



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:31 PM GMT

PDB ID : 5COX
Title : UNINHIBITED MOUSE CYCLOOXYGENASE-2 (PROSTAGLANDIN SYNTHASE-2)
Authors : Kurumbail, R.; Stallings, W.
Deposited on : 1996-12-18
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (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

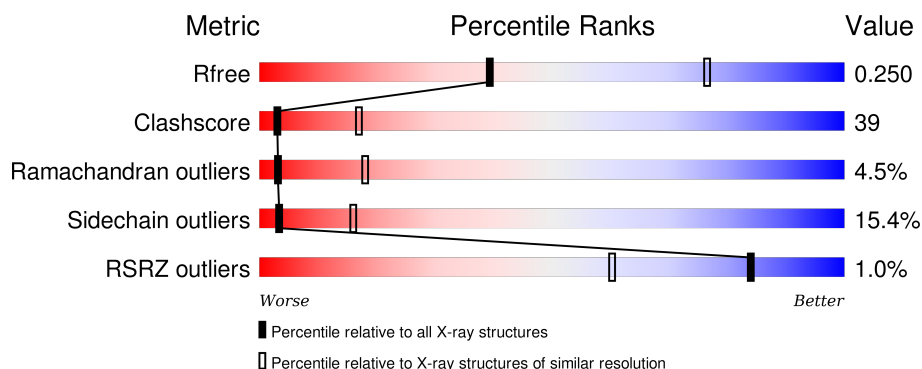
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	587	<div> <div>35%</div> <div>45%</div> <div>13%</div> <div>6%</div> </div>
1	B	587	<div> <div>35%</div> <div>47%</div> <div>11%</div> <div>6%</div> </div>
1	C	587	<div> <div>33%</div> <div>47%</div> <div>13%</div> <div>6%</div> </div>
1	D	587	<div> <div>2%</div> <div>33%</div> <div>49%</div> <div>12%</div> <div>6%</div> </div>

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
2	NAG	A	661	-	-	-	X
2	NAG	A	681	-	-	-	X
2	NAG	B	681	-	-	-	X
2	NAG	C	661	-	-	-	X
2	NAG	C	681	-	-	-	X
2	NAG	D	681	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18232 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 CYCLOOXYGENASE-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	0	0
			4473	2886	748	814	25			
1	B	552	Total	C	N	O	S	0	0	0
			4473	2886	748	814	25			
1	C	552	Total	C	N	O	S	0	0	0
			4473	2886	748	814	25			
1	D	552	Total	C	N	O	S	0	0	0
			4473	2886	748	814	25			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	310	GLN	ASN	CONFLICT	UNP Q05769
A	333	LYS	ARG	CONFLICT	UNP Q05769
B	310	GLN	ASN	CONFLICT	UNP Q05769
B	333	LYS	ARG	CONFLICT	UNP Q05769
C	310	GLN	ASN	CONFLICT	UNP Q05769
C	333	LYS	ARG	CONFLICT	UNP Q05769
D	310	GLN	ASN	CONFLICT	UNP Q05769
D	333	LYS	ARG	CONFLICT	UNP Q05769

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

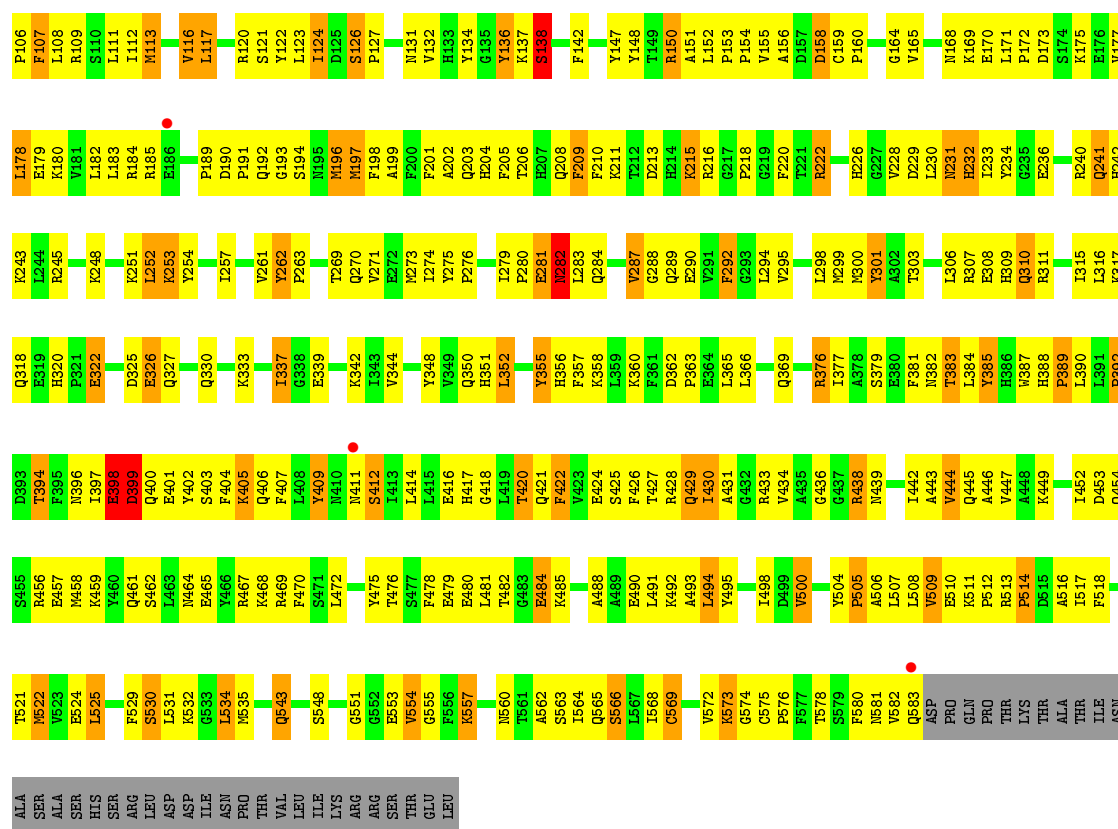


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

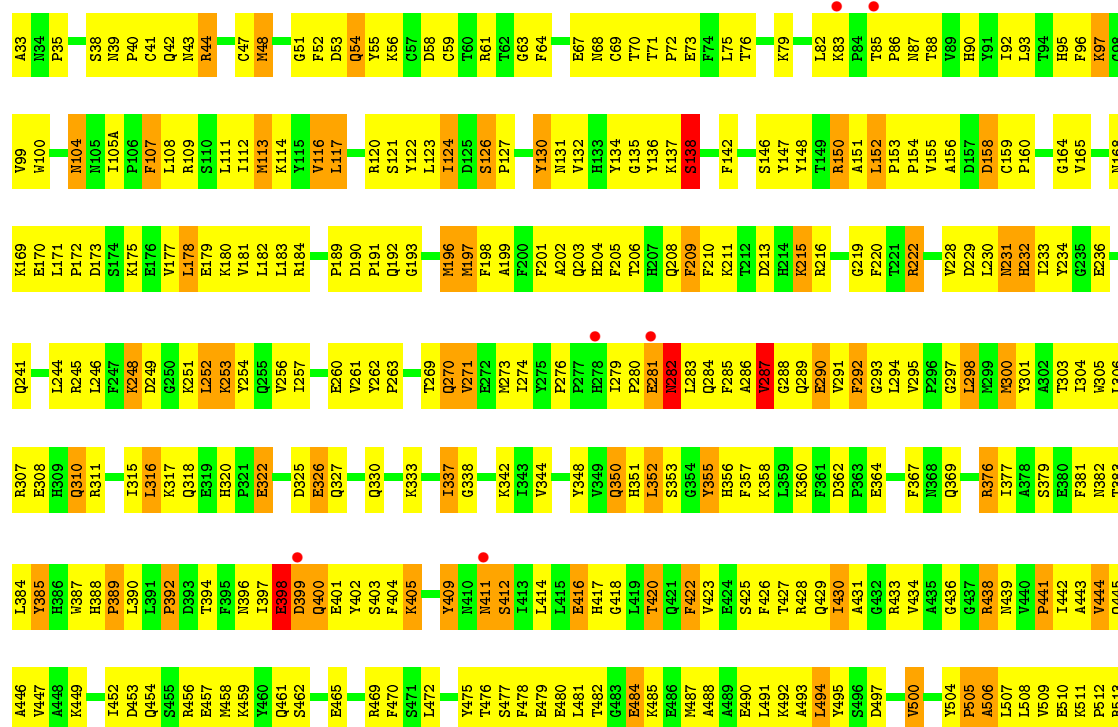
- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

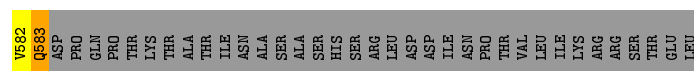
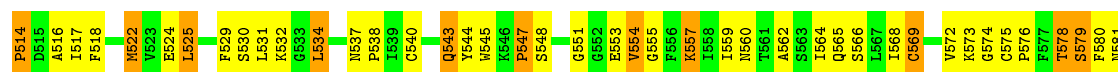


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

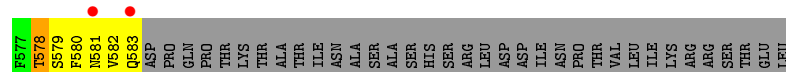
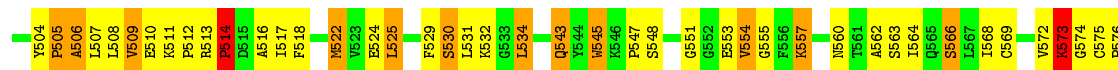
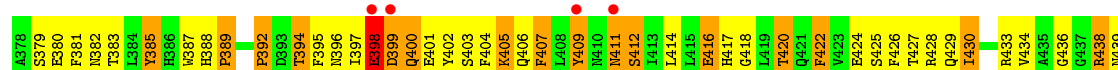
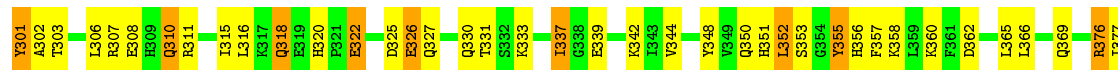
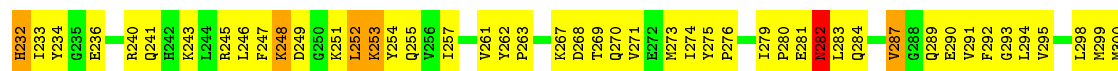
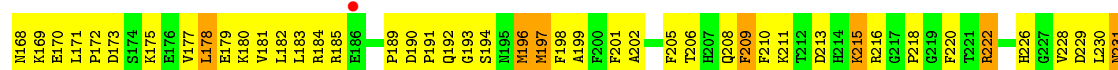
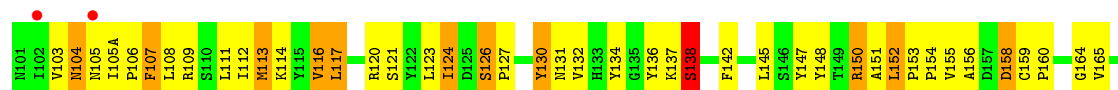


● Molecule 1: CYCLOOXYGENASE-2





Molecule 1: CYCLOOXYGENASE-2



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	180.46 Å 134.42 Å 119.90 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	74.3 (8.00-3.00) 86.0 (20.00-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 2.98 Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.321 , 0.308 0.251 , 0.250	Depositor DCC
R_{free} test set	4811 reflections (11.26%)	DCC
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.932	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 49.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	5 of 50392 reflections (0.010%)	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	18232	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.71 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.1137e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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: HEM, NAG

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	0.73	0/4600	0.87	4/6237 (0.1%)
1	B	0.73	0/4600	0.88	4/6237 (0.1%)
1	C	0.71	0/4600	0.87	3/6237 (0.0%)
1	D	0.72	0/4600	0.88	4/6237 (0.1%)
All	All	0.72	0/18400	0.87	15/24948 (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	2
1	D	0	1
All	All	0	3

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	355	TYR	N-CA-C	6.18	127.69	111.00
1	A	355	TYR	N-CA-C	5.84	126.78	111.00
1	B	355	TYR	N-CA-C	5.79	126.65	111.00
1	D	355	TYR	N-CA-C	5.77	126.58	111.00
1	A	281	GLU	N-CA-C	-5.64	95.78	111.00
1	A	148	TYR	N-CA-C	-5.62	95.83	111.00
1	D	148	TYR	N-CA-C	-5.60	95.88	111.00
1	B	287	VAL	N-CA-C	5.58	126.08	111.00
1	B	148	TYR	N-CA-C	-5.50	96.15	111.00
1	C	281	GLU	N-CA-C	-5.43	96.34	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	287	VAL	N-CA-C	5.42	125.63	111.00
1	A	287	VAL	N-CA-C	5.34	125.42	111.00
1	B	281	GLU	N-CA-C	-5.30	96.68	111.00
1	C	287	VAL	N-CA-C	5.17	124.97	111.00
1	D	573	LYS	N-CA-C	5.09	124.76	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	262	TYR	Sidechain
1	B	301	TYR	Sidechain
1	D	301	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	4473	0	4374	353	0
1	B	4473	0	4375	341	0
1	C	4473	0	4374	343	0
1	D	4473	0	4374	386	0
2	A	42	0	39	0	0
2	B	42	0	39	1	0
2	C	42	0	39	3	0
2	D	42	0	39	5	0
3	A	43	0	30	1	0
3	B	43	0	30	2	0
3	C	43	0	30	2	0
3	D	43	0	30	2	0
All	All	18232	0	17773	1388	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 39.

