



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 12:19 PM GMT

PDB ID : 3ALX  
Title : Crystal structure of the measles virus hemagglutinin bound to its cellular receptor SLAM (MV-H(L482R)-SLAM(N102H/R108Y)fusion)  
Authors : Hashiguchi, T.; Ose, T.; Kubota, M.; Maita, N.; Kamishikiryo, J.; Maenaka, K.; Yanagi, Y.  
Deposited on : 2010-08-09  
Resolution : 3.15 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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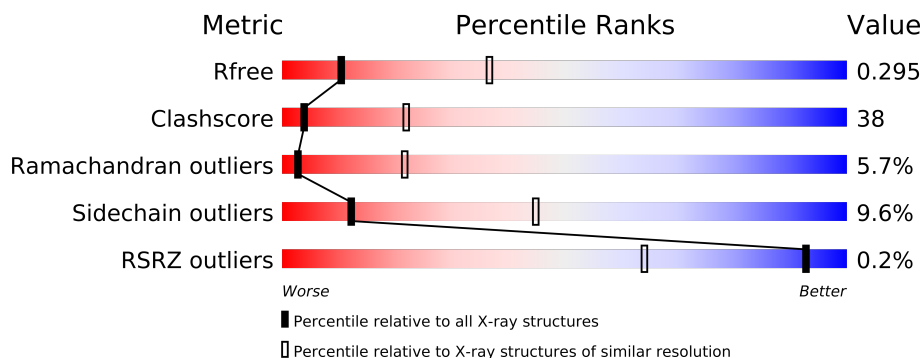
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.15 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))
$R_{free}$	66092	1360 (3.22-3.10)
Clashscore	79885	1681 (3.22-3.10)
Ramachandran outliers	78287	1639 (3.22-3.10)
Sidechain outliers	78261	1638 (3.22-3.10)
RSRZ outliers	66119	1361 (3.22-3.10)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	559	
1	B	559	
1	C	559	
1	D	559	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	NAG	B	801	-	X
2	NAG	C	801	-	X
2	NAG	C	901	-	X
2	NAG	D	901	-	X

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16313 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Hemagglutinin, CDw150.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	515	Total	C	N	O	S	0	0	0
			4053	2598	677	750	28			
1	B	526	Total	C	N	O	S	0	0	0
			4141	2651	695	767	28			
1	C	514	Total	C	N	O	S	0	0	0
			4051	2599	676	748	28			
1	D	504	Total	C	N	O	S	0	0	0
			3984	2562	663	732	27			

There are 60 discrepancies between the modelled and reference sequences:

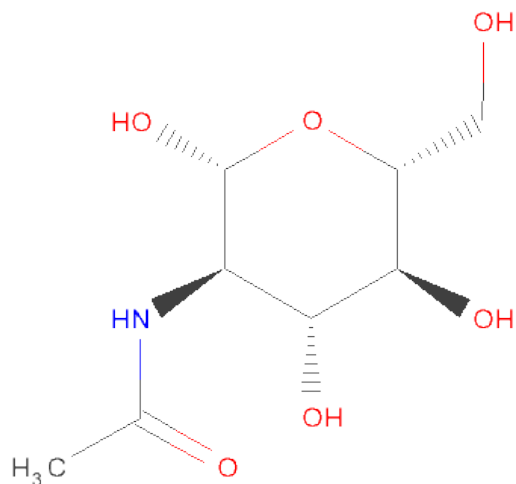
Chain	Residue	Modelled	Actual	Comment	Reference
A	181	GLU	-	EXPRESSION TAG	UNP E2RZS2
A	182	THR	-	EXPRESSION TAG	UNP E2RZS2
A	183	GLY	-	EXPRESSION TAG	UNP E2RZS2
A	482	ARG	LEU	ENGINEERED MUTATION	UNP E2RZS2
A	102	HIS	ASN	ENGINEERED MUTATION	UNP Q9GJT3
A	108	TYR	ARG	ENGINEERED MUTATION	UNP Q9GJT3
A	141	GLY	-	EXPRESSION TAG	UNP Q9GJT3
A	142	THR	-	EXPRESSION TAG	UNP Q9GJT3
A	143	LYS	-	EXPRESSION TAG	UNP Q9GJT3
A	144	HIS	-	EXPRESSION TAG	UNP Q9GJT3
A	145	HIS	-	EXPRESSION TAG	UNP Q9GJT3
A	146	HIS	-	EXPRESSION TAG	UNP Q9GJT3
A	147	HIS	-	EXPRESSION TAG	UNP Q9GJT3
A	148	HIS	-	EXPRESSION TAG	UNP Q9GJT3
A	149	HIS	-	EXPRESSION TAG	UNP Q9GJT3
B	181	GLU	-	EXPRESSION TAG	UNP E2RZS2
B	182	THR	-	EXPRESSION TAG	UNP E2RZS2
B	183	GLY	-	EXPRESSION TAG	UNP E2RZS2
B	482	ARG	LEU	ENGINEERED MUTATION	UNP E2RZS2
B	102	HIS	ASN	ENGINEERED MUTATION	UNP Q9GJT3
B	108	TYR	ARG	ENGINEERED MUTATION	UNP Q9GJT3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	141	GLY	-	EXPRESSION TAG	UNP Q9GJT3
B	142	THR	-	EXPRESSION TAG	UNP Q9GJT3
B	143	LYS	-	EXPRESSION TAG	UNP Q9GJT3
B	144	HIS	-	EXPRESSION TAG	UNP Q9GJT3
B	145	HIS	-	EXPRESSION TAG	UNP Q9GJT3
B	146	HIS	-	EXPRESSION TAG	UNP Q9GJT3
B	147	HIS	-	EXPRESSION TAG	UNP Q9GJT3
B	148	HIS	-	EXPRESSION TAG	UNP Q9GJT3
B	149	HIS	-	EXPRESSION TAG	UNP Q9GJT3
C	181	GLU	-	EXPRESSION TAG	UNP E2RZS2
C	182	THR	-	EXPRESSION TAG	UNP E2RZS2
C	183	GLY	-	EXPRESSION TAG	UNP E2RZS2
C	482	ARG	LEU	ENGINEERED MUTATION	UNP E2RZS2
C	102	HIS	ASN	ENGINEERED MUTATION	UNP Q9GJT3
C	108	TYR	ARG	ENGINEERED MUTATION	UNP Q9GJT3
C	141	GLY	-	EXPRESSION TAG	UNP Q9GJT3
C	142	THR	-	EXPRESSION TAG	UNP Q9GJT3
C	143	LYS	-	EXPRESSION TAG	UNP Q9GJT3
C	144	HIS	-	EXPRESSION TAG	UNP Q9GJT3
C	145	HIS	-	EXPRESSION TAG	UNP Q9GJT3
C	146	HIS	-	EXPRESSION TAG	UNP Q9GJT3
C	147	HIS	-	EXPRESSION TAG	UNP Q9GJT3
C	148	HIS	-	EXPRESSION TAG	UNP Q9GJT3
C	149	HIS	-	EXPRESSION TAG	UNP Q9GJT3
D	181	GLU	-	EXPRESSION TAG	UNP E2RZS2
D	182	THR	-	EXPRESSION TAG	UNP E2RZS2
D	183	GLY	-	EXPRESSION TAG	UNP E2RZS2
D	482	ARG	LEU	ENGINEERED MUTATION	UNP E2RZS2
D	102	HIS	ASN	ENGINEERED MUTATION	UNP Q9GJT3
D	108	TYR	ARG	ENGINEERED MUTATION	UNP Q9GJT3
D	141	GLY	-	EXPRESSION TAG	UNP Q9GJT3
D	142	THR	-	EXPRESSION TAG	UNP Q9GJT3
D	143	LYS	-	EXPRESSION TAG	UNP Q9GJT3
D	144	HIS	-	EXPRESSION TAG	UNP Q9GJT3
D	145	HIS	-	EXPRESSION TAG	UNP Q9GJT3
D	146	HIS	-	EXPRESSION TAG	UNP Q9GJT3
D	147	HIS	-	EXPRESSION TAG	UNP Q9GJT3
D	148	HIS	-	EXPRESSION TAG	UNP Q9GJT3
D	149	HIS	-	EXPRESSION TAG	UNP Q9GJT3

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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	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		







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	187.71Å 170.07Å 110.68Å 90.00° 117.28° 90.00°	Depositor
Resolution (Å)	19.97 – 3.15 19.96 – 3.16	Depositor EDS
% Data completeness (in resolution range)	99.1 (19.97-3.15) 99.2 (19.96-3.16)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.59 (at 3.15Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.231 , 0.292 0.231 , 0.295	Depositor DCC
$R_{free}$ test set	2644 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	71.0	Xtriage
Anisotropy	0.367	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 49.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 52452 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	16313	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.25% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.49	0/4155	0.74	2/5646 (0.0%)
1	B	0.44	0/4243	0.71	2/5763 (0.0%)
1	C	0.46	0/4151	0.71	1/5638 (0.0%)
1	D	0.41	0/4083	0.66	0/5545
All	All	0.45	0/16632	0.70	5/22592 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	48	THR	N-CA-C	-6.29	94.02	111.00
1	C	132	CYS	CA-CB-SG	-6.03	103.15	114.00
1	A	48	THR	N-CA-C	-5.52	96.09	111.00
1	B	92	LEU	N-CA-C	-5.35	96.54	111.00
1	A	92	LEU	N-CA-C	-5.34	96.58	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	541	TYR	Sidechain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4053	0	4023	288	0
1	B	4141	0	4119	297	0
1	C	4051	0	4024	313	0
1	D	3984	0	3964	350	0
2	A	14	0	13	0	0
2	B	28	0	26	0	0
2	C	28	0	26	1	0
2	D	14	0	13	1	0
All	All	16313	0	16208	1224	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 38.

All (1224) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:85:GLU:HG2	1:A:86:ALA:H	1.09	1.16
1:A:236:LYS:HB3	1:A:237:PRO:HD2	1.30	1.14
1:D:503:GLU:HB2	1:D:76:ASN:HD22	1.05	1.09
1:A:60:ILE:HG22	1:A:61:HIS:H	1.13	1.08
1:A:540:TYR:HE1	1:A:568:VAL:HG21	1.22	1.04
1:C:546:SER:HB3	1:C:547:ARG:HH21	1.15	1.04
1:B:483:PHE:HZ	1:B:524:TYR:HH	1.04	0.99
1:C:194:ILE:HG13	1:C:604:VAL:HG12	1.44	0.98
1:D:37:GLN:HE22	1:D:43:VAL:HA	1.28	0.97
1:D:457:PRO:HB3	1:D:513:ASN:HA	1.49	0.95
1:D:503:GLU:HB2	1:D:76:ASN:ND2	1.82	0.94
1:A:589:GLU:HG3	1:A:590:SER:H	1.34	0.93
1:D:37:GLN:NE2	1:D:43:VAL:HA	1.84	0.92
1:C:546:SER:HB3	1:C:547:ARG:NH2	1.84	0.91
1:B:74:VAL:HG13	1:B:75:GLU:H	1.33	0.90
1:B:558:PRO:HG2	1:B:559:ILE:HG23	1.52	0.90
1:D:194:ILE:HG13	1:D:604:VAL:HG12	1.55	0.89
1:C:306:ILE:HD13	1:C:351:LEU:HD21	1.55	0.89
1:C:237:PRO:HG2	1:C:249:LEU:HA	1.54	0.89

