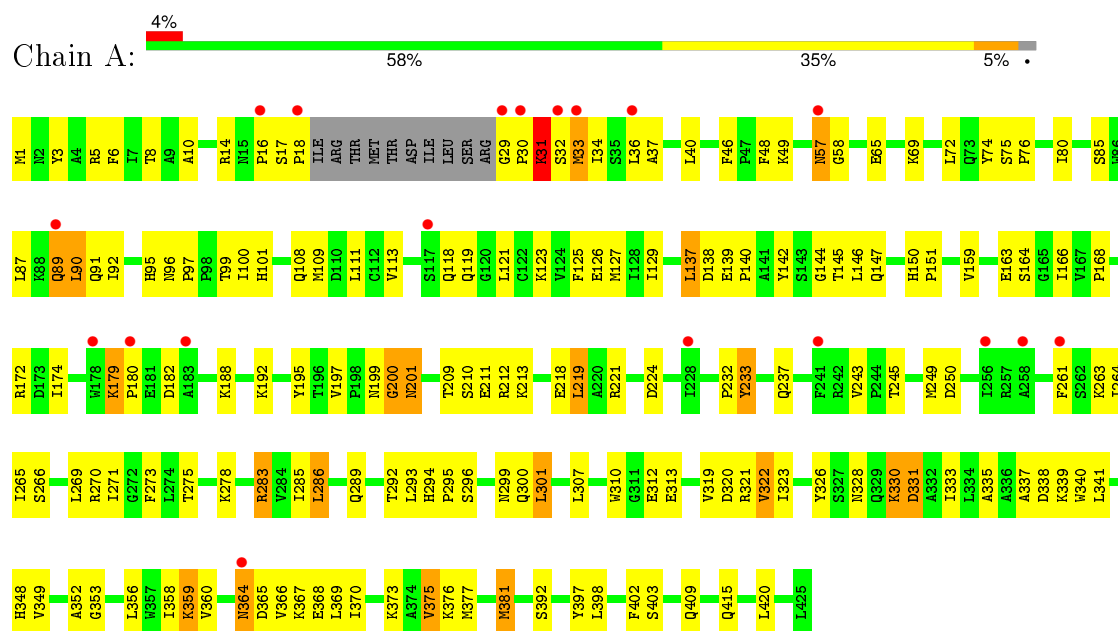
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	225	Total	O	0	0
			225	225		
4	B	226	Total	O	0	0
			226	226		
4	C	202	Total	O	0	0
			202	202		
4	D	175	Total	O	0	0
			175	175		

### 3 Residue-property plots

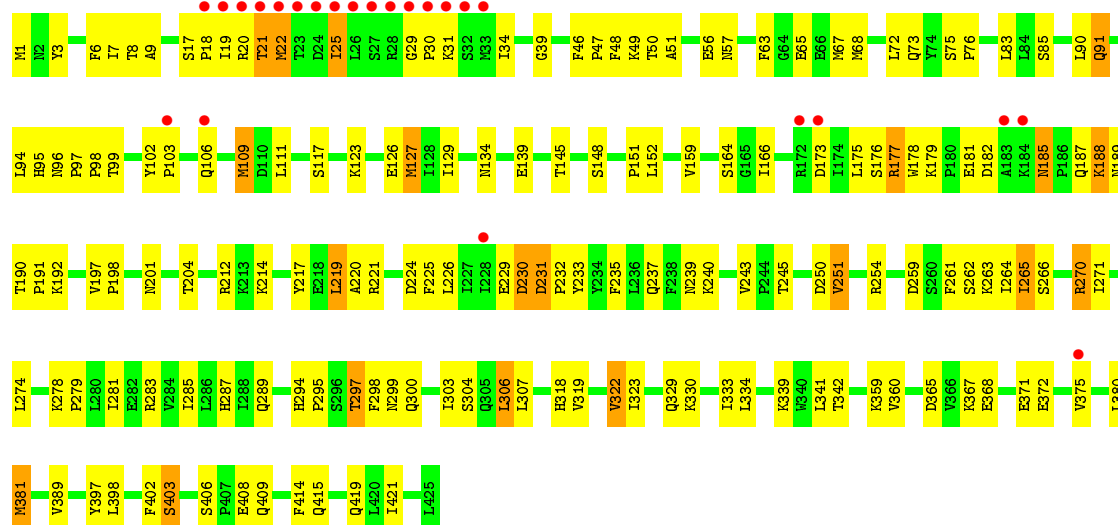
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

- Molecule 1: Kynurenine/alpha-aminoadipate aminotransferase mitochondrial

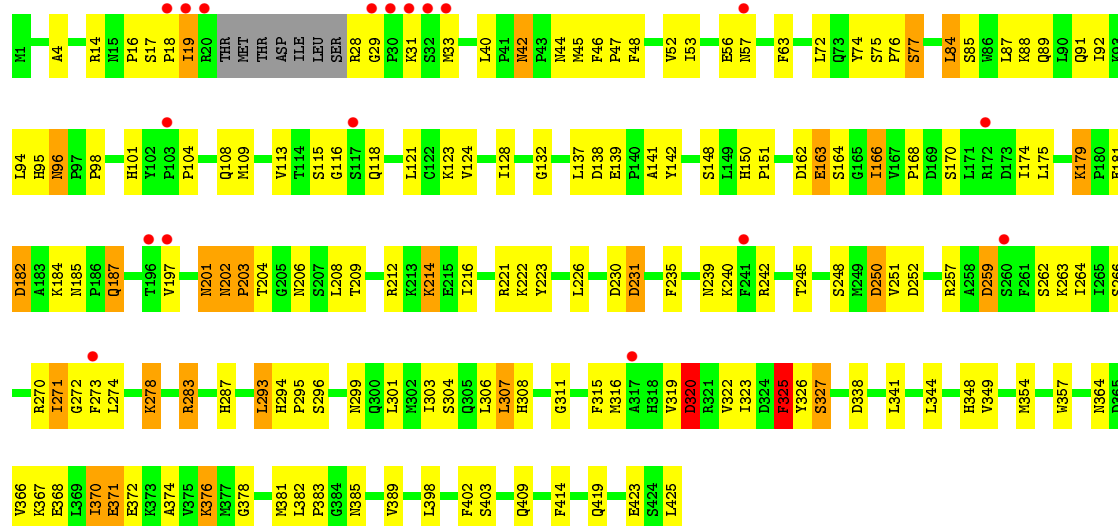




- Molecule 1: Kynurenine/alpha-aminoadipate aminotransferase mitochondrial



- Molecule 1: Kynurenine/alpha-aminoadipate aminotransferase mitochondrial



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.93 Å   72.09 Å   109.08 Å 89.97°   100.65°   93.88°	Depositor
Resolution (Å)	29.69 – 2.50 29.69 – 2.48	Depositor EDS
% Data completeness (in resolution range)	88.7 (29.69-2.50) 88.7 (29.69-2.48)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.32 (at 2.48 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.215   ,   0.244 0.215   ,   0.242	Depositor DCC
$R_{free}$ test set	2867 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.4	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 47.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 57158 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	14067	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.81% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, LLP, AKG

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	0.93	1/3321 (0.0%)	0.87	7/4507 (0.2%)
1	B	0.94	2/3341 (0.1%)	0.92	4/4532 (0.1%)
1	C	0.97	1/3404 (0.0%)	0.92	3/4620 (0.1%)
1	D	0.92	2/3352 (0.1%)	0.89	9/4546 (0.2%)
All	All	0.94	6/13418 (0.0%)	0.90	23/18205 (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	A	0	1
1	B	0	6
1	C	0	1
1	D	0	5
All	All	0	13

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	233	TYR	CD1-CE1	5.77	1.48	1.39
1	B	233	TYR	CD2-CE2	5.56	1.47	1.39
1	D	74	TYR	CE2-CZ	5.27	1.45	1.38
1	D	325	PHE	CE1-CZ	5.20	1.47	1.37
1	B	340	TRP	CB-CG	-5.10	1.41	1.50
1	C	187	GLN	CG-CD	5.06	1.62	1.51

All (23) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	MET	CG-SD-CE	5.80	109.49	100.20
1	A	219	LEU	CA-CB-CG	5.57	128.10	115.30
1	D	320	ASP	CB-CG-OD2	5.47	123.22	118.30
1	D	231	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	D	357	TRP	CA-CB-CG	5.29	123.76	113.70
1	D	250	ASP	CB-CG-OD2	5.28	123.05	118.30
1	D	84	LEU	CB-CG-CD1	-5.26	102.05	111.00
1	C	230	ASP	CB-CG-OD2	5.22	123.00	118.30
1	D	182	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	283	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	D	252	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	224	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	320	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	331	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	194	LEU	CA-CB-CG	5.15	127.15	115.30
1	C	231	ASP	CB-CG-OD2	5.15	122.93	118.30
1	B	334	LEU	CB-CG-CD1	-5.09	102.34	111.00
1	A	250	ASP	CB-CG-OD2	5.08	122.87	118.30
1	B	111	LEU	CA-CB-CG	5.08	126.98	115.30
1	A	286	LEU	CA-CB-CG	5.08	126.98	115.30
1	D	425	LEU	CA-CB-CG	5.08	126.98	115.30
1	C	306	LEU	CA-CB-CG	5.06	126.94	115.30
1	D	40	LEU	C-N-CD	5.02	138.94	128.40

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	31	LYS	Peptide
1	B	18	PRO	Peptide
1	B	19	ILE	Peptide
1	B	202	ASN	Peptide
1	B	30	PRO	Peptide
1	B	31	LYS	Peptide
1	B	32	SER	Peptide
1	C	403	SER	Peptide
1	D	184	LYS	Peptide
1	D	201	ASN	Peptide
1	D	202	ASN	Peptide
1	D	28	ARG	Peptide
1	D	29	GLY	Peptide

## 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	3265	0	3266	180	0
1	B	3285	0	3291	150	0
1	C	3347	0	3358	139	0
1	D	3296	0	3303	161	0
2	A	10	0	4	0	0
3	A	18	0	24	3	0
3	C	12	0	16	6	0
3	D	6	0	8	0	0
4	A	225	0	0	33	0
4	B	226	0	0	18	0
4	C	202	0	0	24	0
4	D	175	0	0	30	0
All	All	14067	0	13270	601	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 23.