All (1388) 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:322:GLU:HG2	1:B:52:PHE:H	1.23	1.00
1:C:322:GLU:HG2	1:D:52:PHE:H	1.29	0.94
1:C:52:PHE:H	1:D:322:GLU:HG2	1.32	0.91
1:A:52:PHE:H	1:B:322:GLU:HG2	1.35	0.90
1:D:189:PRO:HB2	1:D:430:ILE:HD13	1.54	0.90
1:B:189:PRO:HB2	1:B:430:ILE:HD13	1.55	0.88
1:B:273:MET:SD	1:B:290:GLU:HA	2.14	0.88
1:B:85:THR:HG22	1:B:88:THR:OG1	1.75	0.87
1:A:322:GLU:HG2	1:B:52:PHE:N	1.88	0.87
1:A:191:PRO:HD2	1:A:433:ARG:HG3	1.56	0.86
1:C:189:PRO:HB2	1:C:430:ILE:HD13	1.58	0.86
1:C:478:PHE:HE2	1:C:495:TYR:HB2	1.39	0.85
1:B:478:PHE:HE2	1:B:495:TYR:HB2	1.38	0.85
1:C:283:LEU:HD13	1:C:411:ASN:ND2	1.90	0.85
1:A:478:PHE:HE2	1:A:495:TYR:HB2	1.40	0.85
1:B:283:LEU:HD13	1:B:411:ASN:HD21	1.42	0.84
1:A:85:THR:HG22	1:A:88:THR:OG1	1.78	0.84
1:D:85:THR:HG22	1:D:88:THR:OG1	1.78	0.83
1:A:189:PRO:HB2	1:A:430:ILE:HD13	1.59	0.83
1:D:251:LYS:HG2	1:D:310:GLN:HG3	1.60	0.83
1:B:251:LYS:HG2	1:B:310:GLN:HG3	1.59	0.83
1:D:478:PHE:HE2	1:D:495:TYR:HB2	1.43	0.82
1:C:146:SER:OG	2:C:671:NAG:H82	1.79	0.82
1:D:342:LYS:HG2	1:D:562:ALA:HB3	1.61	0.82
1:B:398:GLU:O	1:B:399:ASP:HB2	1.81	0.81
1:D:479:GLU:HG2	1:D:485:LYS:HE3	1.63	0.81
1:D:156:ALA:HB3	1:D:159:CYS:SG	2.20	0.81
1:C:283:LEU:HD13	1:C:411:ASN:HD21	1.45	0.81
1:B:269:THR:OG1	1:B:271:VAL:HG13	1.80	0.80
1:A:52:PHE:N	1:B:322:GLU:HG2	1.96	0.80
1:C:388:HIS:CE1	1:C:447:VAL:HG11	2.15	0.80
1:A:388:HIS:CE1	1:A:447:VAL:HG11	2.17	0.80
1:C:85:THR:HG22	1:C:88:THR:OG1	1.81	0.80
1:C:322:GLU:HG2	1:D:52:PHE:N	1.97	0.80
1:C:88:THR:HG22	1:C:92:ILE:HD11	1.64	0.80
1:C:53:ASP:HB2	1:C:54:GLN:OE1	1.82	0.79
1:B:211:LYS:HZ1	1:B:236:GLU:HG3	1.48	0.79
1:C:273:MET:SD	1:C:290:GLU:HA	2.23	0.79
1:B:281:GLU:HA	1:B:284:GLN:HG3	1.65	0.78
1:C:191:PRO:HD2	1:C:433:ARG:HG3	1.63	0.78
1:B:478:PHE:CE2	1:B:495:TYR:HB2	2.18	0.78
1:D:75:LEU:HG	1:D:79:LYS:HE2	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:399:ASP:HB3	1:C:400:GLN:HE21	1.48	0.78
1:A:283:LEU:HD13	1:A:411:ASN:ND2	1.99	0.78
1:A:75:LEU:HG	1:A:79:LYS:HE2	1.65	0.77
1:B:342:LYS:HG2	1:B:562:ALA:HB3	1.65	0.77
1:C:434:VAL:HG23	1:C:517:ILE:HD11	1.66	0.77
1:A:478:PHE:CE2	1:A:495:TYR:HB2	2.20	0.77
1:C:478:PHE:CE2	1:C:495:TYR:HB2	2.18	0.77
1:D:434:VAL:HG23	1:D:517:ILE:HD11	1.65	0.77
1:C:398:GLU:O	1:C:399:ASP:HB2	1.84	0.76
1:B:283:LEU:HD13	1:B:411:ASN:ND2	1.99	0.76
1:A:434:VAL:HG23	1:A:517:ILE:HD11	1.65	0.76
1:C:205:PHE:CE1	1:C:344:VAL:HG21	2.20	0.76
1:A:97:LYS:HD3	1:A:356:HIS:CD2	2.21	0.76
1:A:281:GLU:HA	1:A:284:GLN:HG3	1.67	0.76
1:A:251:LYS:HG2	1:A:310:GLN:HG3	1.66	0.76
1:D:388:HIS:CE1	1:D:447:VAL:HG11	2.20	0.76
1:A:88:THR:HG22	1:A:92:ILE:HD11	1.67	0.75
1:A:205:PHE:CE1	1:A:344:VAL:HG21	2.21	0.75
1:D:273:MET:SD	1:D:290:GLU:HA	2.26	0.75
1:B:434:VAL:HG23	1:B:517:ILE:HD11	1.69	0.75
1:C:52:PHE:N	1:D:322:GLU:HG2	2.00	0.75
1:D:398:GLU:O	1:D:399:ASP:HB2	1.86	0.74
1:C:156:ALA:HB3	1:C:159:CYS:SG	2.27	0.74
1:D:424:GLU:HA	1:D:428:ARG:NH1	2.02	0.74
1:C:479:GLU:HG2	1:C:485:LYS:HE3	1.69	0.74
1:C:75:LEU:HG	1:C:79:LYS:HE2	1.69	0.74
1:A:211:LYS:NZ	1:A:236:GLU:HG3	2.02	0.74
1:C:283:LEU:HD22	1:C:411:ASN:OD1	1.88	0.74
1:D:88:THR:HG22	1:D:92:ILE:HD11	1.70	0.74
1:B:211:LYS:NZ	1:B:236:GLU:HG3	2.03	0.74
1:A:557:LYS:HD3	1:A:560:ASN:HD22	1.53	0.73
1:C:251:LYS:HG2	1:C:310:GLN:HG3	1.69	0.73
1:B:388:HIS:CE1	1:B:447:VAL:HG11	2.24	0.73
1:A:399:ASP:HB3	1:A:400:GLN:HE21	1.52	0.73
1:D:191:PRO:HG3	1:D:433:ARG:CZ	2.19	0.72
1:B:88:THR:HG22	1:B:92:ILE:HD11	1.70	0.72
1:C:208:GLN:NE2	1:C:228:VAL:HA	2.05	0.72
1:D:245:ARG:HH12	1:D:326:GLU:HG2	1.55	0.72
1:C:108:LEU:O	1:C:112:ILE:HG12	1.89	0.72
1:A:280:PRO:O	1:A:281:GLU:HB3	1.89	0.71
1:D:211:LYS:NZ	1:D:236:GLU:HG3	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:ARG:HE	1:D:438:ARG:HD3	1.55	0.71
1:B:405:LYS:H	1:B:405:LYS:HD2	1.54	0.71
1:D:478:PHE:CE2	1:D:495:TYR:HB2	2.23	0.71
1:C:479:GLU:HG2	1:C:485:LYS:CE	2.20	0.71
1:D:269:THR:OG1	1:D:271:VAL:HG13	1.91	0.71
1:B:134:TYR:HD1	1:B:136:TYR:CE1	2.09	0.71
1:A:283:LEU:HD22	1:A:411:ASN:OD1	1.90	0.71
1:A:184:ARG:HA	1:A:438:ARG:O	1.89	0.71
1:C:182:LEU:O	1:C:438:ARG:HA	1.89	0.71
1:A:211:LYS:HZ1	1:A:236:GLU:HG3	1.56	0.70
1:A:211:LYS:HE2	1:A:222:ARG:HG2	1.73	0.70
1:B:470:PHE:CG	1:B:525:LEU:HD22	2.26	0.70
1:A:273:MET:SD	1:A:290:GLU:HA	2.31	0.70
1:B:73:GLU:O	1:B:76:THR:HB	1.91	0.70
1:A:191:PRO:HG3	1:A:433:ARG:CZ	2.22	0.70
1:A:342:LYS:HG2	1:A:562:ALA:HB3	1.73	0.70
1:D:510:GLU:O	1:D:512:PRO:HD3	1.90	0.70
1:D:506:ALA:O	1:D:510:GLU:HB2	1.92	0.70
1:A:548:SER:OG	1:B:58:ASP:HB2	1.91	0.70
1:D:281:GLU:HA	1:D:284:GLN:HE21	1.56	0.70
1:A:276:PRO:O	1:A:279:ILE:HG12	1.92	0.70
1:B:253:LYS:HE2	1:B:269:THR:HG22	1.74	0.70
1:D:97:LYS:HD3	1:D:356:HIS:CD2	2.27	0.70
1:C:211:LYS:HZ1	1:C:236:GLU:HG3	1.56	0.69
1:B:479:GLU:HG2	1:B:485:LYS:CE	2.21	0.69
1:B:504:TYR:HB3	1:B:505:PRO:HD3	1.74	0.69
1:A:173:ASP:O	1:A:177:VAL:HG23	1.91	0.69
1:D:414:LEU:HA	1:D:422:PHE:CE2	2.26	0.69
1:A:504:TYR:HB3	1:A:505:PRO:HD3	1.74	0.69
1:C:504:TYR:HB3	1:C:505:PRO:HD3	1.72	0.69
1:A:280:PRO:CG	1:A:283:LEU:HD12	2.22	0.69
1:A:283:LEU:HD13	1:A:411:ASN:HD21	1.56	0.69
1:A:398:GLU:O	1:A:399:ASP:HB2	1.91	0.69
1:A:156:ALA:HB3	1:A:159:CYS:SG	2.33	0.69
1:B:75:LEU:HG	1:B:79:LYS:HE2	1.72	0.69
1:B:229:ASP:OD1	1:B:231:ASN:HB3	1.92	0.69
1:B:453:ASP:O	1:B:456:ARG:HB2	1.92	0.69
1:C:173:ASP:O	1:C:177:VAL:HG23	1.93	0.69
1:C:97:LYS:HD3	1:C:356:HIS:CD2	2.28	0.69
1:B:475:TYR:HA	1:B:480:GLU:OE2	1.93	0.69
1:C:211:LYS:HE2	1:C:222:ARG:HG2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:510:GLU:O	1:B:512:PRO:HD3	1.93	0.68
1:A:578:THR:O	1:D:267:LYS:NZ	2.26	0.68
1:D:73:GLU:O	1:D:76:THR:HB	1.93	0.68
1:B:97:LYS:HD3	1:B:356:HIS:CD2	2.28	0.68
1:B:557:LYS:HD3	1:B:560:ASN:HD22	1.58	0.68
1:D:479:GLU:HG2	1:D:485:LYS:CE	2.23	0.68
1:D:453:ASP:O	1:D:456:ARG:HB2	1.94	0.68
1:B:156:ALA:HB3	1:B:159:CYS:SG	2.34	0.68
1:A:35:PRO:HB2	1:A:55:TYR:HB3	1.74	0.68
1:A:470:PHE:CG	1:A:525:LEU:HD22	2.28	0.68
1:D:205:PHE:CE1	1:D:344:VAL:HG21	2.29	0.68
1:D:281:GLU:HA	1:D:284:GLN:HG3	1.76	0.68
1:D:150:ARG:NH2	1:D:154:PRO:HB3	2.08	0.68
1:B:509:VAL:HG12	1:B:509:VAL:O	1.93	0.68
1:C:405:LYS:HD2	1:C:405:LYS:H	1.57	0.68
1:C:454:GLN:HA	1:C:457:GLU:HG2	1.75	0.68
1:C:342:LYS:HG2	1:C:562:ALA:HB3	1.74	0.68
1:D:428:ARG:N	1:D:428:ARG:HD2	2.09	0.68
1:A:182:LEU:O	1:A:438:ARG:HA	1.94	0.67
1:C:184:ARG:HA	1:C:438:ARG:O	1.93	0.67
1:A:506:ALA:O	1:A:510:GLU:HB2	1.93	0.67
1:D:229:ASP:OD1	1:D:231:ASN:HB3	1.95	0.67
1:A:184:ARG:HB2	1:A:439:ASN:HA	1.76	0.67
1:D:406:GLN:HA	2:D:681:NAG:C8	2.24	0.67
1:D:470:PHE:CG	1:D:525:LEU:HD22	2.29	0.67
1:A:507:LEU:HD22	1:A:522:MET:CE	2.25	0.67
1:C:211:LYS:NZ	1:C:236:GLU:HG3	2.09	0.67
1:A:73:GLU:O	1:A:76:THR:HB	1.95	0.67
1:D:208:GLN:NE2	1:D:228:VAL:HA	2.10	0.67
1:A:123:LEU:O	1:A:469:ARG:NH2	2.27	0.67
1:B:184:ARG:HA	1:B:438:ARG:O	1.93	0.67
1:C:507:LEU:HD22	1:C:522:MET:CE	2.25	0.67
1:A:510:GLU:O	1:A:512:PRO:HD3	1.95	0.67
1:D:280:PRO:CG	1:D:283:LEU:HD12	2.25	0.66
1:B:206:THR:HG21	1:B:385:TYR:CE1	2.29	0.66
1:A:281:GLU:O	1:A:283:LEU:N	2.28	0.66
1:C:470:PHE:CG	1:C:525:LEU:HD22	2.31	0.66
1:A:509:VAL:O	1:A:509:VAL:HG12	1.96	0.66
1:C:360:LYS:HE2	1:C:362:ASP:HB2	1.78	0.66
1:D:427:THR:HB	1:D:428:ARG:HD2	1.78	0.66
1:D:185:ARG:HH21	1:D:438:ARG:HE	1.44	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:LEU:O	1:D:112:ILE:HG12	1.96	0.66
1:C:510:GLU:O	1:C:512:PRO:HD3	1.96	0.66
1:D:405:LYS:HD2	1:D:405:LYS:H	1.61	0.65
1:D:283:LEU:HD13	1:D:411:ASN:ND2	2.10	0.65
1:D:35:PRO:HB2	1:D:55:TYR:HB3	1.79	0.65
1:C:398:GLU:HB2	1:C:425:SER:OG	1.95	0.65
1:D:206:THR:HG21	1:D:385:TYR:CE1	2.31	0.65
1:A:206:THR:HG21	1:A:385:TYR:CE1	2.32	0.65
1:D:454:GLN:HA	1:D:457:GLU:HG2	1.77	0.65
1:A:208:GLN:NE2	1:A:228:VAL:HA	2.11	0.65
1:D:434:VAL:H	1:D:517:ILE:HG13	1.62	0.65
1:A:294:LEU:HD22	1:A:409:TYR:CD1	2.32	0.65
1:B:506:ALA:O	1:B:510:GLU:HB2	1.95	0.65
1:D:504:TYR:HB3	1:D:505:PRO:HD3	1.78	0.65
1:A:475:TYR:HA	1:A:480:GLU:OE2	1.96	0.65
1:C:191:PRO:HG3	1:C:433:ARG:CZ	2.27	0.64
1:C:280:PRO:O	1:C:281:GLU:HB3	1.97	0.64
1:D:283:LEU:HD13	1:D:411:ASN:HD21	1.62	0.64
1:B:211:LYS:HZ1	1:B:236:GLU:CG	2.08	0.64
1:D:253:LYS:HE2	1:D:269:THR:HG22	1.79	0.64
1:C:123:LEU:O	1:C:469:ARG:NH2	2.31	0.64
1:C:35:PRO:HB2	1:C:55:TYR:HB3	1.77	0.64
1:D:281:GLU:O	1:D:283:LEU:N	2.31	0.64
1:C:206:THR:HG21	1:C:385:TYR:CE1	2.32	0.64
1:A:134:TYR:HD1	1:A:136:TYR:CE1	2.15	0.64
1:C:73:GLU:O	1:C:76:THR:HB	1.96	0.64
1:B:414:LEU:HA	1:B:422:PHE:CE2	2.33	0.64
1:C:183:LEU:O	1:C:438:ARG:HB3	1.98	0.64
1:D:134:TYR:HD1	1:D:136:TYR:CE1	2.15	0.64
1:C:355:TYR:O	1:C:356:HIS:HB2	1.96	0.64
1:B:281:GLU:O	1:B:283:LEU:N	2.30	0.64
1:D:211:LYS:HZ1	1:D:236:GLU:HG3	1.63	0.64
1:D:280:PRO:O	1:D:281:GLU:HB3	1.97	0.64
1:A:229:ASP:OD1	1:A:231:ASN:HB3	1.97	0.64
1:B:479:GLU:HG2	1:B:485:LYS:HE3	1.79	0.64
1:D:173:ASP:O	1:D:177:VAL:HG23	1.97	0.64
1:D:355:TYR:O	1:D:356:HIS:HB2	1.97	0.63
1:B:205:PHE:CE1	1:B:344:VAL:HG21	2.33	0.63
1:C:405:LYS:H	1:C:405:LYS:CD	2.11	0.63
1:A:364:GLU:HG2	1:A:367:PHE:CE2	2.33	0.63
1:B:454:GLN:HA	1:B:457:GLU:HG2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:LYS:HE2	1:A:269:THR:HG22	1.80	0.63
1:B:557:LYS:HA	1:B:560:ASN:HB2	1.80	0.63
1:C:477:SER:HB2	1:C:479:GLU:OE1	1.98	0.63
1:C:67:GLU:HB3	2:C:661:NAG:H82	1.80	0.63
1:D:294:LEU:HD22	1:D:409:TYR:CD1	2.33	0.63
1:D:215:LYS:N	1:D:215:LYS:HD3	2.14	0.63
1:C:230:LEU:HG	1:C:337:ILE:HG12	1.81	0.63
1:A:213:ASP:OD1	1:A:215:LYS:HG2	1.97	0.63
1:C:197:MET:HE3	1:C:197:MET:HA	1.79	0.63
1:B:342:LYS:CG	1:B:562:ALA:HB3	2.29	0.62
1:B:108:LEU:O	1:B:112:ILE:HG12	1.97	0.62
1:B:482:THR:OG1	1:B:488:ALA:HB2	2.00	0.62
1:D:67:GLU:HB3	2:D:661:NAG:H82	1.82	0.62
1:A:35:PRO:HD3	1:A:52:PHE:O	1.98	0.62
1:B:184:ARG:HB2	1:B:439:ASN:HA	1.82	0.62
1:A:398:GLU:HB2	1:A:425:SER:OG	1.99	0.62
1:A:178:LEU:HA	1:A:182:LEU:HD12	1.81	0.62
1:D:123:LEU:O	1:D:469:ARG:NH2	2.31	0.62
1:A:479:GLU:HG2	1:A:485:LYS:HE3	1.80	0.62
1:C:134:TYR:HD1	1:C:136:TYR:CE1	2.16	0.62
1:D:85:THR:OG1	1:D:86:PRO:HD2	2.00	0.62
1:A:150:ARG:NH2	1:A:458:MET:O	2.33	0.62
1:A:108:LEU:O	1:A:112:ILE:HG12	1.99	0.62
1:D:44:ARG:HH11	1:D:44:ARG:CG	2.12	0.62
1:A:230:LEU:HG	1:A:337:ILE:HG12	1.81	0.62
1:B:39:ASN:N	1:B:40:PRO:HD3	2.15	0.62
1:A:405:LYS:HD2	1:A:405:LYS:H	1.63	0.62
1:A:355:TYR:O	1:A:356:HIS:HB2	2.00	0.62
1:A:454:GLN:HA	1:A:457:GLU:HG2	1.80	0.62
1:B:131:ASN:ND2	1:B:147:TYR:CD2	2.68	0.62
1:C:131:ASN:HA	1:C:150:ARG:HB2	1.82	0.61
1:C:58:ASP:HB2	1:D:548:SER:OG	2.00	0.61
1:B:208:GLN:NE2	1:B:228:VAL:HA	2.16	0.61
1:D:183:LEU:HD22	1:D:442:ILE:HG13	1.80	0.61
1:D:230:LEU:HG	1:D:337:ILE:HG12	1.82	0.61
1:A:142:PHE:O	1:A:376:ARG:NH2	2.29	0.61
1:B:190:ASP:OD1	1:B:517:ILE:HB	2.00	0.61
1:B:281:GLU:HA	1:B:284:GLN:HE21	1.65	0.61
1:A:582:VAL:O	1:A:582:VAL:HG13	1.99	0.61
1:C:198:PHE:HB2	1:C:580:PHE:HB3	1.83	0.61
1:A:58:ASP:HB2	1:B:548:SER:OG	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:THR:OG1	1:C:271:VAL:HG13	2.01	0.61
1:B:424:GLU:HA	1:B:428:ARG:NH1	2.14	0.61
1:C:453:ASP:O	1:C:456:ARG:HB2	1.99	0.61
1:D:160:PRO:HG2	1:D:165:VAL:HA	1.83	0.61
1:D:182:LEU:O	1:D:438:ARG:HA	2.00	0.61
1:B:191:PRO:HG3	1:B:433:ARG:CZ	2.31	0.61
1:C:506:ALA:O	1:C:510:GLU:HB2	2.01	0.61
1:C:39:ASN:N	1:C:40:PRO:HD3	2.16	0.61
1:A:477:SER:HB2	1:A:479:GLU:OE1	2.01	0.61
1:B:112:ILE:HB	1:B:357:PHE:CZ	2.36	0.61
1:A:108:LEU:O	1:A:111:LEU:HB3	2.01	0.61
1:C:434:VAL:H	1:C:517:ILE:HG13	1.65	0.61
1:B:282:ASN:OD1	1:B:282:ASN:N	2.31	0.61
1:A:424:GLU:HA	1:A:428:ARG:NH1	2.16	0.61
1:B:44:ARG:CG	1:B:44:ARG:HH11	2.14	0.61
1:A:434:VAL:H	1:A:517:ILE:HG13	1.66	0.60
1:A:577:PHE:HE1	1:D:267:LYS:HD2	1.65	0.60
1:D:108:LEU:O	1:D:111:LEU:HB3	2.01	0.60
1:C:475:TYR:HA	1:C:480:GLU:OE2	2.00	0.60
1:A:183:LEU:O	1:A:438:ARG:HB3	2.01	0.60
1:C:311:ARG:O	1:C:315:ILE:HG13	2.01	0.60
1:B:257:ILE:HB	1:B:262:TYR:CD2	2.36	0.60
1:B:173:ASP:O	1:B:177:VAL:HG23	2.01	0.60
1:B:398:GLU:HB2	1:B:425:SER:OG	2.00	0.60
1:B:355:TYR:O	1:B:356:HIS:HB2	2.02	0.60
1:D:206:THR:HB	1:D:210:PHE:CD2	2.37	0.60
1:C:160:PRO:HG2	1:C:165:VAL:HA	1.83	0.60
1:D:226:HIS:CE1	1:D:376:ARG:HD2	2.36	0.60
1:B:261:VAL:O	1:B:307:ARG:NH1	2.34	0.60
1:C:190:ASP:OD1	1:C:517:ILE:HB	2.00	0.60
1:A:294:LEU:O	1:A:295:VAL:HG23	2.01	0.60
1:A:131:ASN:HA	1:A:150:ARG:HB2	1.82	0.60
1:C:281:GLU:O	1:C:283:LEU:N	2.35	0.60
1:B:155:VAL:HB	1:B:459:LYS:NZ	2.15	0.60
1:A:160:PRO:HG2	1:A:165:VAL:HA	1.82	0.60
1:C:280:PRO:CG	1:C:283:LEU:HD12	2.32	0.60
1:D:399:ASP:HB3	1:D:400:GLN:HE21	1.67	0.60
1:D:245:ARG:HD2	1:D:247:PHE:CD1	2.37	0.60
1:B:108:LEU:O	1:B:111:LEU:HB3	2.02	0.60
1:B:123:LEU:O	1:B:469:ARG:NH2	2.34	0.60
1:D:43:ASN:HB2	1:D:69:CYS:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:232:HIS:CD2	1:D:233:ILE:HG13	2.37	0.59
1:D:475:TYR:HA	1:D:480:GLU:OE2	2.02	0.59
1:B:160:PRO:HG2	1:B:165:VAL:HA	1.82	0.59
1:D:254:TYR:HD2	1:D:310:GLN:HE21	1.50	0.59
1:C:211:LYS:HZ1	1:C:236:GLU:CG	2.15	0.59
1:A:112:ILE:HB	1:A:357:PHE:CZ	2.37	0.59
1:C:294:LEU:HD22	1:C:409:TYR:CD1	2.36	0.59
1:C:509:VAL:HG12	1:C:509:VAL:O	2.03	0.59
1:B:35:PRO:HB2	1:B:55:TYR:HB3	1.83	0.59
1:D:39:ASN:N	1:D:40:PRO:HD3	2.17	0.59
1:C:482:THR:OG1	1:C:488:ALA:HB2	2.02	0.59
1:C:150:ARG:NH2	1:C:458:MET:O	2.35	0.59
1:D:190:ASP:OD1	1:D:517:ILE:HB	2.02	0.59
1:A:405:LYS:H	1:A:405:LYS:CD	2.14	0.59
1:D:184:ARG:HB2	1:D:439:ASN:HA	1.83	0.59
1:B:206:THR:HB	1:B:210:PHE:CD2	2.36	0.59
1:C:553:GLU:O	1:C:557:LYS:HE3	2.03	0.59
1:A:245:ARG:HH12	1:A:326:GLU:HG2	1.67	0.59
1:D:240:ARG:HH12	1:D:271:VAL:HG23	1.68	0.59
1:C:245:ARG:HH12	1:C:326:GLU:HG2	1.67	0.59
1:D:226:HIS:ND1	1:D:376:ARG:HD2	2.18	0.59
1:C:500:VAL:HG12	1:C:500:VAL:O	2.03	0.59
1:C:414:LEU:HA	1:C:422:PHE:CE1	2.38	0.59
1:B:294:LEU:HD22	1:B:409:TYR:CD1	2.37	0.59
1:C:294:LEU:O	1:C:295:VAL:HG23	2.02	0.59
1:A:191:PRO:CD	1:A:433:ARG:HG3	2.31	0.59
1:D:211:LYS:HZ1	1:D:236:GLU:CG	2.16	0.59
1:B:491:LEU:HD11	1:B:509:VAL:HG11	1.85	0.59
1:A:525:LEU:HD23	1:A:525:LEU:N	2.17	0.59
1:D:554:VAL:HG12	1:D:555:GLY:N	2.18	0.59
1:B:339:GLU:O	1:B:342:LYS:HB3	2.03	0.58
1:C:208:GLN:HE21	1:C:228:VAL:HA	1.64	0.58
1:D:211:LYS:HE2	1:D:222:ARG:HG2	1.85	0.58
1:A:445:GLN:HG3	1:A:446:ALA:N	2.18	0.58
1:D:500:VAL:O	1:D:500:VAL:HG12	2.03	0.58
1:C:43:ASN:ND2	1:C:64:PHE:CD2	2.72	0.58
1:B:35:PRO:HD3	1:B:52:PHE:O	2.02	0.58
1:D:53:ASP:HB2	1:D:54:GLN:OE1	2.03	0.58
1:B:434:VAL:H	1:B:517:ILE:HG13	1.67	0.58
1:B:182:LEU:O	1:B:438:ARG:HA	2.03	0.58
1:C:206:THR:HB	1:C:210:PHE:CD2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:LEU:HA	1:D:182:LEU:HD12	1.84	0.58
1:C:308:GLU:OE1	1:C:311:ARG:HD3	2.03	0.58
1:A:280:PRO:HG3	1:A:283:LEU:HD12	1.84	0.58
1:A:482:THR:OG1	1:A:488:ALA:HB2	2.03	0.58
1:B:150:ARG:NH2	1:B:154:PRO:HB3	2.19	0.58
1:C:142:PHE:O	1:C:376:ARG:NH2	2.33	0.58
1:A:282:ASN:OD1	1:A:282:ASN:N	2.36	0.58
1:D:507:LEU:HD22	1:D:522:MET:CE	2.33	0.58
1:D:104:ASN:CG	1:D:358:LYS:HE2	2.24	0.58
1:D:509:VAL:HG12	1:D:509:VAL:O	2.02	0.58
1:C:95:HIS:O	1:C:100:TRP:HD1	1.87	0.58
1:C:112:ILE:HB	1:C:357:PHE:CZ	2.39	0.58
1:D:418:GLY:O	1:D:422:PHE:HB2	2.04	0.58
1:C:507:LEU:HD22	1:C:522:MET:HE2	1.84	0.58
1:D:230:LEU:HD23	1:D:230:LEU:N	2.19	0.58
1:C:306:LEU:C	1:C:306:LEU:HD23	2.24	0.58
1:B:53:ASP:HB2	1:B:54:GLN:OE1	2.04	0.58
1:A:211:LYS:HZ1	1:A:236:GLU:CG	2.16	0.58
1:A:193:GLY:HA3	1:A:581:ASN:OD1	2.04	0.58
1:D:193:GLY:HA3	1:D:581:ASN:OD1	2.04	0.58
1:A:403:SER:HB2	1:A:405:LYS:HD2	1.85	0.58
1:A:160:PRO:HD2	1:A:164:GLY:O	2.04	0.58
1:C:43:ASN:HB2	1:C:69:CYS:O	2.04	0.58
1:B:452:ILE:O	1:B:456:ARG:HG2	2.04	0.58
1:B:107:PHE:N	1:B:107:PHE:CD1	2.72	0.58
1:B:131:ASN:HA	1:B:150:ARG:HB2	1.86	0.58
1:C:283:LEU:HD22	1:C:411:ASN:CG	2.24	0.57
1:D:112:ILE:HB	1:D:357:PHE:CZ	2.39	0.57
1:A:414:LEU:HA	1:A:422:PHE:CE2	2.38	0.57
1:C:554:VAL:HG12	1:C:555:GLY:N	2.18	0.57
1:D:445:GLN:HG3	1:D:446:ALA:N	2.19	0.57
1:C:281:GLU:HG2	1:C:282:ASN:H	1.68	0.57
1:B:280:PRO:O	1:B:281:GLU:HB3	2.04	0.57
1:B:280:PRO:CG	1:B:283:LEU:HD12	2.34	0.57
1:C:491:LEU:HD11	1:C:509:VAL:HG11	1.85	0.57
1:B:43:ASN:HB2	1:B:69:CYS:O	2.03	0.57
1:D:482:THR:OG1	1:D:488:ALA:HB2	2.04	0.57
1:D:411:ASN:CG	1:D:412:SER:N	2.56	0.57
1:C:403:SER:HB2	1:C:405:LYS:HD2	1.87	0.57
1:B:192:GLN:HG3	1:B:516:ALA:HA	1.86	0.57
1:B:230:LEU:HG	1:B:337:ILE:HG12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:SER:O	1:A:124:ILE:HD12	2.05	0.57
1:C:192:GLN:HG3	1:C:516:ALA:HA	1.86	0.57
1:D:183:LEU:O	1:D:438:ARG:HB3	2.05	0.57
1:A:206:THR:HB	1:A:210:PHE:CD2	2.39	0.57
1:B:160:PRO:HG3	1:B:165:VAL:HG23	1.86	0.57
1:B:472:LEU:HD11	1:B:524:GLU:HB2	1.86	0.57
1:D:282:ASN:OD1	1:D:282:ASN:N	2.36	0.57
1:C:97:LYS:HD3	1:C:356:HIS:NE2	2.19	0.57
1:D:160:PRO:HG3	1:D:165:VAL:HG23	1.86	0.57
1:C:160:PRO:HG3	1:C:165:VAL:HG23	1.87	0.57
1:A:95:HIS:O	1:A:100:TRP:HD1	1.87	0.57
1:A:107:PHE:N	1:A:107:PHE:CD1	2.73	0.57
1:C:44:ARG:HH11	1:C:44:ARG:CG	2.17	0.57
1:A:44:ARG:CG	1:A:44:ARG:HH11	2.17	0.57
1:C:183:LEU:HD22	1:C:442:ILE:HG13	1.85	0.57
1:D:150:ARG:NH2	1:D:458:MET:O	2.37	0.57
1:C:445:GLN:HG3	1:C:446:ALA:N	2.18	0.57
1:B:150:ARG:NH2	1:B:458:MET:O	2.37	0.57
1:C:113:MET:O	1:C:116:VAL:HG13	2.05	0.57
1:A:283:LEU:HD22	1:A:411:ASN:CG	2.24	0.56
1:A:554:VAL:HG12	1:A:555:GLY:N	2.20	0.56
1:C:108:LEU:O	1:C:111:LEU:HB3	2.03	0.56
1:B:311:ARG:O	1:B:315:ILE:HG13	2.05	0.56
1:A:311:ARG:O	1:A:315:ILE:HG13	2.04	0.56
1:C:244:LEU:CD2	1:C:271:VAL:HG11	2.34	0.56
1:D:283:LEU:HD22	1:D:411:ASN:OD1	2.06	0.56
1:B:418:GLY:O	1:B:422:PHE:HB2	2.05	0.56
1:C:136:TYR:CE2	1:D:327:GLN:HG3	2.40	0.56
1:B:64:PHE:CE2	1:B:72:PRO:HB3	2.39	0.56
1:D:394:THR:HA	1:D:402:TYR:O	2.05	0.56
1:A:232:HIS:CD2	1:A:233:ILE:HG13	2.41	0.56
1:D:257:ILE:HB	1:D:262:TYR:CD2	2.40	0.56
1:A:172:PRO:HG2	1:A:495:TYR:CE1	2.41	0.56
1:A:178:LEU:O	1:A:182:LEU:HB2	2.05	0.56
1:B:183:LEU:HD22	1:B:442:ILE:HG13	1.87	0.56
1:C:548:SER:OG	1:D:58:ASP:HB2	2.06	0.56
1:B:500:VAL:HG12	1:B:500:VAL:O	2.05	0.56
1:D:198:PHE:HD1	1:D:199:ALA:N	2.03	0.56
1:D:308:GLU:OE1	1:D:311:ARG:HD3	2.05	0.56
1:B:245:ARG:HH12	1:B:326:GLU:HG2	1.69	0.56
1:A:491:LEU:HD11	1:A:509:VAL:HG11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:582:VAL:O	1:C:582:VAL:HG13	2.05	0.56
1:C:303:THR:HG22	1:C:307:ARG:HD2	1.88	0.56
1:D:261:VAL:O	1:D:307:ARG:NH1	2.39	0.56
1:D:192:GLN:HG3	1:D:516:ALA:HA	1.87	0.56
1:A:39:ASN:N	1:A:40:PRO:HD3	2.20	0.56
1:D:184:ARG:HA	1:D:438:ARG:O	2.04	0.56
1:C:184:ARG:HB2	1:C:439:ASN:HA	1.87	0.56
1:D:436:GLY:HA2	1:D:512:PRO:HD3	1.88	0.56
1:D:279:ILE:HG22	1:D:280:PRO:HD2	1.87	0.56
1:C:452:ILE:O	1:C:456:ARG:HG2	2.06	0.56
1:D:85:THR:HG23	1:D:88:THR:H	1.70	0.56
1:D:191:PRO:HG3	1:D:433:ARG:NH2	2.21	0.56
1:D:208:GLN:HE21	1:D:228:VAL:HA	1.71	0.56
1:B:428:ARG:HD2	1:B:428:ARG:N	2.21	0.56
1:D:397:ILE:HG22	1:D:417:HIS:CD2	2.41	0.56
1:C:35:PRO:HD3	1:C:52:PHE:O	2.06	0.56
1:C:411:ASN:CG	1:C:412:SER:N	2.59	0.56
1:D:582:VAL:HG13	1:D:582:VAL:O	2.05	0.56
1:C:178:LEU:HA	1:C:182:LEU:HD12	1.86	0.56
1:D:131:ASN:HA	1:D:150:ARG:HB2	1.88	0.56
1:A:507:LEU:HD22	1:A:522:MET:HE2	1.87	0.56
1:B:428:ARG:HA	1:B:582:VAL:HG23	1.88	0.56
1:D:557:LYS:HD3	1:D:560:ASN:HD22	1.71	0.56
1:A:404:PHE:H	1:A:405:LYS:HZ2	1.54	0.55
1:A:497:ASP:HB3	1:A:500:VAL:HG23	1.88	0.55
1:B:39:ASN:HD22	1:B:39:ASN:N	2.04	0.55
1:D:180:LYS:HD3	1:D:490:GLU:CD	2.26	0.55
1:A:352:LEU:HD11	1:A:518:PHE:CE2	2.42	0.55
1:D:306:LEU:HD23	1:D:306:LEU:C	2.27	0.55
1:D:107:PHE:CD1	1:D:107:PHE:N	2.75	0.55
1:C:232:HIS:CD2	1:C:233:ILE:HG13	2.41	0.55
1:D:210:PHE:CE1	1:D:382:ASN:HA	2.41	0.55
1:A:418:GLY:O	1:A:422:PHE:HB2	2.06	0.55
1:B:494:LEU:HD12	1:B:494:LEU:H	1.71	0.55
1:B:85:THR:HG23	1:B:88:THR:H	1.71	0.55
1:C:229:ASP:OD1	1:C:231:ASN:HB3	2.07	0.55
1:C:203:GLN:HE22	3:C:682:HEM:HBB2	1.72	0.55
1:D:35:PRO:HD3	1:D:52:PHE:O	2.07	0.55
1:D:279:ILE:CG2	1:D:280:PRO:HD2	2.36	0.55
1:D:406:GLN:HA	2:D:681:NAG:H82	1.88	0.55
1:B:178:LEU:HA	1:B:182:LEU:HD12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ALA:N	1:B:158:ASP:O	2.40	0.55
1:B:185:ARG:HE	1:B:438:ARG:HD3	1.71	0.55
1:D:230:LEU:HD23	1:D:230:LEU:H	1.71	0.55
1:C:276:PRO:HG2	1:C:409:TYR:CD2	2.42	0.55
1:A:500:VAL:HG12	1:A:500:VAL:O	2.05	0.55
1:D:91:TYR:O	1:D:95:HIS:HD2	1.90	0.55
1:B:554:VAL:HG12	1:B:555:GLY:N	2.21	0.55
1:C:197:MET:HA	1:C:197:MET:CE	2.37	0.55
1:B:35:PRO:HG3	1:B:54:GLN:O	2.06	0.55
1:A:411:ASN:CG	1:A:412:SER:N	2.60	0.55
1:A:168:ASN:CG	1:A:169:LYS:N	2.60	0.55
