



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 11:26 AM GMT

PDB ID : 3KM9
Title : Structure of complement C5 in complex with the C-terminal beta-grasp domain of SSL7
Authors : Laursen, N.S.; Gordon, N.; Hermans, S.; Lorenz, N.; Jackson, N.; Wines, B.; Spillner, E.; Christensen, J.B.; Jensen, M.; Fredslund, F.; Bjerre, M.; Sottrup-Jensen, L.; Fraser, J.D.; Andersen, G.R.
Deposited on : 2009-11-10
Resolution : 4.20 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

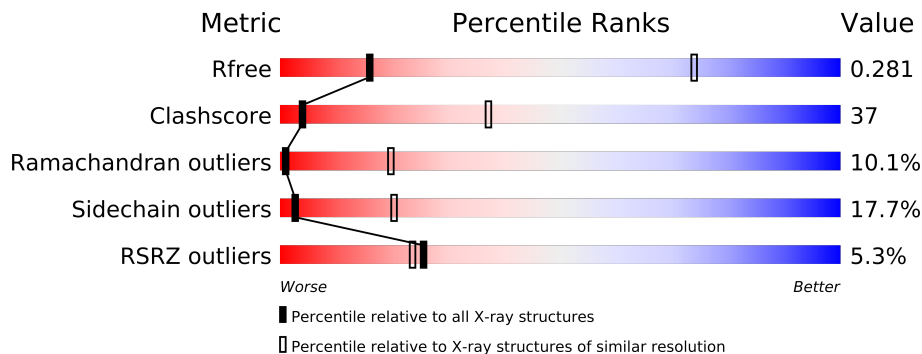
The following versions of software and data (see [references](#)) were used in the production of this report:

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 4.20 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	1001 (4.84-3.50)
Clashscore	79885	1259 (4.84-3.50)
Ramachandran outliers	78287	1192 (4.84-3.50)
Sidechain outliers	78261	1175 (4.84-3.50)
RSRZ outliers	66119	1001 (4.84-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	1676	
1	B	1676	
2	X	103	
2	Y	103	

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

Mol	Type	Chain	Res	Geometry	Electron density
5	NAG	A	1680	-	X
5	NAG	B	1679	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24809 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 Complement C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1459	Total	C	N	O	S	0	0	0
			11541	7396	1903	2200	42			
1	B	1459	Total	C	N	O	S	0	0	0
			11541	7396	1903	2200	42			

- Molecule 2 is a protein called Staphylococcal enterotoxin-like toxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	102	Total	C	N	O	S	0	0	0
			819	517	138	163	1			
2	Y	102	Total	C	N	O	S	0	0	0
			819	517	138	163	1			

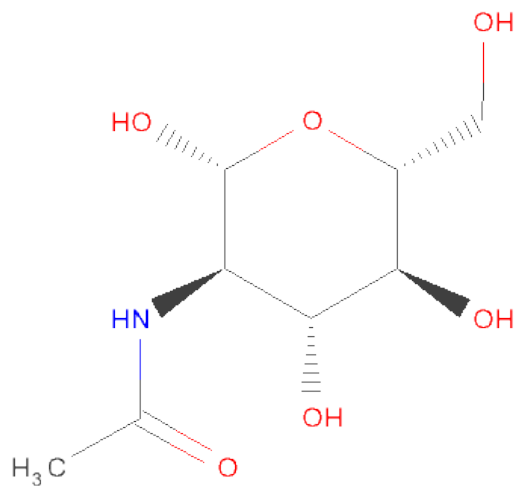
- Molecule 3 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Cd	0	0
			2	2		
3	A	3	Total	Cd	0	0
			3	3		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



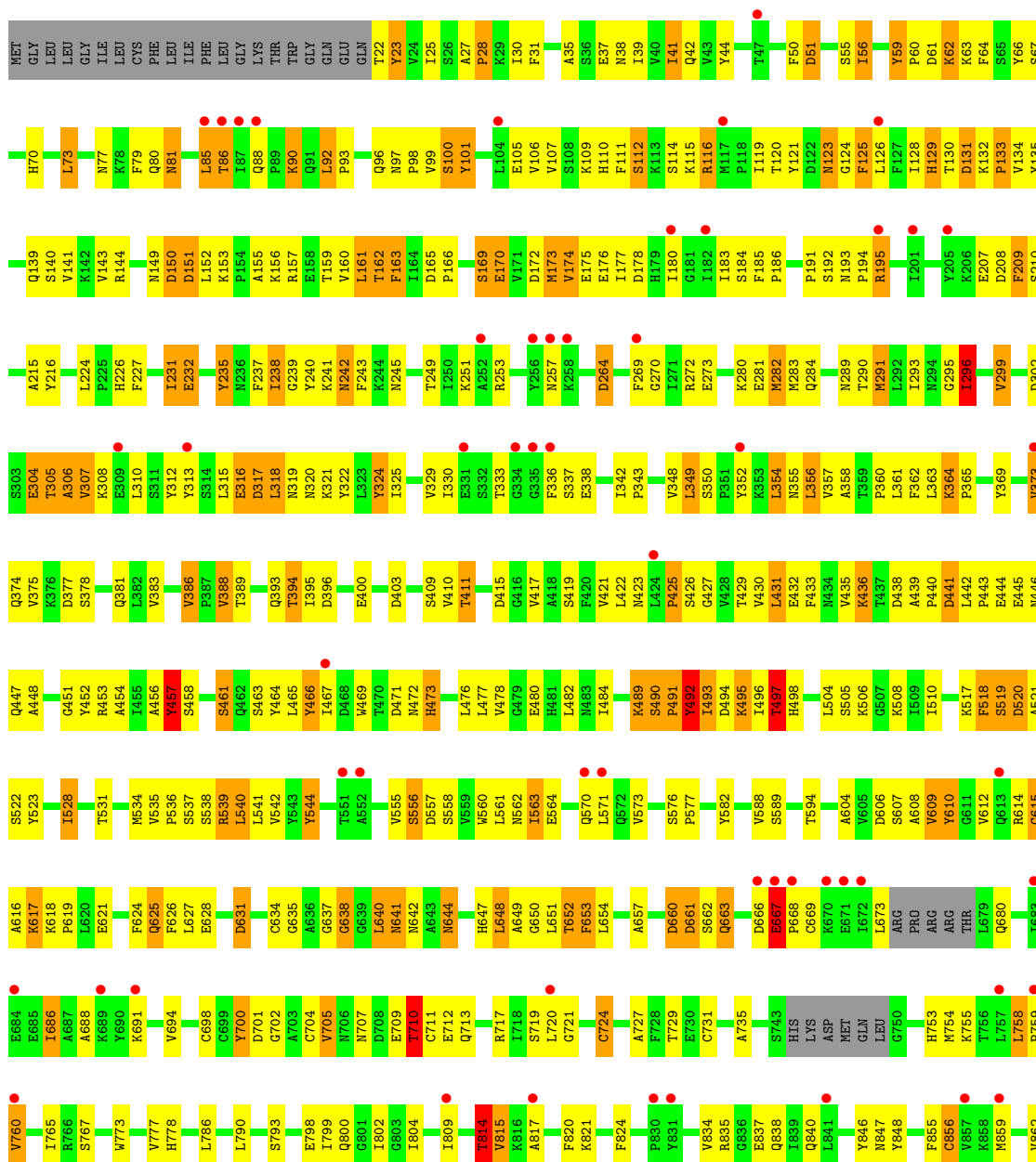
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

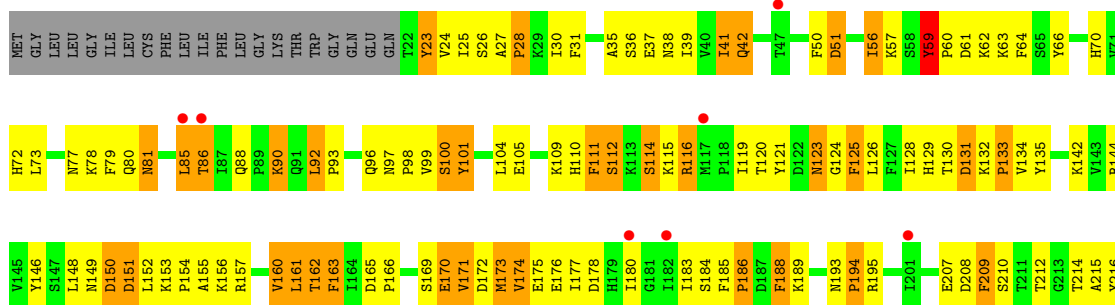
3 Residue-property plots

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

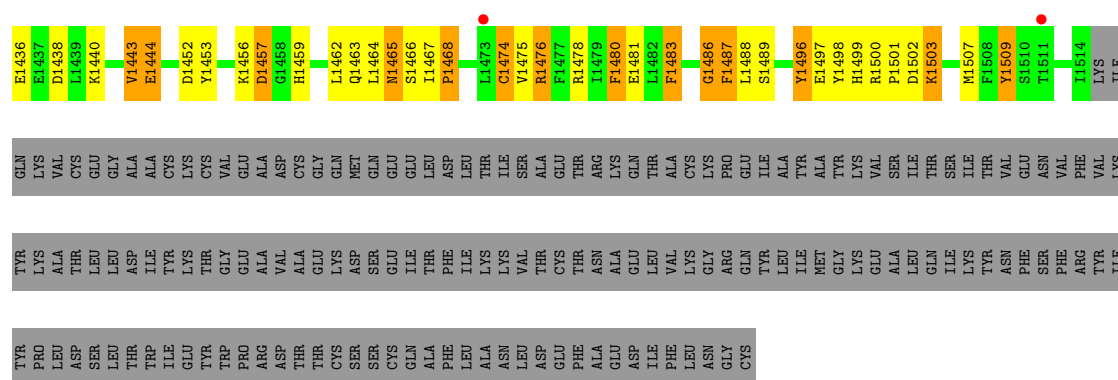
• Molecule 1: Complement C5

Chain A:



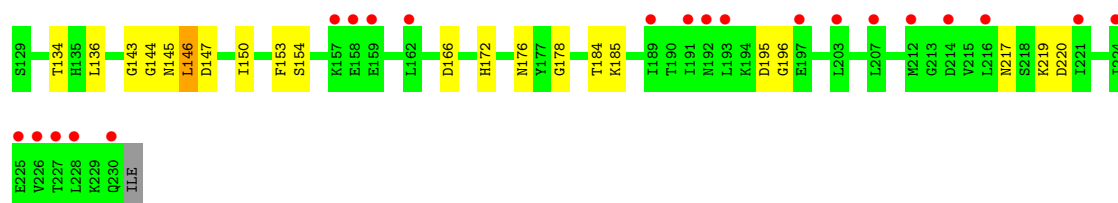






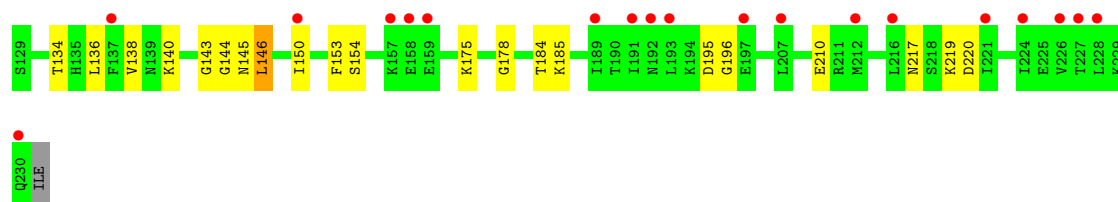
- Molecule 2: Staphylococcal enterotoxin-like toxin