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:472:TRP:H	1:B:472:TRP:HE3	1.19	0.88
1:B:473:ILE:HB	1:B:474:PRO:HD3	1.55	0.88
1:D:47:LEU:HD13	1:D:120:MET:HB2	1.56	0.87
1:B:472:TRP:HA	1:B:476:PHE:HA	1.57	0.86
1:C:81:LEU:HD23	1:C:89:PRO:HB3	1.56	0.85
1:D:520:GLN:NE2	1:D:520:GLN:H	1.73	0.85
1:D:458:PRO:HG2	1:D:511:SER:HB3	1.58	0.85
1:D:437:HIS:HB3	1:D:459:MET:HG2	1.58	0.85
1:B:430:GLY:HA3	1:B:476:PHE:HE2	1.42	0.84
1:B:475:ARG:NH1	1:B:477:LYS:HD3	1.91	0.84
1:C:457:PRO:HB3	1:C:513:ASN:HA	1.58	0.84
1:A:85:GLU:HG2	1:A:86:ALA:N	1.92	0.84
1:A:540:TYR:CE1	1:A:568:VAL:HG21	2.12	0.83
1:B:562:VAL:HB	1:B:586:ALA:HB3	1.60	0.83
1:D:93:LYS:NZ	1:D:93:LYS:HA	1.93	0.83
1:D:222:MET:HE2	1:D:291:LEU:HB2	1.60	0.82
1:D:121:THR:HG23	1:D:128:VAL:HG13	1.59	0.82
1:B:400:ALA:HB3	1:B:401:PRO:HD3	1.60	0.82
1:B:216:VAL:HG22	1:B:234:VAL:HG12	1.61	0.82
1:A:236:LYS:HB3	1:A:237:PRO:CD	2.10	0.82
1:C:135:LEU:HD23	1:C:136:LYS:N	1.95	0.82
1:B:464:LEU:HG	1:B:465:GLY:H	1.45	0.81
1:D:286:ASN:ND2	1:D:304:ASP:HB3	1.95	0.81
1:A:60:ILE:HG22	1:A:61:HIS:N	1.95	0.81
1:C:36:VAL:HG12	1:C:136:LYS:HB3	1.63	0.81
1:A:450:ASN:HA	1:A:472:TRP:CH2	2.16	0.80
1:B:89:PRO:HG2	1:B:91:TYR:CE2	2.17	0.80
1:D:261:ARG:HB2	1:D:261:ARG:NH1	1.97	0.80
1:C:390:ILE:HG23	1:C:393:LEU:HB2	1.64	0.80
1:B:93:LYS:HD2	1:B:94:ASP:C	2.01	0.79
1:C:531:THR:HG22	1:C:536:HIS:CD2	2.17	0.79
1:C:47:LEU:HD13	1:C:120:MET:HB2	1.65	0.79
1:C:378:MET:HB2	1:C:407:ILE:HG21	1.64	0.78
1:D:123:GLU:HB3	1:D:128:VAL:HG22	1.63	0.78
1:C:252:TYR:CE1	1:C:279:PRO:HG3	2.17	0.78
1:C:296:LEU:HD23	1:C:296:LEU:O	1.83	0.78
1:A:93:LYS:HD2	1:A:94:ASP:H	1.48	0.78
1:D:537:ALA:HA	1:D:557:LEU:HD22	1.64	0.78
1:C:545:PRO:HB3	1:C:71:GLU:HA	1.64	0.78
1:D:503:GLU:CB	1:D:76:ASN:HD22	1.91	0.77
1:C:93:LYS:HD2	1:C:94:ASP:N	2.00	0.77
1:C:33:PRO:HD2	1:C:132:CYS:SG	2.25	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:378:MET:HB3	1:A:407:ILE:HG21	1.68	0.77
1:D:38:GLN:HB3	1:D:41:SER:OG	1.85	0.76
1:B:236:LYS:HE3	1:B:238:ASN:HB3	1.65	0.76
1:A:374:ASP:HB2	1:A:407:ILE:HB	1.65	0.76
1:C:68:LYS:HD2	1:C:115:GLU:O	1.86	0.76
1:A:36:VAL:HA	1:A:136:LYS:O	1.84	0.76
1:A:71:GLU:O	1:A:72:ASN:HB2	1.85	0.76
1:A:84:SER:O	1:A:85:GLU:HB2	1.85	0.76
1:A:461:ASN:H	1:A:461:ASN:ND2	1.83	0.76
1:D:525:VAL:HG12	1:D:542:VAL:HA	1.67	0.76
1:B:77:LYS:HB3	1:B:92:LEU:HD11	1.68	0.76
1:D:464:LEU:HG	1:D:465:GLY:H	1.50	0.75
1:A:274:ASN:HD22	1:A:324:LEU:HB3	1.51	0.75
1:D:35:ILE:HD11	1:D:45:LEU:HG	1.68	0.75
1:C:384:GLN:HE22	1:C:490:ALA:HA	1.51	0.75
1:C:194:ILE:CG1	1:C:604:VAL:HG12	2.17	0.75
1:A:461:ASN:H	1:A:461:ASN:HD22	1.34	0.75
1:A:473:ILE:HG22	1:A:474:PRO:N	2.02	0.74
1:B:95:ARG:HH11	1:B:95:ARG:HG3	1.51	0.74
1:D:309:PRO:HG3	1:D:316:GLY:HA2	1.69	0.74
1:D:343:ASP:OD1	1:D:345:VAL:HG12	1.86	0.74
1:D:237:PRO:HA	1:D:249:LEU:HD23	1.69	0.74
1:D:540:TYR:HE1	1:D:568:VAL:HG21	1.53	0.74
1:A:231:THR:HG21	1:A:287:CYS:HB2	1.69	0.74
1:B:139:GLU:O	1:B:140:GLN:HB2	1.87	0.73
1:A:556:ARG:HH12	1:A:125:ASN:HA	1.53	0.73
1:B:140:GLN:HG3	1:C:421:VAL:HA	1.68	0.73
1:A:93:LYS:HD2	1:A:94:ASP:N	2.03	0.73
1:B:570:CYS:HB3	1:B:577:LEU:HD21	1.71	0.73
1:D:354:HIS:CE1	1:D:367:VAL:HG12	2.24	0.73
1:B:93:LYS:HD2	1:B:94:ASP:H	1.53	0.73
1:C:378:MET:CB	1:C:407:ILE:HG21	2.19	0.73
1:A:40:GLY:HA2	1:A:110:SER:O	1.88	0.73
1:A:580:ARG:HG3	1:A:580:ARG:HH11	1.53	0.73
1:A:222:MET:HB3	1:A:355:ARG:HD3	1.71	0.72
1:D:72:ASN:N	1:D:72:ASN:HD22	1.86	0.72
1:B:481:TYR:O	1:B:482:ARG:HG2	1.90	0.72
1:D:93:LYS:HG3	1:D:94:ASP:H	1.54	0.72
1:B:464:LEU:HG	1:B:465:GLY:N	2.04	0.72
1:A:326:VAL:HG23	1:A:327:TRP:CD1	2.25	0.72
1:A:93:LYS:HD2	1:A:94:ASP:C	2.09	0.72
1:D:303:GLU:HG3	1:D:304:ASP:H	1.54	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:91:TYR:HB3	1:B:93:LYS:HB3	1.70	0.72
1:B:35:ILE:O	1:B:35:ILE:HG13	1.89	0.72
1:C:77:LYS:HD2	1:C:80:SER:OG	1.89	0.72
1:A:60:ILE:CG2	1:A:61:HIS:H	1.97	0.72
1:D:65:THR:HG23	1:D:119:PHE:HB2	1.71	0.72
1:C:45:LEU:HD21	1:C:135:LEU:HD12	1.70	0.72
1:C:216:VAL:HG22	1:C:234:VAL:HG13	1.71	0.72
1:B:340:SER:HB3	1:B:426:LYS:HA	1.72	0.72
1:B:461:ASN:H	1:B:461:ASN:HD22	1.35	0.72
1:B:378:MET:CB	1:B:407:ILE:HG21	2.19	0.71
1:A:552:PHE:HE1	1:A:121:THR:HG1	1.37	0.71
1:C:528:THR:HG22	1:C:539:VAL:HB	1.71	0.71
1:A:580:ARG:HB3	1:A:599:MET:HE2	1.73	0.71
1:C:308:ILE:HD11	1:C:349:LEU:HD12	1.71	0.71
1:D:219:ILE:H	1:D:219:ILE:HD12	1.56	0.71
1:B:288:MET:HE3	1:B:299:LEU:HB3	1.73	0.71
1:A:540:TYR:O	1:A:552:PHE:HA	1.91	0.71
1:B:529:TYR:CD1	1:B:563:PRO:HG3	2.26	0.71
1:A:585:LEU:HD23	1:A:585:LEU:H	1.55	0.71
1:A:556:ARG:NH1	1:A:125:ASN:HA	2.06	0.71
1:B:337:VAL:HG12	1:B:423:LEU:HB3	1.72	0.71
1:D:378:MET:HB3	1:D:407:ILE:HG21	1.72	0.71
1:D:37:GLN:CD	1:D:43:VAL:HG23	2.10	0.70
1:B:74:VAL:HG13	1:B:75:GLU:N	2.03	0.70
1:A:398:GLU:O	1:A:403:LYS:HE3	1.91	0.70
1:D:97:ARG:HB3	1:D:106:ALA:HB3	1.71	0.70
1:B:458:PRO:HG3	1:B:465:GLY:H	1.54	0.70
1:A:70:LEU:HD22	1:A:70:LEU:H	1.56	0.70
1:D:253:ARG:HH21	1:D:285:SER:HB2	1.56	0.70
1:C:216:VAL:HG22	1:C:234:VAL:CG1	2.21	0.70
1:C:587:ASP:O	1:C:591:GLY:HA2	1.92	0.69
1:B:399:TRP:CD1	1:B:401:PRO:HD2	2.27	0.69
1:C:222:MET:HB3	1:C:355:ARG:HD3	1.74	0.69
1:B:346:ILE:HG23	1:B:369:THR:HG21	1.73	0.69
1:D:306:ILE:HD12	1:D:306:ILE:N	2.08	0.69
1:B:544:SER:HB2	1:B:549:PHE:HB3	1.73	0.69
1:D:415:VAL:HG12	1:D:425:ILE:HA	1.75	0.68
1:D:194:ILE:HG12	1:D:551:TYR:CD2	2.28	0.68
1:C:464:LEU:CD2	1:C:498:THR:HB	2.24	0.68
1:D:564:ILE:O	1:D:564:ILE:HD12	1.93	0.68
1:C:89:PRO:HG2	1:C:91:TYR:CE2	2.27	0.68
1:D:216:VAL:HG22	1:D:234:VAL:HG22	1.75	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:406:ARG:O	1:C:408:PRO:HD3	1.92	0.68
1:C:261:ARG:HH11	1:C:271:HIS:HB3	1.59	0.67
1:C:389:LYS:HE3	1:C:500:LEU:H	1.58	0.67
1:B:348:ARG:HD3	1:B:350:TYR:OH	1.94	0.67
1:C:43:VAL:CG2	1:C:107:ILE:HB	2.24	0.67
1:B:475:ARG:O	1:B:476:PHE:HB3	1.95	0.67
1:D:194:ILE:HD12	1:D:194:ILE:N	2.09	0.67
1:B:62:ILE:HD13	1:B:83:PRO:HD3	1.75	0.67
1:A:236:LYS:CB	1:A:237:PRO:HD2	2.16	0.67
1:A:461:ASN:N	1:A:461:ASN:HD22	1.88	0.67
1:D:458:PRO:HG2	1:D:511:SER:CB	2.25	0.67
1:B:74:VAL:O	1:B:75:GLU:HB3	1.94	0.67
1:D:288:MET:HB3	1:D:365:TRP:NE1	2.10	0.67
1:D:384:GLN:HA	1:D:387:LYS:HE3	1.77	0.66
1:C:37:GLN:HG2	1:C:43:VAL:HG12	1.77	0.66
1:D:545:PRO:C	1:D:547:ARG:H	1.99	0.66
1:B:549:PHE:O	1:B:549:PHE:HD1	1.78	0.66
1:A:224:SER:O	1:A:225:GLN:HB2	1.95	0.66
1:D:261:ARG:HH11	1:D:261:ARG:CB	2.09	0.66
1:C:546:SER:CB	1:C:547:ARG:HH21	2.02	0.66
1:C:326:VAL:HG13	1:C:327:TRP:H	1.61	0.66
1:A:52:ILE:HD13	1:D:282:ASN:HD21	1.60	0.66
1:D:512:SER:HA	1:D:566:LEU:O	1.96	0.66
1:C:353:SER:OG	1:C:567:GLN:NE2	2.29	0.66
1:B:499:TYR:CD2	1:B:501:PRO:HD3	2.30	0.66
1:D:205:LEU:HB2	1:D:272:MET:HE1	1.78	0.65
1:D:77:LYS:HD2	1:D:80:SER:OG	1.96	0.65
1:A:448:HIS:HB2	1:A:451:VAL:CG1	2.26	0.65
1:A:91:TYR:HB3	1:A:93:LYS:HB3	1.77	0.65
1:B:430:GLY:CA	1:B:476:PHE:HE2	2.09	0.65
1:B:461:ASN:H	1:B:461:ASN:ND2	1.92	0.65
1:C:82:ASP:OD2	1:C:84:SER:HB3	1.96	0.65
1:A:585:LEU:HD23	1:A:585:LEU:N	2.12	0.65
1:D:43:VAL:HG13	1:D:107:ILE:HB	1.79	0.65
1:D:521:ASP:HB2	1:D:546:SER:HB2	1.79	0.65
1:D:514:LEU:CD1	1:D:526:LEU:HD23	2.26	0.65
1:B:140:GLN:HE21	1:C:421:VAL:HA	1.62	0.65
1:D:289:VAL:HG13	1:D:296:LEU:HD11	1.78	0.65
1:B:461:ASN:HD22	1:B:461:ASN:N	1.91	0.65
1:A:499:TYR:CD2	1:A:501:PRO:HD3	2.32	0.65
1:A:51:ARG:HH12	1:A:102:HIS:HB3	1.62	0.65
1:C:273:THR:O	1:C:274:ASN:HB2	1.97	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:439:SER:HB2	1:C:457:PRO:HG2	1.78	0.64
1:B:369:THR:O	1:B:409:SER:HB3	1.97	0.64
1:D:211:GLY:C	1:D:213:GLY:H	2.01	0.64
1:A:430:GLY:HA3	1:A:476:PHE:CE2	2.33	0.64
1:B:101:GLU:CD	1:B:101:GLU:H	2.00	0.64
1:B:216:VAL:HA	1:B:233:LEU:O	1.97	0.64
1:B:467:ILE:O	1:B:481:TYR:HB3	1.96	0.64
1:B:583:CYS:O	1:B:595:THR:HA	1.96	0.64
1:A:52:ILE:CD1	1:D:282:ASN:HD21	2.10	0.64
1:A:520:GLN:HG3	1:A:520:GLN:O	1.97	0.64
1:A:589:GLU:CG	1:A:590:SER:H	2.07	0.64
1:B:61:HIS:CE1	1:B:63:VAL:HG22	2.33	0.64
1:B:215:ASN:CB	1:B:235:GLU:HB2	2.27	0.64
1:B:343:ASP:OD2	1:B:346:ILE:HG13	1.97	0.64
1:B:93:LYS:CG	1:B:94:ASP:N	2.60	0.64
1:B:378:MET:HB2	1:B:407:ILE:HG21	1.79	0.64
1:D:377:ARG:HG3	1:D:377:ARG:HH11	1.63	0.64
1:C:305:SER:C	1:C:306:ILE:HD12	2.19	0.64
1:C:107:ILE:HD11	1:C:118:TYR:CE2	2.32	0.64
1:B:533:ARG:HG2	1:B:61:HIS:CD2	2.32	0.64
1:D:547:ARG:HG3	1:D:548:SER:H	1.63	0.64
1:D:206:LEU:HG	1:D:232:TYR:CE2	2.33	0.64
1:A:337:VAL:CG1	1:A:425:ILE:HG13	2.28	0.64
1:C:410:TYR:CE1	1:C:435:ILE:HD11	2.32	0.63
1:C:65:THR:HG21	1:C:75:GLU:HB3	1.81	0.63
1:C:473:ILE:HG22	1:C:474:PRO:HD3	1.80	0.63
1:B:557:LEU:HD23	1:B:559:ILE:HD11	1.79	0.63
1:A:56:MET:HG2	1:A:57:ASN:H	1.62	0.63
1:D:533:ARG:HB3	1:D:61:HIS:CD2	2.34	0.63
1:A:580:ARG:HH11	1:A:580:ARG:CG	2.12	0.63
1:D:467:ILE:O	1:D:481:TYR:HB3	1.98	0.63
1:A:309:PRO:HG3	1:A:316:GLY:HA3	1.80	0.63
1:B:352:SER:N	1:B:354:HIS:NE2	2.46	0.63
1:B:188:CYS:O	1:B:189:SER:HB3	1.99	0.63
1:C:461:ASN:HD22	1:C:461:ASN:C	2.01	0.63
1:A:358:ILE:HA	1:A:362:GLN:O	1.98	0.63
1:B:386:CYS:HA	1:B:390:ILE:HG13	1.79	0.63
1:D:38:GLN:HB3	1:D:41:SER:CB	2.29	0.63
1:A:189:SER:HB2	1:D:252:TYR:OH	1.98	0.63
1:C:505:ASP:HB3	1:C:508:VAL:HG12	1.80	0.62
1:A:559:ILE:HD13	1:A:559:ILE:H	1.64	0.62
1:A:448:HIS:HB2	1:A:451:VAL:HG12	1.81	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:74:VAL:CG1	1:B:75:GLU:H	2.11	0.62
1:D:449:ASN:O	1:D:450:ASN:HB2	2.00	0.62
1:A:517:LEU:HD11	1:A:525:VAL:CG2	2.28	0.62
1:A:375:LYS:O	1:A:379:GLU:HB2	1.99	0.62
1:B:93:LYS:HD2	1:B:95:ARG:N	2.15	0.62
1:D:124:LYS:HE3	1:D:125:ASN:OD1	1.99	0.62
1:B:36:VAL:HA	1:B:136:LYS:O	1.99	0.62
1:B:357:VAL:HG21	1:B:452:TYR:HE1	1.64	0.62
1:B:103:LEU:HD13	1:B:120:MET:HE3	1.81	0.62
1:C:293:GLU:CB	1:C:295:LYS:HE2	2.30	0.62
1:A:309:PRO:HB2	1:A:341:THR:HG21	1.82	0.62
1:B:229:GLY:N	1:B:291:LEU:HD11	2.14	0.62
1:C:251:MET:CE	1:C:283:ASP:HB3	2.30	0.62
1:A:70:LEU:HD22	1:A:70:LEU:N	2.14	0.61
1:D:295:LYS:NZ	1:D:358:ILE:HG21	2.15	0.61
1:C:345:VAL:HG13	1:C:372:THR:OG1	2.00	0.61
1:B:208:LEU:O	1:B:212:ARG:HG2	2.00	0.61
1:A:530:ASP:OD1	1:A:532:SER:HB3	2.00	0.61
1:D:261:ARG:HH12	1:D:271:HIS:HB3	1.65	0.61
1:C:390:ILE:HG22	1:C:394:CYS:SG	2.40	0.61
1:C:259:VAL:HB	1:C:261:ARG:HH12	1.65	0.61
1:C:205:LEU:HB2	1:C:272:MET:HE1	1.81	0.61
1:C:193:THR:OG1	1:C:607:THR:HG22	1.99	0.61
1:D:349:LEU:HD23	1:D:369:THR:HG23	1.82	0.61
1:A:301:HIS:HB2	1:A:319:PHE:CD2	2.34	0.61
1:D:451:VAL:HA	1:D:470:LEU:O	1.99	0.61
1:B:400:ALA:HB3	1:B:401:PRO:CD	2.30	0.61
1:B:288:MET:CE	1:B:299:LEU:HD23	2.30	0.61
1:C:389:LYS:HG2	1:C:485:VAL:HG21	1.81	0.61
1:C:297:ALA:H	1:C:358:ILE:HD11	1.65	0.61
1:A:349:LEU:HD23	1:A:369:THR:HG22	1.81	0.61
1:D:263:PRO:HG2	1:D:265:LEU:CD1	2.31	0.61
1:D:93:LYS:HA	1:D:93:LYS:HZ1	1.63	0.61
1:B:62:ILE:HD12	1:B:62:ILE:N	2.16	0.61
1:C:210:LEU:HD11	1:C:582:PHE:HE2	1.65	0.61
1:C:546:SER:CB	1:C:547:ARG:HE	2.14	0.61
1:D:45:LEU:O	1:D:104:SER:HA	2.01	0.61
1:A:450:ASN:O	1:A:451:VAL:HB	1.99	0.61
1:C:546:SER:HB3	1:C:547:ARG:HE	1.64	0.61
1:A:77:LYS:O	1:A:92:LEU:HD12	2.00	0.61
1:A:95:ARG:HB2	1:A:95:ARG:NH1	2.16	0.61
1:D:557:LEU:HD12	1:D:596:HIS:CE1	2.36	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:303:GLU:HB2	1:A:306:ILE:CD1	2.31	0.61
1:C:548:SER:O	1:C:550:SER:N	2.33	0.61
1:B:121:THR:HG23	1:B:128:VAL:HG13	1.82	0.61
1:D:293:GLU:CD	1:D:360:ASP:H	2.04	0.61
1:D:70:LEU:HD13	1:D:117:TRP:CZ2	2.36	0.61
1:B:531:THR:HG22	1:B:536:HIS:CD2	2.35	0.61
1:C:48:THR:HG21	1:C:103:LEU:HD12	1.82	0.61
1:B:60:ILE:O	1:B:83:PRO:HD2	2.01	0.61
1:D:263:PRO:HG2	1:D:265:LEU:HD12	1.83	0.61
1:D:87:GLY:O	1:D:89:PRO:HD3	2.01	0.61
1:A:472:TRP:CE3	1:A:473:ILE:HG12	2.37	0.60
1:C:538:VAL:HG23	1:C:557:LEU:HD11	1.82	0.60
1:B:396:ASN:N	1:B:397:PRO:HD3	2.15	0.60
1:B:93:LYS:CD	1:B:94:ASP:H	2.13	0.60
1:D:514:LEU:HD12	1:D:526:LEU:HB3	1.83	0.60
1:C:210:LEU:HD13	1:C:597:SER:CB	2.31	0.60
1:D:303:GLU:HG3	1:D:304:ASP:N	2.17	0.60
1:A:93:LYS:CD	1:A:94:ASP:H	2.15	0.60
1:A:95:ARG:CZ	1:A:95:ARG:HB2	2.32	0.60
1:B:455:THR:HB	1:B:514:LEU:HD22	1.84	0.60
1:D:222:MET:CE	1:D:291:LEU:HB2	2.28	0.60
1:D:377:ARG:HG3	1:D:377:ARG:NH1	2.16	0.60
1:A:212:ARG:HD3	1:C:201:MET:SD	2.42	0.60
1:D:261:ARG:CB	1:D:261:ARG:NH1	2.65	0.60
1:C:388:GLY:O	1:C:391:GLN:HB3	2.01	0.60
1:C:252:TYR:HE1	1:C:279:PRO:HG3	1.66	0.60
1:C:358:ILE:HA	1:C:362:GLN:O	2.01	0.60
1:A:188:CYS:SG	1:A:549:PHE:HZ	2.25	0.60
1:D:505:ASP:HB3	1:D:508:VAL:HG23	1.84	0.60
1:C:236:LYS:HB2	1:C:237:PRO:CD	2.32	0.60
1:C:43:VAL:HG22	1:C:107:ILE:HB	1.83	0.60
1:C:384:GLN:HE22	1:C:490:ALA:CA	2.14	0.60
1:B:549:PHE:O	1:B:549:PHE:CD1	2.55	0.60
1:D:378:MET:CB	1:D:407:ILE:HG21	2.32	0.59
1:B:202:SER:O	1:B:203:LEU:HD23	2.02	0.59
1:A:56:MET:HG2	1:A:57:ASN:N	2.17	0.59
1:C:81:LEU:CD2	1:C:89:PRO:HB3	2.30	0.59
1:A:261:ARG:O	1:A:263:PRO:HD3	2.02	0.59
1:A:46:PRO:O	1:A:48:THR:O	2.21	0.59
1:C:546:SER:HB3	1:C:547:ARG:CZ	2.33	0.59
1:B:121:THR:CG2	1:B:128:VAL:HG13	2.33	0.59
1:D:498:THR:HG22	1:D:499:TYR:N	2.17	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:520:GLN:HE21	1:D:520:GLN:H	1.51	0.59
1:D:514:LEU:CD1	1:D:526:LEU:HB3	2.33	0.59
1:A:507:ASP:HB3	1:A:532:SER:N	2.17	0.59
1:C:413:LEU:HD23	1:C:427:ILE:HB	1.83	0.59
1:A:488:LYS:O	1:A:489:GLU:HB2	2.03	0.59
1:C:542:VAL:HG21	1:C:551:TYR:CZ	2.38	0.59
1:D:121:THR:HG23	1:D:128:VAL:CG1	2.31	0.59