1:B:397:ILE:HG22	1:B:417:HIS:CD2	2.41	0.55
1:B:198:PHE:HD1	1:B:199:ALA:N	2.05	0.55
1:C:420:THR:HG22	1:C:576:PRO:HG3	1.89	0.55
1:B:211:LYS:HE2	1:B:222:ARG:HG2	1.87	0.54
1:D:303:THR:HG22	1:D:307:ARG:HD2	1.88	0.54
1:D:472:LEU:HD11	1:D:524:GLU:HB2	1.89	0.54
1:A:137:LYS:O	1:A:138:SER:O	2.25	0.54
1:A:97:LYS:HB2	1:A:356:HIS:CE1	2.42	0.54
1:D:424:GLU:HA	1:D:428:ARG:HH11	1.72	0.54
1:C:244:LEU:HD21	1:C:271:VAL:HG11	1.89	0.54
1:B:582:VAL:HG13	1:B:582:VAL:O	2.07	0.54
1:A:160:PRO:HG3	1:A:165:VAL:HG23	1.88	0.54
1:A:261:VAL:O	1:A:307:ARG:NH1	2.40	0.54
1:B:306:LEU:C	1:B:306:LEU:HD23	2.27	0.54
1:A:252:LEU:O	1:A:310:GLN:NE2	2.40	0.54
1:C:479:GLU:HG2	1:C:485:LYS:NZ	2.22	0.54
1:D:444:VAL:HG12	1:D:444:VAL:O	2.08	0.54
1:D:494:LEU:H	1:D:494:LEU:HD12	1.72	0.54
1:C:85:THR:HG23	1:C:88:THR:H	1.71	0.54
1:D:398:GLU:H	1:D:425:SER:HB3	1.72	0.54
1:B:427:THR:HB	1:B:428:ARG:HD2	1.90	0.54
1:D:294:LEU:O	1:D:295:VAL:HG23	2.08	0.54
1:C:121:SER:O	1:C:124:ILE:HD12	2.08	0.54
1:A:269:THR:OG1	1:A:271:VAL:HG13	2.08	0.54
1:A:436:GLY:HA2	1:A:512:PRO:HD3	1.89	0.54
1:C:525:LEU:N	1:C:525:LEU:HD23	2.22	0.54
1:A:427:THR:HG22	1:A:583:GLN:HE22	1.73	0.54
1:C:575:CYS:N	1:C:576:PRO:HD3	2.22	0.54
1:A:303:THR:HG22	1:A:307:ARG:HD2	1.90	0.54
1:B:95:HIS:O	1:B:100:TRP:HD1	1.91	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:PHE:HD1	1:B:529:PHE:HD2	1.55	0.54
1:D:131:ASN:ND2	1:D:147:TYR:CD2	2.75	0.54
1:C:436:GLY:HA2	1:C:512:PRO:HD3	1.90	0.54
1:D:507:LEU:HD22	1:D:522:MET:HE2	1.89	0.54
1:B:320:HIS:HE1	1:B:551:GLY:O	1.90	0.54
1:B:190:ASP:O	1:B:430:ILE:HD11	2.08	0.54
1:C:479:GLU:HA	1:C:488:ALA:HB1	1.90	0.54
1:B:303:THR:HG22	1:B:307:ARG:HD2	1.90	0.54
1:D:575:CYS:N	1:D:576:PRO:HD3	2.22	0.54
1:B:406:GLN:HG2	2:B:681:NAG:O7	2.07	0.54
1:D:90:HIS:HD2	1:D:513:ARG:NH1	2.05	0.54
1:D:405:LYS:CD	1:D:405:LYS:H	2.19	0.54
1:D:155:VAL:HB	1:D:459:LYS:NZ	2.23	0.54
1:C:276:PRO:O	1:C:279:ILE:HG12	2.07	0.54
1:A:575:CYS:N	1:A:576:PRO:HD3	2.23	0.54
1:A:394:THR:HA	1:A:402:TYR:O	2.07	0.54
1:B:436:GLY:HA2	1:B:512:PRO:HD3	1.89	0.53
1:B:232:HIS:CD2	1:B:233:ILE:HG13	2.43	0.53
1:B:308:GLU:OE1	1:B:311:ARG:HD3	2.08	0.53
1:A:352:LEU:HD21	1:A:387:TRP:CH2	2.43	0.53
1:C:402:TYR:OH	1:C:417:HIS:HE1	1.91	0.53
1:B:85:THR:OG1	1:B:86:PRO:HD2	2.08	0.53
1:D:281:GLU:HG2	1:D:282:ASN:H	1.73	0.53
1:B:479:GLU:HG3	1:B:488:ALA:HB1	1.91	0.53
1:A:208:GLN:HE21	1:A:228:VAL:HA	1.73	0.53
1:D:491:LEU:HD11	1:D:509:VAL:HG11	1.90	0.53
1:C:85:THR:OG1	1:C:86:PRO:HD2	2.08	0.53
1:B:403:SER:HB2	1:B:405:LYS:HD2	1.90	0.53
1:B:479:GLU:HA	1:B:488:ALA:HB1	1.91	0.53
1:A:90:HIS:HD2	1:A:513:ARG:NH1	2.07	0.53
1:C:364:GLU:HG2	1:C:367:PHE:CE2	2.44	0.53
1:C:107:PHE:CD1	1:C:107:PHE:N	2.77	0.53
1:D:142:PHE:O	1:D:376:ARG:NH2	2.37	0.53
1:B:507:LEU:HD22	1:B:522:MET:CE	2.38	0.53
1:D:33:ALA:N	1:D:158:ASP:O	2.41	0.53
1:A:39:ASN:HD22	1:A:39:ASN:N	2.07	0.53
1:A:192:GLN:HG3	1:A:516:ALA:HA	1.90	0.53
1:D:95:HIS:O	1:D:100:TRP:HD1	1.91	0.53
1:A:210:PHE:CE1	1:A:382:ASN:HA	2.43	0.53
1:A:43:ASN:HB2	1:A:69:CYS:O	2.08	0.53
1:D:320:HIS:HE1	1:D:551:GLY:O	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:SER:O	1:B:416:GLU:N	2.42	0.53
1:A:85:THR:HG23	1:A:88:THR:H	1.74	0.53
1:B:74:PHE:O	1:B:77:ARG:HB2	2.09	0.53
1:B:281:GLU:HG2	1:B:282:ASN:H	1.73	0.52
1:C:39:ASN:N	1:C:39:ASN:HD22	2.07	0.52
1:A:453:ASP:O	1:A:456:ARG:HB2	2.08	0.52
1:C:127:PRO:HD2	1:D:543:GLN:HE22	1.75	0.52
1:A:494:LEU:HD12	1:A:494:LEU:H	1.74	0.52
1:B:172:PRO:HG2	1:B:495:TYR:CE1	2.44	0.52
1:A:88:THR:O	1:A:92:ILE:HG13	2.09	0.52
1:A:444:VAL:HG12	1:A:444:VAL:O	2.09	0.52
1:D:109:ARG:HG3	1:D:357:PHE:CE1	2.45	0.52
1:C:418:GLY:O	1:C:422:PHE:HB2	2.09	0.52
1:D:557:LYS:HA	1:D:560:ASN:HB2	1.90	0.52
1:B:121:SER:O	1:B:124:ILE:HD12	2.09	0.52
1:D:190:ASP:O	1:D:430:ILE:HD11	2.09	0.52
1:D:477:SER:HB2	1:D:479:GLU:OE1	2.08	0.52
1:D:428:ARG:HA	1:D:582:VAL:HG23	1.91	0.52
1:A:510:GLU:HG2	1:A:511:LYS:N	2.23	0.52
1:C:150:ARG:NH2	1:C:154:PRO:HB3	2.24	0.52
1:D:404:PHE:HE2	1:D:444:VAL:HG23	1.75	0.52
1:B:120:ARG:HG2	1:B:531:LEU:HD12	1.90	0.52
1:A:198:PHE:HB2	1:A:580:PHE:HB3	1.91	0.52
1:C:404:PHE:HE2	1:C:444:VAL:HG23	1.74	0.52
1:A:306:LEU:HD23	1:A:306:LEU:C	2.30	0.52
1:C:190:ASP:O	1:C:430:ILE:HD11	2.09	0.52
1:D:403:SER:HB2	1:D:405:LYS:HD2	1.90	0.52
1:A:35:PRO:HG3	1:A:54:GLN:O	2.09	0.52
1:B:507:LEU:HD22	1:B:522:MET:HE2	1.92	0.52
1:A:191:PRO:HG3	1:A:433:ARG:NH1	2.24	0.52
1:A:136:TYR:CE2	1:B:327:GLN:HG3	2.44	0.52
1:C:38:SER:OG	1:C:40:PRO:HG3	2.10	0.52
1:D:150:ARG:HG2	1:D:152:LEU:O	2.10	0.52
1:C:544:TYR:OH	1:D:142:PHE:HB2	2.10	0.52
1:D:198:PHE:HB2	1:D:580:PHE:HB3	1.91	0.52
1:A:114:LYS:HD3	1:A:369:GLN:NE2	2.24	0.52
1:A:320:HIS:HE1	1:A:551:GLY:O	1.93	0.52
1:C:472:LEU:HD21	1:C:524:GLU:HG3	1.91	0.52
1:A:51:GLY:O	1:A:52:PHE:HB2	2.10	0.52
1:D:251:LYS:CG	1:D:310:GLN:HG3	2.37	0.52
1:C:210:PHE:CE1	1:C:382:ASN:HA	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:ARG:HA	1:A:582:VAL:HG23	1.92	0.52
1:D:574:GLY:C	1:D:576:PRO:HD3	2.31	0.52
1:B:420:THR:HG22	1:B:576:PRO:HG3	1.92	0.52
1:A:203:GLN:HE22	3:A:682:HEM:HBB2	1.75	0.52
1:A:172:PRO:HG2	1:A:495:TYR:CD1	2.45	0.52
1:D:342:LYS:CG	1:D:562:ALA:HB3	2.38	0.52
1:A:251:LYS:CG	1:A:310:GLN:HG3	2.38	0.52
1:C:178:LEU:O	1:C:182:LEU:HB2	2.10	0.52
1:B:147:TYR:HE1	1:B:220:PHE:CZ	2.28	0.52
1:A:308:GLU:OE1	1:A:311:ARG:HD3	2.09	0.52
1:C:494:LEU:HD12	1:C:494:LEU:H	1.75	0.52
1:B:193:GLY:HA3	1:B:581:ASN:OD1	2.11	0.51
1:B:575:CYS:N	1:B:576:PRO:HD3	2.24	0.51
1:B:226:HIS:ND1	1:B:376:ARG:HD2	2.25	0.51
1:C:251:LYS:CG	1:C:310:GLN:HG3	2.37	0.51
1:C:252:LEU:O	1:C:310:GLN:NE2	2.43	0.51
1:D:525:LEU:N	1:D:525:LEU:HD23	2.25	0.51
1:A:150:ARG:NH2	1:A:154:PRO:HB3	2.26	0.51
1:C:557:LYS:HD3	1:C:560:ASN:HD22	1.75	0.51
1:B:294:LEU:O	1:B:295:VAL:HG23	2.11	0.51
1:A:420:THR:HG22	1:A:576:PRO:HG3	1.91	0.51
1:D:113:MET:HG2	1:D:360:LYS:HB3	1.92	0.51
1:A:276:PRO:HG2	1:A:409:TYR:CD2	2.45	0.51
1:A:443:ALA:C	1:A:445:GLN:H	2.14	0.51
1:A:322:GLU:HB3	1:B:52:PHE:CD1	2.45	0.51
1:C:412:SER:O	1:C:416:GLU:N	2.41	0.51
1:C:155:VAL:HB	1:C:459:LYS:NZ	2.25	0.51
1:A:464:ASN:O	1:A:468:LYS:HG3	2.10	0.51
1:B:196:MET:CE	1:B:392:PRO:HD3	2.41	0.51
1:D:191:PRO:HG3	1:D:433:ARG:NH1	2.24	0.51
1:C:232:HIS:HD2	1:C:233:ILE:H	1.57	0.51
1:D:147:TYR:HE1	1:D:220:PHE:CZ	2.28	0.51
1:C:192:GLN:OE1	1:C:517:ILE:HG22	2.11	0.51
1:C:389:PRO:HB2	1:C:434:VAL:HA	1.93	0.51
1:B:411:ASN:CG	1:B:412:SER:N	2.64	0.51
1:B:191:PRO:HD2	1:B:433:ARG:HG3	1.92	0.51
1:B:445:GLN:HG3	1:B:446:ALA:N	2.24	0.51
1:D:178:LEU:O	1:D:182:LEU:HB2	2.11	0.51
1:D:481:LEU:HD12	1:D:510:GLU:HG3	1.91	0.51
1:D:215:LYS:CD	1:D:215:LYS:H	2.23	0.51
1:A:198:PHE:HD1	1:A:199:ALA:N	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:MET:O	1:B:48:MET:HG3	2.10	0.51
1:D:88:THR:O	1:D:92:ILE:HG13	2.11	0.51
1:D:482:THR:HB	1:D:484:GLU:HG3	1.91	0.51
1:D:411:ASN:ND2	1:D:412:SER:N	2.59	0.51
1:D:64:PHE:CE2	1:D:72:PRO:HB3	2.46	0.51
1:C:568:ILE:HG13	1:C:572:VAL:HG21	1.93	0.51
1:A:404:PHE:HE2	1:A:444:VAL:HG23	1.76	0.51
1:D:424:GLU:O	1:D:428:ARG:HD3	2.10	0.51
1:C:105(A):ILE:HD12	1:C:108:LEU:HD12	1.93	0.51
1:A:507:LEU:HD22	1:A:522:MET:HE3	1.92	0.51
1:A:152:LEU:HD23	1:A:469:ARG:HG2	1.93	0.51
1:C:68:ASN:ND2	2:C:661:NAG:O7	2.44	0.51
1:D:213:ASP:OD1	1:D:215:LYS:HG2	2.11	0.51
1:D:121:SER:O	1:D:124:ILE:HD12	2.09	0.51
1:A:411:ASN:ND2	1:A:412:SER:N	2.59	0.51
1:A:364:GLU:HG2	1:A:367:PHE:CD2	2.46	0.51
1:A:155:VAL:HB	1:A:459:LYS:NZ	2.26	0.51
1:B:51:GLY:O	1:B:52:PHE:HB2	2.11	0.50
1:D:248:LYS:HG2	1:D:249:ASP:OD2	2.12	0.50
1:D:381:PHE:HD1	1:D:529:PHE:HD2	1.59	0.50
1:C:213:ASP:OD1	1:C:215:LYS:HG2	2.11	0.50
1:A:462:SER:HB3	1:A:465:GLU:HG2	1.93	0.50
1:B:213:ASP:OD1	1:B:215:LYS:HG2	2.11	0.50
1:D:388:HIS:N	1:D:389:PRO:HD2	2.26	0.50
1:C:175:LYS:O	1:C:178:LEU:HB3	2.12	0.50
1:B:510:GLU:HG2	1:B:511:LYS:N	2.26	0.50
1:B:179:GLU:HA	1:B:183:LEU:HD12	1.92	0.50
1:A:150:ARG:HG2	1:A:150:ARG:NH1	2.26	0.50
1:B:105:ASN:O	1:B:106:PRO:HD3	2.12	0.50
1:C:193:GLY:HA3	1:C:581:ASN:OD1	2.11	0.50
1:C:114:LYS:HD3	1:C:369:GLN:NE2	2.27	0.50
1:C:398:GLU:H	1:C:425:SER:HB3	1.77	0.50
1:D:420:THR:HG22	1:D:576:PRO:HG3	1.92	0.50
1:D:120:ARG:HG2	1:D:531:LEU:HD12	1.93	0.50
1:D:464:ASN:O	1:D:468:LYS:HG3	2.11	0.50
1:C:387:TRP:HB2	3:C:682:HEM:CBC	2.41	0.50
1:B:97:LYS:HB2	1:B:356:HIS:CE1	2.47	0.50
1:A:150:ARG:HH11	1:A:150:ARG:CG	2.24	0.50
1:D:44:ARG:HH11	1:D:44:ARG:HG3	1.77	0.50
1:B:251:LYS:CG	1:B:310:GLN:HG3	2.35	0.50
1:A:479:GLU:HG2	1:A:485:LYS:CE	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:VAL:O	1:C:307:ARG:NH1	2.45	0.50
1:B:226:HIS:CE1	1:B:376:ARG:HD2	2.46	0.50
1:B:180:LYS:HD3	1:B:490:GLU:CD	2.32	0.50
1:D:274:ILE:HG13	1:D:290:GLU:HB2	1.94	0.50
1:B:405:LYS:H	1:B:405:LYS:CD	2.17	0.50
1:B:443:ALA:C	1:B:445:GLN:H	2.15	0.50
1:C:352:LEU:HD21	1:C:387:TRP:CH2	2.46	0.50
1:B:281:GLU:CA	1:B:284:GLN:HG3	2.41	0.50
1:A:472:LEU:HD21	1:A:524:GLU:HG3	1.94	0.50
1:A:113:MET:O	1:A:117:LEU:HB2	2.12	0.50
1:D:462:SER:HB3	1:D:465:GLU:HG2	1.93	0.50
1:B:478:PHE:HD1	1:B:478:PHE:H	1.60	0.50
1:A:85:THR:OG1	1:A:86:PRO:HD2	2.11	0.50
1:C:443:ALA:C	1:C:445:GLN:H	2.14	0.50
1:D:452:ILE:O	1:D:456:ARG:HG2	2.11	0.50
1:D:150:ARG:HH11	1:D:150:ARG:CG	2.25	0.50
1:A:105(A):ILE:HD12	1:A:108:LEU:HD12	1.94	0.50
1:A:402:TYR:OH	1:A:417:HIS:HE1	1.95	0.50
1:A:564:ILE:HG12	1:A:580:PHE:CZ	2.47	0.50
1:C:472:LEU:HD11	1:C:524:GLU:HB2	1.94	0.50
1:C:286:ALA:O	1:C:287:VAL:HG22	2.12	0.50
1:D:153:PRO:O	1:D:461:GLN:NE2	2.45	0.50
1:A:82:LEU:N	1:A:82:LEU:HD12	2.26	0.50
1:D:39:ASN:N	1:D:39:ASN:HD22	2.10	0.49
1:A:172:PRO:HG2	1:A:495:TYR:CZ	2.47	0.49
1:A:190:ASP:OD1	1:A:517:ILE:HB	2.12	0.49
1:C:88:THR:O	1:C:92:ILE:HG13	2.11	0.49
1:A:179:GLU:HA	1:A:183:LEU:HD12	1.94	0.49
1:D:454:GLN:HA	1:D:457:GLU:CG	2.41	0.49
1:C:444:VAL:HG12	1:C:444:VAL:O	2.12	0.49
1:D:196:MET:HB3	1:D:426:PHE:CG	2.47	0.49
1:C:282:ASN:OD1	1:C:282:ASN:N	2.44	0.49
1:A:327:GLN:HG3	1:B:136:TYR:CE2	2.47	0.49
1:D:208:GLN:OE1	1:D:232:HIS:CE1	2.64	0.49
1:A:428:ARG:HG3	1:A:583:GLN:OE1	2.12	0.49
1:B:160:PRO:HD2	1:B:164:GLY:O	2.12	0.49
1:C:428:ARG:HD2	1:C:428:ARG:N	2.26	0.49
1:B:381:PHE:CD1	1:B:529:PHE:CB	2.96	0.49
1:D:210:PHE:HB3	1:D:382:ASN:ND2	2.27	0.49
1:C:497:ASP:HB3	1:C:500:VAL:HG23	1.94	0.49
1:C:90:HIS:HD2	1:C:513:ARG:NH1	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:LEU:HD12	1:B:82:LEU:N	2.28	0.49
1:B:197:MET:HA	1:B:197:MET:CE	2.42	0.49
1:A:553:GLU:O	1:A:557:LYS:HE3	2.12	0.49
1:D:43:ASN:ND2	1:D:64:PHE:CD2	2.80	0.49
1:B:230:LEU:N	1:B:230:LEU:HD23	2.28	0.49
1:B:196:MET:HB3	1:B:426:PHE:CG	2.48	0.49
1:B:104:ASN:CG	1:B:358:LYS:HE2	2.33	0.49
1:C:120:ARG:HG2	1:C:531:LEU:HD12	1.94	0.49
1:B:172:PRO:HG2	1:B:495:TYR:CD1	2.47	0.49
1:A:281:GLU:C	1:A:283:LEU:H	2.15	0.49
1:D:411:ASN:ND2	1:D:412:SER:H	2.10	0.49
1:C:481:LEU:HD12	1:C:510:GLU:HG3	1.93	0.49
1:D:395:PHE:CD2	1:D:407:PHE:CD2	3.01	0.49
1:B:388:HIS:N	1:B:389:PRO:HD2	2.26	0.49
1:D:276:PRO:O	1:D:279:ILE:HG12	2.12	0.49
1:D:276:PRO:HG2	1:D:409:TYR:CD2	2.48	0.49
1:D:151:ALA:O	1:D:469:ARG:NH1	2.46	0.49
1:C:180:LYS:HD3	1:C:490:GLU:CD	2.33	0.49
1:D:44:ARG:NH1	1:D:44:ARG:CG	2.75	0.49
1:B:234:TYR:HH	1:B:309:HIS:CE1	2.29	0.49
1:B:263:PRO:HD3	1:B:303:THR:HG23	1.94	0.49
1:D:350:GLN:HE22	1:D:358:LYS:HA	1.77	0.49
1:C:254:TYR:HD2	1:C:310:GLN:HE21	1.61	0.49
1:C:151:ALA:O	1:C:469:ARG:NH1	2.45	0.49
1:C:150:ARG:CG	1:C:150:ARG:HH11	2.26	0.49
1:D:352:LEU:HD21	1:D:387:TRP:CH2	2.47	0.49
1:B:287:VAL:HG23	1:B:288:GLY:N	2.28	0.49
1:A:148:TYR:HD2	1:A:219:GLY:C	2.15	0.49
1:B:240:ARG:HH12	1:B:271:VAL:HG23	1.77	0.49
1:A:109:ARG:HG3	1:A:357:PHE:CE1	2.47	0.49
1:C:198:PHE:HD1	1:C:199:ALA:N	2.11	0.49
1:B:44:ARG:HG3	1:B:44:ARG:HH11	1.78	0.49
1:D:198:PHE:CD1	1:D:199:ALA:N	2.81	0.49
1:A:423:VAL:HG13	1:A:578:THR:HG23	1.95	0.48
1:B:396:ASN:HD22	1:B:401:GLU:HA	1.77	0.48
1:B:522:MET:HG3	1:B:522:MET:O	2.13	0.48
1:B:444:VAL:HG12	1:B:444:VAL:O	2.12	0.48
1:D:254:TYR:CD1	1:D:254:TYR:C	2.87	0.48
1:A:183:LEU:HD22	1:A:442:ILE:HG13	1.95	0.48
1:B:479:GLU:HA	1:B:488:ALA:CB	2.43	0.48
1:D:152:LEU:HD23	1:D:469:ARG:HG2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:GLN:OE1	1:B:232:HIS:CE1	2.67	0.48
1:C:557:LYS:HA	1:C:560:ASN:HB2	1.95	0.48
1:D:198:PHE:CD1	1:D:198:PHE:C	2.86	0.48
1:D:201:PHE:HA	1:D:301:TYR:CE2	2.48	0.48
1:B:398:GLU:H	1:B:425:SER:HB3	1.78	0.48
1:D:281:GLU:CA	1:D:284:GLN:HE21	2.25	0.48
1:B:183:LEU:O	1:B:438:ARG:HB3	2.13	0.48
1:C:198:PHE:CD1	1:C:198:PHE:C	2.87	0.48
1:D:113:MET:O	1:D:116:VAL:HG13	2.13	0.48
1:D:196:MET:HE1	1:D:392:PRO:HD3	1.95	0.48
1:D:202:ALA:HB2	1:D:348:TYR:CE2	2.49	0.48
1:D:197:MET:HA	1:D:197:MET:HE3	1.94	0.48
1:D:172:PRO:HG2	1:D:495:TYR:CD2	2.48	0.48
1:D:97:LYS:HB2	1:D:356:HIS:CE1	2.49	0.48
1:D:215:LYS:HD3	1:D:215:LYS:H	1.75	0.48
1:A:472:LEU:HD11	1:A:524:GLU:HB2	1.95	0.48
1:D:105:ASN:O	1:D:106:PRO:HD3	2.13	0.48
1:C:182:LEU:HD22	1:C:508:LEU:HD12	1.95	0.48
1:B:479:GLU:HG2	1:B:485:LYS:NZ	2.28	0.48
1:C:152:LEU:HD23	1:C:469:ARG:HG2	1.93	0.48
1:D:568:ILE:HG13	1:D:572:VAL:HG21	1.95	0.48
1:B:113:MET:O	1:B:116:VAL:HG13	2.12	0.48
1:C:383:THR:HG22	1:C:384:LEU:N	2.28	0.48
1:A:64:PHE:CE2	1:A:72:PRO:HB3	2.49	0.48
1:A:83:LYS:NZ	1:A:83:LYS:HA	2.28	0.48
1:D:351:HIS:O	1:D:353:SER:N	2.47	0.48
1:C:179:GLU:HA	1:C:183:LEU:HD12	1.95	0.48
1:C:564:ILE:HG12	1:C:580:PHE:CZ	2.49	0.48
1:D:564:ILE:HG12	1:D:580:PHE:CZ	2.49	0.48
1:A:263:PRO:HD3	1:A:303:THR:HG23	1.94	0.48
1:C:330:GLN:HB3	1:D:138:SER:HB2	1.96	0.48
1:B:317:LYS:O	1:B:317:LYS:HG2	2.12	0.48
1:B:201:PHE:HA	1:B:301:TYR:CE2	2.48	0.48
1:D:35:PRO:HG3	1:D:54:GLN:O	2.13	0.48
1:D:398:GLU:HB2	1:D:425:SER:OG	2.13	0.48
1:B:525:LEU:N	1:B:525:LEU:HD23	2.28	0.48
1:B:151:ALA:O	1:B:469:ARG:NH1	2.47	0.48
1:B:462:SER:HB3	1:B:465:GLU:HG2	1.96	0.48
1:B:88:THR:O	1:B:92:ILE:HG13	2.14	0.48
1:C:172:PRO:HG2	1:C:495:TYR:CE2	2.48	0.48
1:A:479:GLU:HA	1:A:488:ALA:HB1	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:TYR:CD1	1:A:136:TYR:CE1	3.00	0.48
1:D:564:ILE:HG12	1:D:580:PHE:CE1	2.49	0.48
1:B:153:PRO:O	1:B:461:GLN:NE2	2.47	0.48
1:A:568:ILE:HG13	1:A:572:VAL:HG21	1.96	0.48
1:C:507:LEU:HD22	1:C:522:MET:HE3	1.95	0.48
1:B:442:ILE:O	1:B:445:GLN:HG2	2.13	0.48
1:A:457:GLU:C	1:A:459:LYS:H	2.17	0.48
1:C:569:CYS:HA	1:C:575:CYS:HA	1.96	0.48
1:C:428:ARG:HA	1:C:582:VAL:HG23	1.96	0.47
1:B:198:PHE:C	1:B:198:PHE:CD1	2.88	0.47
1:B:381:PHE:CD1	1:B:529:PHE:HB3	2.49	0.47
1:A:389:PRO:HB2	1:A:434:VAL:HA	1.96	0.47
1:D:147:TYR:CE1	1:D:220:PHE:CE1	3.02	0.47
1:C:394:THR:HA	1:C:402:TYR:O	2.14	0.47
1:A:257:ILE:HB	1:A:262:TYR:CD2	2.48	0.47
1:A:194:SER:OG	1:A:351:HIS:HE1	1.96	0.47
1:C:578:THR:O	1:C:579:SER:HB2	2.14	0.47
1:B:389:PRO:HB2	1:B:434:VAL:HA	1.96	0.47
1:D:339:GLU:O	1:D:342:LYS:HB3	2.14	0.47
1:D:479:GLU:HA	1:D:488:ALA:HB1	1.96	0.47
1:A:131:ASN:ND2	1:A:147:TYR:CD2	2.81	0.47
1:C:402:TYR:OH	1:C:417:HIS:CE1	2.67	0.47
1:D:197:MET:HA	1:D:197:MET:CE	2.45	0.47
1:D:185:ARG:HH21	1:D:438:ARG:NE	2.11	0.47
1:B:44:ARG:CG	1:B:44:ARG:NH1	2.77	0.47
1:B:124:ILE:HD13	1:B:532:LYS:HG3	1.97	0.47
1:A:113:MET:O	1:A:116:VAL:HG13	2.14	0.47
1:A:209:PHE:O	1:A:377:ILE:HD12	2.14	0.47
1:B:404:PHE:HE2	1:B:444:VAL:HG23	1.80	0.47
1:B:90:HIS:HD2	1:B:513:ARG:NH1	2.11	0.47
1:A:478:PHE:H	1:A:478:PHE:HD1	1.62	0.47
1:D:381:PHE:CD1	1:D:529:PHE:HB3	2.49	0.47
1:C:352:LEU:HD11	1:C:518:PHE:CE2	2.48	0.47
1:B:202:ALA:HB2	1:B:348:TYR:CE2	2.50	0.47
1:D:51:GLY:O	1:D:52:PHE:HB2	2.14	0.47
1:C:172:PRO:HG2	1:C:495:TYR:CD2	2.49	0.47
1:B:243:LYS:O	1:B:269:THR:HB	2.14	0.47
1:C:479:GLU:HA	1:C:488:ALA:CB	2.44	0.47
1:C:234:TYR:CE1	1:C:252:LEU:HD21	2.49	0.47
1:C:253:LYS:HE2	1:C:269:THR:HG22	1.96	0.47
1:C:97:LYS:HB2	1:C:356:HIS:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:PHE:CD1	1:B:199:ALA:N	2.81	0.47
1:B:283:LEU:HD22	1:B:411:ASN:OD1	2.14	0.47
1:B:134:TYR:CD1	1:B:136:TYR:CE1	2.96	0.47
1:A:442:ILE:O	1:A:445:GLN:HG2	2.14	0.47
1:D:501:MET:HE3	1:D:506:ALA:H	1.79	0.47
1:D:280:PRO:HG3	1:D:283:LEU:HD12	1.95	0.47
1:D:232:HIS:HD2	1:D:233:ILE:N	2.12	0.47
1:D:206:THR:HG21	1:D:385:TYR:CD1	2.49	0.47
1:C:230:LEU:N	1:C:230:LEU:HD23	2.29	0.47
1:A:198:PHE:CD1	1:A:198:PHE:C	2.88	0.47
1:B:196:MET:HE1	1:B:392:PRO:HD3	1.96	0.47
1:C:104:ASN:HB3	1:C:358:LYS:HE2	1.96	0.47
1:C:209:PHE:O	1:C:377:ILE:HD12	2.15	0.47
1:C:281:GLU:C	1:C:283:LEU:H	2.18	0.47
1:D:96:PHE:HB3	1:D:99:VAL:CG2	2.44	0.47
1:B:254:TYR:HD2	1:B:310:GLN:HE21	1.63	0.47
1:B:482:THR:HB	1:B:484:GLU:HG3	1.96	0.47
1:B:33:ALA:HB3	1:B:158:ASP:OD2	2.14	0.47
1:C:148:TYR:HD2	1:C:219:GLY:C	2.18	0.47
1:B:209:PHE:O	1:B:377:ILE:HD12	2.15	0.47
1:B:281:GLU:C	1:B:283:LEU:H	2.16	0.47
1:A:280:PRO:O	1:A:281:GLU:CB	2.59	0.47
1:A:175:LYS:O	1:A:178:LEU:HB3	2.15	0.47
1:A:482:THR:HB	1:A:484:GLU:HG3	1.96	0.47
1:A:215:LYS:HD3	1:A:215:LYS:N	2.30	0.47
1:B:394:THR:HA	1:B:402:TYR:O	2.14	0.47
1:D:124:ILE:HD13	1:D:532:LYS:HG3	1.96	0.47
1:A:113:MET:HG2	1:A:360:LYS:HB3	1.97	0.47
1:C:249:ASP:OD1	1:C:317:LYS:HD2	2.15	0.47
1:B:573:LYS:HD2	1:B:573:LYS:O	2.15	0.47
1:A:88:THR:HG22	1:A:92:ILE:CD1	2.41	0.47
1:D:281:GLU:C	1:D:283:LEU:H	2.18	0.47
1:B:210:PHE:CE1	1:B:382:ASN:HA	2.50	0.47
1:B:530:SER:O	1:B:534:LEU:HB2	2.15	0.47
1:C:390:LEU:O	1:C:431:ALA:HB1	2.15	0.47
1:C:51:GLY:O	1:C:52:PHE:HB2	2.15	0.46
1:C:281:GLU:HA	1:C:284:GLN:HG3	1.97	0.46
1:D:403:SER:OG	1:D:406:GLN:HG3	2.15	0.46
1:D:412:SER:HB2	2:D:681:NAG:H62	1.97	0.46
1:D:412:SER:O	1:D:416:GLU:N	2.47	0.46
1:D:97:LYS:HD3	1:D:356:HIS:CG	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:532:LYS:O	1:D:534:LEU:N	2.48	0.46
1:B:201:PHE:N	1:B:301:TYR:HE2	2.13	0.46
1:A:153:PRO:O	1:A:461:GLN:NE2	2.49	0.46
1:C:244:LEU:O	1:C:252:LEU:HD12	2.15	0.46
1:C:350:GLN:HE22	1:C:358:LYS:HA	1.81	0.46
1:C:257:ILE:HB	1:C:262:TYR:CD2	2.50	0.46
1:C:88:THR:HG22	1:C:92:ILE:CD1	2.41	0.46
1:C:287:VAL:HG23	1:C:288:GLY:N	2.31	0.46
1:A:197:MET:CE	1:A:197:MET:HA	2.45	0.46
1:D:191:PRO:HD2	1:D:433:ARG:HG3	1.98	0.46
1:B:97:LYS:HD3	1:B:356:HIS:NE2	2.30	0.46
1:A:522:MET:HG3	1:A:522:MET:O	2.14	0.46
1:D:134:TYR:CD1	1:D:136:TYR:CE1	3.02	0.46
1:C:134:TYR:CD1	1:C:136:TYR:CE1	3.02	0.46
1:A:204:HIS:ND1	1:A:292:PHE:CE2	2.83	0.46
1:D:388:HIS:N	1:D:389:PRO:CD	2.78	0.46
1:A:190:ASP:O	1:A:430:ILE:HD11	2.16	0.46
1:B:203:GLN:HE22	3:B:682:HEM:HBB2	1.80	0.46
1:A:396:ASN:ND2	1:A:401:GLU:HG2	2.31	0.46
1:D:578:THR:O	1:D:579:SER:HB2	2.15	0.46
1:B:388:HIS:N	1:B:389:PRO:CD	2.78	0.46
1:D:381:PHE:CD1	1:D:529:PHE:CB	2.98	0.46
1:C:150:ARG:CG	1:C:150:ARG:NH1	2.78	0.46
1:D:333:LYS:O	1:D:337:ILE:HG13	2.16	0.46
1:C:181:VAL:HB	1:C:509:VAL:HG22	1.98	0.46
1:A:397:ILE:HG22	1:A:417:HIS:CD2	2.50	0.46
1:B:360:LYS:HE2	1:B:362:ASP:HB2	1.98	0.46
1:C:153:PRO:O	1:C:461:GLN:NE2	2.48	0.46
1:C:92:ILE:H	1:C:92:ILE:HG13	1.58	0.46
1:A:150:ARG:CG	1:A:150:ARG:NH1	2.78	0.46
1:C:295:VAL:HG12	1:C:295:VAL:O	2.15	0.46
1:B:350:GLN:HE22	1:B:358:LYS:HA	1.81	0.46
1:C:104:ASN:CG	1:C:358:LYS:HE2	2.36	0.46
1:C:137:LYS:O	1:C:138:SER:O	2.33	0.46
1:C:147:TYR:HE1	1:C:220:PHE:CZ	2.33	0.46
1:C:232:HIS:HD2	1:C:233:ILE:N	2.14	0.46
1:A:274:ILE:HG13	1:A:290:GLU:HB2	1.98	0.46
1:D:276:PRO:HG2	1:D:409:TYR:CG	2.51	0.46
1:A:107:PHE:O	1:A:111:LEU:HB2	2.16	0.46
1:C:475:TYR:CD1	1:C:480:GLU:HG2	2.51	0.46
1:A:44:ARG:HH11	1:A:44:ARG:HG3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:352:LEU:HD11	1:D:518:PHE:CE2	2.51	0.46
1:D:553:GLU:O	1:D:557:LYS:HE3	2.16	0.46
1:A:104:ASN:CG	1:A:358:LYS:HE2	2.36	0.46
1:C:33:ALA:N	1:C:158:ASP:O	2.49	0.46
1:C:196:MET:CE	1:C:392:PRO:HD3	2.46	0.46
1:A:421:GLN:HA	1:A:421:GLN:OE1	2.15	0.46
1:B:38:SER:OG	1:B:40:PRO:HG3	2.16	0.46
1:C:35:PRO:HG3	1:C:54:GLN:O	2.15	0.46
1:B:254:TYR:CD1	1:B:254:TYR:C	2.89	0.46
1:B:232:HIS:HD2	1:B:233:ILE:N	2.14	0.46
1:C:263:PRO:HD3	1:C:303:THR:HG23	1.97	0.46
1:A:352:LEU:HD21	1:A:387:TRP:HH2	1.80	0.46
1:A:394:THR:HB	1:A:401:GLU:HB3	1.97	0.46
1:C:204:HIS:ND1	1:C:292:PHE:CE2	2.83	0.46
1:C:168:ASN:C	1:C:170:GLU:N	2.68	0.46
1:B:464:ASN:O	1:B:468:LYS:HG3	2.15	0.46
1:A:248:LYS:HB2	1:A:248:LYS:HE3	1.54	0.46
1:B:232:HIS:HD2	1:B:233:ILE:H	1.64	0.46
1:D:497:ASP:HB3	1:D:500:VAL:HG23	1.98	0.46
1:A:83:LYS:HA	1:A:83:LYS:HZ1	1.80	0.46
1:B:280:PRO:HG2	1:B:283:LEU:HD12	1.97	0.45
1:A:211:LYS:HE2	1:A:222:ARG:CG	2.45	0.45
1:A:126:SER:CB	1:A:532:LYS:HZ1	2.29	0.45
1:A:92:ILE:HA	1:A:96:PHE:CE2	2.52	0.45