Chain X:



- Molecule 2: Staphylococcal enterotoxin-like toxin

Chain Y: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	144.79Å 144.79Å 245.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.75 – 4.20 49.75 – 4.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.75-4.20) 99.8 (49.75-4.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 4.14Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.233 , 0.297 0.215 , 0.281	Depositor DCC
R_{free} test set	2030 reflections (4.86%)	DCC
Wilson B-factor (Å ²)	115.5	Xtriage
Anisotropy	0.855	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 127.8	EDS
Estimated twinning fraction	0.044 for -h,-k,l 0.397 for h,-h-k,-l 0.045 for -k,-h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 41960 reflections	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	24809	wwPDB-VP
Average B, all atoms (Å ²)	205.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CD

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	0.53	0/11793	0.77	6/16003 (0.0%)
1	B	0.53	0/11793	0.77	5/16003 (0.0%)
2	X	0.34	0/828	0.54	0/1107
2	Y	0.34	0/828	0.56	1/1107 (0.1%)
All	All	0.52	0/25242	0.75	12/34220 (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	A	0	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	264	ASP	CB-CG-OD1	-8.57	110.58	118.30
1	B	640	LEU	CA-CB-CG	7.23	131.94	115.30
1	B	1374	VAL	CB-CA-C	-6.61	98.85	111.40
1	A	640	LEU	CA-CB-CG	6.51	130.28	115.30
1	A	1195	LEU	CA-CB-CG	-5.71	102.17	115.30
1	A	1374	VAL	CB-CA-C	-5.46	101.02	111.40
1	A	1482	LEU	CA-CB-CG	5.38	127.67	115.30
2	Y	175	LYS	CD-CE-NZ	5.25	123.78	111.70
1	B	323	LEU	CA-CB-CG	5.23	127.34	115.30
1	B	1033	ILE	CB-CA-C	-5.14	101.31	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1297	LEU	CA-CB-CG	-5.03	103.74	115.30
1	A	471	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	651	LEU	Peptide
1	B	1179	THR	Peptide
1	B	651	LEU	Peptide

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	11541	0	0	447	0
1	B	11541	0	0	462	0
2	X	819	0	0	9	0
2	Y	819	0	0	7	0
3	A	3	0	0	0	0
3	B	2	0	0	0	0
4	A	28	0	25	1	0
4	B	28	0	25	2	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
All	All	24809	0	76	926	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 37.

All (926) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:698:CYS:SG	1:A:724:CYS:CB	2.33	1.16
1:A:698:CYS:CB	1:A:724:CYS:SG	2.52	0.97
1:B:319:ASN:ND2	1:B:347:TYR:CD1	2.36	0.92