1:B:346:ILE:HG23	1:B:369:THR:CG2	2.33	0.59
1:C:537:ALA:HA	1:C:557:LEU:HG	1.84	0.59
1:A:38:GLN:HE21	1:D:422:GLU:HB3	1.68	0.58
1:C:369:THR:CG2	1:C:411:GLY:HA3	2.32	0.58
1:D:286:ASN:HD21	1:D:304:ASP:HB3	1.67	0.58
1:C:251:MET:HE3	1:C:283:ASP:HB3	1.84	0.58
1:A:521:ASP:CG	1:A:546:SER:HB2	2.23	0.58
1:B:288:MET:HE1	1:B:299:LEU:HD23	1.84	0.58
1:B:570:CYS:HB3	1:B:577:LEU:CD2	2.33	0.58
1:D:398:GLU:O	1:D:403:LYS:HE3	2.03	0.58
1:A:293:GLU:O	1:A:295:LYS:HG2	2.03	0.58
1:B:93:LYS:CG	1:B:94:ASP:H	2.16	0.58
1:C:132:CYS:SG	1:C:133:LEU:N	2.72	0.58
1:D:483:PHE:HZ	1:D:524:TYR:OH	1.87	0.58
1:D:580:ARG:HA	1:D:598:GLY:O	2.03	0.58
1:B:541:TYR:HB3	1:B:543:TYR:HE2	1.68	0.58
1:B:472:TRP:CZ3	1:B:473:ILE:HG13	2.39	0.58
1:A:91:TYR:HB2	1:A:93:LYS:HG2	1.86	0.58
1:D:124:LYS:HG2	1:D:127:SER:HB2	1.83	0.58
1:C:61:HIS:HB3	1:C:123:GLU:HB2	1.85	0.58
1:B:140:GLN:HE22	1:C:422:GLU:HG2	1.68	0.58
1:A:224:SER:O	1:A:227:MET:HG2	2.04	0.58
1:D:472:TRP:CZ3	1:D:473:ILE:HB	2.39	0.58
1:C:540:TYR:HE1	1:C:568:VAL:CG2	2.17	0.58
1:B:430:GLY:HA3	1:B:476:PHE:CE2	2.32	0.57
1:B:472:TRP:HE3	1:B:472:TRP:N	1.96	0.57
1:C:439:SER:CB	1:C:457:PRO:HG2	2.34	0.57
1:B:93:LYS:HD2	1:B:94:ASP:N	2.19	0.57
1:D:540:TYR:CE1	1:D:568:VAL:HG21	2.38	0.57
1:A:41:SER:O	1:A:110:SER:OG	2.19	0.57
1:A:299:LEU:HD21	1:A:425:ILE:HD13	1.85	0.57
1:D:461:ASN:N	1:D:461:ASN:HD22	2.00	0.57
1:A:437:HIS:CE1	1:A:459:MET:HB2	2.38	0.57
1:C:526:LEU:C	1:C:526:LEU:HD12	2.24	0.57
1:C:368:PRO:HD3	1:C:441:MET:HE3	1.86	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:526:LEU:HD12	1:D:526:LEU:C	2.25	0.57
1:B:56:MET:HB3	1:B:101:GLU:HA	1.86	0.57
1:D:520:GLN:HG2	1:D:521:ASP:N	2.19	0.57
1:A:378:MET:CB	1:A:407:ILE:HG21	2.34	0.57
1:B:340:SER:CB	1:B:426:LYS:HA	2.34	0.57
1:A:540:TYR:HE1	1:A:568:VAL:CG2	2.08	0.57
1:B:215:ASN:HB2	1:B:235:GLU:HB2	1.86	0.57
1:C:323:LYS:HB3	1:C:333:MET:HG2	1.87	0.57
1:D:499:TYR:CD2	1:D:501:PRO:HD3	2.40	0.57
1:A:320:GLN:HG3	1:A:336:TRP:CZ2	2.39	0.57
1:D:520:GLN:HG2	1:D:521:ASP:OD2	2.05	0.57
1:B:318:SER:HB3	1:B:337:VAL:O	2.04	0.57
1:D:124:LYS:HE2	1:D:127:SER:CB	2.34	0.57
1:D:298:ALA:O	1:D:321:LEU:HD12	2.04	0.57
1:B:103:LEU:HD13	1:B:120:MET:CE	2.34	0.57
1:B:325:GLY:C	1:B:327:TRP:H	2.08	0.57
1:D:236:LYS:HD3	1:D:252:TYR:CD2	2.40	0.57
1:D:101:GLU:CD	1:D:101:GLU:H	2.08	0.57
1:D:542:VAL:HG21	1:D:551:TYR:CZ	2.40	0.57
1:C:390:ILE:CG2	1:C:393:LEU:HB2	2.34	0.57
1:C:235:GLU:HA	1:C:250:SER:O	2.05	0.57
1:C:38:GLN:HG3	1:C:138:TYR:CE2	2.40	0.57
1:B:303:GLU:O	1:B:306:ILE:HD11	2.04	0.57
1:A:84:SER:O	1:A:85:GLU:CB	2.52	0.57
1:C:319:PHE:HB2	1:C:425:ILE:CD1	2.35	0.57
1:D:552:PHE:HE1	1:D:121:THR:HG1	1.52	0.57
1:A:326:VAL:HG23	1:A:327:TRP:NE1	2.19	0.57
1:A:210:LEU:O	1:A:213:GLY:N	2.32	0.57
1:A:274:ASN:ND2	1:A:324:LEU:HB3	2.17	0.57
1:A:216:VAL:HA	1:A:233:LEU:O	2.05	0.57
1:B:357:VAL:HG21	1:B:452:TYR:CE1	2.39	0.57
1:D:293:GLU:OE1	1:D:360:ASP:N	2.38	0.57
1:B:326:VAL:HG13	1:B:327:TRP:CD1	2.40	0.57
1:B:557:LEU:HB3	1:B:559:ILE:HD13	1.85	0.56
1:C:540:TYR:HE1	1:C:568:VAL:HG21	1.70	0.56
1:C:81:LEU:HD22	1:C:82:ASP:H	1.70	0.56
1:C:259:VAL:HB	1:C:261:ARG:NH1	2.20	0.56
1:C:537:ALA:HB2	1:C:556:ARG:HA	1.87	0.56
1:C:326:VAL:HG13	1:C:327:TRP:N	2.19	0.56
1:D:514:LEU:HD11	1:D:526:LEU:HD23	1.88	0.56
1:C:248:GLN:N	1:C:248:GLN:OE1	2.39	0.56
1:A:399:TRP:CZ3	1:A:435:ILE:HG22	2.41	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:458:PRO:HB2	1:B:511:SER:OG	2.05	0.56
1:B:89:PRO:HG2	1:B:91:TYR:HE2	1.69	0.56
1:D:124:LYS:HE2	1:D:127:SER:HB2	1.87	0.56
1:C:262:ASN:HB2	1:C:573:TRP:HZ2	1.71	0.56
1:B:134:HIS:CE1	1:B:136:LYS:NZ	2.74	0.56
1:B:541:TYR:HB3	1:B:543:TYR:CE2	2.39	0.56
1:C:349:LEU:HD23	1:C:369:THR:HG22	1.87	0.56
1:D:229:GLY:HA2	1:D:256:GLU:O	2.06	0.56
1:D:342:ASP:O	1:D:344:PRO:HD3	2.05	0.56
1:B:100:LEU:O	1:B:100:LEU:HD13	2.06	0.56
1:D:34:LYS:HE3	1:D:134:HIS:HD2	1.70	0.56
1:B:378:MET:HB2	1:B:407:ILE:HD13	1.88	0.56
1:B:418:SER:O	1:B:419:LEU:HD12	2.06	0.56
1:D:565:GLU:HB3	1:D:584:VAL:HB	1.87	0.56
1:C:349:LEU:CD2	1:C:369:THR:HG22	2.36	0.55
1:D:253:ARG:HH21	1:D:285:SER:CB	2.18	0.55
1:C:375:LYS:O	1:C:379:GLU:HB3	2.06	0.55
1:C:546:SER:HB3	1:C:547:ARG:NE	2.21	0.55
1:B:61:HIS:HE1	1:B:63:VAL:HG22	1.68	0.55
1:A:358:ILE:HG12	1:A:363:ALA:HB2	1.89	0.55
1:A:301:HIS:ND1	1:A:302:GLY:N	2.55	0.55
1:D:355:ARG:HB2	1:D:442:ASP:HB3	1.87	0.55
1:A:39:LEU:HB2	1:A:138:TYR:O	2.06	0.55
1:D:559:ILE:HG12	1:D:560:LYS:N	2.21	0.55
1:C:36:VAL:HA	1:C:136:LYS:O	2.06	0.55
1:B:140:GLN:HE21	1:C:422:GLU:H	1.55	0.55
1:D:493:ASP:HB2	1:D:495:HIS:NE2	2.21	0.55
1:D:444:TYR:HB2	1:D:453:TRP:HB2	1.89	0.55
1:A:202:SER:OG	1:A:203:LEU:N	2.39	0.55
1:D:200:ASN:HD22	1:D:200:ASN:H	1.52	0.55
1:C:464:LEU:HD22	1:C:498:THR:HB	1.88	0.55
1:A:337:VAL:HG12	1:A:425:ILE:HG13	1.88	0.55
1:D:81:LEU:HD23	1:D:82:ASP:N	2.22	0.55
1:C:139:GLU:N	1:C:139:GLU:OE2	2.40	0.55
1:C:410:TYR:O	1:C:429:SER:HA	2.07	0.55
1:D:461:ASN:O	1:D:504:VAL:HG21	2.06	0.55
1:C:34:LYS:N	1:C:34:LYS:HD2	2.22	0.55
1:D:515:VAL:HG13	1:D:525:VAL:HG23	1.89	0.55
1:B:475:ARG:O	1:B:476:PHE:CB	2.54	0.55
1:C:392:ALA:C	1:C:394:CYS:H	2.11	0.55
1:D:450:ASN:O	1:D:471:GLU:HA	2.07	0.55
1:A:481:TYR:C	1:A:482:ARG:HG2	2.26	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:64:VAL:HB	1:D:79:VAL:HG13	1.88	0.55
1:D:200:ASN:H	1:D:200:ASN:ND2	2.05	0.55
1:D:503:GLU:HG2	1:D:93:LYS:CD	2.37	0.55
1:B:472:TRP:CE3	1:B:472:TRP:N	2.75	0.55
1:B:389:LYS:HG3	1:B:390:ILE:N	2.21	0.55
1:D:289:VAL:HG13	1:D:296:LEU:CD1	2.38	0.54
1:D:206:LEU:HD22	1:D:210:LEU:HD11	1.89	0.54
1:D:124:LYS:HE2	1:D:127:SER:OG	2.06	0.54
1:B:517:LEU:HB2	1:B:523:GLN:HG3	1.89	0.54
1:A:378:MET:HB3	1:A:407:ILE:HD13	1.89	0.54
1:C:410:TYR:HD2	1:C:454:LEU:HD11	1.73	0.54
1:A:437:HIS:ND1	1:A:459:MET:HB2	2.21	0.54
1:C:321:LEU:N	1:C:335:SER:O	2.31	0.54
1:B:540:TYR:HE1	1:B:568:VAL:HG21	1.72	0.54
1:A:446:SER:OG	1:A:451:VAL:HG13	2.07	0.54
1:D:383:GLN:HA	1:D:386:CYS:HB2	1.89	0.54
1:C:288:MET:HB2	1:C:365:TRP:NE1	2.23	0.54
1:D:376:LEU:HD23	1:D:376:LEU:O	2.08	0.54
1:B:589:GLU:HG2	1:B:590:SER:H	1.72	0.54
1:D:219:ILE:HD12	1:D:219:ILE:N	2.21	0.54
1:A:299:LEU:HD21	1:A:425:ILE:CD1	2.38	0.54
1:A:459:MET:CE	1:A:459:MET:HA	2.38	0.54
1:C:198:PHE:CE1	1:C:600:VAL:HB	2.43	0.54
1:B:542:VAL:O	1:B:550:SER:HA	2.07	0.54
1:B:40:GLY:HA2	1:B:110:SER:O	2.08	0.54
1:B:217:SER:O	1:B:218:SER:HB2	2.06	0.54
1:D:44:LEU:HD11	1:D:104:SER:HB2	1.88	0.54
1:C:461:ASN:HB3	1:C:508:VAL:HG13	1.89	0.54
1:C:215:ASN:O	1:C:234:VAL:HA	2.08	0.54
1:D:483:PHE:HZ	1:D:524:TYR:HH	1.55	0.54
1:C:485:VAL:O	1:C:485:VAL:HG23	2.08	0.54
1:B:132:CYS:SG	1:B:133:LEU:N	2.81	0.54
1:B:255:PHE:HD1	1:B:276:LEU:HD22	1.73	0.54
1:D:93:LYS:HZ2	1:D:93:LYS:HA	1.73	0.54
1:A:121:THR:HG23	1:A:128:VAL:HG13	1.89	0.54
1:A:322:VAL:HG12	1:A:324:LEU:CD1	2.37	0.54
1:D:345:VAL:HG23	1:D:372:THR:OG1	2.08	0.54
1:D:394:CYS:O	1:D:397:PRO:HD3	2.08	0.54
1:C:91:TYR:C	1:C:93:LYS:H	2.07	0.54
1:C:93:LYS:HD2	1:C:94:ASP:H	1.69	0.54
1:D:530:ASP:OD2	1:D:533:ARG:NH1	2.40	0.54
1:A:558:PRO:HG2	1:A:559:ILE:HG23	1.89	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:496:ALA:HB1	1:D:497:PRO:HD2	1.89	0.54
1:A:68:LYS:H	1:A:68:LYS:HD2	1.72	0.54
1:B:208:LEU:HD12	1:B:212:ARG:HD3	1.89	0.54
1:D:537:ALA:HB2	1:D:556:ARG:HA	1.89	0.53
1:B:499:TYR:CZ	1:B:501:PRO:HB3	2.43	0.53
1:C:125:ASN:OD1	1:C:126:ILE:HG13	2.07	0.53
1:D:92:LEU:HD23	1:D:92:LEU:H	1.72	0.53
1:B:73:SER:OG	1:B:74:VAL:N	2.41	0.53
1:B:65:THR:HB	1:B:75:GLU:HG3	1.89	0.53
1:C:341:THR:HA	1:C:427:ILE:HG23	1.89	0.53
1:B:385:ALA:HB2	1:B:487:ILE:HG13	1.91	0.53
1:D:219:ILE:O	1:D:567:GLN:HG3	2.09	0.53
1:D:377:ARG:HD3	1:D:377:ARG:O	2.09	0.53
1:B:140:GLN:NE2	1:C:422:GLU:HG2	2.22	0.53
1:A:47:LEU:HA	1:A:133:LEU:HD12	1.91	0.53
1:C:464:LEU:HD21	1:C:498:THR:HB	1.90	0.53
1:D:265:LEU:HD12	1:D:269:VAL:HG21	1.89	0.53
1:A:438:GLY:O	1:A:440:GLY:N	2.42	0.53
1:D:329:SER:HB2	1:D:330:PRO:HD2	1.90	0.53
1:B:471:GLU:O	1:B:476:PHE:HA	2.09	0.53
1:A:580:ARG:HB3	1:A:599:MET:CE	2.38	0.53
1:D:580:ARG:NH1	1:D:597:SER:OG	2.42	0.53
1:B:464:LEU:HD11	1:B:526:LEU:HD21	1.90	0.53
1:A:519:GLY:O	1:B:520:GLN:HG2	2.08	0.53
1:A:455:THR:CG2	1:A:516:ILE:HD11	2.38	0.53
1:B:308:ILE:HG23	1:B:341:THR:HG22	1.91	0.53
1:D:64:VAL:HB	1:D:79:VAL:CG1	2.39	0.53
1:B:437:HIS:CD2	1:B:459:MET:HB2	2.44	0.53
1:A:268:PRO:HD3	1:A:573:TRP:CE3	2.44	0.53
1:B:36:VAL:O	1:B:37:GLN:HG2	2.09	0.53
1:B:325:GLY:C	1:B:327:TRP:N	2.61	0.53
1:B:526:LEU:C	1:B:526:LEU:HD12	2.29	0.52
1:C:219:ILE:HG21	1:C:582:PHE:CG	2.44	0.52
1:D:461:ASN:O	1:D:462:LEU:HD23	2.08	0.52
1:B:255:PHE:CZ	1:B:322:VAL:HG21	2.44	0.52
1:B:262:ASN:HB2	1:B:573:TRP:HZ2	1.74	0.52
1:B:507:ASP:O	1:B:530:ASP:HA	2.10	0.52
1:A:533:ARG:NH1	1:A:554:PRO:HB3	2.24	0.52
1:C:93:LYS:HD2	1:C:94:ASP:C	2.30	0.52
1:D:231:THR:HG22	1:D:289:VAL:CG2	2.39	0.52
1:D:488:LYS:HG3	1:D:489:GLU:HG2	1.92	0.52
1:D:537:ALA:CB	1:D:556:ARG:HA	2.40	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:277:GLU:O	1:B:278:GLN:HG3	2.09	0.52
1:C:200:ASN:N	1:C:200:ASN:OD1	2.41	0.52
1:D:437:HIS:O	1:D:459:MET:SD	2.68	0.52
1:A:384:GLN:HG3	1:A:490:ALA:HB2	1.90	0.52
1:C:91:TYR:HB3	1:C:93:LYS:HB3	1.90	0.52
1:D:280:VAL:HG12	1:D:282:ASN:H	1.73	0.52
1:A:222:MET:SD	1:A:355:ARG:HG2	2.50	0.52
1:D:472:TRP:CE3	1:D:473:ILE:HB	2.44	0.52
1:A:123:GLU:HG2	1:A:128:VAL:HG22	1.91	0.52
1:B:410:TYR:CD1	1:B:478:VAL:HG11	2.45	0.52
1:A:52:ILE:O	1:A:53:ASN:HB3	2.10	0.52
1:B:262:ASN:HB2	1:B:573:TRP:CZ2	2.45	0.52
1:B:140:GLN:NE2	1:C:422:GLU:H	2.08	0.52
1:C:454:LEU:HD23	1:C:454:LEU:C	2.29	0.52
1:B:389:LYS:HG3	1:B:390:ILE:HG23	1.91	0.52
1:A:215:ASN:O	1:A:234:VAL:HA	2.08	0.52
1:D:93:LYS:HG3	1:D:94:ASP:N	2.25	0.52
1:C:229:GLY:HA3	1:C:296:LEU:HD12	1.92	0.52
1:A:94:ASP:HB3	1:A:95:ARG:HH11	1.75	0.52
1:A:273:THR:HB	1:A:326:VAL:O	2.10	0.52
1:A:430:GLY:HA3	1:A:476:PHE:HE2	1.73	0.52
1:A:132:CYS:O	1:A:133:LEU:HB2	2.09	0.52
1:B:413:LEU:HD12	1:B:427:ILE:CD1	2.40	0.52
1:B:251:MET:SD	1:B:283:ASP:HB3	2.50	0.52
1:B:210:LEU:O	1:B:213:GLY:N	2.36	0.52
1:A:188:CYS:SG	1:A:549:PHE:CZ	3.04	0.52
1:A:393:LEU:HD21	1:A:436:THR:CB	2.40	0.52
1:C:363:ALA:O	1:C:414:SER:HA	2.09	0.52
1:A:38:GLN:OE1	1:A:38:GLN:HA	2.10	0.51
1:D:319:PHE:HB2	1:D:425:ILE:CD1	2.39	0.51
1:B:514:LEU:HD23	1:B:514:LEU:O	2.10	0.51
1:B:459:MET:C	1:B:459:MET:SD	2.89	0.51
1:A:551:TYR:CD2	1:A:552:PHE:N	2.78	0.51
1:B:294:LEU:HB3	1:B:326:VAL:HG12	1.91	0.51
1:D:95:ARG:H	1:D:95:ARG:HE	1.58	0.51
1:A:71:GLU:O	1:A:72:ASN:CB	2.57	0.51
1:D:206:LEU:HD22	1:D:210:LEU:CD1	2.40	0.51
1:C:210:LEU:HD13	1:C:597:SER:HB3	1.92	0.51
1:C:49:HIS:O	1:C:50:GLU:HG3	2.11	0.51
1:A:388:GLY:O	1:A:391:GLN:HB2	2.11	0.51
1:A:193:THR:HG22	1:A:129:GLN:HG3	1.91	0.51
1:B:475:ARG:HH12	1:B:477:LYS:HD3	1.72	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:206:LEU:CD2	1:D:210:LEU:HG	2.40	0.51
1:C:301:HIS:CG	1:C:306:ILE:HD11	2.46	0.51
1:B:238:ASN:O	1:B:239:LEU:HB2	2.10	0.51
1:A:556:ARG:NH2	1:A:125:ASN:O	2.44	0.51
1:C:461:ASN:ND2	1:C:462:LEU:HD23	2.26	0.51
1:D:112:LYS:HB2	1:D:112:LYS:NZ	2.25	0.51
1:B:458:PRO:HG3	1:B:465:GLY:N	2.23	0.51
1:A:378:MET:HE2	1:A:378:MET:HA	1.92	0.51
1:A:461:ASN:N	1:A:461:ASN:ND2	2.47	0.51
1:B:378:MET:CB	1:B:407:ILE:HD13	2.40	0.51
1:A:318:SER:HB3	1:A:337:VAL:O	2.11	0.51
1:C:121:THR:HG22	1:C:128:VAL:CG2	2.41	0.51
1:D:221:THR:HG22	1:D:230:GLY:HA3	1.93	0.51
1:A:79:VAL:HG13	1:A:79:VAL:O	2.11	0.51
1:D:261:ARG:HH12	1:D:271:HIS:CB	2.23	0.51
1:D:38:GLN:HB3	1:D:41:SER:HB3	1.93	0.51
1:B:37:GLN:O	1:B:137:LEU:HA	2.11	0.51
1:C:541:TYR:CE1	1:C:552:PHE:CB	2.94	0.51
1:A:500:LEU:C	1:A:502:ALA:H	2.15	0.51
1:A:533:ARG:NH1	1:A:123:GLU:OE1	2.44	0.51
1:C:391:GLN:HG2	1:C:392:ALA:N	2.25	0.51
1:A:580:ARG:NH1	1:A:580:ARG:CG	2.74	0.51
1:C:472:TRP:CZ3	1:C:473:ILE:HD13	2.46	0.51
1:B:134:HIS:CE1	1:B:136:LYS:HZ2	2.29	0.51
1:C:293:GLU:HB2	1:C:295:LYS:HE2	1.92	0.51
1:D:577:LEU:HD22	1:D:578:TRP:N	2.25	0.51
1:C:451:VAL:CG1	1:C:469:THR:HB	2.41	0.51
1:B:585:LEU:HD12	1:B:585:LEU:N	2.26	0.51
1:C:194:ILE:HA	1:C:603:GLY:O	2.11	0.50
1:D:510:LEU:HD12	1:D:511:SER:H	1.76	0.50
1:B:299:LEU:HD21	1:B:425:ILE:HD13	1.93	0.50
1:B:319:PHE:HB2	1:B:425:ILE:HD11	1.93	0.50
1:C:589:GLU:O	1:C:591:GLY:N	2.43	0.50
1:C:437:HIS:ND1	1:C:459:MET:HG2	2.26	0.50
1:D:233:LEU:HD13	1:D:251:MET:HE3	1.94	0.50
1:B:354:HIS:ND1	1:B:367:VAL:HG12	2.26	0.50
1:C:293:GLU:HB3	1:C:295:LYS:HE2	1.93	0.50
1:B:221:THR:HG22	1:B:230:GLY:HA3	1.93	0.50
1:B:259:VAL:HG12	1:B:260:ILE:N	2.26	0.50
1:D:48:THR:HG21	1:D:103:LEU:HD13	1.93	0.50
1:A:437:HIS:O	1:A:439:SER:N	2.45	0.50
1:A:565:GLU:HB3	1:A:584:VAL:HB	1.94	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:449:ASN:O	1:A:472:TRP:HH2	1.94	0.50
1:C:369:THR:HG23	1:C:411:GLY:HA3	1.91	0.50
1:C:236:LYS:CB	1:C:237:PRO:CD	2.90	0.50
1:C:82:ASP:CG	1:C:84:SER:HB3	2.31	0.50
1:D:219:ILE:HG21	1:D:582:PHE:CD1	2.47	0.50
1:D:378:MET:HG3	1:D:431:PHE:CE2	2.47	0.50
1:A:371:ARG:HD2	1:A:429:SER:HB2	1.93	0.50
1:C:453:TRP:HB3	1:C:516:ILE:HD12	1.93	0.50
1:D:464:LEU:CG	1:D:465:GLY:H	2.23	0.50
1:B:299:LEU:HD11	1:B:425:ILE:HD11	1.94	0.50
1:B:60:ILE:HD12	1:B:124:LYS:HA	1.92	0.50
1:A:50:GLU:HG2	1:A:52:ILE:CG2	2.41	0.50
1:A:499:TYR:CZ	1:A:501:PRO:HB3	2.45	0.50
1:B:500:LEU:CD2	1:B:502:ALA:HB3	2.42	0.50
1:B:337:VAL:CG1	1:B:423:LEU:HB3	2.42	0.50