1:B:191:PRO:HG3	1:B:433:ARG:NH1	2.31	0.45
1:D:40:PRO:HB2	1:D:55:TYR:CE2	2.51	0.45
1:B:88:THR:HG22	1:B:92:ILE:CD1	2.42	0.45
1:C:283:LEU:CD1	1:C:411:ASN:HD21	2.23	0.45
1:A:398:GLU:H	1:A:425:SER:HB3	1.81	0.45
1:B:475:TYR:CD1	1:B:480:GLU:HG2	2.51	0.45
1:D:232:HIS:HD2	1:D:233:ILE:H	1.62	0.45
1:C:510:GLU:HG2	1:C:511:LYS:N	2.32	0.45
1:B:150:ARG:HH11	1:B:150:ARG:CG	2.30	0.45
1:C:295:VAL:HG12	1:C:297:GLY:H	1.81	0.45
1:A:452:ILE:O	1:A:456:ARG:HG2	2.15	0.45
1:A:120:ARG:HG2	1:A:531:LEU:HD12	1.98	0.45
1:D:114:LYS:HD3	1:D:369:GLN:NE2	2.31	0.45
1:C:482:THR:HB	1:C:484:GLU:HG3	1.97	0.45
1:C:232:HIS:CD2	1:C:233:ILE:N	2.85	0.45
1:C:457:GLU:C	1:C:459:LYS:H	2.19	0.45
1:C:152:LEU:CD2	1:C:469:ARG:HG2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:PRO:HG2	1:B:409:TYR:CD2	2.50	0.45
1:D:196:MET:CE	1:D:392:PRO:HD3	2.45	0.45
1:A:197:MET:HA	1:A:197:MET:HE3	1.98	0.45
1:A:350:GLN:HE22	1:A:358:LYS:HA	1.81	0.45
1:A:149:THR:O	1:A:378:ALA:HA	2.17	0.45
1:D:182:LEU:HD22	1:D:508:LEU:HD12	1.98	0.45
1:B:178:LEU:O	1:B:182:LEU:HB2	2.17	0.45
1:D:443:ALA:C	1:D:445:GLN:H	2.20	0.45
1:B:137:LYS:O	1:B:138:SER:O	2.34	0.45
1:A:92:ILE:HA	1:A:96:PHE:HE2	1.80	0.45
1:D:406:GLN:HG2	2:D:681:NAG:O7	2.16	0.45
1:A:151:ALA:O	1:A:469:ARG:NH1	2.49	0.45
1:B:498:ILE:C	1:B:500:VAL:H	2.20	0.45
1:C:86:PRO:HG2	1:C:87:ASN:ND2	2.32	0.45
1:B:470:PHE:CD1	1:B:525:LEU:HD22	2.52	0.45
1:D:150:ARG:HG2	1:D:150:ARG:NH1	2.32	0.45
1:A:215:LYS:HD3	1:A:215:LYS:H	1.82	0.45
1:B:234:TYR:CE1	1:B:252:LEU:HD21	2.52	0.45
1:D:202:ALA:HB2	1:D:348:TYR:HE2	1.80	0.45
1:B:113:MET:HB3	1:B:365:LEU:HD13	1.99	0.45
1:C:532:LYS:O	1:C:534:LEU:N	2.50	0.45
1:C:320:HIS:HE1	1:C:551:GLY:O	1.99	0.45
1:A:333:LYS:O	1:A:337:ILE:HG13	2.16	0.45
1:D:104:ASN:HB3	1:D:358:LYS:HE2	1.99	0.45
1:A:232:HIS:HD2	1:A:233:ILE:H	1.64	0.45
1:B:201:PHE:CA	1:B:301:TYR:CE2	3.00	0.45
1:D:563:SER:OG	1:D:566:SER:HB2	2.17	0.45
1:B:565:GLN:O	1:B:569:CYS:HB2	2.16	0.45
1:D:573:LYS:O	1:D:573:LYS:HD2	2.17	0.45
1:A:510:GLU:HG2	1:A:511:LYS:H	1.82	0.45
1:D:380:GLU:HG2	1:D:466:TYR:CE2	2.52	0.45
1:A:300:MET:O	1:A:304:ILE:HG13	2.17	0.45
1:B:366:LEU:HA	1:B:369:GLN:CG	2.47	0.45
1:B:172:PRO:HG2	1:B:495:TYR:CZ	2.52	0.45
1:C:107:PHE:O	1:C:111:LEU:HB2	2.17	0.45
1:D:184:ARG:HB2	1:D:439:ASN:C	2.37	0.45
1:D:240:ARG:NH1	1:D:271:VAL:HG23	2.31	0.45
1:B:208:GLN:HE21	1:B:228:VAL:HA	1.79	0.45
1:A:569:CYS:HA	1:A:575:CYS:HA	1.99	0.45
1:C:196:MET:HB3	1:C:426:PHE:CG	2.52	0.45
1:D:366:LEU:HA	1:D:369:GLN:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:467:ARG:NH1	1:B:521:THR:OG1	2.48	0.45
1:A:52:PHE:CD1	1:B:322:GLU:HB3	2.52	0.44
1:B:274:ILE:HG13	1:B:290:GLU:HB2	1.99	0.44
1:C:411:ASN:ND2	1:C:412:SER:N	2.65	0.44
1:A:283:LEU:HD22	1:A:411:ASN:ND2	2.32	0.44
1:B:43:ASN:ND2	1:B:64:PHE:CD2	2.85	0.44
1:D:91:TYR:O	1:D:95:HIS:CD2	2.69	0.44
1:B:198:PHE:HB2	1:B:580:PHE:HB3	1.99	0.44
1:B:215:LYS:N	1:B:215:LYS:HD3	2.32	0.44
1:B:209:PHE:O	1:B:377:ILE:CD1	2.65	0.44
1:C:147:TYR:CE1	1:C:220:PHE:CE1	3.05	0.44
1:C:109:ARG:HG3	1:C:357:PHE:CE1	2.52	0.44
1:D:457:GLU:C	1:D:459:LYS:H	2.20	0.44
1:B:107:PHE:O	1:B:111:LEU:HB2	2.17	0.44
1:B:150:ARG:NH1	1:B:150:ARG:CG	2.80	0.44
1:B:366:LEU:HD23	1:B:369:GLN:HG3	2.00	0.44
1:C:543:GLN:NE2	1:D:127:PRO:O	2.50	0.44
1:C:351:HIS:O	1:C:353:SER:N	2.50	0.44
1:A:403:SER:CB	1:A:405:LYS:HD2	2.47	0.44
1:A:182:LEU:HD22	1:A:508:LEU:HD12	1.99	0.44
1:C:210:PHE:HB3	1:C:382:ASN:ND2	2.33	0.44
1:A:230:LEU:N	1:A:230:LEU:HD23	2.31	0.44
1:C:150:ARG:HG2	1:C:150:ARG:NH1	2.31	0.44
1:B:257:ILE:HB	1:B:262:TYR:HD2	1.81	0.44
1:B:490:GLU:O	1:B:493:ALA:HB3	2.18	0.44
1:A:196:MET:HB3	1:A:426:PHE:CG	2.53	0.44
1:A:97:LYS:HD3	1:A:356:HIS:CG	2.50	0.44
1:C:333:LYS:O	1:C:337:ILE:HG13	2.18	0.44
1:B:105(A):ILE:HD12	1:B:108:LEU:HD12	2.00	0.44
1:B:218:PRO:HB2	1:B:458:MET:SD	2.57	0.44
1:A:95:HIS:O	1:A:100:TRP:CD1	2.69	0.44
1:B:352:LEU:HD21	1:B:387:TRP:CH2	2.52	0.44
1:A:360:LYS:HE2	1:A:362:ASP:HB2	1.99	0.44
1:A:537:ASN:O	1:A:540:CYS:HB2	2.18	0.44
1:A:42:GLN:HA	1:A:42:GLN:HE21	1.81	0.44
1:C:388:HIS:N	1:C:389:PRO:HD2	2.33	0.44
1:D:248:LYS:N	1:D:325:ASP:OD1	2.50	0.44
1:B:457:GLU:C	1:B:459:LYS:H	2.20	0.44
1:C:160:PRO:HD2	1:C:164:GLY:O	2.18	0.44
1:D:475:TYR:CD1	1:D:480:GLU:HG2	2.52	0.44
1:B:276:PRO:O	1:B:279:ILE:HG12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:574:GLY:C	1:C:576:PRO:HD3	2.38	0.44
1:D:420:THR:HG22	1:D:576:PRO:CG	2.47	0.44
1:A:53:ASP:HB2	1:A:54:GLN:OE1	2.18	0.44
1:D:92:ILE:HA	1:D:96:PHE:HE2	1.83	0.44
1:D:247:PHE:O	1:D:248:LYS:HB2	2.17	0.44
1:D:275:TYR:CE2	1:D:284:GLN:HA	2.53	0.44
1:B:481:LEU:HD12	1:B:510:GLU:HG3	2.00	0.44
1:B:147:TYR:CE1	1:B:220:PHE:CE1	3.05	0.44
1:B:142:PHE:O	1:B:376:ARG:NH2	2.44	0.44
1:A:532:LYS:O	1:A:534:LEU:N	2.51	0.44
1:A:176:GLU:HG2	1:A:180:LYS:HE3	1.98	0.44
1:A:383:THR:HG22	1:A:384:LEU:N	2.32	0.44
1:A:279:ILE:CG2	1:A:280:PRO:HD2	2.48	0.44
1:A:281:GLU:CA	1:A:284:GLN:HG3	2.40	0.44
1:D:152:LEU:CD2	1:D:469:ARG:HG2	2.47	0.44
1:D:48:MET:O	1:D:56:LYS:N	2.51	0.44
1:B:35:PRO:HB3	1:B:53:ASP:O	2.18	0.44
1:A:211:LYS:NZ	1:A:236:GLU:CG	2.77	0.44
1:C:95:HIS:O	1:C:100:TRP:CD1	2.70	0.44
1:A:44:ARG:CG	1:A:44:ARG:NH1	2.80	0.44
1:B:241:GLN:HG3	1:B:242:HIS:N	2.31	0.44
1:A:192:GLN:OE1	1:A:517:ILE:HG22	2.18	0.44
1:D:478:PHE:HD1	1:D:478:PHE:H	1.64	0.44
1:D:479:GLU:HA	1:D:488:ALA:CB	2.48	0.44
1:A:275:TYR:HA	1:A:276:PRO:HD3	1.91	0.44
1:A:286:ALA:O	1:A:287:VAL:HG22	2.18	0.44
1:B:553:GLU:O	1:B:557:LYS:HE3	2.18	0.44
1:D:215:LYS:CD	1:D:215:LYS:N	2.78	0.44
1:D:91:TYR:CE2	1:D:95:HIS:CE1	3.05	0.44
1:B:381:PHE:CD1	1:B:529:PHE:CD2	3.06	0.44
1:B:104:ASN:HB3	1:B:358:LYS:HE2	1.98	0.44
1:D:103:VAL:C	1:D:105:ASN:H	2.21	0.44
1:C:201:PHE:HA	1:C:301:TYR:CE2	2.53	0.44
1:D:169:LYS:HB3	1:D:170:GLU:OE2	2.17	0.44
1:A:40:PRO:HB2	1:A:55:TYR:CE2	2.53	0.43
1:C:172:PRO:HG2	1:C:495:TYR:CZ	2.52	0.43
1:C:96:PHE:HB3	1:C:99:VAL:CG2	2.48	0.43
1:A:244:LEU:CD2	1:A:271:VAL:HG11	2.47	0.43
1:A:273:MET:CE	1:A:287:VAL:HG22	2.48	0.43
1:D:263:PRO:HD3	1:D:303:THR:HG23	1.99	0.43
1:C:397:ILE:HG22	1:C:417:HIS:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:530:SER:O	1:D:534:LEU:HB2	2.17	0.43
1:A:148:TYR:CD1	1:A:377:ILE:HG13	2.53	0.43
1:D:150:ARG:CG	1:D:150:ARG:NH1	2.81	0.43
1:A:226:HIS:CE1	1:A:376:ARG:HD2	2.53	0.43
1:B:532:LYS:O	1:B:534:LEU:N	2.51	0.43
1:A:295:VAL:HG12	1:A:297:GLY:H	1.83	0.43
1:C:439:ASN:O	1:C:441:PRO:HD3	2.18	0.43
1:C:428:ARG:HG3	1:C:583:GLN:OE1	2.19	0.43
1:A:198:PHE:CD1	1:A:199:ALA:N	2.85	0.43
1:D:113:MET:HB3	1:D:365:LEU:HD13	2.00	0.43
1:D:74:PHE:O	1:D:77:ARG:HB2	2.18	0.43
1:D:252:LEU:HD13	1:D:252:LEU:HA	1.87	0.43
1:D:172:PRO:HG2	1:D:495:TYR:CE2	2.54	0.43
1:B:253:LYS:HB2	1:B:253:LYS:NZ	2.34	0.43
1:A:234:TYR:CE1	1:A:252:LEU:HD21	2.53	0.43
1:D:218:PRO:HB2	1:D:458:MET:SD	2.59	0.43
1:D:231:ASN:C	1:D:231:ASN:OD1	2.57	0.43
1:B:210:PHE:HB3	1:B:382:ASN:ND2	2.33	0.43
1:D:105(A):ILE:HG22	1:D:108:LEU:H	1.83	0.43
1:B:109:ARG:HG3	1:B:357:PHE:CE1	2.54	0.43
1:B:427:THR:HB	1:B:428:ARG:NH1	2.34	0.43
1:C:487:MET:HA	1:C:490:GLU:HB3	2.01	0.43
1:D:402:TYR:OH	1:D:417:HIS:HE1	2.00	0.43
1:B:402:TYR:OH	1:B:417:HIS:HE1	2.01	0.43
1:B:168:ASN:C	1:B:170:GLU:N	2.71	0.43
1:B:390:LEU:O	1:B:431:ALA:HB1	2.19	0.43
1:D:389:PRO:HB2	1:D:434:VAL:HA	1.98	0.43
1:D:510:GLU:HG2	1:D:511:LYS:N	2.33	0.43
1:A:152:LEU:CD2	1:A:469:ARG:HG2	2.48	0.43
1:D:59:CYS:HB3	1:D:64:PHE:O	2.19	0.43
1:D:352:LEU:HD21	1:D:387:TRP:HH2	1.84	0.43
1:A:498:ILE:C	1:A:500:VAL:H	2.22	0.43
1:A:59:CYS:HB3	1:A:64:PHE:O	2.19	0.43
1:B:126:SER:CB	1:B:532:LYS:HZ1	2.31	0.43
1:B:366:LEU:HA	1:B:369:GLN:HG2	2.00	0.43
1:C:478:PHE:HD1	1:C:478:PHE:H	1.67	0.43
1:A:281:GLU:HG2	1:A:282:ASN:H	1.82	0.43
1:A:470:PHE:CD1	1:A:525:LEU:HD22	2.53	0.43
1:C:230:LEU:H	1:C:230:LEU:HD23	1.84	0.43
1:A:196:MET:HE1	1:A:392:PRO:HD3	2.00	0.43
1:D:168:ASN:CG	1:D:169:LYS:N	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:SER:OG	1:B:351:HIS:HE1	2.01	0.43
1:A:48:MET:HG3	1:A:48:MET:O	2.18	0.43
1:B:34:ASN:HA	1:B:35:PRO:HD2	1.85	0.43
1:C:92:ILE:HA	1:C:96:PHE:CE2	2.54	0.43
1:D:179:GLU:HA	1:D:183:LEU:HD12	2.01	0.43
1:A:184:ARG:HB2	1:A:439:ASN:CA	2.47	0.43
1:A:578:THR:O	1:A:579:SER:HB2	2.18	0.43
1:D:232:HIS:CD2	1:D:233:ILE:N	2.87	0.43
1:A:181:VAL:HG12	1:A:487:MET:HB3	2.01	0.43
1:A:130:TYR:CE2	1:A:135:GLY:O	2.71	0.43
1:B:150:ARG:NH1	1:B:150:ARG:HG2	2.33	0.43
1:B:193:GLY:O	1:B:582:VAL:HG12	2.18	0.43
1:D:487:MET:O	1:D:491:LEU:N	2.48	0.43
1:C:44:ARG:CG	1:C:44:ARG:NH1	2.80	0.43
1:B:352:LEU:HD11	1:B:518:PHE:CE2	2.54	0.43
1:D:280:PRO:HG2	1:D:283:LEU:HD12	1.99	0.43
1:A:130:TYR:HB3	1:A:134:TYR:O	2.18	0.43
1:D:42:GLN:O	1:D:69:CYS:HB2	2.19	0.43
1:C:276:PRO:HD2	1:C:279:ILE:CG1	2.48	0.43
1:D:181:VAL:HB	1:D:509:VAL:HG22	2.01	0.43
1:D:490:GLU:O	1:D:493:ALA:HB3	2.19	0.43
1:D:360:LYS:HE2	1:D:362:ASP:HB2	2.01	0.43
1:A:292:PHE:O	1:A:299:MET:HE2	2.18	0.43
1:D:209:PHE:O	1:D:377:ILE:CD1	2.67	0.43
1:A:579:SER:HB2	1:D:267:LYS:HZ1	1.84	0.43
1:A:427:THR:HB	1:A:428:ARG:HD2	2.01	0.43
1:D:498:ILE:C	1:D:500:VAL:H	2.22	0.43
1:D:88:THR:HG22	1:D:92:ILE:CD1	2.46	0.43
1:D:172:PRO:HG2	1:D:495:TYR:CG	2.54	0.43
1:A:477:SER:O	1:A:480:GLU:N	2.52	0.43
1:A:582:VAL:O	1:A:582:VAL:CG1	2.66	0.43
1:D:198:PHE:CZ	1:D:352:LEU:HD13	2.54	0.43
1:C:201:PHE:N	1:C:301:TYR:HE2	2.16	0.43
1:D:234:TYR:CE1	1:D:252:LEU:HD21	2.54	0.43
1:A:226:HIS:ND1	1:A:376:ARG:HD2	2.34	0.42
1:C:180:LYS:HD3	1:C:490:GLU:OE1	2.19	0.42
1:D:137:LYS:O	1:D:138:SER:O	2.36	0.42
1:B:175:LYS:HE2	1:B:449:LYS:HE3	2.01	0.42
1:C:381:PHE:CD1	1:C:529:PHE:HB3	2.54	0.42
1:A:210:PHE:HB3	1:A:382:ASN:ND2	2.34	0.42
1:B:428:ARG:O	1:B:429:GLN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:LYS:O	1:B:337:ILE:HG13	2.19	0.42
1:C:168:ASN:O	1:C:170:GLU:N	2.52	0.42
1:D:92:ILE:HA	1:D:96:PHE:CE2	2.54	0.42
1:D:295:VAL:O	1:D:295:VAL:HG12	2.19	0.42
1:D:450:ALA:O	1:D:453:ASP:N	2.52	0.42
1:A:475:TYR:CD1	1:A:480:GLU:HG2	2.54	0.42
1:B:424:GLU:O	1:B:428:ARG:HD3	2.19	0.42
1:C:449:LYS:HD3	1:C:453:ASP:OD2	2.19	0.42
1:C:260:GLU:HB2	1:C:262:TYR:CE2	2.54	0.42
1:A:196:MET:CE	1:A:392:PRO:HD3	2.49	0.42
1:A:276:PRO:HG2	1:A:409:TYR:CG	2.54	0.42
1:C:522:MET:HG3	1:C:522:MET:O	2.20	0.42
1:C:510:GLU:HG2	1:C:511:LYS:H	1.85	0.42
1:A:147:TYR:HE1	1:A:220:PHE:CZ	2.37	0.42
1:B:564:ILE:HG12	1:B:580:PHE:CZ	2.54	0.42
1:A:137:LYS:NZ	1:B:543:GLN:O	2.44	0.42
1:A:565:GLN:HG2	1:D:268:ASP:HB2	2.02	0.42
1:D:568:ILE:O	1:D:572:VAL:N	2.47	0.42
1:A:74:PHE:O	1:A:77:ARG:HB2	2.18	0.42
1:C:338:GLY:C	1:C:559:ILE:HG23	2.40	0.42
3:D:682:HEM:HHD	3:D:682:HEM:HBC2	2.00	0.42
1:D:35:PRO:HB3	1:D:53:ASP:O	2.20	0.42
1:D:211:LYS:HE2	1:D:222:ARG:CG	2.49	0.42
1:D:175:LYS:O	1:D:178:LEU:HB3	2.19	0.42
1:A:579:SER:HB2	1:D:267:LYS:NZ	2.34	0.42
1:A:232:HIS:HD2	1:A:233:ILE:N	2.17	0.42
1:C:423:VAL:HG13	1:C:578:THR:HG23	2.00	0.42
1:A:543:GLN:NE2	1:B:127:PRO:O	2.52	0.42
1:C:283:LEU:HD22	1:C:411:ASN:ND2	2.35	0.42
1:C:398:GLU:H	1:C:425:SER:CB	2.32	0.42
1:A:411:ASN:ND2	1:A:412:SER:H	2.16	0.42
1:A:244:LEU:O	1:A:252:LEU:HD12	2.19	0.42
1:C:130:TYR:CE2	1:C:135:GLY:O	2.73	0.42
1:C:198:PHE:CD1	1:C:199:ALA:N	2.88	0.42
1:C:181:VAL:HG21	1:C:491:LEU:HD21	2.02	0.42
1:A:352:LEU:HD11	1:A:518:PHE:CZ	2.54	0.42
1:C:352:LEU:HD21	1:C:387:TRP:HH2	1.84	0.42
1:A:168:ASN:O	1:A:170:GLU:N	2.53	0.42
1:D:126:SER:CB	1:D:532:LYS:HZ1	2.32	0.42
1:D:83:LYS:HA	1:D:83:LYS:NZ	2.34	0.42
1:C:82:LEU:N	1:C:82:LEU:HD12	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:GLN:OE1	1:B:421:GLN:HA	2.19	0.42
1:A:171:LEU:HD12	1:A:171:LEU:HA	1.86	0.42
1:C:322:GLU:HB3	1:D:52:PHE:CD1	2.55	0.42
1:C:442:ILE:O	1:C:445:GLN:HG2	2.20	0.42
1:C:505:PRO:O	1:C:507:LEU:N	2.52	0.42
1:B:510:GLU:HG2	1:B:511:LYS:H	1.83	0.42
1:C:403:SER:HB2	1:C:405:LYS:CD	2.50	0.42
1:B:182:LEU:HD22	1:B:508:LEU:HD12	2.01	0.42
1:D:107:PHE:O	1:D:111:LEU:HB2	2.19	0.42
1:C:276:PRO:HG2	1:C:409:TYR:CG	2.55	0.42
1:C:427:THR:HB	1:C:428:ARG:HD2	2.02	0.42
1:B:574:GLY:C	1:B:576:PRO:HD3	2.40	0.42
1:A:544:TYR:OH	1:B:142:PHE:HB2	2.19	0.42
1:C:48:MET:HG3	1:C:48:MET:O	2.19	0.42
1:C:388:HIS:N	1:C:389:PRO:CD	2.82	0.42
1:D:92:ILE:H	1:D:92:ILE:HG13	1.58	0.42
1:A:412:SER:O	1:A:416:GLU:N	2.47	0.42
1:D:294:LEU:HD22	1:D:409:TYR:HD1	1.83	0.42
1:C:59:CYS:HB3	1:C:64:PHE:O	2.20	0.42
1:C:396:ASN:HD22	1:C:401:GLU:HA	1.85	0.42
1:C:256:VAL:HA	1:C:260:GLU:O	2.20	0.42
1:C:202:ALA:HB2	1:C:348:TYR:CE2	2.55	0.42
1:B:204:HIS:ND1	1:B:292:PHE:CE2	2.88	0.42
1:B:478:PHE:N	1:B:478:PHE:CD1	2.87	0.42
1:D:243:LYS:O	1:D:269:THR:HB	2.20	0.42
1:A:175:LYS:HD3	1:A:175:LYS:HA	1.88	0.42
1:D:487:MET:HA	1:D:490:GLU:HB3	2.01	0.42
1:A:320:HIS:CE1	1:A:551:GLY:O	2.72	0.42
1:B:197:MET:HE3	1:B:197:MET:HA	2.01	0.42
1:A:563:SER:OG	1:A:566:SER:HB2	2.20	0.42
1:C:298:LEU:HD12	1:C:298:LEU:HA	1.81	0.42
1:C:61:ARG:NH2	1:D:545:TRP:O	2.51	0.42
1:D:82:LEU:N	1:D:82:LEU:HD12	2.35	0.42
1:B:40:PRO:HB2	1:B:55:TYR:CE2	2.55	0.42
1:A:388:HIS:N	1:A:389:PRO:HD2	2.34	0.42
1:A:388:HIS:CG	1:A:444:VAL:HG11	2.54	0.42
1:C:105(A):ILE:O	1:C:108:LEU:HB2	2.20	0.42
1:B:73:GLU:O	1:B:76:THR:N	2.52	0.42
1:D:145:LEU:HD23	1:D:376:ARG:CZ	2.50	0.42
1:C:113:MET:O	1:C:117:LEU:HB2	2.20	0.42
1:D:201:PHE:CA	1:D:301:TYR:CE2	3.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:SER:OG	1:D:351:HIS:HE1	2.02	0.42
1:A:300:MET:HB3	1:A:300:MET:HE3	1.85	0.42
1:C:537:ASN:O	1:C:540:CYS:HB2	2.19	0.42
1:A:478:PHE:CD1	1:A:478:PHE:N	2.88	0.41
1:B:206:THR:HG21	1:B:385:TYR:CD1	2.55	0.41
1:B:275:TYR:HA	1:B:276:PRO:HD3	1.93	0.41
1:B:230:LEU:H	1:B:230:LEU:HD23	1.84	0.41
1:D:201:PHE:N	1:D:301:TYR:HE2	2.18	0.41
1:C:462:SER:HB3	1:C:465:GLU:HG2	2.02	0.41
1:C:248:LYS:N	1:C:325:ASP:OD1	2.53	0.41
1:D:38:SER:OG	1:D:40:PRO:HG3	2.20	0.41
1:D:105(A):ILE:HD12	1:D:108:LEU:HD12	2.01	0.41
1:C:206:THR:HG21	1:C:385:TYR:CD1	2.56	0.41
1:A:168:ASN:ND2	1:A:169:LYS:H	2.18	0.41
1:A:565:GLN:O	1:A:569:CYS:HB2	2.20	0.41
1:C:138:SER:HB2	1:D:330:GLN:HB3	2.01	0.41
1:C:300:MET:O	1:C:304:ILE:HG13	2.21	0.41
1:A:390:LEU:O	1:A:431:ALA:HB1	2.20	0.41
1:A:96:PHE:HB3	1:A:99:VAL:CG2	2.50	0.41
1:C:211:LYS:HE2	1:C:222:ARG:CG	2.45	0.41
1:B:433:ARG:HH21	1:B:512:PRO:CB	2.33	0.41
1:D:210:PHE:HZ	1:D:381:PHE:CD2	2.38	0.41
1:A:138:SER:HB2	1:B:330:GLN:HB3	2.01	0.41
1:B:381:PHE:HD1	1:B:529:PHE:CD2	2.35	0.41
1:A:43:ASN:ND2	1:A:64:PHE:CD2	2.88	0.41
1:B:215:LYS:H	1:B:215:LYS:HD3	1.85	0.41
1:B:568:ILE:HG13	1:B:572:VAL:HG21	2.01	0.41
1:B:475:TYR:CD2	1:B:481:LEU:HB2	2.56	0.41
1:D:522:MET:O	1:D:522:MET:HG3	2.20	0.41
1:D:130:TYR:HB3	1:D:134:TYR:O	2.21	0.41
1:B:208:GLN:HB3	1:B:232:HIS:ND1	2.36	0.41
1:D:104:ASN:CB	1:D:358:LYS:HE2	2.51	0.41
1:B:42:GLN:O	1:B:69:CYS:HB2	2.21	0.41
1:D:83:LYS:HZ1	1:D:84:PRO:HD2	1.85	0.41
1:A:490:GLU:O	1:A:493:ALA:HB3	2.21	0.41
1:A:86:PRO:HG2	1:A:87:ASN:ND2	2.36	0.41
1:A:294:LEU:HD22	1:A:409:TYR:HD1	1.83	0.41
1:C:403:SER:HB2	1:C:405:LYS:HZ3	1.85	0.41
1:A:215:LYS:CD	1:A:215:LYS:H	2.32	0.41
1:B:402:TYR:OH	1:B:417:HIS:CE1	2.73	0.41
1:C:565:GLN:O	1:C:569:CYS:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:513:ARG:O	1:D:514:PRO:O	2.39	0.41
1:A:113:MET:HE2	1:A:360:LYS:O	2.20	0.41
1:A:260:GLU:HB2	1:A:262:TYR:CE2	2.55	0.41
1:A:330:GLN:HB3	1:B:138:SER:HB2	2.03	0.41
1:D:209:PHE:O	1:D:377:ILE:HD12	2.19	0.41
1:B:96:PHE:O	1:B:98:GLY:N	2.53	0.41
1:A:41:CYS:SG	1:A:47:CYS:HB2	2.61	0.41
1:C:41:CYS:SG	1:C:47:CYS:HB2	2.61	0.41
1:B:481:LEU:HD11	1:B:506:ALA:HB1	2.03	0.41
1:B:232:HIS:CD2	1:B:233:ILE:N	2.89	0.41
1:D:160:PRO:HD2	1:D:164:GLY:O	2.21	0.41
1:C:491:LEU:HD11	1:C:509:VAL:CG1	2.49	0.41
1:C:117:LEU:HD12	1:C:117:LEU:HA	1.92	0.41
1:D:352:LEU:HD11	1:D:518:PHE:CZ	2.56	0.41
1:C:352:LEU:HD11	1:C:518:PHE:CZ	2.55	0.41
1:A:168:ASN:C	1:A:170:GLU:N	2.73	0.41
1:C:209:PHE:O	1:C:377:ILE:CD1	2.69	0.41
1:D:291:VAL:O	1:D:293:GLY:N	2.54	0.41
1:B:39:ASN:N	1:B:40:PRO:CD	2.83	0.41
1:A:96:PHE:O	1:A:99:VAL:N	2.54	0.41
1:C:246:LEU:HD23	1:C:251:LYS:HB2	2.02	0.41
1:D:311:ARG:O	1:D:315:ILE:HG13	2.20	0.41
1:C:394:THR:HB	1:C:401:GLU:HB3	2.02	0.41
1:A:338:GLY:HA3	1:A:559:ILE:HD13	2.03	0.41
1:D:299:MET:HA	1:D:302:ALA:HB3	2.03	0.41
1:C:280:PRO:HG2	1:C:283:LEU:HD12	2.02	0.41
1:A:92:ILE:HG13	1:A:92:ILE:H	1.61	0.41
1:D:130:TYR:CD1	1:D:130:TYR:N	2.88	0.41
1:A:396:ASN:N	1:A:396:ASN:ND2	2.69	0.41
3:D:682:HEM:HHH	3:D:682:HEM:CBC	2.51	0.41
1:C:208:GLN:OE1	1:C:232:HIS:CE1	2.74	0.41
1:C:184:ARG:HB2	1:C:439:ASN:C	2.42	0.41
1:B:479:GLU:HG3	1:B:488:ALA:CB	2.50	0.41
1:B:482:THR:HG22	1:B:509:VAL:HG12	2.03	0.41
1:D:150:ARG:CG	1:D:152:LEU:O	2.69	0.41
1:A:481:LEU:HD12	1:A:510:GLU:HG3	2.03	0.41
1:B:184:ARG:HB2	1:B:439:ASN:C	2.41	0.41
1:A:424:GLU:HA	1:A:428:ARG:HH11	1.86	0.41
1:C:490:GLU:O	1:C:493:ALA:HB3	2.21	0.41
1:B:394:THR:HB	1:B:396:ASN:HD21	1.86	0.41
1:B:320:HIS:CE1	1:B:551:GLY:O	2.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:MET:O	1:B:117:LEU:HB2	2.21	0.41
1:B:168:ASN:O	1:B:170:GLU:N	2.54	0.41
1:C:316:LEU:HD12	1:C:316:LEU:HA	1.86	0.41
1:B:248:LYS:N	1:B:325:ASP:OD1	2.54	0.41
1:A:573:LYS:O	1:A:573:LYS:HD2	2.21	0.41
1:D:254:TYR:HD1	1:D:255:GLN:N	2.19	0.41
1:A:295:VAL:HG12	1:A:295:VAL:O	2.20	0.41
1:D:273:MET:CE	1:D:287:VAL:HG22	2.51	0.41
1:A:399:ASP:HB3	1:A:400:GLN:NE2	2.28	0.41
1:A:181:VAL:HB	1:A:509:VAL:HG22	2.02	0.41
1:D:109:ARG:HG3	1:D:357:PHE:HE1	1.86	0.41
1:D:381:PHE:CD1	1:D:529:PHE:CD2	3.09	0.41
1:A:232:HIS:CD2	1:A:233:ILE:N	2.89	0.41
1:A:574:GLY:C	1:A:576:PRO:HD3	2.40	0.41
1:B:113:MET:HE2	1:B:360:LYS:O	2.21	0.41
1:C:433:ARG:NH2	1:C:516:ALA:O	2.54	0.40
1:C:172:PRO:HG2	1:C:495:TYR:CG	2.56	0.40
1:C:269:THR:O	1:C:270:GLN:CB	2.69	0.40
1:C:538:PRO:HG3	1:D:142:PHE:CE2	2.57	0.40
1:B:198:PHE:CZ	1:B:352:LEU:HD13	2.56	0.40
1:D:201:PHE:HD2	1:D:301:TYR:CZ	2.39	0.40
1:B:153:PRO:HG2	1:B:461:GLN:HE22	1.86	0.40
1:B:202:ALA:HB2	1:B:348:TYR:HE2	1.85	0.40
1:C:126:SER:CB	1:C:532:LYS:HZ1	2.34	0.40
1:D:48:MET:HG3	1:D:48:MET:O	2.20	0.40
1:C:389:PRO:CB	1:C:434:VAL:HA	2.51	0.40
1:B:412:SER:O	1:B:416:GLU:HB2	2.20	0.40
1:C:92:ILE:HA	1:C:96:PHE:HE2	1.85	0.40
1:C:274:ILE:HG13	1:C:290:GLU:HB2	2.01	0.40
1:A:281:GLU:HA	1:A:284:GLN:HE21	1.86	0.40
1:A:253:LYS:NZ	1:A:253:LYS:HB2	2.37	0.40
1:A:184:ARG:HB2	1:A:439:ASN:C	2.42	0.40
1:D:281:GLU:HA	1:D:284:GLN:NE2	2.30	0.40
1:D:505:PRO:O	1:D:507:LEU:N	2.55	0.40
1:D:487:MET:O	1:D:490:GLU:HB3	2.21	0.40
1:B:472:LEU:HD21	1:B:524:GLU:HG3	2.02	0.40
1:D:394:THR:HB	1:D:401:GLU:HB3	2.04	0.40
1:B:531:LEU:O	1:B:535:MET:HB2	2.21	0.40
1:B:420:THR:HG22	1:B:576:PRO:CG	2.51	0.40
1:D:318:GLN:CD	1:D:318:GLN:C	2.79	0.40
1:D:478:PHE:N	1:D:478:PHE:CD1	2.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:184:ARG:HB2	1:D:439:ASN:CA	2.49	0.40
1:A:273:MET:HE2	1:A:287:VAL:HG22	2.02	0.40
1:A:577:PHE:CE1	1:D:267:LYS:HD2	2.51	0.40
1:C:210:PHE:CG	1:C:382:ASN:ND2	2.85	0.40
1:B:295:VAL:HG21	3:B:682:HEM:CBB	2.51	0.40
1:D:472:LEU:HD21	1:D:524:GLU:HG3	2.03	0.40
1:A:402:TYR:OH	1:A:417:HIS:CE1	2.73	0.40
1:C:204:HIS:ND1	1:C:292:PHE:HE2	2.18	0.40
1:D:366:LEU:HD23	1:D:369:GLN:HG3	2.03	0.40
1:B:292:PHE:O	1:B:299:MET:HE2	2.22	0.40
1:B:563:SER:OG	1:B:566:SER:HB2	2.21	0.40
1:D:479:GLU:HG2	1:D:485:LYS:NZ	2.36	0.40
1:C:479:GLU:HG2	1:C:485:LYS:HZ1	1.85	0.40
1:A:210:PHE:CG	1:A:382:ASN:ND2	2.88	0.40
1:C:63:GLY:HA2	1:C:73:GLU:CD	2.42	0.40
1:C:327:GLN:HG3	1:D:136:TYR:CE2	2.57	0.40
1:C:130:TYR:HB3	1:C:134:TYR:O	2.21	0.40
1:B:564:ILE:HG12	1:B:580:PHE:CE1	2.57	0.40
1:D:113:MET:O	1:D:117:LEU:HB2	2.22	0.40
1:C:33:ALA:HB3	1:C:158:ASP:OD2	2.20	0.40
1:B:299:MET:HG3	1:B:299:MET:O	2.21	0.40
1:C:291:VAL:O	1:C:293:GLY:N	2.54	0.40
1:D:41:CYS:SG	1:D:47:CYS:HB2	2.62	0.40
1:D:246:LEU:HD23	1:D:251:LYS:HB2	2.03	0.40
1:A:97:LYS:HD3	1:A:356:HIS:NE2	2.37	0.40
1:A:269:THR:O	1:A:270:GLN:CB	2.68	0.40
1:C:233:ILE:HD13	1:C:305:TRP:HB3	2.03	0.40
1:C:181:VAL:HG12	1:C:487:MET:HB3	2.03	0.40
1:C:64:PHE:CE2	1:C:72:PRO:HB3	2.57	0.40
1:B:498:ILE:O	1:B:500:VAL:N	2.52	0.40
1:D:320:HIS:CE1	1:D:551:GLY:O	2.73	0.40
1:D:103:VAL:O	1:D:105:ASN:N	2.54	0.40
1:B:383:THR:HG22	1:B:384:LEU:N	2.36	0.40
1:C:285:PHE:CD1	1:C:285:PHE:N	2.89	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	550/587 (94%)	446 (81%)	78 (14%)	26 (5%)	3	17
1	B	550/587 (94%)	442 (80%)	87 (16%)	21 (4%)	4	22
1	C	550/587 (94%)	443 (80%)	80 (14%)	27 (5%)	3	16
1	D	550/587 (94%)	440 (80%)	85 (16%)	25 (4%)	3	18
All	All	2200/2348 (94%)	1771 (80%)	330 (15%)	99 (4%)	3	18