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:319:ASN:O	1:B:320:ASN:ND2	2.06	0.89
1:A:653:PHE:N	1:A:653:PHE:CD2	2.48	0.81
1:B:242:ASN:CB	1:B:245:ASN:O	2.29	0.80
1:B:653:PHE:N	1:B:653:PHE:CD2	2.50	0.79
1:A:386:VAL:N	1:A:411:THR:CG2	2.46	0.79
1:B:938:SER:OG	1:B:1279:ARG:CZ	2.32	0.76
1:B:429:THR:OG1	1:B:430:VAL:N	2.14	0.76
1:A:1030:HIS:NE2	1:A:1306:GLN:NE2	2.34	0.76
1:A:317:ASP:O	1:A:319:ASN:N	2.18	0.76
1:A:429:THR:OG1	1:A:430:VAL:N	2.20	0.75
1:A:938:SER:OG	1:A:1279:ARG:CZ	2.35	0.75
1:A:293:ILE:N	1:A:296:ILE:O	2.22	0.73
1:A:609:VAL:CG2	1:A:610:TYR:N	2.51	0.73
1:A:492:TYR:CD2	1:A:493:ILE:N	2.57	0.73
1:B:386:VAL:N	1:B:411:THR:CG2	2.52	0.72
1:B:492:TYR:CD2	1:B:493:ILE:N	2.57	0.72
1:A:1024:TYR:CD2	1:A:1024:TYR:C	2.63	0.72
1:B:1421:HIS:CE1	1:B:1498:TYR:CD2	2.78	0.72
1:A:1030:HIS:CE1	1:A:1306:GLN:NE2	2.58	0.72
1:B:1024:TYR:CE2	1:B:1030:HIS:CD2	2.78	0.72
1:B:1024:TYR:CD2	1:B:1024:TYR:C	2.63	0.71
1:B:354:LEU:N	1:B:354:LEU:CD2	2.53	0.71
1:A:425:PRO:O	1:A:427:GLY:N	2.23	0.71
1:B:120:THR:CG2	1:B:121:TYR:N	2.54	0.71
1:B:1239:VAL:O	1:B:1241:ASN:N	2.24	0.71
1:A:855:PHE:CZ	1:A:886:GLN:CB	2.73	0.71
1:A:1080:ALA:O	1:A:1083:LEU:N	2.24	0.71
1:A:1296:GLY:O	1:A:1298:THR:N	2.24	0.71
1:A:1180:LEU:O	1:A:1182:ALA:N	2.24	0.70
1:A:1421:HIS:CE1	1:A:1498:TYR:CD2	2.79	0.70
1:A:194:PRO:O	1:A:1070:LYS:NZ	2.25	0.70
1:A:242:ASN:CB	1:A:245:ASN:O	2.39	0.70
1:B:131:ASP:OD1	1:B:132:LYS:N	2.25	0.69
1:A:719:SER:O	1:A:721:GLY:N	2.25	0.69
1:B:194:PRO:O	1:B:1070:LYS:NZ	2.25	0.69
1:B:242:ASN:ND2	1:B:242:ASN:N	2.41	0.69
1:A:1239:VAL:O	1:A:1241:ASN:N	2.26	0.69
1:A:156:LYS:O	1:A:157:ARG:CG	2.41	0.69
1:A:1487:PHE:N	1:A:1487:PHE:CD2	2.60	0.68
1:A:354:LEU:CD2	1:A:354:LEU:N	2.57	0.68
1:B:947:ARG:O	1:B:949:ILE:N	2.25	0.68
1:B:1487:PHE:N	1:B:1487:PHE:CD2	2.61	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:151:ASP:OD2	1:B:508:LYS:NZ	2.27	0.68
1:B:1019:PHE:CE2	1:B:1020:TYR:CE1	2.82	0.68
1:B:855:PHE:CZ	1:B:886:GLN:CB	2.77	0.68
1:A:1029:ASN:O	1:A:1029:ASN:ND2	2.27	0.68
1:B:425:PRO:O	1:B:427:GLY:N	2.27	0.68
1:A:131:ASP:CG	1:A:132:LYS:N	2.48	0.67
1:A:316:GLU:O	1:A:317:ASP:C	2.33	0.67
1:A:51:ASP:OD2	1:A:70:HIS:NE2	2.27	0.67
1:B:932:GLU:OE1	1:B:932:GLU:N	2.28	0.67
1:B:1296:GLY:O	1:B:1298:THR:N	2.27	0.67
1:B:350:SER:CB	1:B:446:ASN:O	2.43	0.67
1:A:1440:LYS:NZ	1:A:1453:TYR:OH	2.27	0.67
1:B:293:ILE:N	1:B:296:ILE:O	2.28	0.66
1:B:719:SER:O	1:B:721:GLY:N	2.28	0.66
1:A:1024:TYR:OH	1:A:1306:GLN:NE2	2.29	0.66
1:A:1054:LEU:O	1:A:1056:ILE:N	2.29	0.66
1:A:120:THR:CG2	1:A:121:TYR:N	2.59	0.66
1:A:77:ASN:ND2	1:A:81:ASN:ND2	2.43	0.66
1:A:1136:GLU:OE1	1:A:1415:SER:CB	2.43	0.66
1:A:710:THR:N	1:A:713:GLN:OE1	2.29	0.66
2:X:143:GLY:O	2:X:145:ASN:N	2.28	0.66
1:B:708:ASP:OD2	1:B:1401:ARG:NH2	2.29	0.66
1:B:1024:TYR:OH	1:B:1306:GLN:NE2	2.29	0.65
1:A:350:SER:CB	1:A:446:ASN:O	2.44	0.65
1:B:710:THR:N	1:B:713:GLN:OE1	2.29	0.65
1:B:1028:GLY:O	1:B:1029:ASN:C	2.33	0.65
1:B:653:PHE:CZ	1:B:660:ASP:CA	2.79	0.65
1:A:952:THR:OG1	1:A:953:ILE:N	2.29	0.65
1:B:1263:ASP:O	1:B:1265:ASN:N	2.30	0.65
1:B:163:PHE:CD1	1:B:163:PHE:N	2.65	0.65
1:B:133:PRO:O	1:B:134:VAL:CG2	2.43	0.65
1:A:325:ILE:O	1:A:342:ILE:N	2.30	0.65
1:B:364:LYS:CD	1:B:364:LYS:N	2.60	0.65
1:B:1047:LYS:O	1:B:1049:LEU:N	2.30	0.64
1:B:1029:ASN:O	1:B:1029:ASN:ND2	2.30	0.64
1:A:169:SER:O	1:A:170:GLU:O	2.15	0.64
1:B:838:GLN:O	1:B:1486:GLY:N	2.30	0.64
1:B:906:GLY:O	1:B:908:HIS:CE1	2.51	0.64
1:A:1279:ARG:CD	1:A:1284:PHE:CG	2.81	0.64
1:A:1435:ASN:O	1:A:1438:ASP:N	2.30	0.64
1:B:319:ASN:ND2	1:B:347:TYR:CG	2.65	0.64
1:B:494:ASP:O	1:B:496:ILE:N	2.31	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:906:GLY:O	1:A:908:HIS:CE1	2.50	0.64
1:A:1081:PHE:CE1	1:A:1288:GLN:NE2	2.66	0.64
1:B:440:PRO:CD	1:B:441:ASP:OD2	2.46	0.64
1:A:617:LYS:O	1:A:618:LYS:CG	2.46	0.64
1:B:641:ASN:O	1:B:644:ASN:N	2.31	0.64
1:B:490:SER:O	1:B:491:PRO:C	2.34	0.63
1:B:1226:ARG:N	1:B:1269:PRO:O	2.31	0.63
1:B:609:VAL:CG2	1:B:610:TYR:N	2.61	0.63
1:B:1206:ARG:CG	1:B:1206:ARG:NH1	2.61	0.63
1:B:441:ASP:OD2	1:B:441:ASP:N	2.30	0.63
1:B:922:ILE:CD1	4:B:2001:NAG:H82	2.28	0.63
1:A:491:PRO:O	1:A:493:ILE:N	2.32	0.63
1:A:59:TYR:CB	1:A:60:PRO:CD	2.76	0.63
1:A:1202:HIS:O	1:A:1203:PRO:C	2.37	0.63
1:B:491:PRO:O	1:B:493:ILE:N	2.32	0.63
1:A:1263:ASP:O	1:A:1265:ASN:N	2.31	0.63
1:A:451:GLY:C	1:A:452:TYR:CD2	2.73	0.63
1:B:59:TYR:CB	1:B:60:PRO:CD	2.77	0.62
1:A:92:LEU:N	1:A:93:PRO:CD	2.62	0.62
1:A:364:LYS:CD	1:A:364:LYS:N	2.61	0.62
1:A:315:LEU:O	1:A:316:GLU:O	2.17	0.62
1:A:1136:GLU:O	1:A:1140:ASN:N	2.32	0.62
1:B:156:LYS:O	1:B:157:ARG:CG	2.48	0.62
1:B:1202:HIS:O	1:B:1203:PRO:C	2.37	0.62
1:B:1097:GLN:O	1:B:1099:SER:N	2.33	0.62
1:A:490:SER:O	1:A:491:PRO:C	2.36	0.62
1:A:932:GLU:OE1	1:A:932:GLU:N	2.33	0.62
1:A:124:GLY:O	1:A:125:PHE:CD2	2.53	0.62
2:X:153:PHE:CD2	2:X:154:SER:N	2.68	0.62
1:B:131:ASP:CG	1:B:132:LYS:N	2.53	0.61
1:A:131:ASP:OD1	1:A:132:LYS:N	2.33	0.61
1:B:30:ILE:CG2	1:B:31:PHE:N	2.64	0.61
1:B:1080:ALA:O	1:B:1083:LEU:N	2.33	0.61
1:B:617:LYS:O	1:B:618:LYS:CG	2.49	0.61
1:A:1226:ARG:CZ	1:A:1266:TYR:CE1	2.84	0.61
1:B:92:LEU:N	1:B:93:PRO:CD	2.63	0.61
1:B:1423:VAL:CG2	1:B:1496:TYR:CE1	2.83	0.61
1:B:1279:ARG:O	1:B:1280:TYR:C	2.38	0.61
1:A:984:VAL:CG1	1:A:1024:TYR:CE1	2.84	0.61
1:A:1019:PHE:CE2	1:A:1020:TYR:CE1	2.88	0.61
2:Y:143:GLY:O	2:Y:145:ASN:N	2.33	0.60
1:B:855:PHE:CE1	1:B:886:GLN:CB	2.84	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:438:ASP:O	1:B:439:ALA:C	2.39	0.60
1:B:451:GLY:C	1:B:452:TYR:CD2	2.75	0.60
1:B:243:PHE:CE2	1:B:316:GLU:CG	2.85	0.60
1:A:242:ASN:ND2	1:A:242:ASN:N	2.49	0.60
1:B:1180:LEU:O	1:B:1182:ALA:N	2.34	0.60
1:A:838:GLN:O	1:A:1486:GLY:N	2.34	0.60
1:A:1028:GLY:O	1:A:1029:ASN:C	2.40	0.60
1:B:243:PHE:CZ	1:B:316:GLU:CG	2.85	0.60
1:A:257:ASN:OD1	1:A:893:SER:O	2.20	0.60
1:B:961:TYR:OH	1:B:1343:ASN:ND2	2.35	0.60
1:B:1250:THR:O	1:B:1253:TYR:N	2.35	0.60
1:B:66:TYR:CE1	1:B:90:LYS:CG	2.84	0.59
1:B:457:TYR:CD2	1:B:457:TYR:C	2.76	0.59
1:B:322:TYR:CD2	1:B:322:TYR:N	2.70	0.59
1:A:647:HIS:O	1:A:649:ALA:N	2.34	0.59
1:B:239:GLY:O	1:B:241:LYS:N	2.36	0.59
1:B:981:GLY:O	1:B:982:LEU:CB	2.49	0.59
1:B:163:PHE:CD2	1:B:188:PHE:CD2	2.91	0.59
1:B:1304:VAL:CG1	1:B:1305:LYS:N	2.66	0.59
1:B:1054:LEU:O	1:B:1056:ILE:N	2.36	0.59