All (601) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:LYS:C	1:A:31:LYS:HD3	1.35	1.33
1:B:31:LYS:HB3	1:B:31:LYS:NZ	1.46	1.23
1:B:31:LYS:HB3	1:B:31:LYS:HZ3	0.99	1.06
1:B:31:LYS:HG2	1:B:32:SER:H	1.17	1.05
1:C:283:ARG:HD3	4:C:509:HOH:O	1.52	1.05
1:B:185:ASN:HD21	1:B:187:GLN:HG3	1.19	1.02
1:A:31:LYS:C	1:A:31:LYS:CD	2.26	1.02
1:A:270:ARG:NH2	1:B:293:LEU:HD12	1.74	1.01
1:A:31:LYS:HD3	1:A:32:SER:N	1.75	1.01
1:A:89:GLN:HG3	4:A:456:HOH:O	1.58	1.01
1:C:31:LYS:HG3	1:C:31:LYS:O	1.59	1.00
1:A:30:PRO:O	1:A:31:LYS:HG3	1.62	0.98
1:B:185:ASN:ND2	1:B:187:GLN:HG3	1.77	0.98
1:D:166:ILE:HD11	1:D:216:ILE:CD1	1.95	0.97
1:C:30:PRO:HD3	3:C:427:GOL:O1	1.67	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:GLU:OE2	1:D:389:VAL:HG23	1.66	0.95
1:A:30:PRO:O	1:A:31:LYS:CG	2.15	0.94
1:B:31:LYS:CB	1:B:31:LYS:NZ	2.32	0.93
1:A:366:VAL:HG21	1:A:398:LEU:HD21	1.48	0.93
1:C:1:MET:HB3	4:C:582:HOH:O	1.67	0.93
1:A:16:PRO:HA	1:A:286:LEU:HD22	1.51	0.91
1:A:31:LYS:O	1:A:31:LYS:HD3	1.71	0.90
1:D:214:LYS:HD2	4:D:579:HOH:O	1.70	0.90
1:A:57:ASN:HA	4:A:579:HOH:O	1.72	0.88
1:A:366:VAL:CG2	1:A:398:LEU:HD21	2.03	0.88
1:C:65:GLU:HG3	4:C:552:HOH:O	1.75	0.86
1:A:37:ALA:HB1	1:B:382:LEU:HB2	1.57	0.86
1:C:177:ARG:HB2	1:C:177:ARG:HH11	1.39	0.85
1:C:67:MET:HG2	4:C:464:HOH:O	1.75	0.85
1:A:349:VAL:O	1:A:349:VAL:HG13	1.77	0.84
1:B:31:LYS:HG2	1:B:32:SER:N	1.88	0.84
1:C:20:ARG:HA	4:C:624:HOH:O	1.76	0.84
1:A:100:ILE:HB	4:A:625:HOH:O	1.78	0.83
1:B:185:ASN:HD21	1:B:187:GLN:CG	1.91	0.83
1:A:213:LYS:HB3	1:A:249:MET:HE1	1.61	0.83
1:B:281:ILE:O	1:B:284:VAL:HG22	1.80	0.81
1:D:259:ASP:HB3	1:D:273:PHE:CZ	2.14	0.81
1:A:30:PRO:O	1:A:31:LYS:CD	2.29	0.81
1:C:30:PRO:CD	3:C:427:GOL:O1	2.30	0.80
1:D:19:ILE:O	1:D:19:ILE:CG2	2.30	0.80
1:A:89:GLN:HG2	4:A:518:HOH:O	1.81	0.80
1:C:270:ARG:NH2	1:D:293:LEU:HD22	1.97	0.79
1:B:292:THR:O	1:B:293:LEU:HB2	1.82	0.79
1:D:42:ASN:HD21	1:D:44:ASN:HD22	1.30	0.79
1:D:166:ILE:HD11	1:D:216:ILE:HD13	1.65	0.79
1:A:270:ARG:O	1:A:271:ILE:HG12	1.83	0.78
1:C:265:ILE:HD11	1:C:303:ILE:HG12	1.64	0.78
1:C:31:LYS:CG	1:C:31:LYS:O	2.30	0.78
1:D:89:GLN:HG3	4:D:595:HOH:O	1.83	0.77
1:C:75:SER:HB2	1:C:76:PRO:HD3	1.64	0.77
1:B:34:ILE:O	1:B:34:ILE:HG22	1.85	0.77
1:D:19:ILE:O	1:D:19:ILE:HG22	1.86	0.76
1:B:31:LYS:HB3	1:B:31:LYS:HZ2	1.47	0.76
1:C:91:GLN:O	1:C:95:HIS:HB2	1.86	0.76
1:C:19:ILE:HG23	3:C:426:GOL:O1	1.86	0.75
1:C:381:MET:HE2	1:C:398:LEU:HD13	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:ASN:HB3	4:B:638:HOH:O	1.87	0.73
1:C:188:LYS:O	1:C:189:ASN:HB2	1.89	0.73
1:D:370:ILE:HD11	1:D:398:LEU:HD21	1.69	0.73
1:A:80:ILE:HD12	1:A:301:LEU:HD13	1.70	0.73
1:C:197:VAL:HB	1:C:201:ASN:HD22	1.52	0.73
1:A:31:LYS:CD	1:A:32:SER:N	2.50	0.73
1:A:349:VAL:HG13	4:A:517:HOH:O	1.88	0.73
1:C:262:SER:HA	1:C:266:SER:O	1.89	0.72
1:D:166:ILE:HD11	1:D:216:ILE:HD11	1.72	0.72
1:A:57:ASN:CA	4:A:579:HOH:O	2.31	0.72
1:D:370:ILE:HD11	1:D:398:LEU:CD2	2.20	0.72
1:A:218:GLU:HG3	1:A:221:ARG:HH12	1.55	0.72
1:A:30:PRO:O	1:A:31:LYS:HD2	1.90	0.71
1:A:213:LYS:HB3	1:A:249:MET:CE	2.20	0.71
1:B:174:ILE:O	1:B:177:ARG:HD3	1.90	0.71
1:D:402:PHE:O	1:D:402:PHE:CD1	2.43	0.71
1:C:299:ASN:HD21	1:D:299:ASN:HD21	1.39	0.71
1:C:21:THR:HG23	1:C:22:MET:H	1.55	0.70
1:D:42:ASN:HD22	1:D:44:ASN:H	1.38	0.70
1:B:192:LYS:NZ	4:B:619:HOH:O	2.24	0.70
1:B:89:GLN:HG3	4:B:532:HOH:O	1.90	0.70
1:C:330:LYS:O	1:C:334:LEU:HB2	1.91	0.70
1:D:45:MET:HG2	4:D:554:HOH:O	1.92	0.70
1:B:20:ARG:O	1:B:20:ARG:CG	2.40	0.70
1:B:164:SER:HB2	1:B:212:ARG:CZ	2.22	0.69
1:D:294:HIS:HD2	1:D:295:PRO:O	1.76	0.69
1:B:283:ARG:HD3	4:B:533:HOH:O	1.93	0.69
1:A:37:ALA:HB2	1:B:382:LEU:N	2.09	0.68
1:B:163:GLU:HG2	1:B:348:HIS:CE1	2.28	0.68
1:C:294:HIS:HD2	1:C:295:PRO:O	1.75	0.68
1:A:75:SER:HB2	1:A:76:PRO:CD	2.23	0.68
1:D:124:VAL:O	1:D:128:ILE:HG13	1.94	0.68
1:B:373:LYS:HE2	4:B:603:HOH:O	1.94	0.68
1:A:16:PRO:HA	1:A:286:LEU:CD2	2.22	0.68
1:B:381:MET:HE3	1:B:398:LEU:HB3	1.74	0.68
1:D:95:HIS:O	1:D:96:ASN:C	2.33	0.68
1:D:257:ARG:HD3	1:D:259:ASP:OD2	1.94	0.68
1:A:111:LEU:HD13	1:A:275:THR:HB	1.75	0.67
1:A:1:MET:N	4:A:569:HOH:O	2.27	0.67
1:C:109:MET:HE1	4:C:563:HOH:O	1.94	0.67
1:A:366:VAL:HG21	1:A:398:LEU:CD2	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:ARG:O	1:B:20:ARG:HG3	1.95	0.67
1:A:37:ALA:HB2	1:B:381:MET:HA	1.76	0.67
1:A:373:LYS:HB3	1:A:420:LEU:HD22	1.76	0.67
1:A:197:VAL:HB	1:A:201:ASN:HD22	1.59	0.67
4:A:559:HOH:O	1:B:354:MET:SD	2.53	0.66
1:A:111:LEU:HD11	1:A:273:PHE:HD2	1.59	0.66
1:B:44:ASN:OD1	1:B:69:LYS:HE3	1.96	0.66
1:A:261:PHE:HB3	1:A:265:ILE:HB	1.76	0.66
1:C:96:ASN:HB2	4:C:536:HOH:O	1.95	0.66
1:B:67:MET:HE3	4:B:552:HOH:O	1.94	0.66
1:D:308:HIS:HE1	4:D:458:HOH:O	1.78	0.66
1:B:95:HIS:CE1	1:B:245:THR:HG21	2.31	0.66
1:B:6:PHE:CD2	1:B:226:LEU:HD22	2.30	0.66
1:D:402:PHE:O	1:D:402:PHE:HD1	1.79	0.65
1:D:370:ILE:HD12	1:D:383:PRO:HG3	1.79	0.65
1:A:294:HIS:HD2	1:A:295:PRO:O	1.80	0.65
1:A:349:VAL:CG1	1:A:349:VAL:O	2.44	0.65
1:D:231:ASP:OD2	1:D:257:ARG:NH2	2.30	0.65
1:B:90:LEU:HG	1:B:94:LEU:HD22	1.79	0.65
1:C:75:SER:HB2	1:C:76:PRO:CD	2.26	0.64
1:A:99:THR:HG23	1:A:109:MET:HB2	1.80	0.63
1:A:58:GLY:N	4:A:579:HOH:O	2.25	0.63
1:D:263:LLP:HG2	1:D:354:MET:HE1	1.80	0.63
1:B:294:HIS:HD2	1:B:295:PRO:O	1.81	0.63
1:D:316:MET:HA	1:D:319:VAL:HG13	1.81	0.63
1:D:31:LYS:NZ	4:D:532:HOH:O	2.28	0.63
1:C:177:ARG:CB	1:C:177:ARG:HH11	2.09	0.62
1:C:177:ARG:HB2	1:C:177:ARG:NH1	2.14	0.62
1:A:349:VAL:CG1	4:A:517:HOH:O	2.45	0.62
1:A:17:SER:N	1:A:18:PRO:HD3	2.14	0.62
1:B:15:ASN:HB3	1:B:16:PRO:HD2	1.80	0.62
1:A:49:LYS:HD2	4:B:583:HOH:O	2.00	0.62
1:C:271:ILE:HD12	1:C:300:GLN:HG3	1.82	0.62
1:A:36:LEU:O	1:B:401:SER:N	2.24	0.61
1:C:65:GLU:H	1:C:65:GLU:CD	2.03	0.61
1:D:75:SER:HB2	1:D:76:PRO:HD2	1.82	0.61
1:B:5:ARG:NH2	1:B:224:ASP:OD2	2.33	0.61
1:A:340:TRP:CE2	1:A:415:GLN:HB3	2.35	0.61
1:A:263:LLP:NZ	1:A:263:LLP:H5'2	2.15	0.61
1:D:163:GLU:HG3	1:D:348:HIS:CE1	2.35	0.61
1:A:37:ALA:CB	1:B:382:LEU:HB2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:LYS:HE3	1:A:32:SER:H	1.64	0.61
1:C:375:VAL:HG12	1:C:380:LEU:HD21	1.83	0.61
1:B:295:PRO:HD3	4:B:526:HOH:O	2.00	0.60
1:D:75:SER:HB2	1:D:76:PRO:CD	2.31	0.60
1:D:349:VAL:HG22	4:D:544:HOH:O	2.01	0.60
1:D:42:ASN:ND2	1:D:44:ASN:H	1.99	0.60
1:C:126:GLU:HA	4:C:587:HOH:O	2.00	0.60
1:A:87:LEU:O	1:A:91:GLN:HG2	2.01	0.60
1:A:377:MET:HB3	4:A:572:HOH:O	2.00	0.60
1:D:168:PRO:HD3	1:D:212:ARG:HD3	1.82	0.60
1:B:99:THR:HG22	1:B:102:TYR:CE1	2.35	0.60
1:A:37:ALA:HB2	1:B:381:MET:C	2.22	0.60
1:A:338:ASP:HB3	4:A:491:HOH:O	2.01	0.60