All (99) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	SER
1	A	429	GLN
1	A	438	ARG
1	A	514	PRO
1	A	573	LYS
1	B	138	SER
1	B	429	GLN
1	B	438	ARG
1	B	514	PRO
1	B	573	LYS
1	C	138	SER
1	C	429	GLN
1	C	514	PRO
1	C	573	LYS
1	D	138	SER
1	D	429	GLN
1	D	514	PRO
1	D	573	LYS
1	A	97	LYS
1	A	282	ASN
1	A	398	GLU
1	A	399	ASP

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Mol	Chain	Res	Type
1	B	97	LYS
1	B	282	ASN
1	B	398	GLU
1	B	399	ASP
1	B	444	VAL
1	C	97	LYS
1	C	292	PHE
1	C	398	GLU
1	C	399	ASP
1	C	438	ARG
1	D	97	LYS
1	D	282	ASN
1	D	292	PHE
1	D	352	LEU
1	D	398	GLU
1	D	399	ASP
1	D	438	ARG
1	A	292	PHE
1	A	352	LEU
1	A	444	VAL
1	A	506	ALA
1	B	169	LYS
1	B	292	PHE
1	B	500	VAL
1	B	554	VAL
1	C	132	VAL
1	C	282	ASN
1	C	500	VAL
1	D	104	ASN
1	D	392	PRO
1	D	460	TYR
1	A	169	LYS
1	A	392	PRO
1	A	460	TYR
1	B	392	PRO
1	C	352	LEU
1	C	392	PRO
1	C	444	VAL
1	C	506	ALA
1	C	554	VAL
1	D	132	VAL
1	D	248	LYS