1:D:441:MET:HA	1:D:455:THR:O	2.12	0.50
1:A:458:PRO:HB2	1:A:511:SER:CB	2.41	0.50
1:B:282:ASN:OD1	1:B:284:LEU:HB2	2.12	0.50
1:A:485:VAL:O	1:A:495:HIS:HB3	2.12	0.50
1:A:93:LYS:HD2	1:A:94:ASP:CA	2.43	0.49
1:D:306:ILE:CD1	1:D:306:ILE:N	2.75	0.49
1:B:47:LEU:HD13	1:B:120:MET:HB2	1.93	0.49
1:D:326:VAL:HG13	1:D:327:TRP:N	2.28	0.49
1:B:51:ARG:O	1:B:53:ASN:N	2.45	0.49
1:D:457:PRO:O	1:D:459:MET:HE2	2.10	0.49
1:D:415:VAL:CG1	1:D:425:ILE:HA	2.42	0.49
1:B:453:TRP:CE2	1:B:522:LEU:HD13	2.47	0.49
1:A:378:MET:CE	1:A:378:MET:HA	2.43	0.49
1:D:354:HIS:ND1	1:D:367:VAL:HG12	2.26	0.49
1:D:547:ARG:HG3	1:D:549:PHE:H	1.76	0.49
1:C:205:LEU:HB2	1:C:272:MET:CE	2.43	0.49
1:B:326:VAL:HG22	1:B:326:VAL:O	2.12	0.49
1:A:466:VAL:CG1	1:A:468:ASN:HD21	2.26	0.49
1:C:459:MET:SD	1:C:460:LYS:HB2	2.53	0.49
1:D:579:CYS:SG	1:D:602:MET:HE1	2.53	0.49
1:D:481:TYR:CD2	1:D:482:ARG:HG2	2.47	0.49
1:C:367:VAL:HG13	1:C:368:PRO:HD2	1.93	0.49
1:B:308:ILE:N	1:B:308:ILE:HD12	2.27	0.49
1:A:320:GLN:HB2	1:A:336:TRP:CH2	2.47	0.49
1:B:85:GLU:HG3	1:B:87:GLY:H	1.77	0.49
1:D:458:PRO:HB3	1:D:465:GLY:N	2.28	0.49
1:A:233:LEU:HD23	1:A:253:ARG:HA	1.95	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:135:LEU:HD12	1:D:136:LYS:H	1.76	0.49
1:B:514:LEU:HD23	1:B:514:LEU:C	2.33	0.49
1:B:540:TYR:HE1	1:B:568:VAL:CG2	2.25	0.49
1:D:503:GLU:HG2	1:D:93:LYS:HD2	1.93	0.49
1:D:523:GLN:O	1:D:524:TYR:HB3	2.12	0.49
1:D:72:ASN:N	1:D:72:ASN:ND2	2.59	0.49
1:D:295:LYS:HA	1:D:325:GLY:HA2	1.94	0.49
1:B:280:VAL:HG12	1:B:282:ASN:H	1.77	0.49
1:C:287:CYS:HA	1:C:299:LEU:O	2.13	0.49
1:B:293:GLU:O	1:B:295:LYS:HG2	2.13	0.49
1:C:509:LYS:HB2	1:C:563:PRO:HG3	1.94	0.49
1:D:231:THR:HG21	1:D:287:CYS:HB2	1.95	0.49
1:C:472:TRP:N	1:C:472:TRP:CD1	2.81	0.49
1:C:541:TYR:CE1	1:C:552:PHE:HB3	2.48	0.49
1:D:559:ILE:CG1	1:D:560:LYS:N	2.76	0.49
1:C:227:MET:HB2	1:C:258:GLY:O	2.13	0.49
1:B:559:ILE:HG12	1:B:560:LYS:N	2.28	0.48
1:D:464:LEU:HG	1:D:465:GLY:N	2.23	0.48
1:C:206:LEU:CD2	1:C:210:LEU:HG	2.42	0.48
1:A:261:ARG:C	1:A:263:PRO:HD3	2.33	0.48
1:A:192:THR:HG22	1:A:606:CYS:SG	2.53	0.48
1:C:255:PHE:O	1:C:275:TYR:HB2	2.13	0.48
1:D:545:PRO:C	1:D:547:ARG:N	2.67	0.48
1:D:547:ARG:CG	1:D:548:SER:H	2.26	0.48
1:B:306:ILE:HD12	1:B:306:ILE:N	2.27	0.48
1:C:99:TYR:HB3	1:C:101:GLU:HG2	1.95	0.48
1:B:562:VAL:CB	1:B:586:ALA:HB3	2.39	0.48
1:C:68:LYS:HD3	1:C:113:LYS:O	2.12	0.48
1:A:257:VAL:HG13	1:A:274:ASN:HB3	1.94	0.48
1:A:337:VAL:HG11	1:A:425:ILE:HG13	1.94	0.48
1:D:399:TRP:O	1:D:403:LYS:HG3	2.14	0.48
1:D:75:GLU:OE2	1:D:130:ARG:NH2	2.41	0.48
1:C:230:GLY:HA2	1:C:289:VAL:HG11	1.95	0.48
1:B:95:ARG:NH1	1:B:95:ARG:HG3	2.22	0.48
1:A:52:ILE:HG12	1:A:52:ILE:O	2.13	0.48
1:B:513:ASN:OD1	1:B:568:VAL:HG12	2.13	0.48
1:B:540:TYR:O	1:B:552:PHE:HA	2.14	0.48
1:A:466:VAL:CG1	1:A:468:ASN:ND2	2.76	0.48
1:D:332:ASP:O	1:D:333:MET:HB3	2.13	0.48
1:C:236:LYS:C	1:C:249:LEU:HB3	2.34	0.48
1:C:82:ASP:C	1:C:84:SER:H	2.17	0.48
1:A:222:MET:HB3	1:A:355:ARG:CD	2.41	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:253:ARG:HG3	1:D:253:ARG:HH11	1.78	0.48
1:C:548:SER:O	1:C:549:PHE:C	2.51	0.48
1:C:541:TYR:CD1	1:C:552:PHE:HB3	2.49	0.48
1:B:227:MET:HE2	1:B:294:LEU:HD13	1.96	0.48
1:D:307:THR:HA	1:D:348:ARG:HG2	1.95	0.48
1:A:95:ARG:H	1:A:95:ARG:HH11	1.62	0.48
1:A:580:ARG:HB2	1:A:580:ARG:CZ	2.44	0.48
1:D:321:LEU:N	1:D:335:SER:O	2.36	0.48
1:A:520:GLN:CG	1:A:520:GLN:O	2.61	0.48
1:B:206:LEU:HD13	1:B:232:TYR:CD1	2.49	0.48
1:C:480:PRO:HB2	1:C:484:THR:HG21	1.95	0.48
1:C:249:LEU:HD22	1:C:249:LEU:H	1.78	0.48
1:C:37:GLN:CA	1:C:37:GLN:HE21	2.27	0.48
1:C:374:ASP:HB2	1:C:407:ILE:HB	1.95	0.48
1:B:38:GLN:HG3	1:C:422:GLU:HB3	1.96	0.48
1:C:210:LEU:HD11	1:C:582:PHE:CE2	2.48	0.48
1:B:263:PRO:HB2	1:B:265:LEU:HD13	1.96	0.48
1:C:363:ALA:HB3	1:C:415:VAL:HG23	1.94	0.48
1:B:441:MET:HE2	1:B:456:ILE:HD11	1.96	0.48
1:D:194:ILE:CD1	1:D:194:ILE:N	2.77	0.48
1:A:399:TRP:CD1	1:A:401:PRO:HD2	2.49	0.48
1:B:43:VAL:HG21	1:B:135:LEU:HD21	1.95	0.48
1:A:91:TYR:CB	1:A:93:LYS:HB3	2.42	0.48
1:A:135:LEU:HG	1:A:136:LYS:N	2.28	0.48
1:B:374:ASP:HB2	1:B:407:ILE:HB	1.96	0.48
1:B:533:ARG:HG3	1:B:533:ARG:HH11	1.79	0.48
1:D:280:VAL:HG12	1:D:281:SER:N	2.29	0.48
1:A:303:GLU:HB2	1:A:306:ILE:HD13	1.95	0.48
1:D:198:PHE:CE1	1:D:600:VAL:HB	2.49	0.48
1:D:255:PHE:O	1:D:275:TYR:HA	2.14	0.48
1:B:301:HIS:ND1	1:B:302:GLY:N	2.62	0.48
1:B:399:TRP:NE1	1:B:401:PRO:HD2	2.28	0.48
1:B:93:LYS:HB2	1:B:96:TYR:HD1	1.78	0.48
1:D:482:ARG:HD2	1:D:72:ASN:HD21	1.79	0.48
1:A:55:SER:HB3	1:A:57:ASN:HD21	1.79	0.48
1:A:515:VAL:HG12	1:A:525:VAL:HB	1.96	0.48
1:C:48:THR:HG22	1:C:103:LEU:HB2	1.95	0.48
1:D:59:SER:HB2	1:D:123:GLU:O	2.14	0.47
1:B:91:TYR:CB	1:B:93:LYS:HB3	2.41	0.47
1:A:309:PRO:HB2	1:A:341:THR:CG2	2.43	0.47
1:B:392:ALA:HA	1:B:395:GLU:CD	2.35	0.47
1:C:458:PRO:HD2	1:C:511:SER:HB3	1.95	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:467:ILE:HD12	1:D:483:PHE:HE2	1.79	0.47
1:B:308:ILE:HD13	1:B:348:ARG:HA	1.95	0.47
1:C:461:ASN:HD22	1:C:462:LEU:N	2.11	0.47
1:D:514:LEU:HD13	1:D:526:LEU:HD23	1.96	0.47
1:B:37:GLN:HB2	1:B:137:LEU:HD23	1.97	0.47
1:B:47:LEU:HA	1:B:133:LEU:HD12	1.97	0.47
1:A:510:LEU:O	1:A:528:THR:HA	2.14	0.47
1:C:37:GLN:O	1:C:137:LEU:HA	2.15	0.47
1:C:390:ILE:CG2	1:C:394:CYS:SG	3.03	0.47
1:A:80:SER:O	1:A:81:LEU:HB2	2.14	0.47
1:D:552:PHE:HE1	1:D:121:THR:OG1	1.97	0.47
1:D:537:ALA:HA	1:D:557:LEU:CD2	2.41	0.47
1:A:125:ASN:OD1	1:A:126:ILE:N	2.48	0.47
1:C:589:GLU:C	1:C:591:GLY:H	2.17	0.47
1:C:219:ILE:HG21	1:C:582:PHE:CD2	2.50	0.47
1:C:288:MET:HB3	1:C:354:HIS:HB2	1.95	0.47
1:C:480:PRO:CB	1:C:484:THR:HG21	2.44	0.47
1:D:202:SER:O	1:D:203:LEU:HD23	2.14	0.47
1:A:101:GLU:CD	1:A:101:GLU:H	2.18	0.47
1:C:91:TYR:HB3	1:C:93:LYS:HG2	1.95	0.47
1:A:472:TRP:CZ3	1:A:473:ILE:HG12	2.49	0.47
1:D:261:ARG:HB2	1:D:261:ARG:CZ	2.45	0.47
1:C:531:THR:HG22	1:C:536:HIS:CG	2.48	0.47
1:C:384:GLN:HE22	1:C:490:ALA:CB	2.28	0.47
1:C:369:THR:HG21	1:C:411:GLY:HA3	1.96	0.47
1:D:347:ASP:H	1:D:371:ARG:HA	1.80	0.47
1:A:519:GLY:C	1:A:521:ASP:H	2.17	0.47
1:B:294:LEU:N	1:B:294:LEU:HD22	2.29	0.47
1:B:206:LEU:HD13	1:B:232:TYR:CG	2.49	0.47
1:A:139:GLU:N	1:A:139:GLU:OE2	2.47	0.47
1:C:569:GLU:O	1:C:569:GLU:HG3	2.15	0.47
1:A:255:PHE:CZ	1:A:322:VAL:HG21	2.49	0.47
1:B:339:LEU:HD12	1:B:425:ILE:HB	1.95	0.47
1:B:264:GLY:C	1:B:265:LEU:HD12	2.35	0.47
1:D:374:ASP:HB3	1:D:407:ILE:HG12	1.97	0.47
1:D:526:LEU:HD12	1:D:526:LEU:O	2.15	0.47
1:C:522:LEU:HD12	1:C:523:GLN:N	2.29	0.47
1:A:524:TYR:N	1:A:524:TYR:CD2	2.83	0.47
1:B:471:GLU:OE2	1:B:477:LYS:O	2.32	0.47
1:C:81:LEU:HD22	1:C:82:ASP:N	2.30	0.47
1:A:517:LEU:HD11	1:A:525:VAL:HG23	1.97	0.47
1:A:293:GLU:OE2	1:A:359:ALA:HA	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:459:MET:HE2	1:A:459:MET:HA	1.96	0.47
1:D:577:LEU:C	1:D:577:LEU:HD22	2.35	0.47
1:D:261:ARG:HB3	1:D:261:ARG:HH11	1.80	0.46
1:A:569:GLU:OE2	1:A:582:PHE:HE1	1.97	0.46
1:D:501:PRO:O	1:D:504:VAL:HG12	2.15	0.46
1:D:324:LEU:HD23	1:D:332:ASP:HB3	1.96	0.46
1:D:223:THR:O	1:D:224:SER:HB2	2.15	0.46
1:A:98:PHE:HZ	1:A:103:LEU:HD22	1.79	0.46
1:B:77:LYS:NZ	1:B:80:SER:HB2	2.30	0.46
1:B:92:LEU:HD23	1:B:92:LEU:N	2.31	0.46
1:C:540:TYR:CE1	1:C:568:VAL:HG21	2.50	0.46
1:A:98:PHE:CG	1:A:99:TYR:N	2.83	0.46
1:D:389:LYS:C	1:D:391:GLN:H	2.19	0.46
1:C:329:SER:OG	1:C:331:THR:HG23	2.14	0.46
1:D:228:TYR:CE1	1:D:258:GLY:HA3	2.51	0.46
1:D:43:VAL:HG22	1:D:45:LEU:CD1	2.45	0.46
1:C:35:ILE:HD13	1:C:45:LEU:HD23	1.97	0.46
1:A:299:LEU:CD1	1:A:321:LEU:HD13	2.46	0.46
1:D:293:GLU:O	1:D:295:LYS:HE3	2.14	0.46
1:D:295:LYS:HZ2	1:D:358:ILE:HG21	1.80	0.46
1:D:498:THR:HG22	1:D:499:TYR:H	1.80	0.46
1:D:36:VAL:HG22	1:D:136:LYS:HB3	1.97	0.46
1:D:410:TYR:CE1	1:D:435:ILE:HD11	2.50	0.46
1:D:419:LEU:HD21	1:D:423:LEU:HD11	1.97	0.46
1:A:38:GLN:NE2	1:D:422:GLU:HB3	2.31	0.46
1:D:514:LEU:HD12	1:D:514:LEU:HA	1.74	0.46
1:D:63:VAL:HG12	1:D:64:VAL:N	2.30	0.46
1:A:437:HIS:C	1:A:439:SER:H	2.18	0.46
1:B:126:ILE:HG13	1:B:126:ILE:O	2.15	0.46
1:D:569:GLU:O	1:D:569:GLU:HG3	2.15	0.46
1:C:135:LEU:HD23	1:C:135:LEU:C	2.35	0.46
1:D:538:VAL:HG21	1:D:581:HIS:CD2	2.50	0.46
1:D:556:ARG:HH21	1:D:556:ARG:HG3	1.81	0.46
1:A:231:THR:OG1	1:A:253:ARG:HD2	2.16	0.46
1:A:38:GLN:HG3	1:D:422:GLU:HB3	1.98	0.46
1:D:205:LEU:HB2	1:D:272:MET:CE	2.46	0.46
1:A:507:ASP:OD1	1:A:90:ARG:NH1	2.47	0.46
1:C:50:GLU:O	1:C:51:ARG:C	2.54	0.46
1:D:461:ASN:ND2	1:D:461:ASN:N	2.62	0.46
1:B:52:ILE:HD13	1:C:282:ASN:OD1	2.16	0.46
1:D:39:LEU:HB2	1:D:138:TYR:O	2.16	0.46
1:D:521:ASP:HB2	1:D:546:SER:CB	2.44	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:107:ILE:HD11	1:C:118:TYR:HE2	1.78	0.46
1:A:95:ARG:N	1:A:95:ARG:HH11	2.14	0.46
1:A:415:VAL:CG1	1:A:425:ILE:HG12	2.46	0.46
1:A:47:LEU:HD21	1:A:105:LEU:HB2	1.98	0.46
1:B:51:ARG:C	1:B:53:ASN:H	2.19	0.46
1:B:222:MET:HB3	1:B:355:ARG:HD3	1.98	0.46
1:A:377:ARG:HH11	1:A:377:ARG:HG2	1.80	0.46
1:A:230:GLY:HA2	1:A:289:VAL:HG11	1.98	0.46
1:D:35:ILE:HG12	1:D:133:LEU:HD22	1.97	0.46
1:B:374:ASP:C	1:B:376:LEU:H	2.19	0.46
1:D:504:VAL:O	1:D:504:VAL:HG13	2.16	0.46
1:C:121:THR:HG22	1:C:128:VAL:HG22	1.98	0.46
1:A:45:LEU:HD13	1:A:133:LEU:HD13	1.98	0.46
1:B:473:ILE:HB	1:B:474:PRO:CD	2.37	0.46
1:C:421:VAL:O	1:C:422:GLU:C	2.53	0.46
1:D:65:THR:OG1	1:D:66:MET:N	2.49	0.46
1:C:543:TYR:OH	1:C:75:GLU:HB2	2.16	0.46
1:C:236:LYS:HB2	1:C:237:PRO:HD2	1.97	0.46
1:D:464:LEU:CG	1:D:465:GLY:N	2.79	0.46
1:A:93:LYS:HD2	1:A:94:ASP:O	2.15	0.46
1:D:516:ILE:HD13	1:D:524:TYR:HB3	1.98	0.46
1:C:461:ASN:ND2	1:C:461:ASN:C	2.67	0.46
1:D:463:ALA:HB2	1:D:498:THR:O	2.15	0.46
1:C:542:VAL:HG21	1:C:551:TYR:OH	2.16	0.46
1:D:572:THR:HG22	1:D:576:LYS:O	2.16	0.46
1:C:79:VAL:HG23	1:C:90:ARG:O	2.16	0.46
1:D:107:ILE:HD11	1:D:118:TYR:CE2	2.51	0.46
1:D:194:ILE:HA	1:D:603:GLY:O	2.15	0.46
1:B:247:SER:O	1:B:249:LEU:HD13	2.16	0.46
1:B:61:HIS:C	1:B:62:ILE:HD12	2.37	0.46
1:C:233:LEU:HD21	1:C:253:ARG:NH2	2.31	0.46
1:A:264:GLY:O	1:A:265:LEU:HD23	2.16	0.46
1:C:208:LEU:O	1:C:212:ARG:HG2	2.16	0.45
1:C:123:GLU:HG2	1:C:128:VAL:HG23	1.98	0.45
1:C:434:LEU:HD13	1:C:495:HIS:O	2.16	0.45
1:A:395:GLU:O	1:A:395:GLU:OE1	2.34	0.45
1:C:481:TYR:CD2	1:C:482:ARG:HG2	2.51	0.45
1:C:488:LYS:C	1:C:489:GLU:HG2	2.37	0.45
1:A:589:GLU:CG	1:A:590:SER:N	2.78	0.45
1:A:589:GLU:O	1:A:591:GLY:N	2.46	0.45
1:C:236:LYS:NZ	1:C:277:GLU:OE1	2.42	0.45
1:C:36:VAL:C	1:C:37:GLN:HE21	2.19	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:585:LEU:CD2	1:A:585:LEU:N	2.79	0.45
1:A:393:LEU:O	1:A:393:LEU:HD12	2.16	0.45
1:A:282:ASN:OD1	1:A:284:LEU:HB2	2.16	0.45
1:D:593:HIS:HB2	2:D:901:NAG:O7	2.16	0.45
1:D:304:ASP:HB2	1:D:351:LEU:O	2.17	0.45
1:B:215:ASN:HB3	1:B:235:GLU:HB2	1.99	0.45
1:C:219:ILE:HG22	1:C:219:ILE:O	2.16	0.45
1:D:461:ASN:H	1:D:461:ASN:ND2	2.15	0.45
1:B:294:LEU:O	1:B:326:VAL:HG12	2.17	0.45
1:B:522:LEU:O	1:B:545:PRO:HD2	2.17	0.45
1:A:395:GLU:H	1:A:395:GLU:HG3	1.56	0.45
1:A:366:ALA:O	1:A:441:MET:HB3	2.16	0.45
1:A:473:ILE:HG22	1:A:474:PRO:CD	2.46	0.45
1:B:35:ILE:HA	1:C:334:GLN:O	2.16	0.45
1:C:533:ARG:HB3	1:C:61:HIS:CD2	2.51	0.45
1:A:573:TRP:O	1:A:574:ASP:CB	2.62	0.45
1:B:406:ARG:O	1:B:408:PRO:HD3	2.17	0.45
1:D:379:GLU:HG3	1:D:380:THR:H	1.82	0.45
1:C:236:LYS:HD3	1:C:252:TYR:CD2	2.52	0.45
1:D:306:ILE:HD12	1:D:306:ILE:H	1.81	0.45
1:D:206:LEU:HG	1:D:232:TYR:CZ	2.52	0.45
1:B:36:VAL:HG11	1:C:333:MET:SD	2.57	0.45
1:A:301:HIS:HB2	1:A:319:PHE:CE2	2.51	0.45
1:D:200:ASN:N	1:D:200:ASN:HD22	2.10	0.45
1:B:276:LEU:HD23	1:B:277:GLU:N	2.31	0.45
1:B:265:LEU:HD11	1:D:209:TYR:CE2	2.52	0.45
1:C:510:LEU:HD12	1:C:563:PRO:HB2	1.99	0.45
1:C:467:ILE:HD12	1:C:483:PHE:HE2	1.82	0.45
1:C:315:LYS:O	1:C:315:LYS:HG3	2.16	0.45
1:D:499:TYR:CE2	1:D:501:PRO:HD3	2.51	0.45
1:C:123:GLU:HA	1:C:128:VAL:HG23	1.99	0.45
1:C:119:PHE:HA	1:C:131:PHE:O	2.15	0.45
1:C:570:CYS:HA	1:C:578:TRP:O	2.16	0.45
1:D:99:TYR:O	1:D:103:LEU:N	2.50	0.45
1:C:536:HIS:CE1	1:C:560:LYS:HB3	2.51	0.45
1:D:211:GLY:C	1:D:213:GLY:N	2.68	0.45
1:A:559:ILE:CD1	1:A:559:ILE:H	2.28	0.45
1:C:540:TYR:O	1:C:552:PHE:HA	2.17	0.45
1:A:32:CYS:SG	1:A:133:LEU:N	2.90	0.45
1:A:466:VAL:HG12	1:A:468:ASN:ND2	2.32	0.45
1:B:274:ASN:ND2	1:B:324:LEU:HG	2.32	0.45
1:B:473:ILE:CB	1:B:474:PRO:HD3	2.34	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:580:ARG:NH1	1:A:580:ARG:HB2	2.31	0.45
1:D:369:THR:OG1	1:D:411:GLY:HA3	2.17	0.45
1:C:253:ARG:HD3	1:C:287:CYS:SG	2.57	0.45
1:C:223:THR:O	1:C:224:SER:HB2	2.17	0.45
1:B:529:TYR:CE1	1:B:563:PRO:HD3	2.51	0.45
1:C:558:PRO:HD2	1:C:596:HIS:NE2	2.32	0.45
1:A:505:ASP:OD2	1:A:77:LYS:HD3	2.18	0.44
1:C:564:ILE:HD11	1:C:584:VAL:CG1	2.47	0.44
1:B:362:GLN:HB3	1:B:364:LYS:HE2	1.99	0.44
1:B:252:TYR:N	1:B:252:TYR:CD2	2.85	0.44
1:B:194:ILE:HD12	1:B:194:ILE:N	2.32	0.44
1:B:558:PRO:HG2	1:B:559:ILE:N	2.32	0.44
1:C:386:CYS:O	1:C:391:GLN:HA	2.16	0.44
1:A:93:LYS:CD	1:A:94:ASP:N	2.76	0.44
1:A:36:VAL:O	1:A:37:GLN:HG2	2.18	0.44
1:C:367:VAL:O	1:C:369:THR:HG23	2.17	0.44
1:A:52:ILE:HB	1:D:302:GLY:HA3	2.00	0.44
1:D:498:THR:CG2	1:D:499:TYR:N	2.80	0.44
1:A:444:TYR:CD2	1:A:516:ILE:HG12	2.52	0.44
1:D:254:VAL:HG12	1:D:255:PHE:N	2.32	0.44
1:B:48:THR:O	1:B:50:GLU:N	2.48	0.44
1:C:406:ARG:HG3	1:C:406:ARG:HH11	1.82	0.44
1:A:308:ILE:HG23	1:A:309:PRO:HD2	1.98	0.44
1:C:38:GLN:O	1:C:41:SER:OG	2.32	0.44
1:C:565:GLU:HB3	1:C:584:VAL:CG2	2.47	0.44