1:A:324:TYR:CD2	1:A:324:TYR:C	2.75	0.59
1:A:1304:VAL:CG1	1:A:1305:LYS:N	2.66	0.59
1:B:161:LEU:CG	1:B:185:PHE:CE1	2.86	0.59
1:A:30:ILE:CG2	1:A:31:PHE:N	2.65	0.59
1:A:986:GLU:CA	1:A:986:GLU:OE2	2.50	0.59
1:A:1228:TRP:N	1:A:1228:TRP:CE3	2.71	0.58
1:A:1068:VAL:CG1	1:A:1069:TRP:N	2.66	0.58
1:A:1226:ARG:NE	1:A:1266:TYR:CE1	2.71	0.58
1:A:239:GLY:O	1:A:241:LYS:N	2.36	0.58
1:A:936:ARG:NH1	1:A:1002:HIS:CE1	2.71	0.58
1:B:491:PRO:C	1:B:493:ILE:N	2.55	0.58
1:A:457:TYR:CD2	1:A:457:TYR:C	2.77	0.58
1:B:96:GLN:O	1:B:98:PRO:CD	2.51	0.58
1:A:641:ASN:O	1:A:644:ASN:N	2.36	0.58
1:B:444:GLU:O	1:B:445:GLU:C	2.39	0.58
1:A:1279:ARG:O	1:A:1280:TYR:C	2.41	0.58
1:B:1226:ARG:CZ	1:B:1266:TYR:CE1	2.87	0.58
1:B:256:TYR:O	1:B:257:ASN:ND2	2.37	0.58
1:B:27:ALA:O	1:B:28:PRO:O	2.22	0.58
1:B:952:THR:OG1	1:B:953:ILE:N	2.37	0.57
1:B:1019:PHE:CD2	1:B:1020:TYR:CD1	2.92	0.57
1:A:290:THR:CG2	1:A:290:THR:O	2.51	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1047:LYS:O	1:A:1049:LEU:N	2.37	0.57
1:B:1408:TYR:CD1	1:B:1409:LYS:N	2.72	0.57
1:A:441:ASP:OD2	1:A:441:ASP:N	2.37	0.57
1:B:814:THR:OG1	1:B:815:VAL:N	2.36	0.57
1:A:1210:SER:O	1:A:1214:ARG:N	2.38	0.57
1:A:61:ASP:O	1:A:63:LYS:N	2.36	0.57
1:A:124:GLY:C	1:A:125:PHE:CG	2.78	0.57
1:A:1423:VAL:CG2	1:A:1496:TYR:CE1	2.87	0.57
1:A:634:CYS:SG	1:A:635:GLY:N	2.78	0.57
1:A:284:GLN:OE1	1:A:284:GLN:N	2.37	0.57
1:A:1465:ASN:ND2	1:A:1465:ASN:N	2.53	0.57
1:A:133:PRO:O	1:A:134:VAL:CG2	2.53	0.57
2:Y:153:PHE:CD2	2:Y:154:SER:N	2.72	0.57
1:A:208:ASP:O	1:A:209:PHE:CB	2.53	0.57
1:B:1056:ILE:O	1:B:1058:SER:N	2.38	0.57
1:B:27:ALA:O	1:B:652:THR:O	2.23	0.57
1:B:77:ASN:ND2	1:B:81:ASN:ND2	2.52	0.57
1:A:172:ASP:OD2	1:A:173:MET:N	2.38	0.57
1:A:1008:ALA:N	1:A:1068:VAL:O	2.37	0.57
1:A:25:ILE:O	1:A:654:LEU:N	2.38	0.57
1:A:1274:LEU:O	1:A:1276:GLU:N	2.38	0.57
1:A:824:PHE:CE1	1:A:846:TYR:CD1	2.93	0.57
1:A:1278:GLN:NE2	1:A:1278:GLN:CA	2.68	0.57
1:B:451:GLY:O	1:B:452:TYR:CD2	2.58	0.56
1:A:1307:LEU:O	1:A:1308:ARG:C	2.43	0.56
1:A:304:GLU:O	1:A:305:THR:O	2.22	0.56
1:A:814:THR:OG1	1:A:815:VAL:N	2.38	0.56
1:A:614:ARG:NH2	1:A:798:GLU:OE2	2.38	0.56
1:B:169:SER:O	1:B:170:GLU:O	2.23	0.56
1:B:835:ARG:CG	1:B:835:ARG:NH1	2.67	0.56
1:B:1509:TYR:CD2	1:B:1509:TYR:O	2.58	0.56
1:B:1217:LEU:O	1:B:1218:VAL:CG1	2.53	0.56
1:A:1056:ILE:O	1:A:1057:MET:C	2.43	0.56
1:B:208:ASP:O	1:B:209:PHE:CB	2.53	0.56
1:B:1465:ASN:ND2	1:B:1465:ASN:N	2.52	0.56
1:A:96:GLN:O	1:A:98:PRO:CD	2.52	0.56
1:B:456:ALA:O	1:B:458:SER:N	2.38	0.56
1:B:61:ASP:O	1:B:63:LYS:N	2.37	0.56
1:B:240:TYR:CZ	1:B:443:PRO:CD	2.88	0.56
1:A:215:ALA:C	1:A:216:TYR:CD2	2.79	0.56
1:B:1435:ASN:O	1:B:1438:ASP:N	2.38	0.56
1:A:1024:TYR:CE2	1:A:1030:HIS:CD2	2.93	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:451:GLY:O	1:A:452:TYR:CD2	2.58	0.56
1:B:1143:TYR:CE1	1:B:1186:PHE:CZ	2.94	0.56
1:A:438:ASP:O	1:A:439:ALA:C	2.43	0.56
1:B:226:HIS:CD2	1:B:336:PHE:CE2	2.93	0.56
1:A:647:HIS:O	1:A:650:GLY:N	2.38	0.56
1:A:1250:THR:O	1:A:1253:TYR:N	2.39	0.56
1:B:478:VAL:N	1:B:564:GLU:OE1	2.39	0.56
1:A:1023:HIS:CD2	1:A:1092:TYR:OH	2.59	0.56
1:B:707:ASN:OD1	1:B:707:ASN:N	2.39	0.56
1:B:1019:PHE:CD2	1:B:1020:TYR:CE1	2.95	0.55
1:A:396:ASP:N	1:A:400:GLU:O	2.39	0.55
1:A:85:LEU:O	1:A:86:THR:CB	2.54	0.55
1:A:1225:TYR:CE1	1:A:1272:LYS:CG	2.89	0.55
1:A:295:GLY:O	1:A:296:ILE:CD1	2.55	0.55
1:A:444:GLU:O	1:A:445:GLU:C	2.44	0.55
1:B:163:PHE:CE2	1:B:188:PHE:CD2	2.95	0.55
1:B:1290:THR:O	1:B:1294:ILE:CG1	2.54	0.55
1:B:1056:ILE:O	1:B:1057:MET:C	2.44	0.55
1:A:163:PHE:N	1:A:163:PHE:CD1	2.73	0.55
1:B:442:LEU:O	1:B:443:PRO:C	2.41	0.55
1:B:1143:TYR:CE1	1:B:1186:PHE:CE2	2.94	0.55
1:A:432:GLU:OE2	1:A:453:ARG:NH2	2.40	0.55
1:B:614:ARG:NH2	1:B:798:GLU:OE2	2.39	0.55
1:B:940:SER:CB	1:B:959:PHE:CD1	2.90	0.55
1:B:1126:PRO:O	1:B:1499:HIS:ND1	2.40	0.55
1:B:606:ASP:O	1:B:608:ALA:N	2.40	0.55
1:A:1066:TYR:N	1:A:1066:TYR:CD1	2.74	0.55
1:A:1320:LYS:N	1:A:1344:ASP:OD2	2.40	0.55
1:B:348:VAL:CG1	1:B:349:LEU:N	2.70	0.55
1:A:561:LEU:O	1:A:563:ILE:CG2	2.55	0.55
1:B:101:TYR:CE1	1:B:116:ARG:NE	2.75	0.55
1:B:306:ALA:O	1:B:307:VAL:CG2	2.55	0.55
1:B:1028:GLY:O	1:B:1029:ASN:O	2.25	0.54
1:B:1136:GLU:O	1:B:1140:ASN:N	2.40	0.54
1:B:1300:TYR:CD2	1:B:1300:TYR:C	2.80	0.54
1:B:235:TYR:CD2	1:B:235:TYR:N	2.74	0.54
1:A:226:HIS:CD2	1:A:336:PHE:CE2	2.96	0.54
1:A:556:SER:OG	1:A:557:ASP:N	2.40	0.54
1:B:38:ASN:O	1:B:39:ILE:CD1	2.54	0.54
1:A:1289:ASP:O	1:A:1293:ALA:N	2.41	0.54
1:B:373:VAL:CG2	1:B:374:GLN:N	2.70	0.54
1:B:457:TYR:CD2	1:B:457:TYR:O	2.61	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:388:VAL:O	1:A:388:VAL:CG1	2.54	0.54
1:B:1068:VAL:CG1	1:B:1069:TRP:N	2.71	0.54
1:A:1325:ASN:ND2	1:A:1325:ASN:O	2.41	0.54
1:A:491:PRO:C	1:A:493:ILE:N	2.60	0.54
1:A:961:TYR:OH	1:A:1343:ASN:ND2	2.41	0.54
1:A:1456:LYS:O	1:A:1457:ASP:C	2.46	0.54
1:A:463:SER:OG	1:A:544:TYR:OH	2.26	0.54
1:A:1286:SER:OG	1:A:1287:THR:N	2.41	0.54
1:A:1056:ILE:O	1:A:1059:TYR:N	2.41	0.54
1:B:647:HIS:O	1:B:650:GLY:N	2.41	0.54
1:A:235:TYR:CD2	1:A:235:TYR:N	2.76	0.54
1:B:1082:ALA:O	1:B:1083:LEU:C	2.46	0.53
1:B:149:ASN:O	1:B:152:LEU:N	2.41	0.53
1:B:608:ALA:O	1:B:609:VAL:C	2.47	0.53
1:B:1334:LEU:N	1:B:1334:LEU:CD2	2.71	0.53
1:B:944:LEU:N	1:B:1357:ALA:O	2.41	0.53
1:B:686:ILE:C	1:B:688:ALA:N	2.58	0.53
1:B:124:GLY:C	1:B:125:PHE:CG	2.81	0.53
1:B:1008:ALA:O	1:B:1009:GLU:C	2.47	0.53
1:B:1090:ASN:O	1:B:1090:ASN:OD1	2.27	0.53
1:B:284:GLN:N	1:B:284:GLN:OE1	2.42	0.53
1:B:290:THR:O	1:B:290:THR:CG2	2.57	0.53
1:A:968:VAL:CG1	1:A:1368:THR:CG2	2.86	0.53
1:A:922:ILE:CD1	4:A:2001:NAG:H82	2.39	0.53
1:A:456:ALA:O	1:A:458:SER:N	2.42	0.53
1:B:350:SER:OG	1:B:446:ASN:O	2.27	0.53
1:A:1090:ASN:OD1	1:A:1090:ASN:O	2.26	0.53
1:A:440:PRO:CD	1:A:441:ASP:OD2	2.57	0.53
1:A:306:ALA:O	1:A:307:VAL:CG2	2.56	0.53
1:A:435:VAL:CG1	1:A:436:LYS:N	2.72	0.53
1:A:240:TYR:CZ	1:A:443:PRO:CD	2.92	0.53
1:B:700:TYR:C	1:B:702:GLY:N	2.60	0.53
1:A:707:ASN:N	1:A:707:ASN:OD1	2.41	0.53
1:A:653:PHE:CZ	1:A:660:ASP:CA	2.92	0.53
1:B:561:LEU:O	1:B:563:ILE:CG2	2.57	0.53
1:A:1115:ASN:C	1:A:1115:ASN:ND2	2.63	0.53
1:A:319:ASN:O	1:A:320:ASN:ND2	2.43	0.52
1:B:1028:GLY:O	1:B:1030:HIS:CD2	2.62	0.52
1:B:1136:GLU:OE1	1:B:1415:SER:CB	2.57	0.52
1:B:50:PHE:CE2	1:B:79:PHE:CE2	2.97	0.52
1:B:1210:SER:OG	1:B:1211:ALA:N	2.40	0.52