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Mol	Chain	Res	Type
1	D	444	VAL
1	D	500	VAL
1	D	506	ALA
1	A	132	VAL
1	A	248	LYS
1	A	500	VAL
1	C	169	LYS
1	C	290	GLU
1	C	545	TRP
1	C	579	SER
1	D	545	TRP
1	D	554	VAL
1	A	554	VAL
1	B	352	LEU
1	C	104	ASN
1	C	248	LYS
1	D	505	PRO
1	A	430	ILE
1	A	509	VAL
1	B	132	VAL
1	C	547	PRO
1	D	509	VAL
1	D	547	PRO
1	A	505	PRO
1	B	505	PRO
1	C	505	PRO
1	A	228	VAL
1	B	509	VAL
1	D	430	ILE
1	A	447	VAL
1	B	363	PRO
1	B	430	ILE
1	C	287	VAL
1	C	430	ILE
1	A	287	VAL

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	493/525 (94%)	417 (85%)	76 (15%)	3	16
1	B	493/525 (94%)	418 (85%)	75 (15%)	3	16
1	C	493/525 (94%)	416 (84%)	77 (16%)	3	16
1	D	493/525 (94%)	417 (85%)	76 (15%)	3	16
All	All	1972/2100 (94%)	1668 (85%)	304 (15%)	3	16