1:D:96:TYR:CD2	1:D:107:ILE:HG12	2.53	0.44
1:C:306:ILE:HG12	1:C:319:PHE:HE1	1.83	0.44
1:A:93:LYS:CG	1:A:94:ASP:N	2.80	0.44
1:B:386:CYS:SG	1:B:386:CYS:O	2.74	0.44
1:D:453:TRP:CH2	1:D:522:LEU:HD13	2.53	0.44
1:D:572:THR:HA	1:D:577:LEU:HA	1.98	0.44
1:A:100:LEU:O	1:A:103:LEU:HD23	2.17	0.44
1:C:276:LEU:HA	1:C:276:LEU:HD12	1.85	0.44
1:A:310:TYR:O	1:A:312:GLY:N	2.47	0.44
1:D:103:LEU:HD22	1:D:120:MET:SD	2.57	0.44
1:B:458:PRO:HB3	1:B:464:LEU:HA	1.98	0.44
1:D:545:PRO:O	1:D:547:ARG:N	2.51	0.44
1:B:418:SER:O	1:B:419:LEU:HB2	2.18	0.44
1:A:384:GLN:CG	1:A:490:ALA:HB2	2.46	0.44
1:D:135:LEU:HD12	1:D:136:LYS:N	2.31	0.44
1:A:472:TRP:HE3	1:A:473:ILE:HG12	1.81	0.44
1:B:337:VAL:HA	1:B:338:PRO:HD3	1.88	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:533:ARG:HG3	1:B:533:ARG:NH1	2.31	0.44
1:C:48:THR:CG2	1:C:103:LEU:HB2	2.47	0.44
1:A:455:THR:HG22	1:A:516:ILE:HD11	1.98	0.44
1:D:136:LYS:HG2	1:D:137:LEU:N	2.33	0.44
1:C:503:GLU:OE1	1:C:76:ASN:HB3	2.18	0.44
1:D:288:MET:O	1:D:298:ALA:HA	2.18	0.44
1:D:450:ASN:ND2	1:D:473:ILE:CG2	2.81	0.44
1:A:399:TRP:HZ3	1:A:435:ILE:HG22	1.81	0.44
1:D:585:LEU:HD12	1:D:594:ILE:HG22	1.99	0.44
1:D:400:ALA:HB3	1:D:401:PRO:CD	2.48	0.44
1:D:260:ILE:HG12	1:D:270:PHE:CE1	2.52	0.44
1:C:91:TYR:HB3	1:C:93:LYS:CG	2.48	0.44
1:A:38:GLN:HB3	1:A:41:SER:HB3	2.00	0.44
1:A:569:GLU:HG3	1:A:580:ARG:HG2	2.00	0.44
1:D:206:LEU:HD23	1:D:210:LEU:HG	1.99	0.44
1:C:206:LEU:HD22	1:C:210:LEU:CD1	2.48	0.44
1:C:288:MET:HB2	1:C:365:TRP:CD1	2.52	0.44
1:C:569:GLU:O	1:C:579:CYS:HA	2.18	0.44
1:C:131:PHE:N	1:C:131:PHE:CD1	2.85	0.44
1:D:46:PRO:O	1:D:48:THR:N	2.51	0.44
1:D:303:GLU:CG	1:D:304:ASP:H	2.29	0.44
1:A:36:VAL:C	1:A:37:GLN:HG2	2.38	0.44
1:B:299:LEU:HD11	1:B:425:ILE:CD1	2.48	0.44
1:B:229:GLY:H	1:B:291:LEU:HD11	1.81	0.44
1:D:574:ASP:O	1:D:576:LYS:N	2.51	0.44
1:D:375:LYS:CA	1:D:379:GLU:HB3	2.47	0.44
1:C:74:VAL:HG12	1:C:74:VAL:O	2.17	0.44
1:D:94:ASP:HB3	1:D:95:ARG:H	1.41	0.43
1:D:585:LEU:HD12	1:D:585:LEU:O	2.18	0.43
1:C:390:ILE:O	1:C:390:ILE:HG22	2.18	0.43
1:D:309:PRO:HG3	1:D:316:GLY:CA	2.44	0.43
1:C:499:TYR:CE2	1:C:501:PRO:HB3	2.53	0.43
1:C:444:TYR:CZ	1:C:515:VAL:HA	2.54	0.43
1:A:570:CYS:HA	1:A:578:TRP:O	2.19	0.43
1:D:538:VAL:HG23	1:D:557:LEU:HD11	2.00	0.43
1:A:580:ARG:HA	1:A:599:MET:HA	2.00	0.43
1:C:505:ASP:OD2	1:C:77:LYS:HE2	2.19	0.43
1:C:77:LYS:HG2	1:C:92:LEU:HD13	2.00	0.43
1:B:352:SER:OG	1:B:440:GLY:HA2	2.18	0.43
1:D:358:ILE:HA	1:D:362:GLN:O	2.18	0.43
1:C:345:VAL:HG11	1:C:373:ASP:OD1	2.18	0.43
1:A:46:PRO:O	1:A:46:PRO:HG2	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:405:ASN:N	1:D:405:ASN:HD22	2.15	0.43
1:A:310:TYR:C	1:A:312:GLY:H	2.22	0.43
1:B:196:GLY:HA3	1:B:553:TYR:CZ	2.54	0.43
1:C:392:ALA:O	1:C:394:CYS:N	2.43	0.43
1:C:490:ALA:HB3	1:C:494:CYS:HB3	2.00	0.43
1:D:232:TYR:CD1	1:D:232:TYR:N	2.86	0.43
1:A:312:GLY:O	1:A:314:GLY:N	2.44	0.43
1:B:93:LYS:HD3	1:B:96:TYR:N	2.33	0.43
1:D:514:LEU:HD13	1:D:526:LEU:CD2	2.48	0.43
1:D:451:VAL:CG1	1:D:469:THR:HB	2.48	0.43
1:C:70:LEU:HD12	1:C:117:TRP:CE2	2.53	0.43
1:A:206:LEU:HD13	1:A:232:TYR:CD1	2.53	0.43
1:B:551:TYR:N	1:B:551:TYR:CD1	2.87	0.43
1:D:516:ILE:CD1	1:D:524:TYR:HB3	2.48	0.43
1:D:346:ILE:HG23	1:D:369:THR:CG2	2.49	0.43
1:C:514:LEU:HG	1:C:526:LEU:HD23	2.00	0.43
1:B:400:ALA:CB	1:B:401:PRO:HD3	2.42	0.43
1:B:481:TYR:O	1:B:482:ARG:CG	2.64	0.43
1:A:46:PRO:HA	1:A:104:SER:HA	2.00	0.43
1:C:39:LEU:HG	1:C:138:TYR:O	2.19	0.43
1:C:117:TRP:NE1	1:C:134:HIS:HB2	2.34	0.43
1:A:296:LEU:HD12	1:A:297:ALA:N	2.34	0.43
1:D:412:VAL:N	1:D:428:ALA:O	2.36	0.43
1:D:139:GLU:OE1	1:D:139:GLU:HA	2.19	0.43
1:A:556:ARG:HH22	1:A:125:ASN:HB2	1.83	0.43
1:C:462:LEU:HB2	1:C:463:ALA:H	1.69	0.43
1:C:39:LEU:C	1:C:41:SER:H	2.22	0.43
1:A:573:TRP:O	1:A:574:ASP:HB3	2.19	0.43
1:B:508:VAL:HG13	1:B:528:THR:HG23	2.00	0.43
1:C:593:HIS:HD2	2:C:901:NAG:H81	1.83	0.43
1:A:58:LYS:HG3	1:A:58:LYS:O	2.18	0.43
1:C:319:PHE:HB2	1:C:425:ILE:HD12	2.01	0.43
1:C:508:VAL:HG23	1:C:528:THR:OG1	2.17	0.43
1:A:69:SER:OG	1:A:70:LEU:N	2.51	0.43
1:A:50:GLU:HG2	1:A:52:ILE:HG23	2.00	0.43
1:C:580:ARG:NH1	1:C:597:SER:OG	2.52	0.43
1:C:39:LEU:O	1:C:41:SER:N	2.51	0.43
1:C:467:ILE:HB	1:C:482:ARG:HB2	2.00	0.43
1:B:48:THR:C	1:B:50:GLU:H	2.20	0.43
1:B:66:MET:HG3	1:B:118:TYR:CZ	2.54	0.43
1:D:74:VAL:O	1:D:74:VAL:HG12	2.19	0.43
1:A:387:LYS:HA	1:A:387:LYS:CE	2.49	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:374:ASP:CG	1:C:406:ARG:HE	2.22	0.43
1:D:482:ARG:HD2	1:D:72:ASN:ND2	2.34	0.43
1:B:533:ARG:NH2	1:B:554:PRO:HB3	2.34	0.43
1:D:473:ILE:N	1:D:474:PRO:HD2	2.34	0.43
1:D:346:ILE:HG23	1:D:369:THR:HG22	2.01	0.43
1:D:346:ILE:HA	1:D:371:ARG:HG2	2.01	0.43
1:A:551:TYR:HD2	1:A:552:PHE:N	2.16	0.42
1:B:538:VAL:HG23	1:B:557:LEU:HD11	2.01	0.42
1:A:473:ILE:HA	1:A:473:ILE:HD13	1.88	0.42
1:A:70:LEU:HA	1:A:73:SER:HB2	2.01	0.42
1:B:343:ASP:OD2	1:B:345:VAL:HB	2.19	0.42
1:D:566:LEU:HG	1:D:566:LEU:O	2.19	0.42
1:B:443:LEU:HD22	1:B:452:TYR:HB3	2.01	0.42
1:D:200:ASN:N	1:D:200:ASN:ND2	2.64	0.42
1:D:388:GLY:O	1:D:391:GLN:HB2	2.18	0.42
1:D:375:LYS:NZ	1:D:405:ASN:HB3	2.33	0.42
1:B:340:SER:HB2	1:B:424:LYS:HD3	2.01	0.42
1:C:209:TYR:O	1:C:210:LEU:C	2.56	0.42
1:D:461:ASN:O	1:D:504:VAL:CG2	2.67	0.42
1:C:290:ALA:HB2	1:C:365:TRP:CZ2	2.54	0.42
1:C:286:ASN:O	1:C:300:CYS:HA	2.18	0.42
1:B:558:PRO:HG2	1:B:559:ILE:H	1.84	0.42
1:B:559:ILE:H	1:B:559:ILE:CD1	2.32	0.42
1:D:61:HIS:HE1	1:D:63:VAL:CG2	2.32	0.42
1:B:395:GLU:O	1:B:396:ASN:HB2	2.19	0.42
1:B:418:SER:O	1:B:419:LEU:CB	2.67	0.42
1:A:440:GLY:O	1:A:457:PRO:HD2	2.19	0.42
1:A:427:ILE:HG12	1:A:428:ALA:N	2.35	0.42
1:A:539:VAL:HA	1:A:553:TYR:O	2.18	0.42
1:B:470:LEU:HD11	1:B:476:PHE:CE1	2.55	0.42
1:B:400:ALA:CB	1:B:401:PRO:CD	2.95	0.42
1:D:543:TYR:C	1:D:545:PRO:HD3	2.40	0.42
1:B:265:LEU:HD11	1:D:209:TYR:HE2	1.83	0.42
1:D:437:HIS:HB3	1:D:459:MET:CG	2.39	0.42
1:B:233:LEU:HD23	1:B:253:ARG:HA	2.01	0.42
1:A:406:ARG:O	1:A:408:PRO:HD3	2.20	0.42
1:D:301:HIS:CE1	1:D:306:ILE:HG13	2.54	0.42
1:D:252:TYR:CE1	1:D:279:PRO:HB3	2.54	0.42
1:C:99:TYR:O	1:C:100:LEU:C	2.58	0.42
1:C:337:VAL:CG1	1:C:338:PRO:HD2	2.49	0.42
1:D:320:GLN:HB2	1:D:336:TRP:CZ3	2.53	0.42
1:C:229:GLY:HA2	1:C:256:GLU:O	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:464:LEU:HD22	1:C:498:THR:O	2.19	0.42
1:D:564:ILE:C	1:D:564:ILE:HD12	2.40	0.42
1:B:59:SER:O	1:B:61:HIS:N	2.53	0.42
1:C:537:ALA:CB	1:C:556:ARG:HA	2.50	0.42
1:D:385:ALA:O	1:D:390:ILE:HG12	2.20	0.42
1:D:111:THR:OG1	1:D:112:LYS:N	2.53	0.42
1:D:326:VAL:HG13	1:D:327:TRP:H	1.84	0.42
1:B:371:ARG:HH11	1:B:429:SER:HB3	1.84	0.42
1:B:464:LEU:CG	1:B:465:GLY:N	2.79	0.42
1:A:475:ARG:O	1:A:476:PHE:C	2.58	0.42
1:A:400:ALA:HB3	1:A:401:PRO:CD	2.50	0.42
1:B:487:ILE:HG22	1:B:490:ALA:HB3	2.01	0.42
1:C:453:TRP:CB	1:C:516:ILE:HD12	2.50	0.42
1:D:49:HIS:O	1:D:50:GLU:HG3	2.19	0.42
1:D:262:ASN:HB2	1:D:573:TRP:HZ2	1.84	0.42
1:A:552:PHE:HE1	1:A:121:THR:OG1	2.00	0.42
1:C:473:ILE:HG22	1:C:474:PRO:CD	2.49	0.42
1:B:229:GLY:HA3	1:B:291:LEU:HD21	2.02	0.42
1:C:61:HIS:CE1	1:C:63:VAL:CG2	3.03	0.42
1:D:559:ILE:CG1	1:D:560:LYS:H	2.33	0.42
1:D:307:THR:HA	1:D:348:ARG:CG	2.50	0.42
1:A:265:LEU:HD22	1:C:214:TYR:CZ	2.55	0.42
1:A:356:GLY:HA3	1:A:364:LYS:O	2.19	0.42
1:D:340:SER:HB3	1:D:426:LYS:HA	2.01	0.42
1:D:37:GLN:NE2	1:D:43:VAL:CA	2.70	0.42
1:A:38:GLN:CG	1:D:422:GLU:HB3	2.49	0.42
1:C:293:GLU:OE2	1:C:358:ILE:HG22	2.19	0.42
1:B:548:SER:O	1:B:550:SER:N	2.53	0.42
1:D:586:ALA:HB2	1:D:593:HIS:CE1	2.55	0.42
1:A:124:LYS:HB2	1:A:127:SER:HB2	2.02	0.42
1:D:445:LYS:HA	1:D:452:TYR:CD2	2.55	0.42
1:B:470:LEU:HD13	1:B:478:VAL:CG2	2.50	0.41
1:D:516:ILE:HD13	1:D:524:TYR:CB	2.50	0.41
1:D:384:GLN:NE2	1:D:489:GLU:HB2	2.35	0.41
1:D:81:LEU:CD1	1:D:89:PRO:HG2	2.50	0.41
1:D:233:LEU:HD13	1:D:251:MET:CE	2.50	0.41
1:A:81:LEU:C	1:A:81:LEU:HD23	2.39	0.41
1:A:538:VAL:HB	1:A:555:PHE:HB3	2.02	0.41
1:C:97:ARG:HB3	1:C:106:ALA:HB3	2.02	0.41
1:A:365:TRP:O	1:A:412:VAL:HA	2.19	0.41
1:D:222:MET:HE2	1:D:291:LEU:N	2.35	0.41
1:A:222:MET:CE	1:A:291:LEU:HB2	2.50	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:379:GLU:HA	1:B:407:ILE:HD11	2.01	0.41
1:C:205:LEU:N	1:C:272:MET:HE2	2.35	0.41
1:C:205:LEU:O	1:C:208:LEU:HB3	2.20	0.41
1:A:205:LEU:HG	1:A:209:TYR:CE1	2.54	0.41
1:C:95:ARG:HG2	1:C:95:ARG:NH1	2.35	0.41
1:A:533:ARG:NH1	1:A:554:PRO:CB	2.82	0.41
1:B:62:ILE:CD1	1:B:62:ILE:N	2.82	0.41
1:C:293:GLU:OE1	1:C:360:ASP:N	2.48	0.41
1:A:47:LEU:HD13	1:A:47:LEU:N	2.34	0.41
1:A:383:GLN:HA	1:A:386:CYS:HB2	2.02	0.41
1:B:524:TYR:CD2	1:B:524:TYR:N	2.88	0.41
1:C:536:HIS:CD2	1:C:560:LYS:HG2	2.56	0.41
1:A:327:TRP:CZ3	1:C:328:LYS:HD3	2.56	0.41
1:A:318:SER:HB3	1:A:337:VAL:C	2.40	0.41
1:A:379:GLU:HA	1:A:379:GLU:OE1	2.20	0.41
1:B:36:VAL:C	1:B:37:GLN:HG2	2.40	0.41
1:D:357:VAL:HG22	1:D:358:ILE:N	2.35	0.41
1:B:546:SER:OG	1:B:547:ARG:N	2.53	0.41
1:A:325:GLY:C	1:A:327:TRP:N	2.73	0.41
1:D:298:ALA:HB3	1:D:322:VAL:HB	2.01	0.41
1:D:125:ASN:OD1	1:D:126:ILE:N	2.46	0.41
1:B:548:SER:C	1:B:550:SER:N	2.73	0.41
1:C:124:LYS:O	1:C:125:ASN:C	2.59	0.41
1:B:262:ASN:C	1:B:264:GLY:H	2.24	0.41
1:C:233:LEU:HD21	1:C:253:ARG:CZ	2.50	0.41
1:D:248:GLN:HG2	1:D:249:LEU:N	2.36	0.41
1:B:139:GLU:O	1:B:140:GLN:CB	2.63	0.41
1:C:389:LYS:HE3	1:C:500:LEU:N	2.30	0.41
1:B:348:ARG:HD3	1:B:350:TYR:CZ	2.56	0.41
1:C:30:MET:O	1:C:32:CYS:N	2.53	0.41
1:A:198:PHE:CD2	1:A:198:PHE:N	2.89	0.41
1:A:418:SER:O	1:A:419:LEU:HB2	2.21	0.41
1:D:542:VAL:HB	1:D:551:TYR:CE1	2.56	0.41
1:C:406:ARG:HG3	1:C:406:ARG:NH1	2.35	0.41
1:A:455:THR:HG21	1:A:516:ILE:HD11	2.03	0.41
1:B:466:VAL:CG1	1:B:468:ASN:HD21	2.34	0.41
1:A:255:PHE:HB2	1:A:276:LEU:HB3	2.01	0.41
1:A:229:GLY:N	1:A:291:LEU:HD11	2.35	0.41
1:C:261:ARG:NH1	1:C:271:HIS:ND1	2.68	0.41
1:B:208:LEU:O	1:B:209:TYR:C	2.56	0.41
1:D:559:ILE:HG12	1:D:560:LYS:O	2.21	0.41
1:D:386:CYS:HA	1:D:390:ILE:HG13	2.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:348:ARG:HH11	1:D:348:ARG:HG2	1.86	0.41
1:C:575:GLN:HB2	1:C:575:GLN:HE21	1.70	0.41
1:B:486:PRO:HA	1:B:495:HIS:ND1	2.36	0.41
1:D:99:TYR:HB2	1:D:104:SER:OG	2.21	0.41
1:D:542:VAL:HG21	1:D:551:TYR:OH	2.21	0.41
1:C:88:PRO:HA	1:C:89:PRO:HD2	1.81	0.41
1:D:520:GLN:CG	1:D:521:ASP:N	2.83	0.41
1:A:378:MET:HB3	1:A:407:ILE:CD1	2.51	0.41
1:A:569:GLU:O	1:A:579:CYS:HA	2.20	0.41
1:A:569:GLU:CG	1:A:580:ARG:HG2	2.50	0.41
1:A:224:SER:C	1:A:226:GLY:H	2.24	0.41
1:A:308:ILE:HA	1:A:309:PRO:HD3	1.94	0.41
1:B:352:SER:H	1:B:354:HIS:CD2	2.38	0.41
1:B:36:VAL:O	1:B:37:GLN:CG	2.69	0.41
1:B:209:TYR:O	1:B:210:LEU:C	2.59	0.41
1:C:48:THR:OG1	1:C:49:HIS:N	2.54	0.41
1:B:392:ALA:HA	1:B:395:GLU:OE1	2.21	0.41
1:B:203:LEU:HB2	1:B:271:HIS:HA	2.03	0.41
1:C:61:HIS:HE1	1:C:63:VAL:CG2	2.34	0.41
1:B:500:LEU:HD22	1:B:502:ALA:HB3	2.02	0.41
1:B:545:PRO:O	1:B:546:SER:C	2.59	0.41
1:A:103:LEU:HD13	1:A:120:MET:SD	2.61	0.41
1:C:260:ILE:HG12	1:C:270:PHE:CE1	2.56	0.41
1:C:572:THR:HA	1:C:577:LEU:HA	2.03	0.41
1:D:30:MET:HG3	1:D:30:MET:O	2.21	0.41
1:C:37:GLN:CG	1:C:43:VAL:HG12	2.47	0.41
1:C:407:ILE:N	1:C:407:ILE:HD12	2.35	0.41
1:C:308:ILE:CD1	1:C:349:LEU:HD12	2.47	0.41
1:D:530:ASP:OD1	1:D:532:SER:HB3	2.21	0.41
1:D:347:ASP:CG	1:D:406:ARG:HH22	2.24	0.41
1:B:129:GLN:HG2	1:B:131:PHE:CE1	2.55	0.41
1:D:37:GLN:OE1	1:D:43:VAL:HG23	2.21	0.40
1:B:562:VAL:HG23	1:B:586:ALA:O	2.21	0.40
1:A:72:ASN:O	1:A:74:VAL:N	2.55	0.40
1:B:570:CYS:HA	1:B:578:TRP:O	2.21	0.40
1:A:580:ARG:HA	1:A:598:GLY:O	2.21	0.40
1:B:337:VAL:O	1:B:337:VAL:HG23	2.19	0.40
1:D:231:THR:OG1	1:D:253:ARG:NH1	2.54	0.40
1:B:540:TYR:CE1	1:B:568:VAL:HG21	2.54	0.40
1:D:574:ASP:C	1:D:576:LYS:H	2.25	0.40
1:C:516:ILE:O	1:C:516:ILE:HG22	2.20	0.40
1:A:387:LYS:HE2	1:A:387:LYS:HA	2.03	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:197:GLN:NE2	1:A:266:GLY:O	2.51	0.40
1:B:65:THR:OG1	1:B:119:PHE:HB2	2.21	0.40
1:B:93:LYS:HB2	1:B:96:TYR:H	1.86	0.40
1:C:473:ILE:N	1:C:474:PRO:CD	2.84	0.40
1:B:392:ALA:HA	1:B:395:GLU:HG2	2.03	0.40
1:A:107:ILE:HD11	1:A:118:TYR:CE2	2.57	0.40
1:C:91:TYR:HB3	1:C:93:LYS:CB	2.51	0.40
1:D:472:TRP:C	1:D:474:PRO:HD2	2.42	0.40
1:D:474:PRO:O	1:D:475:ARG:HB3	2.21	0.40
1:B:395:GLU:O	1:B:395:GLU:HG3	2.21	0.40
1:C:488:LYS:O	1:C:489:GLU:HG2	2.22	0.40
1:A:310:TYR:N	1:A:310:TYR:CD2	2.89	0.40
1:D:562:VAL:HA	1:D:563:PRO:HD2	1.92	0.40
1:B:579:CYS:O	1:B:599:MET:HA	2.20	0.40
1:C:306:ILE:N	1:C:306:ILE:HD12	2.37	0.40
1:D:345:VAL:O	1:D:345:VAL:HG22	2.21	0.40
1:C:508:VAL:O	1:C:508:VAL:HG13	2.20	0.40
1:D:230:GLY:HA2	1:D:289:VAL:HG11	2.02	0.40
1:B:358:ILE:HA	1:B:362:GLN:O	2.21	0.40
1:C:236:LYS:O	1:C:249:LEU:HB3	2.21	0.40
1:B:236:LYS:O	1:B:249:LEU:O	2.39	0.40
1:B:308:ILE:N	1:B:308:ILE:CD1	2.85	0.40
1:C:65:THR:CG2	1:C:75:GLU:HB3	2.48	0.40
1:C:535:GLU:OE2	1:C:556:ARG:HD3	2.22	0.40
1:B:294:LEU:HD12	1:B:326:VAL:HG11	2.03	0.40
1:C:493:ASP:HB2	1:C:495:HIS:NE2	2.36	0.40
1:D:262:ASN:HB2	1:D:573:TRP:CZ2	2.57	0.40
1:C:416:ASP:OD1	1:C:416:ASP:C	2.60	0.40
1:C:412:VAL:CG2	1:C:476:PHE:HE1	2.34	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	509/559 (91%)	416 (82%)	62 (12%)	31 (6%)	2	19
1	B	520/559 (93%)	412 (79%)	86 (16%)	22 (4%)	4	31
1	C	504/559 (90%)	407 (81%)	67 (13%)	30 (6%)	2	20
1	D	492/559 (88%)	389 (79%)	70 (14%)	33 (7%)	2	16
All	All	2025/2236 (91%)	1624 (80%)	285 (14%)	116 (6%)	3	22