1:A:1019:PHE:CD2	1:A:1020:TYR:CD1	2.98	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1456:LYS:O	1:B:1457:ASP:C	2.48	0.52
1:A:661:ASP:OD2	1:A:663:GLN:NE2	2.43	0.52
1:B:1081:PHE:CE1	1:B:1288:GLN:NE2	2.77	0.52
1:B:1288:GLN:O	1:B:1292:ASN:ND2	2.43	0.52
1:B:1226:ARG:NE	1:B:1266:TYR:CE1	2.77	0.52
1:A:348:VAL:CG1	1:A:349:LEU:N	2.72	0.52
1:A:1113:LEU:N	1:A:1117:SER:O	2.43	0.52
1:B:1289:ASP:O	1:B:1293:ALA:N	2.42	0.52
1:A:577:PRO:O	1:A:582:TYR:OH	2.28	0.52
1:A:173:MET:O	1:A:174:VAL:CB	2.57	0.52
1:B:968:VAL:CG1	1:B:1368:THR:CG2	2.88	0.52
1:B:362:PHE:CE1	1:B:638:GLY:O	2.62	0.52
1:A:322:TYR:N	1:A:322:TYR:CD2	2.78	0.52
1:A:618:LYS:CG	1:A:621:GLU:CD	2.78	0.52
1:A:1128:LYS:O	1:A:1246:ARG:NH2	2.42	0.52
1:B:388:VAL:CG1	1:B:388:VAL:O	2.55	0.52
1:A:243:PHE:CZ	1:A:316:GLU:CG	2.92	0.52
1:B:66:TYR:CD1	1:B:90:LYS:CE	2.92	0.52
1:A:431:LEU:CD2	1:A:431:LEU:C	2.78	0.52
1:B:51:ASP:OD2	1:B:70:HIS:NE2	2.43	0.52
1:B:948:GLY:O	1:B:950:TYR:N	2.42	0.52
1:B:661:ASP:OD2	1:B:663:GLN:NE2	2.42	0.52
1:B:25:ILE:O	1:B:654:LEU:N	2.43	0.52
1:B:1066:TYR:N	1:B:1066:TYR:CD1	2.75	0.52
1:A:1206:ARG:NH1	1:A:1206:ARG:CG	2.73	0.52
1:B:978:SER:N	1:B:1360:HIS:O	2.43	0.52
1:A:1334:LEU:N	1:A:1334:LEU:CD2	2.72	0.52
1:B:576:SER:OG	1:B:589:SER:CB	2.58	0.52
1:B:984:VAL:CG1	1:B:1024:TYR:CE1	2.92	0.52
1:A:1421:HIS:CE1	1:A:1498:TYR:CG	2.97	0.52
1:B:626:PHE:O	1:B:628:GLU:N	2.44	0.52
1:B:169:SER:O	1:B:170:GLU:C	2.49	0.52
1:A:362:PHE:CE1	1:A:638:GLY:O	2.63	0.52
1:B:269:PHE:CB	1:B:283:MET:CE	2.88	0.52
1:B:1030:HIS:CE1	1:B:1306:GLN:NE2	2.78	0.51
1:A:149:ASN:O	1:A:152:LEU:N	2.43	0.51
1:B:227:PHE:CZ	1:B:329:VAL:O	2.63	0.51
1:A:162:THR:OG1	1:A:162:THR:O	2.27	0.51
1:A:1133:LEU:N	1:A:1134:PRO:CD	2.73	0.51
1:B:215:ALA:C	1:B:216:TYR:CD2	2.83	0.51
1:B:1018:VAL:O	1:B:1021:VAL:N	2.44	0.51
1:A:269:PHE:CB	1:A:283:MET:CE	2.89	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:491:PRO:O	1:B:492:TYR:C	2.49	0.51
1:B:647:HIS:O	1:B:649:ALA:N	2.43	0.51
1:B:121:TYR:O	1:B:210:SER:N	2.43	0.51
1:A:1296:GLY:O	1:A:1299:GLU:N	2.42	0.51
1:B:1049:LEU:O	1:B:1050:LYS:C	2.47	0.51
1:B:325:ILE:O	1:B:342:ILE:N	2.44	0.51
1:B:528:ILE:CD1	1:B:528:ILE:N	2.74	0.51
1:A:1080:ALA:O	1:A:1081:PHE:C	2.47	0.51
1:A:169:SER:O	1:A:170:GLU:C	2.49	0.51
1:B:1008:ALA:O	1:B:1011:GLU:N	2.44	0.51
1:A:1432:ILE:O	1:A:1433:SER:C	2.49	0.51
1:B:1307:LEU:O	1:B:1308:ARG:C	2.48	0.51
1:A:478:VAL:N	1:A:564:GLU:OE1	2.44	0.51
1:A:1118:PHE:CE2	1:A:1148:THR:OG1	2.64	0.51
1:B:847:ASN:O	1:B:848:TYR:CD1	2.63	0.51
1:B:1022:PHE:CE2	1:B:1092:TYR:CG	2.99	0.51
2:Y:219:LYS:N	2:Y:219:LYS:CD	2.73	0.51
1:A:493:ILE:CG2	1:A:494:ASP:N	2.73	0.51
1:B:618:LYS:CB	1:B:621:GLU:CB	2.88	0.51
1:A:700:TYR:C	1:A:702:GLY:N	2.62	0.51
1:A:316:GLU:O	1:A:319:ASN:N	2.43	0.51
1:B:1030:HIS:NE2	1:B:1306:GLN:NE2	2.59	0.51
1:B:155:ALA:O	1:B:156:LYS:C	2.49	0.51
1:A:701:ASP:OD1	1:A:702:GLY:N	2.44	0.51
1:A:1126:PRO:O	1:A:1499:HIS:ND1	2.44	0.51
1:A:27:ALA:O	1:A:652:THR:O	2.29	0.51
1:B:165:ASP:C	1:B:165:ASP:OD1	2.49	0.51
1:B:1202:HIS:CD2	1:B:1204:GLN:CB	2.94	0.51
1:A:38:ASN:O	1:A:39:ILE:CD1	2.58	0.51
1:B:1210:SER:O	1:B:1214:ARG:N	2.45	0.50
1:A:161:LEU:CG	1:A:185:PHE:CE1	2.94	0.50
1:B:1432:ILE:O	1:B:1433:SER:O	2.28	0.50
1:B:936:ARG:NH1	1:B:1002:HIS:CE1	2.78	0.50
1:A:150:ASP:N	1:A:150:ASP:OD2	2.44	0.50
1:A:1199:ASP:OD1	1:A:1201:THR:OG1	2.29	0.50
1:A:491:PRO:O	1:A:492:TYR:C	2.48	0.50
1:B:1069:TRP:NE1	1:B:1463:GLN:NE2	2.60	0.50
1:B:1404:ALA:C	1:B:1474:CYS:SG	2.89	0.50
1:A:1210:SER:OG	1:A:1211:ALA:N	2.44	0.50
1:B:42:GLN:OE1	1:B:543:TYR:OH	2.29	0.50
1:B:1217:LEU:C	1:B:1218:VAL:CG2	2.80	0.50
1:B:1151:GLY:O	1:B:1152:ILE:C	2.48	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:896:VAL:O	1:B:897:THR:CG2	2.60	0.50
1:B:1440:LYS:NZ	1:B:1453:TYR:OH	2.45	0.50
1:A:1082:ALA:O	1:A:1083:LEU:C	2.48	0.50
1:B:234:GLU:C	1:B:235:TYR:CD2	2.85	0.50
1:A:944:LEU:N	1:A:1357:ALA:O	2.45	0.50
1:A:1022:PHE:CE2	1:A:1092:TYR:CG	3.00	0.50
1:A:316:GLU:O	1:A:318:LEU:N	2.45	0.50
1:B:150:ASP:OD2	1:B:150:ASP:N	2.45	0.50
1:A:227:PHE:CE1	1:A:338:GLU:CB	2.94	0.50
1:B:1212:LEU:O	1:B:1215:GLU:N	2.44	0.50
1:A:395:ILE:O	1:A:429:THR:CG2	2.60	0.50
1:B:1334:LEU:O	1:B:1335:GLY:O	2.29	0.50
1:A:558:SER:OG	1:A:638:GLY:N	2.44	0.50
1:B:1115:ASN:ND2	1:B:1115:ASN:C	2.65	0.50
1:A:317:ASP:C	1:A:319:ASN:N	2.64	0.49
1:B:553:GLU:OE1	1:B:555:VAL:CG2	2.60	0.49
1:B:466:TYR:C	1:B:466:TYR:CD1	2.85	0.49
1:B:1421:HIS:CE1	1:B:1498:TYR:CG	2.99	0.49
1:B:188:PHE:CD1	1:B:188:PHE:C	2.86	0.49
1:B:618:LYS:CG	1:B:621:GLU:CD	2.80	0.49
1:B:982:LEU:CD2	1:B:1309:LEU:CD1	2.90	0.49
1:A:727:ALA:O	1:A:731:CYS:SG	2.71	0.49
1:B:493:ILE:CG2	1:B:494:ASP:N	2.75	0.49
1:B:232:GLU:OE2	1:B:251:LYS:CE	2.60	0.49
1:B:1251:THR:OG1	1:B:1273:TRP:CZ3	2.65	0.49
1:B:395:ILE:O	1:B:429:THR:CG2	2.60	0.49
1:A:1213:LYS:NZ	1:A:1263:ASP:OD2	2.44	0.49
1:B:534:MET:O	1:B:537:SER:O	2.30	0.49
1:B:634:CYS:SG	1:B:635:GLY:N	2.85	0.49
1:A:1332:ASN:CG	1:A:1332:ASN:O	2.51	0.49
1:B:1056:ILE:O	1:B:1059:TYR:N	2.46	0.49
1:B:1202:HIS:O	1:B:1204:GLN:N	2.45	0.49
1:A:243:PHE:CE2	1:A:316:GLU:CG	2.95	0.49
2:X:143:GLY:C	2:X:145:ASN:N	2.66	0.49
1:A:1268:ASN:N	1:A:1269:PRO:CD	2.75	0.49
1:B:172:ASP:OD2	1:B:173:MET:N	2.44	0.49
1:B:1435:ASN:O	1:B:1436:GLU:C	2.51	0.49
1:A:281:GLU:O	1:A:282:MET:O	2.29	0.49
1:B:1113:LEU:N	1:B:1117:SER:O	2.46	0.49
1:A:625:GLN:O	1:A:626:PHE:C	2.51	0.49
1:B:100:SER:O	1:B:101:TYR:CD2	2.66	0.49
1:A:1456:LYS:O	1:A:1459:HIS:N	2.46	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1432:ILE:O	1:B:1433:SER:C	2.50	0.49
1:B:173:MET:O	1:B:174:VAL:CB	2.61	0.49
1:A:606:ASP:O	1:A:608:ALA:N	2.45	0.49
1:B:1199:ASP:OD1	1:B:1201:THR:OG1	2.30	0.49
1:A:494:ASP:O	1:A:496:ILE:N	2.46	0.49
1:A:1153:ARG:O	1:A:1156:PHE:N	2.46	0.49
1:B:1255:LEU:CD2	1:B:1271:ILE:CG2	2.91	0.49
1:A:505:SER:OG	1:A:506:LYS:NZ	2.46	0.49
1:A:386:VAL:CG2	1:A:411:THR:CG2	2.90	0.48
1:A:855:PHE:C	1:A:855:PHE:CD1	2.86	0.48
1:A:621:GLU:O	1:A:625:GLN:N	2.46	0.48
1:B:438:ASP:C	1:B:439:ALA:O	2.51	0.48
1:A:457:TYR:CD2	1:A:457:TYR:O	2.66	0.48
1:A:129:HIS:O	1:A:129:HIS:CD2	2.66	0.48
1:A:124:GLY:O	1:A:125:PHE:CG	2.66	0.48
1:B:1153:ARG:O	1:B:1156:PHE:N	2.46	0.48
1:B:897:THR:C	1:B:898:PHE:CD2	2.87	0.48
1:A:1008:ALA:CB	1:A:1059:TYR:CD2	2.96	0.48
1:B:1047:LYS:C	1:B:1049:LEU:N	2.64	0.48