1:D:179:LYS:HB2	1:D:181:GLU:OE2	2.01	0.59
1:D:33:MET:CE	4:D:599:HOH:O	2.50	0.59
1:A:121:LEU:HD11	1:A:195:TYR:HE1	1.65	0.59
1:C:406:SER:OG	1:C:409:GLN:HG3	2.02	0.59
1:D:187:GLN:H	1:D:187:GLN:CD	2.06	0.59
1:A:218:GLU:HG3	1:A:221:ARG:NH1	2.17	0.59
1:A:285:ILE:O	1:A:289:GLN:HG3	2.03	0.59
1:D:94:LEU:O	1:D:95:HIS:ND1	2.35	0.59
3:C:426:GOL:H31	1:D:263:LLP:H4'1	1.84	0.59
1:A:49:LYS:HE3	1:B:56:GLU:HB2	1.83	0.59
1:D:137:LEU:HD13	1:D:141:ALA:HB2	1.85	0.59
1:D:139:GLU:OE2	1:D:389:VAL:CG2	2.47	0.58
1:D:259:ASP:CB	1:D:273:PHE:CE2	2.85	0.58
1:D:95:HIS:CE1	1:D:245:THR:HG21	2.38	0.58
1:B:147:GLN:OE1	1:B:147:GLN:HA	2.03	0.58
1:B:257:ARG:HD3	1:B:259:ASP:OD2	2.02	0.58
1:A:270:ARG:C	1:A:271:ILE:HG12	2.23	0.58
1:B:263:LLP:HG3	4:B:521:HOH:O	2.04	0.58
1:A:159:VAL:HG22	1:A:174:ILE:HD12	1.86	0.58
1:A:99:THR:CG2	1:A:109:MET:HB2	2.34	0.58
1:A:80:ILE:HD13	1:A:300:GLN:HB3	1.86	0.58
1:B:55:VAL:HG12	1:B:56:GLU:O	2.03	0.58
1:B:419:GLN:O	1:B:423:GLU:HB2	2.03	0.57
1:C:175:LEU:HD12	1:C:219:LEU:HG	1.85	0.57
1:D:150:HIS:HD2	4:D:593:HOH:O	1.86	0.57
1:A:237:GLN:HE22	1:A:243:VAL:H	1.52	0.57
1:C:90:LEU:HG	1:C:94:LEU:HD22	1.87	0.57
1:D:263:LLP:HG2	1:D:354:MET:CE	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:VAL:HG12	1:A:295:PRO:HG2	1.86	0.57
1:D:179:LYS:HG2	1:D:182:ASP:OD2	2.02	0.57
1:A:138:ASP:HB3	1:A:166:ILE:HG12	1.86	0.57
1:B:42:ASN:C	1:B:42:ASN:HD22	2.08	0.56
1:B:412:VAL:O	1:B:416:VAL:HG23	2.06	0.56
1:A:18:PRO:HD2	3:A:428:GOL:O2	2.04	0.56
1:D:95:HIS:CE1	1:D:245:THR:CG2	2.88	0.56
1:C:73:GLN:O	1:C:297:THR:HG21	2.05	0.56
1:A:137:LEU:HG	4:A:576:HOH:O	2.04	0.56
1:A:37:ALA:HB2	1:B:381:MET:CA	2.36	0.56
1:B:163:GLU:CG	1:B:348:HIS:CE1	2.88	0.56
1:C:90:LEU:O	1:C:94:LEU:HB2	2.05	0.56
1:C:139:GLU:OE1	1:C:389:VAL:HG23	2.05	0.56
1:C:148:SER:O	1:C:151:PRO:HD2	2.06	0.56
1:D:283:ARG:HD3	4:D:478:HOH:O	2.06	0.56
1:B:8:THR:HG22	1:B:10:ALA:H	1.71	0.56
1:B:281:ILE:O	1:B:284:VAL:CG2	2.53	0.55
1:A:283:ARG:HD3	4:A:548:HOH:O	2.06	0.55
1:D:16:PRO:C	1:D:18:PRO:HD3	2.27	0.55
1:B:294:HIS:HB2	1:B:295:PRO:CD	2.37	0.55
1:B:356:LEU:HD12	4:B:457:HOH:O	2.06	0.55
1:D:16:PRO:O	1:D:18:PRO:HD3	2.05	0.55
1:C:34:ILE:HG21	1:D:409:GLN:HB3	1.87	0.55
1:C:303:ILE:O	1:C:307:LEU:HG	2.07	0.55
1:C:179:LYS:O	1:C:182:ASP:HB2	2.06	0.55
1:A:96:ASN:N	1:A:97:PRO:HD3	2.22	0.55
1:D:33:MET:HE3	4:D:599:HOH:O	2.05	0.55
1:C:360:VAL:HG13	1:C:421:ILE:HD13	1.88	0.55
1:D:259:ASP:CB	1:D:273:PHE:CZ	2.89	0.55
1:D:197:VAL:HB	1:D:201:ASN:HD22	1.71	0.55
1:D:245:THR:HB	1:D:257:ARG:HH21	1.71	0.55
1:D:326:TYR:CE1	1:D:354:MET:HE2	2.42	0.54
1:D:259:ASP:HB2	1:D:273:PHE:CE2	2.42	0.54
1:A:337:ALA:O	1:A:341:LEU:HB2	2.08	0.54
1:B:140:PRO:HD2	4:B:596:HOH:O	2.08	0.54
1:D:101:HIS:HE1	4:D:476:HOH:O	1.89	0.54
1:A:97:PRO:O	1:A:100:ILE:HG12	2.08	0.54
1:D:235:PHE:HB2	1:D:264:ILE:HD11	1.90	0.54
1:C:111:LEU:HA	1:C:274:LEU:O	2.08	0.54
1:B:42:ASN:HD22	1:B:43:PRO:N	2.06	0.53
1:B:264:ILE:HG12	1:B:265:ILE:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:121:LEU:HD11	1:D:230:ASP:CG	2.29	0.53
1:B:31:LYS:CB	1:B:31:LYS:HZ3	1.94	0.53
1:B:365:ASP:OD1	1:B:367:LYS:HB2	2.08	0.53
1:A:321:ARG:HD3	4:A:545:HOH:O	2.07	0.53
1:A:31:LYS:CD	1:A:32:SER:H	2.22	0.53
1:B:8:THR:HG22	1:B:10:ALA:N	2.24	0.53
1:C:1:MET:HG3	4:C:564:HOH:O	2.09	0.53
1:D:240:LYS:CE	4:D:519:HOH:O	2.56	0.53
1:C:359:LYS:HB2	1:C:397:TYR:CE2	2.44	0.53
1:A:283:ARG:CD	4:A:548:HOH:O	2.56	0.53
1:C:381:MET:CE	1:C:398:LEU:HD13	2.36	0.53
1:D:209:THR:OG1	1:D:212:ARG:HG3	2.09	0.53
1:D:251:VAL:O	1:D:251:VAL:HG12	2.08	0.53
1:C:270:ARG:HH22	1:D:293:LEU:HD22	1.73	0.53
1:C:341:LEU:HD11	1:C:414:PHE:CE2	2.44	0.52
1:B:197:VAL:HB	1:B:201:ASN:ND2	2.24	0.52
1:D:240:LYS:HE2	4:D:519:HOH:O	2.09	0.52
1:A:263:LLP:N1	4:A:610:HOH:O	2.34	0.52
1:D:84:LEU:O	1:D:88:LYS:HG3	2.09	0.52
1:D:166:ILE:CD1	1:D:216:ILE:CD1	2.80	0.52
1:A:359:LYS:HG3	1:A:397:TYR:CZ	2.44	0.52
1:A:118:GLN:NE2	3:A:427:GOL:O1	2.42	0.52
1:A:366:VAL:HG22	1:A:398:LEU:HD21	1.90	0.52
1:A:264:ILE:HG13	1:A:265:ILE:N	2.25	0.52
1:B:175:LEU:HD13	1:B:219:LEU:HD22	1.92	0.52
1:C:197:VAL:HB	1:C:201:ASN:ND2	2.20	0.52
1:C:339:LYS:HB2	4:C:533:HOH:O	2.10	0.52
1:C:365:ASP:OD1	1:C:367:LYS:HB2	2.10	0.52
1:B:139:GLU:HA	1:B:140:PRO:C	2.30	0.52
1:C:56:GLU:O	1:C:57:ASN:HB2	2.10	0.52
1:A:16:PRO:CA	1:A:286:LEU:HD22	2.33	0.51
1:D:245:THR:HB	1:D:257:ARG:NH2	2.25	0.51
1:C:99:THR:HG22	1:C:102:TYR:CE1	2.45	0.51
1:B:67:MET:HG2	4:B:552:HOH:O	2.08	0.51
1:B:204:THR:HG21	4:B:596:HOH:O	2.11	0.51
1:C:368:GLU:HB2	4:C:462:HOH:O	2.10	0.51
1:A:75:SER:HB2	1:A:76:PRO:HD3	1.93	0.51
1:C:375:VAL:CG1	1:C:380:LEU:HD21	2.40	0.51
1:B:338:ASP:O	1:B:342:THR:HG23	2.10	0.51
1:D:206:ASN:ND2	4:D:528:HOH:O	2.36	0.51
1:A:150:HIS:HA	4:A:526:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:MET:HE2	1:A:398:LEU:HD13	1.92	0.51
1:A:29:GLY:N	4:A:646:HOH:O	2.42	0.51
1:A:48:PHE:HB2	1:A:72:LEU:HD11	1.93	0.51
1:A:330:LYS:HB2	1:A:402:PHE:CZ	2.45	0.51
1:B:92:ILE:HG12	1:B:100:ILE:HD13	1.91	0.51
1:C:408:GLU:H	1:C:408:GLU:CD	2.13	0.51
1:C:91:GLN:HA	1:C:91:GLN:HE21	1.75	0.51
1:A:376:LYS:O	1:B:30:PRO:HG3	2.10	0.51
1:A:40:LEU:HD23	1:A:40:LEU:N	2.26	0.51
1:A:199:ASN:O	1:A:200:GLY:C	2.49	0.51
1:A:330:LYS:HB2	1:A:402:PHE:CE1	2.46	0.51
1:A:366:VAL:HG11	1:A:398:LEU:HD23	1.94	0.51
1:A:92:ILE:HG12	1:A:100:ILE:HG21	1.93	0.51
1:A:125:PHE:HB3	1:A:129:ILE:HD12	1.92	0.51
1:B:304:SER:O	1:B:308:HIS:HD2	1.93	0.51
1:A:31:LYS:CE	1:A:32:SER:H	2.23	0.50
1:B:223:TYR:O	1:B:224:ASP:C	2.49	0.50
1:D:98:PRO:HB2	1:D:251:VAL:HA	1.94	0.50
1:C:51:ALA:HA	1:D:52:VAL:O	2.12	0.50
1:A:245:THR:HG22	4:A:522:HOH:O	2.12	0.50
1:B:31:LYS:CB	1:B:31:LYS:HZ2	2.11	0.50
1:A:403:SER:O	1:B:42:ASN:HB2	2.12	0.50
1:D:242:ARG:NH2	1:D:316:MET:CE	2.75	0.50
1:B:265:ILE:HG22	1:B:266:SER:N	2.26	0.50
1:B:197:VAL:HB	1:B:201:ASN:HD22	1.75	0.50
1:D:239:ASN:HB3	4:D:553:HOH:O	2.11	0.50
1:D:338:ASP:HB3	4:D:523:HOH:O	2.10	0.50
1:C:181:GLU:HG2	4:C:537:HOH:O	2.10	0.50
1:C:95:HIS:HD2	4:C:531:HOH:O	1.93	0.50
1:C:265:ILE:CD1	1:C:303:ILE:HG12	2.39	0.50
1:D:354:MET:HA	1:D:402:PHE:CZ	2.47	0.50
1:B:16:PRO:HA	1:B:286:LEU:HD22	1.93	0.50
1:C:264:ILE:HD12	4:C:449:HOH:O	2.11	0.50
1:C:318:HIS:O	1:C:322:VAL:HG13	2.11	0.50
1:B:60:THR:HG22	4:B:517:HOH:O	2.10	0.50
1:D:370:ILE:CD1	1:D:398:LEU:CD2	2.89	0.50
1:D:222:LYS:HD3	1:D:223:TYR:CE2	2.46	0.50
1:A:14:ARG:HB2	1:A:283:ARG:HH21	1.77	0.50
1:C:17:SER:N	1:C:18:PRO:HD3	2.27	0.50
1:D:187:GLN:N	1:D:187:GLN:CD	2.65	0.49
1:D:52:VAL:C	1:D:53:ILE:HD12	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:ILE:O	1:B:307:LEU:HG	2.12	0.49