All (304) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	39	ASN
1	A	42	GLN
1	A	44	ARG
1	A	48	MET
1	A	54	GLN
1	A	70	THR
1	A	71	THR
1	A	83	LYS
1	A	93	LEU
1	A	107	PHE
1	A	113	MET
1	A	116	VAL
1	A	122	TYR
1	A	124	ILE
1	A	126	SER
1	A	130	TYR
1	A	138	SER
1	A	150	ARG
1	A	152	LEU
1	A	158	ASP
1	A	171	LEU
1	A	178	LEU
1	A	196	MET
1	A	197	MET
1	A	209	PHE
1	A	215	LYS
1	A	216	ARG
1	A	222	ARG
1	A	231	ASN
1	A	232	HIS

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Mol	Chain	Res	Type
1	A	241	GLN
1	A	252	LEU
1	A	253	LYS
1	A	270	GLN
1	A	271	VAL
1	A	282	ASN
1	A	289	GLN
1	A	298	LEU
1	A	300	MET
1	A	310	GLN
1	A	316	LEU
1	A	318	GLN
1	A	322	GLU
1	A	326	GLU
1	A	337	ILE
1	A	350	GLN
1	A	376	ARG
1	A	379	SER
1	A	385	TYR
1	A	389	PRO
1	A	398	GLU
1	A	400	GLN
1	A	405	LYS
1	A	409	TYR
1	A	411	ASN
1	A	412	SER
1	A	416	GLU
1	A	420	THR
1	A	422	PHE
1	A	476	THR
1	A	484	GLU
1	A	492	LYS
1	A	494	LEU
1	A	514	PRO
1	A	522	MET
1	A	525	LEU
1	A	530	SER
1	A	534	LEU
1	A	543	GLN
1	A	547	PRO
1	A	557	LYS
1	A	566	SER