All (116) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	311	GLN
1	A	389	LYS
1	A	439	SER
1	A	490	ALA
1	A	494	CYS
1	A	502	ALA
1	A	548	SER
1	A	39	LEU
1	A	60	ILE
1	A	72	ASN
1	A	73	SER
1	A	85	GLU
1	A	93	LYS
1	A	94	ASP
1	B	476	PHE
1	B	512	SER
1	B	60	ILE
1	B	73	SER
1	B	74	VAL
1	B	93	LYS
1	C	236	LYS
1	C	237	PRO
1	C	449	ASN
1	C	549	PHE
1	C	31	ASN
1	C	39	LEU
1	C	93	LYS
1	D	309	PRO
1	D	347	ASP
1	D	376	LEU
1	D	460	LYS
1	D	497	PRO
1	D	547	ARG

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Mol	Chain	Res	Type
1	D	38	GLN
1	D	86	ALA
1	D	94	ASP
1	A	438	GLY
1	A	475	ARG
1	A	574	ASP
1	A	590	SER
1	A	592	GLY
1	A	52	ILE
1	A	79	VAL
1	B	239	LEU
1	B	397	PRO
1	B	474	PRO
1	B	490	ALA
1	B	52	ILE
1	B	94	ASP
1	C	274	ASN
1	C	315	LYS
1	C	347	ASP
1	C	422	GLU
1	C	475	ARG
1	C	548	SER
1	C	50	GLU
1	D	374	ASP
1	D	437	HIS
1	D	465	GLY
1	D	475	ARG
1	D	522	LEU
1	D	546	SER
1	D	548	SER
1	D	575	GLN
1	D	39	LEU
1	D	47	LEU
1	D	59	SER
1	D	109	GLU
1	A	189	SER
1	A	451	VAL
1	A	53	ASN
1	A	133	LEU
1	B	222	MET
1	B	250	SER
1	B	489	GLU