1:A:108:GLN:O	1:A:109:MET:C	2.50	0.49
1:B:315:PHE:O	1:B:319:VAL:HG13	2.12	0.49
1:D:382:LEU:HD12	1:D:383:PRO:HD2	1.94	0.49
1:C:281:ILE:O	1:C:285:ILE:HG13	2.12	0.49
1:C:185:ASN:HD22	1:C:185:ASN:C	2.16	0.49
1:D:138:ASP:CG	1:D:166:ILE:HG22	2.33	0.49
1:B:230:ASP:OD1	1:B:232:PRO:HD3	2.12	0.49
1:D:123:LYS:HD3	1:D:287:HIS:CG	2.47	0.49
1:A:356:LEU:HD23	1:A:358:ILE:HD11	1.95	0.49
1:A:163:GLU:HG3	1:A:348:HIS:CE1	2.48	0.49
1:A:172:ARG:HG3	1:A:219:LEU:HD11	1.93	0.49
1:C:8:THR:HG22	1:C:9:ALA:N	2.27	0.49
1:B:398:LEU:CD1	1:B:417:LEU:HD21	2.43	0.48
1:D:166:ILE:CD1	1:D:216:ILE:HD11	2.42	0.48
1:A:36:LEU:HB2	1:B:381:MET:HB3	1.95	0.48
1:A:210:SER:HB3	4:A:564:HOH:O	2.12	0.48
1:B:188:LYS:HD3	1:B:188:LYS:HA	1.42	0.48
1:D:263:LLP:H5'2	1:D:263:LLP:H4'2	1.68	0.48
1:B:339:LYS:HD3	1:B:340:TRP:NE1	2.28	0.48
1:B:359:LYS:HB2	1:B:397:TYR:CE1	2.48	0.48
1:A:270:ARG:HH22	1:B:293:LEU:HD12	1.72	0.48
1:C:271:ILE:HD12	1:C:300:GLN:CG	2.43	0.48
1:C:220:ALA:HA	1:C:225:PHE:CZ	2.49	0.48
1:C:198:PRO:HG3	1:C:229:GLU:HG3	1.95	0.48
1:D:98:PRO:CB	1:D:251:VAL:HA	2.44	0.48
1:A:278:LYS:HG2	4:A:531:HOH:O	2.13	0.48
1:A:211:GLU:OE1	4:A:564:HOH:O	2.20	0.48
1:C:283:ARG:N	1:C:283:ARG:HD2	2.28	0.48
1:C:224:ASP:OD1	1:C:254:ARG:NH1	2.34	0.48
1:C:159:VAL:HG11	1:C:166:ILE:HG23	1.95	0.48
1:C:3:TYR:O	1:C:7:ILE:HD12	2.14	0.48
1:D:89:GLN:CD	4:D:488:HOH:O	2.52	0.48
1:C:278:LYS:HB3	1:C:279:PRO:HD3	1.95	0.48
1:D:166:ILE:CD1	1:D:216:ILE:HD13	2.40	0.47
1:A:197:VAL:HB	1:A:201:ASN:ND2	2.29	0.47
1:A:365:ASP:OD1	1:A:367:LYS:HB2	2.14	0.47
1:B:182:ASP:CG	1:B:188:LYS:HG3	2.34	0.47
1:C:217:TYR:OH	1:C:250:ASP:HA	2.15	0.47
1:D:132:GLY:C	4:D:489:HOH:O	2.52	0.47
1:D:150:HIS:N	1:D:151:PRO:HD2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:PRO:HG2	1:D:250:ASP:C	2.34	0.47
1:D:301:LEU:HA	1:D:301:LEU:HD23	1.69	0.47
1:D:341:LEU:HD22	1:D:414:PHE:CE2	2.49	0.47
1:D:278:LYS:HE3	4:D:518:HOH:O	2.13	0.47
1:D:142:TYR:CD2	1:D:263:LLP:H2'3	2.50	0.47
1:D:77:SER:HA	1:D:294:HIS:HB3	1.97	0.47
1:B:410:MET:O	1:B:414:PHE:HD1	1.97	0.47
1:C:415:GLN:NE2	4:C:592:HOH:O	2.46	0.47
1:C:237:GLN:HE22	1:C:243:VAL:H	1.62	0.47
1:A:263:LLP:HZ1	1:A:263:LLP:H5'2	1.79	0.47
1:C:30:PRO:CG	3:C:427:GOL:O1	2.63	0.47
1:A:150:HIS:N	1:A:151:PRO:HD2	2.30	0.47
1:C:188:LYS:O	1:C:189:ASN:CB	2.59	0.47
1:C:126:GLU:OE2	1:C:287:HIS:HE1	1.97	0.47
1:D:270:ARG:C	1:D:271:ILE:HG12	2.35	0.47
1:C:271:ILE:CD1	1:C:300:GLN:HG3	2.45	0.46
1:B:19:ILE:HG13	1:B:19:ILE:H	1.45	0.46
1:A:335:ALA:HB1	4:A:620:HOH:O	2.15	0.46
1:A:97:PRO:C	1:A:99:THR:H	2.19	0.46
1:B:175:LEU:HD22	1:B:223:TYR:CG	2.50	0.46
1:B:231:ASP:OD2	1:B:257:ARG:NH2	2.48	0.46
1:C:29:GLY:HA2	4:C:620:HOH:O	2.16	0.46
1:D:92:ILE:CG2	1:D:92:ILE:O	2.63	0.46
1:C:265:ILE:O	1:C:266:SER:HB2	2.16	0.46
1:D:367:LYS:O	1:D:371:GLU:HB3	2.16	0.46
1:A:310:TRP:O	1:A:313:GLU:O	2.33	0.46
1:B:316:MET:HE3	4:B:537:HOH:O	2.16	0.46
1:D:271:ILE:O	1:D:271:ILE:HG22	2.15	0.46
1:B:270:ARG:C	1:B:271:ILE:HG12	2.35	0.46
1:A:370:ILE:HG21	1:A:381:MET:O	2.16	0.46
1:C:75:SER:CB	1:C:76:PRO:CD	2.94	0.46
1:B:89:GLN:NE2	4:B:616:HOH:O	2.43	0.46
1:B:148:SER:O	1:B:152:LEU:HD23	2.16	0.46
1:C:25:ILE:CG2	4:C:621:HOH:O	2.63	0.46
1:B:201:ASN:ND2	4:B:539:HOH:O	2.49	0.46
1:D:118:GLN:HE22	1:D:142:TYR:HE2	1.63	0.46
1:D:163:GLU:HG3	1:D:348:HIS:ND1	2.31	0.46
1:B:165:GLY:O	1:B:166:ILE:C	2.53	0.46
1:B:185:ASN:HD21	1:B:187:GLN:CD	2.19	0.45
1:D:113:VAL:HG12	1:D:295:PRO:HG2	1.98	0.45
1:A:294:HIS:CD2	1:A:295:PRO:O	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:VAL:HG12	1:B:295:PRO:HG2	1.98	0.45
1:C:285:ILE:O	1:C:289:GLN:HG3	2.15	0.45
1:C:6:PHE:CD2	1:C:226:LEU:HG	2.51	0.45
1:C:48:PHE:HB2	1:C:72:LEU:HD11	1.98	0.45
1:A:366:VAL:HG23	1:A:369:LEU:HD23	1.98	0.45
1:B:381:MET:HE2	1:B:398:LEU:CD1	2.46	0.45
1:C:63:PHE:HB3	1:C:68:MET:HE2	1.98	0.45
1:D:263:LLP:HD2	1:D:263:LLP:N	2.32	0.45
1:B:260:SER:OG	1:B:262:SER:HB2	2.16	0.45
1:B:46:PHE:O	1:B:49:LYS:HE2	2.15	0.45
1:D:162:ASP:O	1:D:164:SER:N	2.49	0.45
1:A:142:TYR:CE1	1:A:144:GLY:HA3	2.50	0.45
1:A:364:ASN:HD22	1:A:365:ASP:N	2.14	0.45
1:A:370:ILE:O	1:A:375:VAL:HG22	2.17	0.45
1:D:316:MET:O	1:D:320:ASP:HB2	2.17	0.45
1:A:359:LYS:HB2	1:A:397:TYR:CE2	2.52	0.45
4:C:584:HOH:O	1:D:378:GLY:HA3	2.17	0.45
1:B:381:MET:HE2	1:B:398:LEU:HD13	1.99	0.45
1:D:257:ARG:HG2	4:D:452:HOH:O	2.17	0.45
1:C:294:HIS:CD2	1:C:295:PRO:O	2.64	0.45
1:B:42:ASN:ND2	1:B:44:ASN:H	2.14	0.45
1:A:145:THR:HG21	1:A:195:TYR:CE2	2.52	0.45
1:A:145:THR:HG21	1:A:195:TYR:CZ	2.52	0.45
1:B:179:LYS:O	1:B:182:ASP:HB2	2.17	0.45
1:A:209:THR:OG1	1:A:212:ARG:HG3	2.17	0.45
1:A:356:LEU:HD12	4:A:453:HOH:O	2.17	0.45
1:C:217:TYR:CZ	1:C:250:ASP:HA	2.52	0.45
1:B:269:LEU:O	1:B:271:ILE:HG12	2.17	0.45
1:D:116:GLY:H	1:D:272:GLY:H	1.65	0.45
1:A:65:GLU:O	1:A:69:LYS:HG3	2.17	0.45
1:B:149:LEU:HA	1:B:149:LEU:HD23	1.72	0.45
1:C:6:PHE:CE2	1:C:226:LEU:HG	2.52	0.45
1:A:270:ARG:CZ	1:B:293:LEU:HD12	2.42	0.44
1:A:328:ASN:O	1:A:331:ASP:HB2	2.16	0.44
1:C:197:VAL:HG22	1:C:230:ASP:HB3	1.99	0.44
1:B:295:PRO:O	1:B:296:SER:C	2.54	0.44
1:C:17:SER:N	1:C:18:PRO:CD	2.79	0.44
1:D:87:LEU:O	1:D:91:GLN:HG2	2.16	0.44
1:A:126:GLU:HG2	4:A:560:HOH:O	2.17	0.44
1:D:19:ILE:O	1:D:19:ILE:HG23	2.15	0.44
1:C:34:ILE:CG2	1:D:409:GLN:HB3	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:ALA:HA	1:C:225:PHE:CE2	2.52	0.44
1:A:182:ASP:CG	1:A:188:LYS:HG3	2.37	0.44
1:D:4:ALA:HA	4:D:570:HOH:O	2.18	0.44
1:C:49:LYS:C	1:C:68:MET:HG2	2.38	0.44
1:A:89:GLN:O	1:A:90:LEU:C	2.54	0.44
1:C:341:LEU:HD11	1:C:414:PHE:HE2	1.83	0.44
1:A:99:THR:HG23	1:A:109:MET:H	1.83	0.44
1:D:370:ILE:CD1	1:D:398:LEU:HD21	2.43	0.44
1:A:111:LEU:HD11	1:A:273:PHE:CD2	2.47	0.44
1:D:304:SER:O	1:D:308:HIS:HD2	2.01	0.44
1:A:46:PHE:O	1:A:49:LYS:HE2	2.17	0.44
1:D:341:LEU:HD22	1:D:414:PHE:CD2	2.53	0.44
1:D:56:GLU:O	1:D:57:ASN:HB2	2.17	0.44
1:A:14:ARG:HB2	1:A:283:ARG:NH2	2.33	0.44
1:C:263:LLP:O	4:C:491:HOH:O	2.21	0.44
1:B:2:ASN:HD21	1:B:4:ALA:HB3	1.82	0.44
1:C:263:LLP:N	1:C:263:LLP:HD3	2.32	0.44
1:C:329:GLN:HB3	1:C:402:PHE:O	2.18	0.44
1:C:97:PRO:HA	1:C:98:PRO:HD3	1.86	0.44
1:A:5:ARG:NH2	1:A:224:ASP:OD2	2.51	0.44
1:B:18:PRO:HB2	1:B:20:ARG:H	1.82	0.44
1:D:109:MET:HA	4:D:495:HOH:O	2.18	0.44
1:A:33:MET:HG3	1:A:34:ILE:N	2.31	0.44
1:D:368:GLU:HB3	1:D:372:GLU:OE2	2.17	0.44
1:A:292:THR:HG23	1:B:119:GLN:HG3	2.00	0.43
1:B:381:MET:HE3	1:B:398:LEU:CB	2.46	0.43
1:D:95:HIS:CE1	1:D:245:THR:HG23	2.52	0.43
1:B:197:VAL:HA	1:B:230:ASP:O	2.18	0.43
1:A:264:ILE:HG13	1:A:265:ILE:HG13	2.00	0.43
1:A:295:PRO:O	1:A:296:SER:C	2.57	0.43
1:D:179:LYS:C	1:D:181:GLU:H	2.21	0.43