1:B:1203:PRO:O	1:B:1206:ARG:CB	2.61	0.48
1:A:352:TYR:O	1:A:448:ALA:CB	2.61	0.48
1:B:727:ALA:O	1:B:731:CYS:SG	2.71	0.48
1:A:1381:ILE:CG2	1:A:1509:TYR:CD1	2.97	0.48
1:B:281:GLU:O	1:B:282:MET:O	2.31	0.48
1:B:489:LYS:O	1:B:490:SER:CB	2.62	0.48
1:B:304:GLU:O	1:B:305:THR:C	2.52	0.48
1:B:1007:SER:OG	1:B:1008:ALA:N	2.47	0.48
1:A:686:ILE:C	1:A:688:ALA:N	2.65	0.48
1:A:123:ASN:C	1:A:123:ASN:ND2	2.66	0.48
1:A:165:ASP:C	1:A:165:ASP:OD1	2.51	0.48
1:A:489:LYS:O	1:A:490:SER:CB	2.60	0.48
1:A:208:ASP:O	1:A:209:PHE:CG	2.67	0.48
1:B:352:TYR:O	1:B:448:ALA:CB	2.61	0.48
1:B:1271:ILE:CD1	1:B:1271:ILE:O	2.61	0.48
1:A:1509:TYR:CD2	1:A:1509:TYR:C	2.86	0.48
1:A:151:ASP:OD1	1:A:508:LYS:NZ	2.47	0.48
1:A:373:VAL:CG2	1:A:374:GLN:N	2.75	0.48
1:B:377:ASP:O	1:B:379:LEU:N	2.47	0.48
1:A:837:GLU:OE2	1:A:1488:LEU:CA	2.61	0.48
1:A:1408:TYR:CD1	1:A:1409:LYS:N	2.81	0.48
2:X:153:PHE:CG	2:X:154:SER:N	2.81	0.48
1:B:616:ALA:O	1:B:617:LYS:C	2.51	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:558:SER:OG	1:B:638:GLY:N	2.46	0.48
1:A:66:TYR:CE1	1:A:90:LYS:CG	2.97	0.48
1:A:946:PRO:CB	1:A:1352:PHE:O	2.62	0.48
1:A:1082:ALA:O	1:A:1086:LEU:N	2.46	0.48
1:A:1226:ARG:CD	1:A:1266:TYR:CE1	2.96	0.48
1:A:1509:TYR:CD2	1:A:1509:TYR:O	2.66	0.48
1:A:618:LYS:CB	1:A:621:GLU:CB	2.91	0.48
1:B:100:SER:O	1:B:101:TYR:CB	2.61	0.48
1:A:544:TYR:CD1	1:A:544:TYR:N	2.81	0.48
1:B:1296:GLY:O	1:B:1299:GLU:N	2.47	0.48
1:B:305:THR:O	1:B:307:VAL:N	2.47	0.48
1:B:560:TRP:CH2	1:B:562:ASN:CB	2.97	0.48
1:B:214:THR:CG2	1:B:215:ALA:N	2.77	0.48
1:A:409:SER:OG	1:A:410:VAL:N	2.47	0.48
1:B:938:SER:OG	1:B:1279:ARG:NH1	2.47	0.48
1:A:1003:LEU:CD1	1:A:1498:TYR:CE1	2.97	0.48
1:A:59:TYR:CG	1:A:60:PRO:CD	2.97	0.48
1:B:304:GLU:O	1:B:305:THR:O	2.32	0.48
1:B:131:ASP:OD1	1:B:135:TYR:OH	2.31	0.47
1:A:1056:ILE:O	1:A:1058:SER:N	2.47	0.47
1:A:59:TYR:CD2	1:A:60:PRO:CD	2.97	0.47
1:A:637:GLY:O	1:A:638:GLY:O	2.32	0.47
1:A:1118:PHE:O	1:A:1144:LEU:CD2	2.62	0.47
1:A:66:TYR:CD1	1:A:90:LYS:CE	2.97	0.47
2:Y:143:GLY:C	2:Y:145:ASN:N	2.68	0.47
1:A:305:THR:O	1:A:307:VAL:N	2.47	0.47
1:B:1320:LYS:N	1:B:1344:ASP:OD2	2.47	0.47
1:A:940:SER:CB	1:A:959:PHE:CD1	2.97	0.47
1:B:162:THR:O	1:B:162:THR:OG1	2.32	0.47
1:B:1244:THR:O	1:B:1285:TYR:CD2	2.67	0.47
1:B:1024:TYR:CD2	1:B:1025:LEU:N	2.83	0.47
1:A:1204:GLN:O	1:A:1207:SER:N	2.47	0.47
1:A:647:HIS:C	1:A:649:ALA:N	2.67	0.47
1:B:466:TYR:CD1	1:B:467:ILE:N	2.82	0.47
1:A:1153:ARG:O	1:A:1154:LYS:C	2.52	0.47
1:B:1173:ASN:O	1:B:1174:PHE:C	2.52	0.47
1:B:820:PHE:CE2	1:B:848:TYR:CD2	3.03	0.47
1:B:520:ASP:CG	1:B:521:ALA:N	2.66	0.47
1:B:431:LEU:C	1:B:431:LEU:CD2	2.83	0.47
1:B:1050:LYS:O	1:B:1053:MET:CB	2.63	0.47
1:B:606:ASP:C	1:B:608:ALA:N	2.68	0.47
1:A:129:HIS:C	1:A:129:HIS:CD2	2.86	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:23:TYR:CD1	1:A:23:TYR:N	2.81	0.47
1:B:394:THR:CG2	1:B:395:ILE:N	2.78	0.47
1:A:157:ARG:NH1	1:A:209:PHE:CD1	2.82	0.47
1:A:183:ILE:CG2	1:A:185:PHE:CE2	2.97	0.47
2:Y:217:ASN:ND2	2:Y:220:ASP:OD2	2.47	0.47
1:B:571:LEU:CD1	1:B:572:GLN:N	2.77	0.47
1:A:1283:GLY:CA	1:A:1290:THR:CG2	2.92	0.47
1:B:1325:ASN:ND2	1:B:1325:ASN:O	2.48	0.47
1:B:1280:TYR:C	1:B:1280:TYR:CD2	2.86	0.47
1:A:394:THR:CG2	1:A:395:ILE:N	2.77	0.47
1:B:1047:LYS:O	1:B:1048:LYS:C	2.53	0.47
1:B:1404:ALA:O	1:B:1474:CYS:SG	2.73	0.47
1:A:837:GLU:OE2	1:A:1488:LEU:CB	2.63	0.47
1:B:1503:LYS:CD	1:B:1503:LYS:N	2.78	0.47
2:X:217:ASN:ND2	2:X:220:ASP:OD2	2.47	0.47
1:A:1438:ASP:OD2	1:A:1478:ARG:CG	2.63	0.47
1:A:1434:ALA:CB	1:A:1477:PHE:CE1	2.98	0.47
1:B:1279:ARG:CD	1:B:1284:PHE:CG	2.98	0.47
1:B:59:TYR:CG	1:B:60:PRO:CD	2.98	0.47
1:A:304:GLU:O	1:A:305:THR:C	2.52	0.47
1:B:1153:ARG:O	1:B:1154:LYS:C	2.52	0.47
1:A:835:ARG:NH1	1:A:835:ARG:CG	2.77	0.47
1:B:1193:TYR:O	1:B:1196:SER:CB	2.63	0.47
2:X:219:LYS:CD	2:X:219:LYS:N	2.78	0.47
1:A:110:HIS:O	1:A:110:HIS:CD2	2.68	0.47
1:A:155:ALA:O	1:A:156:LYS:C	2.53	0.46
1:A:539:ARG:NH1	1:A:631:ASP:OD1	2.49	0.46
1:B:1278:GLN:O	1:B:1360:HIS:NE2	2.48	0.46
1:A:1432:ILE:O	1:A:1433:SER:O	2.33	0.46
1:A:537:SER:O	1:A:538:SER:OG	2.32	0.46
1:B:1370:THR:CG2	1:B:1370:THR:O	2.63	0.46
1:B:1016:VAL:O	1:B:1018:VAL:N	2.48	0.46
1:A:520:ASP:CG	1:A:521:ALA:N	2.68	0.46
1:A:1217:LEU:O	1:A:1218:VAL:CG1	2.63	0.46
1:B:1003:LEU:CD1	1:B:1498:TYR:CE1	2.98	0.46
1:A:855:PHE:CE1	1:A:886:GLN:CB	2.98	0.46
1:A:1466:SER:OG	1:A:1468:PRO:CD	2.62	0.46
1:A:1310:SER:O	1:A:1311:MET:O	2.32	0.46
1:A:350:SER:OG	1:A:446:ASN:O	2.34	0.46
1:A:1050:LYS:O	1:A:1053:MET:CB	2.63	0.46
1:B:240:TYR:C	1:B:240:TYR:CD1	2.86	0.46
1:A:478:VAL:CG1	1:A:478:VAL:O	2.62	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:544:TYR:CE1	1:B:555:VAL:CG1	2.99	0.46
1:B:1030:HIS:O	1:B:1033:ILE:CG1	2.64	0.46
1:A:1008:ALA:O	1:A:1009:GLU:C	2.53	0.46
1:A:1452:ASP:O	1:A:1463:GLN:N	2.49	0.46
1:B:157:ARG:NH1	1:B:209:PHE:CD1	2.84	0.46
1:B:987:ILE:CD1	1:B:1294:ILE:CD1	2.93	0.46
1:A:191:PRO:C	1:A:193:ASN:N	2.69	0.46
1:B:608:ALA:O	1:B:609:VAL:O	2.34	0.46
1:A:940:SER:OG	1:A:1361:VAL:CG1	2.63	0.46
1:A:820:PHE:CE2	1:A:848:TYR:CD2	3.04	0.46
1:B:799:ILE:O	1:B:799:ILE:CG1	2.64	0.46
1:B:41:ILE:CG2	1:B:81:ASN:O	2.64	0.46
1:A:700:TYR:CE1	1:A:758:LEU:CB	2.99	0.46
1:B:544:TYR:N	1:B:544:TYR:CD1	2.84	0.46
1:A:987:ILE:CD1	1:A:1294:ILE:CD1	2.94	0.46
1:A:1097:GLN:O	1:A:1099:SER:N	2.49	0.46
1:A:560:TRP:CH2	1:A:562:ASN:CB	2.99	0.46
1:A:1028:GLY:O	1:A:1030:HIS:CD2	2.69	0.46
1:B:272:ARG:O	1:B:273:GLU:OE2	2.34	0.46
1:B:1244:THR:CG2	1:B:1245:ALA:N	2.78	0.46
1:A:131:ASP:OD1	1:A:135:TYR:OH	2.34	0.46
1:A:41:ILE:O	1:A:81:ASN:N	2.49	0.46
1:A:824:PHE:O	1:A:846:TYR:N	2.49	0.46
1:B:324:TYR:C	1:B:324:TYR:CD2	2.88	0.46
1:A:694:VAL:O	1:A:698:CYS:SG	2.74	0.46
1:A:1273:TRP:CZ3	1:A:1274:LEU:CD2	2.99	0.46
1:A:834:VAL:O	1:A:835:ARG:C	2.52	0.46
1:B:1019:PHE:CE2	1:B:1088:GLN:NE2	2.84	0.45
1:B:1202:HIS:CD2	1:B:1204:GLN:N	2.84	0.45
1:B:157:ARG:O	1:B:178:ASP:CB	2.63	0.45
1:A:539:ARG:NH2	1:A:634:CYS:C	2.69	0.45
1:B:1162:VAL:CG2	1:B:1163:LYS:N	2.78	0.45
1:A:466:TYR:CD1	1:A:467:ILE:N	2.83	0.45
1:A:100:SER:O	1:A:101:TYR:CB	2.63	0.45
1:A:540:LEU:CD1	1:A:540:LEU:C	2.84	0.45
1:B:51:ASP:OD1	1:B:72:HIS:ND1	2.49	0.45
1:A:1169:ILE:C	1:A:1171:ALA:N	2.67	0.45
1:B:129:HIS:ND1	1:B:146:TYR:OH	2.49	0.45
1:A:1090:ASN:ND2	1:A:1158:ILE:CD1	2.79	0.45