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Mol	Chain	Res	Type
1	A	569	CYS
1	A	578	THR
1	A	583	GLN
1	B	39	ASN
1	B	42	GLN
1	B	44	ARG
1	B	48	MET
1	B	56	LYS
1	B	70	THR
1	B	71	THR
1	B	83	LYS
1	B	93	LEU
1	B	107	PHE
1	B	113	MET
1	B	116	VAL
1	B	117	LEU
1	B	122	TYR
1	B	124	ILE
1	B	126	SER
1	B	136	TYR
1	B	138	SER
1	B	150	ARG
1	B	152	LEU
1	B	158	ASP
1	B	171	LEU
1	B	178	LEU
1	B	196	MET
1	B	197	MET
1	B	209	PHE
1	B	215	LYS
1	B	216	ARG
1	B	222	ARG
1	B	231	ASN
1	B	232	HIS
1	B	241	GLN
1	B	252	LEU
1	B	253	LYS
1	B	270	GLN
1	B	282	ASN
1	B	289	GLN
1	B	298	LEU
1	B	300	MET

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Mol	Chain	Res	Type
1	B	310	GLN
1	B	316	LEU
1	B	318	GLN
1	B	322	GLU
1	B	326	GLU
1	B	337	ILE
1	B	376	ARG
1	B	379	SER
1	B	383	THR
1	B	385	TYR
1	B	389	PRO
1	B	394	THR
1	B	398	GLU
1	B	399	ASP
1	B	400	GLN
1	B	405	LYS
1	B	407	PHE
1	B	409	TYR
1	B	412	SER
1	B	420	THR
1	B	422	PHE
1	B	476	THR
1	B	484	GLU
1	B	492	LYS
1	B	494	LEU
1	B	514	PRO
1	B	522	MET
1	B	525	LEU
1	B	530	SER
1	B	534	LEU
1	B	543	GLN
1	B	557	LYS
1	B	566	SER
1	B	569	CYS
1	B	578	THR
1	B	583	GLN
1	C	42	GLN
1	C	44	ARG
1	C	48	MET
1	C	54	GLN
1	C	56	LYS
1	C	70	THR

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Mol	Chain	Res	Type
1	C	71	THR
1	C	83	LYS
1	C	93	LEU
1	C	107	PHE
1	C	113	MET
1	C	116	VAL
1	C	117	LEU
1	C	122	TYR
1	C	124	ILE
1	C	126	SER
1	C	130	TYR
1	C	138	SER
1	C	150	ARG
1	C	152	LEU
1	C	158	ASP
1	C	171	LEU
1	C	178	LEU
1	C	196	MET
1	C	197	MET
1	C	209	PHE
1	C	215	LYS
1	C	216	ARG
1	C	222	ARG
1	C	231	ASN
1	C	232	HIS
1	C	241	GLN
1	C	252	LEU
1	C	253	LYS
1	C	270	GLN
1	C	271	VAL
1	C	282	ASN
1	C	289	GLN
1	C	298	LEU
1	C	300	MET
1	C	310	GLN
1	C	316	LEU
1	C	318	GLN
1	C	322	GLU
1	C	326	GLU
1	C	337	ILE
1	C	350	GLN
1	C	376	ARG

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Mol	Chain	Res	Type
1	C	379	SER
1	C	385	TYR
1	C	389	PRO
1	C	398	GLU
1	C	400	GLN
1	C	405	LYS
1	C	409	TYR
1	C	411	ASN
1	C	412	SER
1	C	416	GLU
1	C	420	THR
1	C	422	PHE
1	C	441	PRO
1	C	476	THR
1	C	484	GLU
1	C	492	LYS
1	C	494	LEU
1	C	514	PRO
1	C	522	MET
1	C	525	LEU
1	C	530	SER
1	C	534	LEU
1	C	543	GLN
1	C	547	PRO
1	C	557	LYS
1	C	566	SER
1	C	569	CYS
1	C	578	THR
1	C	583	GLN
1	D	42	GLN
1	D	44	ARG
1	D	48	MET
1	D	70	THR
1	D	71	THR
1	D	83	LYS
1	D	93	LEU
1	D	107	PHE
1	D	113	MET
1	D	116	VAL
1	D	117	LEU
1	D	124	ILE
1	D	126	SER

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Mol	Chain	Res	Type
1	D	130	TYR
1	D	138	SER
1	D	150	ARG
1	D	152	LEU
1	D	158	ASP
1	D	171	LEU
1	D	178	LEU
1	D	196	MET
1	D	197	MET
1	D	209	PHE
1	D	215	LYS
1	D	216	ARG
1	D	222	ARG
1	D	231	ASN
1	D	232	HIS
1	D	241	GLN
1	D	252	LEU
1	D	253	LYS
1	D	270	GLN
1	D	282	ASN
1	D	289	GLN
1	D	298	LEU
1	D	300	MET
1	D	310	GLN
1	D	316	LEU
1	D	318	GLN
1	D	322	GLU
1	D	326	GLU
1	D	331	THR
1	D	337	ILE
1	D	376	ARG
1	D	379	SER
1	D	383	THR
1	D	385	TYR
1	D	389	PRO
1	D	394	THR
1	D	396	ASN
1	D	398	GLU
1	D	400	GLN
1	D	405	LYS
1	D	407	PHE
1	D	409	TYR

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Mol	Chain	Res	Type
1	D	411	ASN
1	D	412	SER
1	D	416	GLU
1	D	420	THR
1	D	422	PHE
1	D	441	PRO
1	D	476	THR
1	D	484	GLU
1	D	492	LYS
1	D	494	LEU
1	D	514	PRO
1	D	522	MET
1	D	525	LEU
1	D	530	SER
1	D	534	LEU
1	D	543	GLN
1	D	557	LYS
1	D	566	SER
1	D	569	CYS
1	D	578	THR
1	D	583	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	87	ASN
1	A	95	HIS
1	A	203	GLN
1	A	232	HIS
1	A	278	HIS
1	A	284	GLN
1	A	320	HIS
1	A	350	GLN
1	A	351	HIS
1	A	369	GLN
1	A	396	ASN
1	A	400	GLN
1	A	417	HIS
1	A	454	GLN
1	A	560	ASN
1	B	42	GLN

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Mol	Chain	Res	Type
1	B	87	ASN
1	B	95	HIS
1	B	203	GLN
1	B	232	HIS
1	B	278	HIS
1	B	284	GLN
1	B	320	HIS
1	B	350	GLN
1	B	351	HIS
1	B	396	ASN
1	B	400	GLN
1	B	411	ASN
1	B	417	HIS
1	B	454	GLN
1	B	543	GLN
1	B	560	ASN
1	C	39	ASN
1	C	42	GLN
1	C	95	HIS
1	C	203	GLN
1	C	232	HIS
1	C	242	HIS
1	C	320	HIS
1	C	350	GLN
1	C	369	GLN
1	C	396	ASN
1	C	400	GLN
1	C	411	ASN
1	C	417	HIS
1	C	454	GLN
1	C	543	GLN
1	C	560	ASN
1	D	42	GLN
1	D	90	HIS
1	D	95	HIS
1	D	203	GLN
1	D	232	HIS
1	D	284	GLN
1	D	350	GLN
1	D	351	HIS
1	D	369	GLN
1	D	396	ASN

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Mol	Chain	Res	Type
1	D	400	GLN
1	D	411	ASN
1	D	417	HIS
1	D	454	GLN
1	D	543	GLN
1	D	560	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

16 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	NAG	A	661	1	14,14,15	0.63	0	15,19,21	0.79	0
2	NAG	A	671	1	14,14,15	0.83	0	15,19,21	1.69	3 (20%)
2	NAG	A	681	1	14,14,15	0.38	0	15,19,21	0.88	1 (6%)
3	HEM	A	682	1	30,50,50	2.95	10 (33%)	24,82,82	1.90	6 (25%)
2	NAG	B	661	1	14,14,15	0.69	1 (7%)	15,19,21	0.90	0
2	NAG	B	671	1	14,14,15	0.81	0	15,19,21	1.55	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	681	1	14,14,15	0.55	0	15,19,21	1.00	2 (13%)
3	HEM	B	682	1	30,50,50	2.85	10 (33%)	24,82,82	1.96	6 (25%)
2	NAG	C	661	1	14,14,15	0.55	0	15,19,21	1.04	1 (6%)
2	NAG	C	671	1	14,14,15	0.82	0	15,19,21	1.73	3 (20%)
2	NAG	C	681	1	14,14,15	0.61	0	15,19,21	0.92	1 (6%)
3	HEM	C	682	1	30,50,50	2.81	8 (26%)	24,82,82	1.92	6 (25%)
2	NAG	D	661	1	14,14,15	0.60	0	15,19,21	0.96	1 (6%)
2	NAG	D	671	1	14,14,15	0.62	0	15,19,21	1.38	2 (13%)
2	NAG	D	681	1	14,14,15	0.62	0	15,19,21	0.88	1 (6%)
3	HEM	D	682	1	30,50,50	2.82	10 (33%)	24,82,82	1.98	6 (25%)

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	NAG	A	661	1	-	0/6/23/26	0/1/1/1
2	NAG	A	671	1	-	0/6/23/26	0/1/1/1
2	NAG	A	681	1	-	0/6/23/26	0/1/1/1
3	HEM	A	682	1	-	0/10/54/54	0/0/8/8
2	NAG	B	661	1	-	0/6/23/26	0/1/1/1
2	NAG	B	671	1	-	0/6/23/26	0/1/1/1
2	NAG	B	681	1	-	0/6/23/26	0/1/1/1
3	HEM	B	682	1	-	0/10/54/54	0/0/8/8
2	NAG	C	661	1	-	0/6/23/26	0/1/1/1
2	NAG	C	671	1	-	0/6/23/26	0/1/1/1
2	NAG	C	681	1	-	0/6/23/26	0/1/1/1
3	HEM	C	682	1	-	0/10/54/54	0/0/8/8
2	NAG	D	661	1	-	0/6/23/26	0/1/1/1
2	NAG	D	671	1	-	0/6/23/26	0/1/1/1
2	NAG	D	681	1	-	0/6/23/26	0/1/1/1
3	HEM	D	682	1	-	0/10/54/54	0/0/8/8

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	682	HEM	C3C-CAC	-7.11	1.38	1.51
3	A	682	HEM	C3D-C4D	-6.96	1.42	1.51
3	A	682	HEM	C2D-C3D	-6.70	1.34	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	682	HEM	C3C-CAC	-6.48	1.39	1.51
3	B	682	HEM	C2D-C3D	-6.46	1.35	1.54
3	A	682	HEM	C3B-CAB	-6.45	1.39	1.51
3	C	682	HEM	C2D-C3D	-6.44	1.35	1.54
3	A	682	HEM	C3C-CAC	-6.38	1.39	1.51
3	C	682	HEM	C3B-CAB	-6.30	1.39	1.51
3	B	682	HEM	C3C-CAC	-6.22	1.39	1.51
3	B	682	HEM	C3B-CAB	-6.21	1.39	1.51
3	D	682	HEM	C3B-CAB	-6.18	1.39	1.51
3	D	682	HEM	C2D-C3D	-6.13	1.36	1.54
3	C	682	HEM	C3D-C4D	-6.08	1.43	1.51
3	B	682	HEM	C3D-C4D	-5.97	1.43	1.51
3	D	682	HEM	C3D-C4D	-5.84	1.44	1.51
3	B	682	HEM	C3B-C4B	-5.66	1.46	1.51
3	A	682	HEM	C3B-C4B	-5.19	1.47	1.51
3	C	682	HEM	C3B-C4B	-5.00	1.47	1.51
3	D	682	HEM	C3B-C4B	-4.80	1.47	1.51
3	B	682	HEM	C2C-C1C	-4.64	1.43	1.52
3	A	682	HEM	C2C-C1C	-4.50	1.44	1.52
3	C	682	HEM	C2C-C1C	-3.99	1.45	1.52
3	D	682	HEM	C2C-C1C	-3.19	1.46	1.52
3	A	682	HEM	C2B-C1B	-2.45	1.43	1.51
3	B	682	HEM	CBC-CAC	2.01	1.40	1.29
3	D	682	HEM	C1C-NC	2.09	1.38	1.36
2	B	661	NAG	C1-C2	2.10	1.55	1.52
3	D	682	HEM	CBC-CAC	2.14	1.41	1.29
3	B	682	HEM	C1C-NC	2.14	1.38	1.36
3	B	682	HEM	CBB-CAB	2.30	1.42	1.29
3	A	682	HEM	C4C-NC	2.37	1.38	1.36
3	B	682	HEM	C4C-NC	2.38	1.38	1.36
3	A	682	HEM	CBC-CAC	2.54	1.44	1.29
3	C	682	HEM	CBC-CAC	2.73	1.45	1.29
3	D	682	HEM	CBB-CAB	2.83	1.45	1.29
3	C	682	HEM	CBB-CAB	2.93	1.46	1.29
3	A	682	HEM	CBB-CAB	2.95	1.46	1.29
3	D	682	HEM	C4C-NC	3.94	1.40	1.36

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	671	NAG	C4-C3-C2	-4.94	103.55	111.23
2	C	671	NAG	C4-C3-C2	-4.59	104.10	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	671	NAG	C4-C3-C2	-4.47	104.28	111.23
2	B	671	NAG	C4-C3-C2	-4.40	104.38	111.23
2	C	671	NAG	C2-N2-C7	-3.64	118.36	123.04
2	A	681	NAG	C2-N2-C7	-3.00	119.19	123.04
2	A	671	NAG	C2-N2-C7	-2.93	119.27	123.04
2	C	681	NAG	C2-N2-C7	-2.91	119.30	123.04
2	D	661	NAG	C2-N2-C7	-2.70	119.57	123.04
2	B	681	NAG	C2-N2-C7	-2.59	119.71	123.04
2	B	671	NAG	C2-N2-C7	-2.51	119.81	123.04
2	D	681	NAG	C2-N2-C7	-2.43	119.92	123.04
2	B	681	NAG	C1-O5-C5	-2.24	109.40	112.25
2	D	671	NAG	C2-N2-C7	-2.13	120.30	123.04
2	C	661	NAG	C1-O5-C5	2.12	114.94	112.25
2	B	671	NAG	C1-O5-C5	2.32	115.20	112.25
2	A	671	NAG	C1-O5-C5	2.53	115.45	112.25
2	C	671	NAG	C1-O5-C5	2.57	115.51	112.25
3	D	682	HEM	CMD-C2D-C3D	2.68	126.21	114.35
3	B	682	HEM	CMD-C2D-C3D	2.69	126.23	114.35
3	A	682	HEM	CMD-C2D-C3D	2.70	126.28	114.35
3	C	682	HEM	CMD-C2D-C3D	2.71	126.34	114.35
3	A	682	HEM	CMC-C2C-C3C	2.90	123.77	116.53
3	D	682	HEM	CMB-C2B-C3B	3.01	124.04	116.53
3	A	682	HEM	C2D-C3D-C4D	3.05	106.66	101.50
3	D	682	HEM	C2D-C3D-C4D	3.05	106.68	101.50
3	C	682	HEM	C2D-C3D-C4D	3.17	106.88	101.50
3	B	682	HEM	CMB-C2B-C3B	3.20	124.51	116.53
3	C	682	HEM	CMB-C2B-C3B	3.24	124.61	116.53
3	B	682	HEM	C2D-C3D-C4D	3.30	107.10	101.50
3	A	682	HEM	CMB-C2B-C3B	3.35	124.90	116.53
3	D	682	HEM	CAD-C3D-C4D	3.36	124.33	112.47
3	C	682	HEM	CAD-C3D-C4D	3.38	124.40	112.47
3	A	682	HEM	CAD-C3D-C4D	3.40	124.46	112.47
3	B	682	HEM	CAD-C3D-C4D	3.41	124.49	112.47
3	C	682	HEM	CMC-C2C-C3C	3.61	125.55	116.53
3	D	682	HEM	CMC-C2C-C3C	3.92	126.31	116.53
3	B	682	HEM	CMC-C2C-C3C	4.15	126.88	116.53
3	B	682	HEM	CAD-C3D-C2D	5.05	127.73	113.22
3	C	682	HEM	CAD-C3D-C2D	5.12	127.93	113.22
3	D	682	HEM	CAD-C3D-C2D	5.21	128.19	113.22
3	A	682	HEM	CAD-C3D-C2D	5.29	128.41	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	682	HEM	1	0
2	B	681	NAG	1	0
3	B	682	HEM	2	0
2	C	661	NAG	2	0
2	C	671	NAG	1	0
3	C	682	HEM	2	0
2	D	661	NAG	1	0
2	D	681	NAG	4	0
3	D	682	HEM	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	552/587 (94%)	-0.27	5 (0%) 85 64	2, 8, 25, 40	0
1	B	552/587 (94%)	-0.25	3 (0%) 91 76	2, 8, 26, 38	0
1	C	552/587 (94%)	-0.18	6 (1%) 82 58	2, 8, 28, 38	0
1	D	552/587 (94%)	-0.15	9 (1%) 74 47	2, 9, 27, 41	0
All	All	2208/2348 (94%)	-0.21	23 (1%) 84 60	2, 8, 27, 41	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	411	ASN	4.0
1	D	583	GLN	3.8
1	D	398	GLU	3.2
1	D	105	ASN	3.0
1	C	411	ASN	3.0
1	C	83	LYS	2.9
1	C	399	ASP	2.8
1	A	583	GLN	2.7
1	C	278	HIS	2.7
1	D	399	ASP	2.6
1	D	186	GLU	2.5
1	A	83	LYS	2.4
1	A	280	PRO	2.3
1	C	281	GLU	2.2
1	B	583	GLN	2.2
1	D	409	TYR	2.1
1	A	444	VAL	2.1
1	B	411	ASN	2.1
1	D	581	ASN	2.1
1	C	85	THR	2.1
1	D	102	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	411	ASN	2.1
1	B	186	GLU	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 [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NAG	C	661	14/15	0.79	0.33	4.88	24,26,29,30	0
2	NAG	A	681	14/15	0.82	0.32	4.81	23,29,34,36	0
2	NAG	A	661	14/15	0.84	0.31	3.66	21,25,30,32	0
2	NAG	D	681	14/15	0.72	0.38	3.18	21,31,33,37	0
2	NAG	B	681	14/15	0.76	0.42	2.89	22,32,33,33	0
2	NAG	C	681	14/15	0.89	0.35	2.73	24,29,32,36	0
2	NAG	A	671	14/15	0.77	0.33	1.74	2,6,18,20	0
2	NAG	B	661	14/15	0.88	0.30	1.46	22,25,31,33	0
2	NAG	D	661	14/15	0.82	0.28	1.39	20,25,29,31	0
2	NAG	D	671	14/15	0.85	0.24	1.03	4,7,18,21	0
2	NAG	C	671	14/15	0.73	0.31	0.85	4,7,17,21	0
3	HEM	A	682	43/43	0.91	0.21	0.14	2,4,24,31	0
3	HEM	D	682	43/43	0.91	0.20	-0.08	2,9,26,27	0
3	HEM	B	682	43/43	0.93	0.19	-0.11	2,8,24,28	0
2	NAG	B	671	14/15	0.88	0.18	-0.31	4,7,17,20	0
3	HEM	C	682	43/43	0.92	0.20	-0.32	2,5,25,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.