1:D:104:PRO:HA	1:D:108:GLN:CB	2.48	0.43
1:D:175:LEU:HD23	1:D:175:LEU:HA	1.92	0.43
1:B:199:ASN:O	1:B:233:TYR:HB2	2.18	0.43
1:A:339:LYS:HE3	4:C:526:HOH:O	2.18	0.43
1:B:95:HIS:CE1	1:B:245:THR:CG2	3.01	0.43
1:A:294:HIS:HB2	1:A:295:PRO:CD	2.49	0.43
1:A:263:LLP:HZ1	1:A:263:LLP:C5'	2.32	0.43
1:D:303:ILE:HG22	1:D:307:LEU:HD22	2.01	0.43
1:C:103:PRO:HB2	1:C:106:GLN:HB2	1.99	0.43
1:A:263:LLP:O	4:A:645:HOH:O	2.20	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:GLY:HA2	1:B:30:PRO:HD2	1.89	0.43
1:B:269:LEU:HD22	1:B:299:ASN:CG	2.39	0.43
1:A:8:THR:HG22	1:A:10:ALA:H	1.83	0.43
1:C:173:ASP:O	1:C:176:SER:OG	2.35	0.43
1:A:213:LYS:C	1:A:249:MET:HE1	2.39	0.43
1:A:200:GLY:N	1:A:352:ALA:HB3	2.33	0.43
1:B:171:LEU:HG	1:B:219:LEU:HD13	1.99	0.43
1:C:368:GLU:CD	1:C:368:GLU:H	2.22	0.43
1:D:115:SER:HA	1:D:270:ARG:O	2.18	0.43
1:D:262:SER:HA	1:D:266:SER:O	2.19	0.43
1:C:261:PHE:HA	1:C:261:PHE:HD1	1.72	0.43
1:A:263:LLP:NZ	1:A:263:LLP:C5'	2.81	0.43
1:C:123:LYS:HG2	1:C:287:HIS:ND1	2.33	0.43
1:B:322:VAL:HG23	1:B:323:ILE:N	2.33	0.43
1:C:217:TYR:CE1	1:C:250:ASP:HA	2.53	0.43
1:B:242:ARG:NH2	1:B:316:MET:HE2	2.34	0.43
1:C:319:VAL:HG12	1:C:323:ILE:HD12	2.01	0.43
1:A:95:HIS:HD2	4:A:537:HOH:O	2.00	0.43
1:A:74:TYR:CE1	1:A:293:LEU:HD12	2.54	0.43
1:D:14:ARG:O	1:D:283:ARG:NH2	2.52	0.43
1:B:111:LEU:HA	1:B:274:LEU:O	2.18	0.43
1:A:409:GLN:HB3	1:B:34:ILE:HD13	2.00	0.43
1:C:233:TYR:OH	1:C:263:LLP:O3	2.29	0.43
1:D:46:PHE:HA	1:D:47:PRO:HD3	1.78	0.43
1:B:124:VAL:O	1:B:128:ILE:HD12	2.19	0.43
1:B:292:THR:O	1:B:293:LEU:CB	2.56	0.42
1:A:299:ASN:HD21	1:B:299:ASN:HD21	1.67	0.42
1:C:83:LEU:HB2	1:C:304:SER:HB2	2.00	0.42
1:A:18:PRO:HD2	3:A:428:GOL:C2	2.49	0.42
1:A:85:SER:O	1:A:89:GLN:HB2	2.19	0.42
1:A:16:PRO:C	1:A:18:PRO:HD3	2.40	0.42
1:B:373:LYS:HB3	1:B:420:LEU:HD22	2.01	0.42
1:B:294:HIS:HB2	1:B:295:PRO:HD2	2.00	0.42
1:D:311:GLY:HA2	4:D:479:HOH:O	2.19	0.42
1:D:372:GLU:O	1:D:376:LYS:HE2	2.20	0.42
1:C:240:LYS:HB3	4:C:594:HOH:O	2.18	0.42
1:D:323:ILE:O	1:D:327:SER:HB2	2.19	0.42
1:B:225:PHE:O	1:B:254:ARG:NH1	2.52	0.42
1:A:292:THR:CG2	1:B:119:GLN:HG3	2.49	0.42
1:A:119:GLN:NE2	1:A:292:THR:OG1	2.50	0.42
1:A:147:GLN:OE1	1:B:15:ASN:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:SER:HB2	1:C:212:ARG:CZ	2.50	0.42
1:D:325:PHE:HB2	4:D:542:HOH:O	2.20	0.42
1:D:42:ASN:HD21	1:D:44:ASN:ND2	2.07	0.42
1:A:199:ASN:HB2	4:A:497:HOH:O	2.19	0.42
1:D:33:MET:HE2	4:D:599:HOH:O	2.16	0.42
1:B:2:ASN:HD22	1:B:3:TYR:N	2.18	0.42
1:A:266:SER:OG	1:A:269:LEU:HG	2.19	0.42
1:D:170:SER:O	1:D:174:ILE:HG13	2.19	0.42
1:D:295:PRO:O	1:D:296:SER:C	2.58	0.42
1:B:193:PHE:HA	1:B:226:LEU:O	2.20	0.42
1:A:172:ARG:HD2	4:A:448:HOH:O	2.19	0.42
1:D:325:PHE:C	1:D:325:PHE:CD2	2.93	0.42
1:A:139:GLU:HA	1:A:140:PRO:C	2.41	0.42
1:B:142:TYR:O	1:B:143:SER:C	2.57	0.42
1:D:366:VAL:O	1:D:366:VAL:HG22	2.20	0.42
1:D:257:ARG:O	1:D:274:LEU:HD12	2.19	0.41
1:D:91:GLN:OE1	1:D:91:GLN:HA	2.20	0.41
1:D:202:ASN:HA	1:D:203:PRO:HA	1.87	0.41
1:B:119:GLN:NE2	1:B:292:THR:OG1	2.52	0.41
1:B:232:PRO:HG2	1:B:233:TYR:CD2	2.55	0.41
1:C:245:THR:HG22	4:C:508:HOH:O	2.19	0.41
1:D:419:GLN:O	1:D:423:GLU:HG3	2.20	0.41
1:C:342:THR:HG23	1:C:342:THR:O	2.19	0.41
1:C:270:ARG:NH2	1:D:293:LEU:CD2	2.78	0.41
1:C:299:ASN:ND2	1:D:299:ASN:HD21	2.11	0.41
1:B:179:LYS:HB3	1:B:181:GLU:OE2	2.20	0.41
1:A:233:TYR:CD2	1:A:353:GLY:HA2	2.55	0.41
1:D:85:SER:O	1:D:89:GLN:HB2	2.20	0.41
1:A:168:PRO:HD3	1:A:212:ARG:HD3	2.02	0.41
1:C:145:THR:HG22	1:C:145:THR:O	2.21	0.41
1:C:39:GLY:O	3:C:426:GOL:O3	2.36	0.41
1:A:80:ILE:CD1	1:A:300:GLN:HB3	2.50	0.41
1:C:231:ASP:HA	4:C:540:HOH:O	2.21	0.41
1:A:3:TYR:O	1:A:6:PHE:HB2	2.20	0.41
1:D:89:GLN:HA	4:D:488:HOH:O	2.19	0.41
1:C:298:PHE:HD1	1:C:299:ASN:HD22	1.69	0.41
1:D:240:LYS:HE3	4:D:578:HOH:O	2.20	0.41
1:B:242:ARG:NH2	1:B:316:MET:CE	2.83	0.41
1:A:392:SER:O	4:A:600:HOH:O	2.22	0.41
1:A:146:LEU:HD23	1:A:146:LEU:HA	1.81	0.41
1:B:171:LEU:O	1:B:175:LEU:HD12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:201:ASN:O	1:D:204:THR:N	2.54	0.41
1:B:190:THR:HA	1:B:191:PRO:HD3	1.93	0.41
1:D:364:ASN:HD22	1:D:364:ASN:HA	1.53	0.41
1:D:381:MET:O	1:D:383:PRO:HD3	2.20	0.41
1:C:261:PHE:HB2	1:C:271:ILE:O	2.21	0.41
1:D:179:LYS:H	1:D:179:LYS:HG2	1.57	0.41
1:B:261:PHE:HB3	1:B:265:ILE:HB	2.02	0.41
1:C:235:PHE:HB2	1:C:264:ILE:HD11	2.02	0.41
1:D:270:ARG:O	1:D:271:ILE:HG12	2.20	0.41
1:A:232:PRO:HG2	1:A:233:TYR:CD1	2.56	0.41
1:B:7:ILE:HB	4:B:542:HOH:O	2.20	0.41
1:A:319:VAL:O	1:A:323:ILE:HG13	2.21	0.41
1:A:101:HIS:CD2	4:A:625:HOH:O	2.74	0.41
1:D:370:ILE:HA	1:D:374:ALA:HB3	2.01	0.41
1:C:201:ASN:HB3	1:C:204:THR:OG1	2.21	0.41
1:B:174:ILE:O	1:B:177:ARG:CD	2.64	0.41
1:B:95:HIS:O	1:B:96:ASN:C	2.58	0.41
1:C:231:ASP:N	1:C:232:PRO:CD	2.84	0.41
1:C:239:ASN:HB3	4:C:522:HOH:O	2.21	0.41
1:D:63:PHE:N	1:D:63:PHE:CD2	2.89	0.41
1:B:203:PRO:HG3	1:B:387:PHE:CG	2.55	0.41
1:A:179:LYS:O	1:A:180:PRO:C	2.59	0.41
1:C:129:ILE:HB	1:C:152:LEU:HD23	2.03	0.41
1:A:322:VAL:HB	1:B:45:MET:SD	2.61	0.41
1:C:178:TRP:CH2	1:C:191:PRO:HD3	2.56	0.41
1:A:200:GLY:H	1:A:352:ALA:HB3	1.86	0.41
1:A:91:GLN:OE1	1:A:91:GLN:HA	2.21	0.41
1:D:283:ARG:CD	4:D:478:HOH:O	2.67	0.41
1:D:368:GLU:O	1:D:372:GLU:HB2	2.21	0.41
1:A:368:GLU:HB2	4:A:554:HOH:O	2.21	0.41
1:D:166:ILE:HD13	1:D:208:LEU:HD21	2.03	0.40
1:D:315:PHE:O	1:D:319:VAL:CG1	2.68	0.40
1:C:98:PRO:HB2	1:C:251:VAL:HA	2.03	0.40
1:C:127:MET:SD	1:C:283:ARG:HB2	2.61	0.40
1:C:177:ARG:HD2	1:C:178:TRP:CZ2	2.56	0.40
1:C:197:VAL:HG13	1:C:230:ASP:O	2.21	0.40
1:D:240:LYS:HE3	4:D:519:HOH:O	2.19	0.40
1:B:356:LEU:HD23	1:B:358:ILE:HD11	2.04	0.40
1:C:50:THR:O	1:D:53:ILE:HA	2.21	0.40
1:C:63:PHE:CB	1:C:68:MET:HE2	2.51	0.40
1:B:107:GLY:O	1:B:108:GLN:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:PHE:HA	1:C:47:PRO:HD3	1.83	0.40
1:A:200:GLY:O	1:A:201:ASN:C	2.58	0.40
1:A:330:LYS:HA	1:A:333:ILE:HG22	2.03	0.40
1:B:319:VAL:HA	1:B:322:VAL:HG22	2.04	0.40
1:A:322:VAL:HG23	1:A:326:TYR:HD2	1.87	0.40
1:B:278:LYS:N	1:B:279:PRO:CD	2.84	0.40
1:C:134:ASN:O	1:C:191:PRO:HA	2.21	0.40
1:A:301:LEU:HD12	1:A:301:LEU:HA	1.82	0.40
1:C:294:HIS:HB2	1:C:295:PRO:CD	2.52	0.40
1:D:14:ARG:HG2	4:D:467:HOH:O	2.21	0.40
1:A:164:SER:HB2	1:A:212:ARG:CZ	2.51	0.40
1:D:48:PHE:HB2	1:D:72:LEU:HD11	2.03	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	410/425 (96%)	376 (92%)	32 (8%)	2 (0%)	34	55
1	B	412/425 (97%)	382 (93%)	29 (7%)	1 (0%)	52	75
1	C	422/425 (99%)	395 (94%)	27 (6%)	0	100	100
1	D	413/425 (97%)	375 (91%)	34 (8%)	4 (1%)	19	34
All	All	1657/1700 (98%)	1528 (92%)	122 (7%)	7 (0%)	39	61