1:A:361:LEU:O	1:A:454:ALA:CA	2.64	0.45
1:A:1244:THR:N	1:A:1285:TYR:CE2	2.85	0.45
1:B:1202:HIS:O	1:B:1205:PHE:N	2.49	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1049:LEU:O	1:A:1050:LYS:C	2.54	0.45
1:B:41:ILE:O	1:B:80:GLN:CA	2.64	0.45
1:B:1008:ALA:N	1:B:1068:VAL:O	2.50	0.45
1:A:544:TYR:CE1	1:A:555:VAL:CG1	2.98	0.45
1:B:1023:HIS:CD2	1:B:1092:TYR:OH	2.69	0.45
1:B:531:THR:N	1:B:534:MET:SD	2.90	0.45
1:B:432:GLU:OE2	1:B:453:ARG:NH2	2.50	0.45
1:A:754:MET:O	1:A:755:LYS:CG	2.65	0.45
1:B:123:ASN:C	1:B:123:ASN:ND2	2.70	0.45
1:B:599:TRP:CE3	1:B:778:HIS:O	2.70	0.45
1:B:1076:THR:N	1:B:1120:GLU:OE2	2.49	0.45
1:B:947:ARG:C	1:B:949:ILE:N	2.70	0.45
1:A:1438:ASP:OD2	1:A:1478:ARG:N	2.49	0.45
1:B:1509:TYR:CD2	1:B:1509:TYR:C	2.87	0.45
1:B:240:TYR:CD1	1:B:240:TYR:O	2.70	0.45
1:A:27:ALA:O	1:A:28:PRO:O	2.35	0.45
1:B:824:PHE:O	1:B:846:TYR:N	2.50	0.45
1:B:492:TYR:CD2	1:B:492:TYR:C	2.87	0.45
1:A:1007:SER:OG	1:A:1008:ALA:N	2.50	0.45
1:B:144:ARG:NH2	1:B:602:LEU:O	2.50	0.45
2:Y:140:LYS:O	2:Y:146:LEU:CD2	2.65	0.45
1:B:1125:GLN:O	1:B:1421:HIS:N	2.49	0.45
1:B:605:VAL:CG1	1:B:606:ASP:N	2.80	0.45
1:B:978:SER:OG	1:B:986:GLU:OE1	2.35	0.45
1:A:101:TYR:CE1	1:A:116:ARG:NE	2.85	0.45
1:B:505:SER:OG	1:B:506:LYS:NZ	2.50	0.45
1:B:435:VAL:CG1	1:B:436:LYS:N	2.80	0.45
1:B:1204:GLN:O	1:B:1207:SER:N	2.50	0.45
1:A:519:SER:O	1:A:520:ASP:C	2.55	0.45
2:X:172:HIS:O	2:X:176:ASN:N	2.49	0.45
1:B:142:LYS:CD	1:B:775:TRP:CG	3.00	0.45
1:A:50:PHE:CE2	1:A:79:PHE:CE2	3.05	0.45
1:A:604:ALA:N	1:A:773:TRP:O	2.50	0.45
1:B:104:LEU:O	1:B:114:SER:CB	2.65	0.45
1:A:227:PHE:O	1:A:227:PHE:CD1	2.70	0.45
1:A:1467:ILE:N	1:A:1468:PRO:CD	2.80	0.45
1:A:528:ILE:N	1:A:528:ILE:CD1	2.80	0.45
1:B:1332:ASN:O	1:B:1332:ASN:CG	2.53	0.45
1:B:1082:ALA:O	1:B:1086:LEU:N	2.49	0.44
1:B:621:GLU:O	1:B:625:GLN:N	2.49	0.44
2:Y:153:PHE:CG	2:Y:154:SER:N	2.85	0.44
1:A:576:SER:CB	1:A:577:PRO:CD	2.95	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:758:LEU:O	1:A:760:VAL:N	2.50	0.44
1:A:492:TYR:C	1:A:492:TYR:CD2	2.90	0.44
1:B:577:PRO:O	1:B:582:TYR:OH	2.35	0.44
1:B:1271:ILE:CD1	1:B:1271:ILE:C	2.86	0.44
1:A:531:THR:N	1:A:534:MET:SD	2.90	0.44
1:A:44:TYR:CE1	1:A:497:THR:OG1	2.69	0.44
1:B:396:ASP:N	1:B:400:GLU:O	2.50	0.44
1:A:1300:TYR:CD2	1:A:1300:TYR:C	2.90	0.44
1:A:195:ARG:NH1	1:A:195:ARG:CG	2.80	0.44
1:B:540:LEU:CD1	1:B:540:LEU:C	2.85	0.44
1:B:1012:LEU:O	1:B:1015:VAL:CG1	2.65	0.44
1:B:537:SER:O	1:B:538:SER:OG	2.36	0.44
1:B:1107:LEU:O	1:B:1111:TYR:N	2.51	0.44
1:B:183:ILE:CG2	1:B:185:PHE:CE2	3.01	0.44
1:B:950:TYR:OH	1:B:1300:TYR:OH	2.35	0.44
1:B:50:PHE:CE2	1:B:79:PHE:CD2	3.06	0.44
1:A:847:ASN:O	1:A:848:TYR:CD1	2.71	0.44
1:B:1323:LEU:CG	1:B:1324:HIS:N	2.80	0.44
1:B:754:MET:O	1:B:755:LYS:CG	2.65	0.44
1:A:1047:LYS:C	1:A:1049:LEU:N	2.68	0.44
1:B:835:ARG:NH2	1:B:905:ILE:CD1	2.80	0.44
1:B:61:ASP:CG	1:B:61:ASP:O	2.56	0.44
1:A:968:VAL:O	1:A:971:THR:CG2	2.65	0.44
1:A:360:PRO:O	1:A:369:TYR:OH	2.36	0.44
1:B:297:ALA:O	1:B:298:GLN:CG	2.65	0.44
1:B:1228:TRP:N	1:B:1228:TRP:CE3	2.86	0.44
1:B:1497:GLU:O	1:B:1498:TYR:C	2.55	0.44
1:A:157:ARG:O	1:A:178:ASP:CB	2.66	0.44
1:B:1018:VAL:O	1:B:1019:PHE:C	2.56	0.44
1:A:1047:LYS:O	1:A:1048:LYS:C	2.56	0.44
1:B:42:GLN:CG	1:B:80:GLN:NE2	2.81	0.44
1:B:1037:ASP:OD1	1:B:1038:PRO:N	2.51	0.44
1:B:193:ASN:OD1	1:B:1070:LYS:NZ	2.51	0.44
1:A:290:THR:O	1:A:291:MET:O	2.35	0.44
1:A:1368:THR:O	1:A:1508:PHE:CE2	2.71	0.44
1:A:365:PRO:CD	1:A:464:TYR:CD2	3.00	0.44
1:B:973:ILE:CG2	1:B:1365:VAL:CG2	2.95	0.44
1:B:1286:SER:OG	1:B:1287:THR:N	2.50	0.44
1:B:1239:VAL:CG2	1:B:1239:VAL:O	2.65	0.44
1:A:153:LYS:O	1:A:155:ALA:N	2.51	0.44
1:B:1016:VAL:O	1:B:1017:PRO:C	2.56	0.44
1:B:253:ARG:NH2	1:B:257:ASN:CA	2.79	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1438:ASP:OD2	1:B:1478:ARG:CG	2.66	0.44
1:A:159:THR:CG2	1:A:160:VAL:N	2.81	0.44
1:A:938:SER:OG	1:A:1279:ARG:NE	2.50	0.44
1:A:609:VAL:CG2	1:A:610:TYR:CD2	3.01	0.44
1:B:621:GLU:O	1:B:622:ARG:C	2.56	0.44
1:B:576:SER:N	1:B:589:SER:O	2.51	0.44
1:A:56:ILE:O	1:A:66:TYR:CD2	2.70	0.44
1:A:959:PHE:O	1:A:1346:LEU:N	2.51	0.44
1:B:272:ARG:CG	1:B:273:GLU:N	2.81	0.44
1:B:1133:LEU:N	1:B:1134:PRO:CD	2.81	0.44
1:B:667:GLU:N	1:B:667:GLU:OE1	2.51	0.44
1:A:724:CYS:O	1:A:727:ALA:N	2.51	0.43
1:B:352:TYR:CD1	1:B:375:VAL:CG1	3.01	0.43
1:A:439:ALA:O	1:A:447:GLN:NE2	2.50	0.43
1:A:442:LEU:O	1:A:443:PRO:C	2.52	0.43
1:B:701:ASP:OD1	1:B:702:GLY:N	2.51	0.43
1:B:1081:PHE:O	1:B:1081:PHE:CD2	2.71	0.43
1:A:1429:PRO:O	1:A:1432:ILE:CG1	2.66	0.43
1:A:606:ASP:C	1:A:608:ALA:N	2.71	0.43
1:B:1328:MET:O	1:B:1329:THR:CG2	2.66	0.43
1:B:515:ARG:NH2	1:B:527:ASN:N	2.66	0.43
1:A:1107:LEU:O	1:A:1111:TYR:N	2.51	0.43
1:A:319:ASN:OD1	1:A:321:LYS:CG	2.66	0.43
1:B:356:LEU:CD1	1:B:452:TYR:CD1	3.00	0.43
1:B:257:ASN:ND2	1:B:893:SER:O	2.51	0.43
1:B:1144:LEU:O	1:B:1148:THR:CG2	2.66	0.43
1:B:896:VAL:C	1:B:897:THR:CG2	2.86	0.43
1:A:777:VAL:CG1	1:A:778:HIS:N	2.81	0.43
2:X:146:LEU:C	2:X:146:LEU:CD2	2.85	0.43
1:A:1096:ASN:C	1:A:1096:ASN:ND2	2.71	0.43
1:A:377:ASP:N	1:A:377:ASP:OD1	2.51	0.43
1:B:840:GLN:O	1:B:1483:PHE:CD2	2.70	0.43
1:A:1203:PRO:O	1:A:1206:ARG:N	2.52	0.43
1:A:227:PHE:CZ	1:A:329:VAL:O	2.72	0.43
1:A:1169:ILE:O	1:A:1170:LYS:C	2.57	0.43
1:A:1120:GLU:OE2	1:A:1121:ASN:N	2.51	0.43
1:A:253:ARG:NH2	1:A:257:ASN:CA	2.81	0.43
1:B:1090:ASN:ND2	1:B:1158:ILE:CD1	2.81	0.43
1:B:758:LEU:O	1:B:760:VAL:N	2.50	0.43
1:B:216:TYR:N	1:B:216:TYR:CD2	2.86	0.43
1:A:1352:PHE:CG	1:A:1353:GLY:N	2.83	0.43
1:B:85:LEU:O	1:B:86:THR:CB	2.67	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1480:PHE:O	1:B:1481:GLU:C	2.56	0.43
1:A:496:ILE:CD1	1:A:517:LYS:NZ	2.82	0.43
1:B:625:GLN:O	1:B:626:PHE:C	2.56	0.43
1:A:641:ASN:O	1:A:642:ASN:C	2.57	0.43
1:B:699:CYS:SG	1:B:727:ALA:O	2.76	0.43
1:A:560:TRP:CZ3	1:A:562:ASN:CB	3.02	0.43
1:B:1424:MET:N	1:B:1462:LEU:O	2.51	0.43
1:A:41:ILE:O	1:A:80:GLN:CA	2.67	0.43
1:B:1352:PHE:CG	1:B:1353:GLY:N	2.84	0.43
1:A:106:VAL:CG1	1:A:107:VAL:N	2.81	0.43
1:B:488:PRO:CG	1:B:499:TYR:OH	2.66	0.43
1:B:1284:PHE:CD2	1:B:1285:TYR:CE1	3.06	0.43
1:B:982:LEU:N	1:B:982:LEU:CD2	2.81	0.43
1:B:700:TYR:CE1	1:B:758:LEU:CB	3.02	0.43
1:B:820:PHE:CZ	1:B:821:LYS:O	2.72	0.43
1:A:352:TYR:CD1	1:A:375:VAL:CG1	3.01	0.43
1:A:995:GLU:O	1:A:996:GLY:O	2.36	0.43
1:B:472:ASN:OD1	1:B:473:HIS:CE1	2.72	0.43