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Mol	Chain	Res	Type
1	C	393	LEU
1	C	40	GLY
1	C	101	GLU
1	D	390	ILE
1	D	92	LEU
1	A	390	ILE
1	B	238	ASN
1	B	481	TYR
1	C	460	LYS
1	C	125	ASN
1	C	133	LEU
1	D	224	SER
1	D	502	ALA
1	D	46	PRO
1	A	352	SER
1	A	75	GLU
1	A	84	SER
1	B	400	ALA
1	B	549	PHE
1	C	400	ALA
1	C	74	VAL
1	D	212	ARG
1	D	381	CYS
1	D	422	GLU
1	D	441	MET
1	D	68	LYS
1	A	473	ILE
1	B	390	ILE
1	C	462	LEU
1	C	46	PRO
1	C	83	PRO
1	C	94	ASP
1	D	492	GLY
1	C	316	GLY
1	C	500	LEU
1	D	43	VAL
1	B	401	PRO
1	C	35	ILE
1	A	492	GLY
1	C	60	ILE
1	B	226	GLY

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	457/489 (94%)	403 (88%)	54 (12%)	8 32
1	B	468/489 (96%)	433 (92%)	35 (8%)	19 61
1	C	457/489 (94%)	400 (88%)	57 (12%)	7 29
1	D	449/489 (92%)	419 (93%)	30 (7%)	23 66
All	All	1831/1956 (94%)	1655 (90%)	176 (10%)	12 45