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	200	GLY
1	B	203	PRO
1	D	203	PRO

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Mol	Chain	Res	Type
1	A	201	ASN
1	D	163	GLU
1	D	96	ASN
1	D	271	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	359/369 (97%)	340 (95%)	19 (5%)	28	50
1	B	361/369 (98%)	327 (91%)	34 (9%)	11	20
1	C	369/369 (100%)	340 (92%)	29 (8%)	15	28
1	D	362/369 (98%)	333 (92%)	29 (8%)	15	28
All	All	1451/1476 (98%)	1340 (92%)	111 (8%)	16	30

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LYS
1	A	33	MET
1	A	57	ASN
1	A	89	GLN
1	A	90	LEU
1	A	123	LYS
1	A	137	LEU
1	A	179	LYS
1	A	192	LYS
1	A	301	LEU
1	A	307	LEU
1	A	312	GLU
1	A	322	VAL
1	A	330	LYS
1	A	359	LYS
1	A	360	VAL
1	A	364	ASN

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Mol	Chain	Res	Type
1	A	375	VAL
1	A	381	MET
1	B	2	ASN
1	B	5	ARG
1	B	17	SER
1	B	19	ILE
1	B	31	LYS
1	B	33	MET
1	B	42	ASN
1	B	57	ASN
1	B	60	THR
1	B	89	GLN
1	B	94	LEU
1	B	143	SER
1	B	148	SER
1	B	172	ARG
1	B	176	SER
1	B	187	GLN
1	B	188	LYS
1	B	190	THR
1	B	192	LYS
1	B	226	LEU
1	B	262	SER
1	B	264	ILE
1	B	265	ILE
1	B	278	LYS
1	B	283	ARG
1	B	320	ASP
1	B	330	LYS
1	B	341	LEU
1	B	349	VAL
1	B	372	GLU
1	B	379	VAL
1	B	380	LEU
1	B	392	SER
1	B	423	GLU
1	C	21	THR
1	C	22	MET
1	C	25	ILE
1	C	85	SER
1	C	91	GLN
1	C	109	MET

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Mol	Chain	Res	Type
1	C	117	SER
1	C	127	MET
1	C	177	ARG
1	C	185	ASN
1	C	188	LYS
1	C	190	THR
1	C	192	LYS
1	C	214	LYS
1	C	219	LEU
1	C	221	ARG
1	C	251	VAL
1	C	259	ASP
1	C	265	ILE
1	C	270	ARG
1	C	297	THR
1	C	306	LEU
1	C	322	VAL
1	C	333	ILE
1	C	371	GLU
1	C	372	GLU
1	C	381	MET
1	C	403	SER
1	C	419	GLN
1	D	17	SER
1	D	19	ILE
1	D	42	ASN
1	D	77	SER
1	D	148	SER
1	D	166	ILE
1	D	179	LYS
1	D	185	ASN
1	D	187	GLN
1	D	214	LYS
1	D	221	ARG
1	D	226	LEU
1	D	248	SER
1	D	259	ASP
1	D	278	LYS
1	D	283	ARG
1	D	293	LEU
1	D	306	LEU
1	D	307	LEU

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Mol	Chain	Res	Type
1	D	320	ASP
1	D	322	VAL
1	D	325	PHE
1	D	327	SER
1	D	344	LEU
1	D	370	ILE
1	D	371	GLU
1	D	376	LYS
1	D	385	ASN
1	D	403	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	95	HIS
1	A	108	GLN
1	A	118	GLN
1	A	150	HIS
1	A	201	ASN
1	A	237	GLN
1	A	294	HIS
1	A	299	ASN
1	A	305	GLN
1	A	364	ASN
1	B	2	ASN
1	B	42	ASN
1	B	57	ASN
1	B	62	GLN
1	B	95	HIS
1	B	108	GLN
1	B	118	GLN
1	B	119	GLN
1	B	155	ASN
1	B	185	ASN
1	B	201	ASN
1	B	206	ASN
1	B	294	HIS
1	B	305	GLN
1	B	308	HIS
1	B	348	HIS
1	C	91	GLN

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Mol	Chain	Res	Type
1	C	101	HIS
1	C	108	GLN
1	C	118	GLN
1	C	150	HIS
1	C	185	ASN
1	C	189	ASN
1	C	201	ASN
1	C	206	ASN
1	C	237	GLN
1	C	294	HIS
1	C	299	ASN
1	C	419	GLN
1	D	2	ASN
1	D	42	ASN
1	D	95	HIS
1	D	101	HIS
1	D	106	GLN
1	D	108	GLN
1	D	201	ASN
1	D	237	GLN
1	D	294	HIS
1	D	299	ASN
1	D	308	HIS
1	D	318	HIS
1	D	364	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
1	LLP	A	263	1	23,24,25	1.92	6 (26%)	28,32,34	1.88	4 (14%)
1	LLP	B	263	1	23,24,25	1.73	3 (13%)	28,32,34	1.83	5 (17%)
1	LLP	C	263	1	23,24,25	1.87	6 (26%)	28,32,34	1.83	4 (14%)
1	LLP	D	263	1	23,24,25	1.98	6 (26%)	28,32,34	1.71	4 (14%)