All (176) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	188	CYS
1	A	193	THR
1	A	195	ARG
1	A	215	ASN
1	A	221	THR
1	A	224	SER
1	A	261	ARG
1	A	273	THR
1	A	275	TYR
1	A	293	GLU
1	A	296	LEU
1	A	311	GLN
1	A	331	THR
1	A	333	MET
1	A	341	THR
1	A	360	ASP
1	A	378	MET
1	A	379	GLU
1	A	381	CYS
1	A	384	GLN
1	A	387	LYS
1	A	395	GLU
1	A	398	GLU
1	A	413	LEU
1	A	449	ASN
1	A	461	ASN

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Mol	Chain	Res	Type
1	A	471	GLU
1	A	472	TRP
1	A	479	SER
1	A	482	ARG
1	A	484	THR
1	A	488	LYS
1	A	489	GLU
1	A	494	CYS
1	A	514	LEU
1	A	518	PRO
1	A	520	GLN
1	A	521	ASP
1	A	549	PHE
1	A	552	PHE
1	A	559	ILE
1	A	580	ARG
1	A	38	GLN
1	A	45	LEU
1	A	47	LEU
1	A	48	THR
1	A	56	MET
1	A	70	LEU
1	A	80	SER
1	A	93	LYS
1	A	95	ARG
1	A	100	LEU
1	A	103	LEU
1	A	133	LEU
1	B	193	THR
1	B	217	SER
1	B	235	GLU
1	B	246	LEU
1	B	249	LEU
1	B	275	TYR
1	B	304	ASP
1	B	305	SER
1	B	310	TYR
1	B	342	ASP
1	B	387	LYS
1	B	419	LEU
1	B	449	ASN
1	B	459	MET

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Mol	Chain	Res	Type
1	B	461	ASN
1	B	464	LEU
1	B	472	TRP
1	B	479	SER
1	B	484	THR
1	B	500	LEU
1	B	510	LEU
1	B	526	LEU
1	B	559	ILE
1	B	577	LEU
1	B	605	SER
1	B	34	LYS
1	B	38	GLN
1	B	45	LEU
1	B	48	THR
1	B	52	ILE
1	B	80	SER
1	B	92	LEU
1	B	93	LYS
1	B	101	GLU
1	B	133	LEU
1	C	192	THR
1	C	200	ASN
1	C	206	LEU
1	C	207	ASP
1	C	221	THR
1	C	223	THR
1	C	227	MET
1	C	231	THR
1	C	234	VAL
1	C	248	GLN
1	C	249	LEU
1	C	282	ASN
1	C	286	ASN
1	C	319	PHE
1	C	320	GLN
1	C	349	LEU
1	C	351	LEU
1	C	355	ARG
1	C	365	TRP
1	C	391	GLN
1	C	405	ASN

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Mol	Chain	Res	Type
1	C	414	SER
1	C	415	VAL
1	C	422	GLU
1	C	436	THR
1	C	437	HIS
1	C	449	ASN
1	C	455	THR
1	C	459	MET
1	C	461	ASN
1	C	464	LEU
1	C	472	TRP
1	C	479	SER
1	C	510	LEU
1	C	514	LEU
1	C	528	THR
1	C	533	ARG
1	C	547	ARG
1	C	555	PHE
1	C	568	VAL
1	C	572	THR
1	C	589	GLU
1	C	607	THR
1	C	34	LYS
1	C	37	GLN
1	C	50	GLU
1	C	58	LYS
1	C	65	THR
1	C	66	MET
1	C	70	LEU
1	C	72	ASN
1	C	85	GLU
1	C	93	LYS
1	C	95	ARG
1	C	102	HIS
1	C	132	CYS
1	C	136	LYS
1	D	193	THR
1	D	200	ASN
1	D	206	LEU
1	D	223	THR
1	D	232	TYR
1	D	315	LYS

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Mol	Chain	Res	Type
1	D	331	THR
1	D	360	ASP
1	D	365	TRP
1	D	377	ARG
1	D	416	ASP
1	D	437	HIS
1	D	455	THR
1	D	461	ASN
1	D	464	LEU
1	D	515	VAL
1	D	520	GLN
1	D	528	THR
1	D	549	PHE
1	D	555	PHE
1	D	572	THR
1	D	577	LEU
1	D	42	ASP
1	D	46	PRO
1	D	65	THR
1	D	72	ASN
1	D	85	GLU
1	D	93	LYS
1	D	95	ARG
1	D	112	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	274	ASN
1	A	278	GLN
1	A	320	GLN
1	A	448	HIS
1	A	449	ASN
1	A	461	ASN
1	A	468	ASN
1	A	567	GLN
1	A	581	HIS
1	A	37	GLN
1	A	57	ASN
1	A	76	ASN
1	B	278	GLN
1	B	320	GLN

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Mol	Chain	Res	Type
1	B	334	GLN
1	B	383	GLN
1	B	461	ASN
1	B	468	ASN
1	B	567	GLN
1	B	575	GLN
1	B	37	GLN
1	B	61	HIS
1	B	72	ASN
1	B	125	ASN
1	B	140	GLN
1	C	286	ASN
1	C	334	GLN
1	C	383	GLN
1	C	384	GLN
1	C	461	ASN
1	C	468	ASN
1	C	523	GLN
1	C	567	GLN
1	C	575	GLN
1	C	593	HIS
1	C	37	GLN
1	C	61	HIS
1	D	197	GLN
1	D	200	ASN
1	D	248	GLN
1	D	286	ASN
1	D	320	GLN
1	D	383	GLN
1	D	405	ASN
1	D	461	ASN
1	D	468	ASN
1	D	520	GLN
1	D	523	GLN
1	D	575	GLN
1	D	593	HIS
1	D	37	GLN
1	D	49	HIS
1	D	61	HIS
1	D	72	ASN
1	D	76	ASN
1	D	102	HIS

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Mol	Chain	Res	Type
1	D	129	GLN
1	D	134	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

6 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	901	1	12,14,15	0.85	1 (8%)	15,19,21	1.29	3 (20%)
2	NAG	B	801	1	12,14,15	0.59	0	15,19,21	1.07	2 (13%)
2	NAG	B	901	1	12,14,15	0.55	0	15,19,21	0.79	1 (6%)
2	NAG	C	801	1	12,14,15	0.66	0	15,19,21	0.60	0
2	NAG	C	901	1	12,14,15	0.61	0	15,19,21	0.94	1 (6%)
2	NAG	D	901	1	12,14,15	0.76	0	15,19,21	0.81	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	NAG	A	901	1	-	0/6/23/26	0/1/1/1
2	NAG	B	801	1	-	1/6/23/26	0/1/1/1
2	NAG	B	901	1	-	0/6/23/26	0/1/1/1
2	NAG	C	801	1	-	0/6/23/26	0/1/1/1
2	NAG	C	901	1	-	0/6/23/26	0/1/1/1
2	NAG	D	901	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	NAG	C4-C5	2.07	1.57	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	NAG	C3-C4-C5	3.01	115.58	110.20
2	C	901	NAG	C3-C2-N2	-2.41	108.09	111.76
2	A	901	NAG	O5-C5-C4	2.41	113.72	110.65
2	A	901	NAG	C2-N2-C7	-2.20	119.39	123.09
2	B	801	NAG	C3-C2-N2	-2.10	108.56	111.76
2	B	901	NAG	C2-N2-C7	-2.07	119.62	123.09
2	B	801	NAG	C3-C4-C5	-2.01	106.61	110.20

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	NAG	O7-C7-N2-C2

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	515/559 (92%)	-0.26	1 (0%) 93 64	33, 57, 97, 115	0
1	B	526/559 (94%)	-0.18	2 (0%) 90 49	38, 66, 109, 122	0
1	C	514/559 (91%)	-0.20	1 (0%) 93 64	39, 66, 101, 118	0
1	D	504/559 (90%)	-0.15	0 100 100	49, 75, 114, 130	0
All	All	2059/2236 (92%)	-0.20	4 (0%) 93 64	33, 67, 108, 130	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	589	GLU	2.8
1	B	314	GLY	2.4
1	A	310	TYR	2.3
1	C	314	GLY	2.1

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

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

### 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	D	901	14/15	0.43	13.97	95,98,103,105	0
2	NAG	C	801	14/15	0.48	7.38	90,94,98,98	0
2	NAG	B	801	14/15	0.43	5.55	89,91,93,93	0
2	NAG	C	901	14/15	0.33	4.76	94,97,99,99	0
2	NAG	B	901	14/15	0.27	0.94	100,102,104,104	0
2	NAG	A	901	14/15	0.27	0.72	88,90,91,91	0

## 6.5 Other polymers

There are no such residues in this entry.