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
1	LLP	A	263	1	-	0/15/17/19	0/1/1/1
1	LLP	B	263	1	-	0/15/17/19	0/1/1/1
1	LLP	C	263	1	-	0/15/17/19	0/1/1/1
1	LLP	D	263	1	-	0/15/17/19	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	263	LLP	O3-C3	-6.26	1.22	1.37
1	D	263	LLP	O3-C3	-6.22	1.22	1.37
1	C	263	LLP	O3-C3	-6.10	1.22	1.37
1	B	263	LLP	O3-C3	-5.81	1.23	1.37
1	C	263	LLP	P-OP3	-2.97	1.44	1.54
1	D	263	LLP	P-OP3	-2.93	1.44	1.54
1	A	263	LLP	P-OP3	-2.89	1.44	1.54
1	A	263	LLP	P-OP2	-2.79	1.44	1.54
1	D	263	LLP	P-OP2	-2.74	1.44	1.54
1	C	263	LLP	P-OP2	-2.65	1.45	1.54
1	A	263	LLP	C4-C5	-2.31	1.38	1.42
1	A	263	LLP	C3-C2	-2.30	1.39	1.40
1	D	263	LLP	C3-C2	-2.30	1.39	1.40
1	C	263	LLP	C3-C2	-2.22	1.39	1.40
1	D	263	LLP	P-OP1	-2.05	1.44	1.51
1	C	263	LLP	P-OP1	-2.05	1.44	1.51
1	A	263	LLP	C4-C4'	2.04	1.50	1.46
1	B	263	LLP	C2-N1	2.09	1.38	1.34
1	B	263	LLP	C4-C4'	2.22	1.50	1.46
1	C	263	LLP	C4-C4'	2.30	1.50	1.46
1	D	263	LLP	C4-C4'	3.15	1.52	1.46

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	263	LLP	CE-NZ-C4'	-3.27	109.52	118.97
1	A	263	LLP	CE-NZ-C4'	-3.13	109.92	118.97
1	B	263	LLP	C4-C4'-NZ	-2.80	109.48	125.06
1	A	263	LLP	C4-C4'-NZ	-2.73	109.84	125.06
1	C	263	LLP	C4-C4'-NZ	-2.69	110.11	125.06
1	C	263	LLP	CE-NZ-C4'	-2.54	111.63	118.97
1	B	263	LLP	C5-C6-N1	-2.19	120.06	123.86
1	A	263	LLP	OP3-P-OP2	2.02	115.06	107.38
1	D	263	LLP	OP3-P-OP2	2.04	115.14	107.38
1	C	263	LLP	OP3-P-OP2	2.17	115.64	107.38
1	B	263	LLP	C3-C4-C5	2.31	119.84	118.11
1	D	263	LLP	C3-C4-C4'	3.06	124.13	120.16
1	D	263	LLP	CD-CE-NZ	3.69	117.03	110.98
1	D	263	LLP	OP4-C5'-C5	4.99	117.24	108.99
1	B	263	LLP	OP4-C5'-C5	6.66	120.00	108.99
1	A	263	LLP	OP4-C5'-C5	7.57	121.50	108.99
1	C	263	LLP	OP4-C5'-C5	7.83	121.93	108.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	263	LLP	6	0
1	B	263	LLP	1	0
1	C	263	LLP	3	0
1	D	263	LLP	6	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

7 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	AKG	A	426	-	3,9,9	0.76	0	4,11,11	2.11	2 (50%)
3	GOL	A	427	-	5,5,5	0.54	0	5,5,5	0.47	0
3	GOL	A	428	-	5,5,5	0.83	0	5,5,5	1.13	0
3	GOL	A	429	-	5,5,5	0.68	0	5,5,5	0.62	0
3	GOL	C	426	-	5,5,5	0.62	0	5,5,5	1.51	1 (20%)
3	GOL	C	427	-	5,5,5	0.48	0	5,5,5	0.61	0
3	GOL	D	426	-	5,5,5	0.26	0	5,5,5	0.90	0

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	AKG	A	426	-	-	0/3/9/9	0/0/0/0
3	GOL	A	427	-	-	0/4/4/4	0/0/0/0
3	GOL	A	428	-	-	0/4/4/4	0/0/0/0
3	GOL	A	429	-	-	0/4/4/4	0/0/0/0
3	GOL	C	426	-	-	0/4/4/4	0/0/0/0
3	GOL	C	427	-	-	0/4/4/4	0/0/0/0
3	GOL	D	426	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	426	GOL	O2-C2-C1	-2.16	98.74	108.65
2	A	426	AKG	O5-C2-C3	2.39	124.78	120.28
2	A	426	AKG	C3-C4-C5	3.11	118.45	112.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	427	GOL	1	0
3	A	428	GOL	2	0
3	C	426	GOL	3	0
3	C	427	GOL	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	414/425 (97%)	0.30	19 (4%) 36 41	18, 32, 47, 84	0
1	B	416/425 (97%)	0.36	23 (5%) 29 32	19, 32, 50, 76	0
1	C	424/425 (99%)	0.41	24 (5%) 27 31	16, 31, 47, 88	0
1	D	417/425 (98%)	0.32	18 (4%) 39 44	17, 33, 51, 73	0
All	All	1671/1700 (98%)	0.35	84 (5%) 32 37	16, 32, 49, 88	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	29	GLY	12.3
1	C	21	THR	9.0
1	A	29	GLY	6.7
1	C	22	MET	6.7
1	C	23	THR	6.3
1	C	28	ARG	6.2
1	C	27	SER	5.8
1	A	30	PRO	5.8
1	B	29	GLY	5.1
1	C	30	PRO	5.0
1	B	30	PRO	4.9
1	D	33	MET	4.7
1	A	18	PRO	4.7
1	C	20	ARG	4.5
1	C	26	LEU	4.4
1	C	32	SER	4.4
1	B	31	LYS	4.2
1	C	24	ASP	4.0
1	B	19	ILE	4.0
1	D	18	PRO	3.9
1	B	18	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	31	LYS	3.8
1	C	25	ILE	3.7
1	C	18	PRO	3.6
1	A	33	MET	3.6
1	C	19	ILE	3.6
1	B	57	ASN	3.5
1	A	258	ALA	3.5
1	D	172	ARG	3.4
1	D	20	ARG	3.4
1	A	241	PHE	3.4
1	A	57	ASN	3.4
1	B	20	ARG	3.3
1	A	228	ILE	3.3
1	B	241	PHE	3.1
1	D	29	GLY	3.1
1	C	33	MET	3.1
1	C	183	ALA	3.1
1	A	364	ASN	3.0
1	C	228	ILE	3.0
1	B	258	ALA	2.9
1	A	32	SER	2.8
1	D	196	THR	2.8
1	A	183	ALA	2.8
1	D	30	PRO	2.8
1	D	32	SER	2.8
1	A	178	TRP	2.6
1	D	57	ASN	2.6
1	D	19	ILE	2.6
1	D	317	ALA	2.6
1	A	256	ILE	2.6
1	B	17	SER	2.5
1	B	231	ASP	2.5
1	B	197	VAL	2.5
1	B	186	PRO	2.4
1	A	36	LEU	2.4
1	A	180	PRO	2.3
1	B	187	GLN	2.3
1	A	16	PRO	2.3
1	B	273	PHE	2.3
1	A	89	GLN	2.3
1	D	103	PRO	2.3
1	D	260	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	106	GLN	2.2
1	B	182	ASP	2.2
1	B	392	SER	2.2
1	C	103	PRO	2.2
1	B	228	ILE	2.2
1	C	31	LYS	2.2
1	B	407	PRO	2.1
1	B	196	THR	2.1
1	C	173	ASP	2.1
1	A	261	PHE	2.1
1	D	197	VAL	2.1
1	C	184	LYS	2.1
1	A	117	SER	2.1
1	D	273	PHE	2.1
1	B	65	GLU	2.0
1	D	241	PHE	2.0
1	B	32	SER	2.0
1	C	375	VAL	2.0
1	D	117	SER	2.0
1	C	172	ARG	2.0
1	B	375	VAL	2.0

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

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
1	LLP	B	263	24/25	0.94	0.21	-	13,29,34,35	0
1	LLP	C	263	24/25	0.96	0.19	-	17,29,33,34	0
1	LLP	A	263	24/25	0.94	0.18	-	23,30,33,34	0
1	LLP	D	263	24/25	0.95	0.19	-	21,27,31,31	0

## 6.3 Carbohydrates ⓘ

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
3	GOL	C	426	6/6	0.69	0.33	1.92	24,26,27,29	0
3	GOL	A	428	6/6	0.75	0.36	1.20	40,42,44,46	0
2	AKG	A	426	10/10	0.80	0.23	0.28	33,41,47,48	0
3	GOL	D	426	6/6	0.89	0.20	0.20	29,36,37,38	0
3	GOL	A	427	6/6	0.92	0.22	0.18	39,42,43,46	0
3	GOL	C	427	6/6	0.88	0.15	-1.32	38,42,47,48	0
3	GOL	A	429	6/6	0.75	0.42	-	45,47,49,49	0

## 6.5 Other polymers

There are no such residues in this entry.