1:B:647:HIS:C	1:B:649:ALA:N	2.71	0.43
1:A:968:VAL:O	1:A:969:PRO:O	2.37	0.43
1:B:1456:LYS:O	1:B:1459:HIS:N	2.52	0.43
1:A:1175:LEU:O	1:A:1179:THR:OG1	2.36	0.43
1:A:35:ALA:O	1:A:37:GLU:N	2.52	0.43
1:A:859:MET:CE	1:A:912:PHE:CZ	3.02	0.43
1:A:1016:VAL:O	1:A:1017:PRO:C	2.55	0.43
1:B:1342:LEU:CD2	1:B:1342:LEU:N	2.82	0.43
1:B:208:ASP:O	1:B:209:PHE:CG	2.72	0.43
1:B:1438:ASP:OD2	1:B:1478:ARG:N	2.50	0.43
1:A:1217:LEU:C	1:A:1218:VAL:CG2	2.84	0.43
1:B:1175:LEU:O	1:B:1179:THR:OG1	2.36	0.43
1:A:62:LYS:CD	1:A:105:GLU:OE2	2.67	0.43
1:B:834:VAL:CG2	1:B:1489:SER:OG	2.66	0.43
1:B:641:ASN:C	1:B:643:ALA:N	2.67	0.43
1:B:1283:GLY:O	1:B:1290:THR:OG1	2.36	0.43
1:A:971:THR:OG1	1:A:971:THR:O	2.36	0.43
1:A:1144:LEU:O	1:A:1148:THR:CG2	2.67	0.43
1:B:1193:TYR:CD1	1:B:1256:LEU:CB	3.02	0.43
1:A:820:PHE:CZ	1:A:821:LYS:O	2.72	0.43
1:A:330:ILE:CG2	1:A:337:SER:OG	2.67	0.43
1:A:465:LEU:CD2	1:A:542:VAL:O	2.66	0.43
4:B:2001:NAG:HO3	4:B:2002:NAG:C1	2.32	0.42
1:B:562:ASN:OD1	1:B:563:ILE:N	2.52	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:576:SER:CB	1:B:577:PRO:CD	2.97	0.42
1:B:1440:LYS:O	1:B:1444:GLU:CB	2.67	0.42
1:A:1290:THR:O	1:A:1294:ILE:CG1	2.67	0.42
1:B:270:GLY:N	1:B:324:TYR:O	2.52	0.42
1:A:1162:VAL:CG2	1:A:1163:LYS:N	2.82	0.42
1:A:1143:TYR:CE1	1:A:1186:PHE:CZ	3.07	0.42
1:A:132:LYS:NZ	1:A:139:GLN:NE2	2.67	0.42
1:A:1050:LYS:O	1:A:1053:MET:N	2.52	0.42
1:B:115:LYS:CG	1:B:116:ARG:N	2.82	0.42
1:B:968:VAL:O	1:B:971:THR:CG2	2.66	0.42
1:A:735:ALA:O	1:A:754:MET:SD	2.77	0.42
1:A:472:ASN:OD1	1:A:473:HIS:CE1	2.72	0.42
1:B:1467:ILE:N	1:B:1468:PRO:CD	2.82	0.42
1:A:111:PHE:CD2	1:A:112:SER:N	2.86	0.42
1:A:1057:MET:O	1:A:1060:ARG:N	2.52	0.42
1:A:61:ASP:O	1:A:61:ASP:CG	2.57	0.42
1:B:61:ASP:OD1	1:B:61:ASP:O	2.38	0.42
1:A:758:LEU:C	1:A:760:VAL:N	2.73	0.42
1:B:1148:THR:O	1:B:1152:ILE:CG1	2.67	0.42
1:A:100:SER:O	1:A:101:TYR:CD2	2.72	0.42
1:B:1093:VAL:O	1:B:1094:GLU:C	2.58	0.42
1:A:1028:GLY:O	1:A:1029:ASN:O	2.38	0.42
1:A:1203:PRO:O	1:A:1206:ARG:CB	2.68	0.42
1:B:1080:ALA:O	1:B:1084:ARG:N	2.53	0.42
1:A:961:TYR:OH	1:A:1343:ASN:CG	2.58	0.42
1:B:377:ASP:OD1	1:B:377:ASP:N	2.52	0.42
1:B:735:ALA:O	1:B:754:MET:SD	2.77	0.42
1:A:73:LEU:N	1:A:73:LEU:CD2	2.82	0.42
1:A:1239:VAL:CG2	1:A:1239:VAL:O	2.64	0.42
1:B:350:SER:OG	1:B:448:ALA:N	2.52	0.42
1:A:461:SER:C	1:A:463:SER:N	2.72	0.42
1:A:330:ILE:CG2	1:A:337:SER:CB	2.97	0.42
1:A:981:GLY:O	1:A:982:LEU:CB	2.68	0.42
1:A:55:SER:CB	1:A:67:SER:O	2.68	0.42
1:B:111:PHE:CD2	1:B:112:SER:N	2.87	0.42
1:A:1019:PHE:CE2	1:A:1020:TYR:CD1	3.08	0.42
1:A:284:GLN:O	1:A:310:LEU:CD1	2.68	0.42
1:B:758:LEU:C	1:B:760:VAL:N	2.73	0.42
1:B:1199:ASP:OD1	1:B:1199:ASP:C	2.58	0.42
1:B:518:PHE:O	1:B:519:SER:C	2.58	0.42
1:A:571:LEU:C	1:A:571:LEU:CD1	2.86	0.42
1:B:862:VAL:O	1:B:863:GLU:C	2.58	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1282:GLY:O	1:B:1284:PHE:N	2.53	0.42
1:A:626:PHE:O	1:A:628:GLU:N	2.53	0.42
1:B:438:ASP:O	1:B:439:ALA:O	2.38	0.42
1:B:1278:GLN:CA	1:B:1278:GLN:NE2	2.83	0.42
1:B:975:ARG:O	1:B:1340:VAL:N	2.52	0.42
1:B:585:GLY:CA	1:B:790:LEU:O	2.68	0.42
1:B:1159:CYS:N	1:B:1160:PRO:CD	2.82	0.42
1:B:1429:PRO:O	1:B:1430:THR:C	2.58	0.42
1:A:935:LYS:O	1:A:1365:VAL:O	2.36	0.42
1:A:1277:GLU:CA	1:A:1277:GLU:OE2	2.67	0.42
1:A:1496:TYR:CD1	1:A:1496:TYR:C	2.93	0.42
1:A:968:VAL:CG2	1:A:968:VAL:O	2.67	0.42
1:B:1318:LYS:CG	1:B:1319:HIS:CE1	3.03	0.42
1:B:57:LYS:NZ	1:B:105:GLU:OE1	2.52	0.42
1:A:1279:ARG:CG	1:A:1284:PHE:CB	2.98	0.42
1:B:354:LEU:CD1	1:B:435:VAL:CG1	2.98	0.42
1:A:855:PHE:CD1	1:A:856:CYS:N	2.87	0.42
1:A:1069:TRP:NE1	1:A:1463:GLN:NE2	2.68	0.42
1:B:564:GLU:O	1:B:566:LYS:N	2.53	0.42
1:B:125:PHE:CD1	1:B:125:PHE:N	2.87	0.42
1:A:497:THR:OG1	1:A:498:HIS:ND1	2.52	0.42
1:B:415:ASP:OD1	1:B:417:VAL:CG2	2.67	0.42
1:A:1054:LEU:C	1:A:1056:ILE:N	2.71	0.42
1:A:616:ALA:O	1:A:617:LYS:C	2.57	0.42
1:B:1207:SER:O	1:B:1210:SER:OG	2.37	0.42
1:B:157:ARG:CZ	1:B:209:PHE:CE1	3.03	0.42
1:B:321:LYS:C	1:B:322:TYR:CD2	2.93	0.42
1:A:1212:LEU:O	1:A:1215:GLU:N	2.53	0.42
1:A:1279:ARG:CD	1:A:1284:PHE:CD2	3.03	0.41
1:A:1435:ASN:O	1:A:1436:GLU:C	2.59	0.41
1:A:356:LEU:CD1	1:A:452:TYR:CD1	3.03	0.41
1:A:1227:PHE:CA	1:A:1228:TRP:CE3	3.03	0.41
1:A:270:GLY:N	1:A:283:MET:CE	2.83	0.41
1:B:35:ALA:O	1:B:37:GLU:N	2.53	0.41
1:B:110:HIS:O	1:B:110:HIS:CD2	2.73	0.41
1:A:667:GLU:N	1:A:667:GLU:OE1	2.53	0.41
1:A:1019:PHE:CD2	1:A:1020:TYR:CE1	3.08	0.41
1:B:1162:VAL:O	1:B:1165:ASP:N	2.52	0.41
1:B:1324:HIS:CE1	1:B:1326:TYR:CE2	3.07	0.41
2:X:146:LEU:CD2	2:X:147:ASP:N	2.83	0.41
1:A:1084:ARG:NE	1:A:1088:GLN:OE1	2.53	0.41
1:A:862:VAL:O	1:A:863:GLU:C	2.57	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:415:ASP:OD1	1:A:417:VAL:CG2	2.68	0.41
1:A:232:GLU:OE2	1:A:251:LYS:CE	2.68	0.41
1:A:295:GLY:C	1:A:296:ILE:CG1	2.88	0.41
1:B:1081:PHE:CD2	1:B:1081:PHE:C	2.93	0.41
1:A:1076:THR:N	1:A:1120:GLU:OE2	2.52	0.41
1:A:319:ASN:C	1:A:320:ASN:ND2	2.73	0.41
1:A:1496:TYR:CD1	1:A:1496:TYR:O	2.74	0.41
1:A:1118:PHE:CD2	1:A:1148:THR:OG1	2.73	0.41
1:B:1118:PHE:O	1:B:1144:LEU:CD2	2.68	0.41
1:B:1152:ILE:O	1:B:1153:ARG:C	2.58	0.41
1:B:160:VAL:CG2	1:B:174:VAL:O	2.69	0.41
1:A:115:LYS:CG	1:A:116:ARG:N	2.83	0.41
1:A:1503:LYS:CD	1:A:1503:LYS:N	2.83	0.41
1:B:1466:SER:OG	1:B:1468:PRO:CD	2.68	0.41
1:A:1380:LYS:O	1:A:1405:CYS:N	2.53	0.41
1:B:386:VAL:CG2	1:B:411:THR:CG2	2.98	0.41
1:B:41:ILE:O	1:B:81:ASN:N	2.53	0.41
1:A:1148:THR:O	1:A:1152:ILE:CD1	2.69	0.41
1:A:700:TYR:O	1:A:702:GLY:N	2.53	0.41
1:A:1244:THR:O	1:A:1285:TYR:CD2	2.73	0.41
1:B:752:LEU:C	1:B:753:HIS:CG	2.93	0.41
1:A:1440:LYS:O	1:A:1444:GLU:CB	2.68	0.41
1:A:644:ASN:C	1:A:644:ASN:ND2	2.74	0.41
1:B:169:SER:C	1:B:170:GLU:O	2.57	0.41
1:A:563:ILE:CG1	1:A:564:GLU:N	2.84	0.41
1:A:1153:ARG:O	1:A:1155:ALA:N	2.53	0.41
1:B:1162:VAL:O	1:B:1164:ILE:N	2.53	0.41
1:A:1445:GLY:O	1:A:1448:GLN:CB	2.69	0.41
1:B:23:TYR:N	1:B:23:TYR:CD1	2.88	0.41
1:B:56:ILE:O	1:B:66:TYR:CD2	2.74	0.41
1:B:349:LEU:CD2	1:B:349:LEU:C	2.88	0.41
1:B:1022:PHE:CD2	1:B:1092:TYR:CD2	3.09	0.41
1:B:1405:CYS:N	1:B:1474:CYS:SG	2.87	0.41
1:A:897:THR:C	1:A:898:PHE:CD2	2.94	0.41
1:B:1176:LEU:O	1:B:1178:ASN:N	2.54	0.41
1:A:1424:MET:N	1:A:1462:LEU:O	2.54	0.41
1:A:1313:ILE:CG2	1:A:1314:ASP:N	2.84	0.41
1:A:237:PHE:O	1:A:238:ILE:CG1	2.69	0.41
1:B:1284:PHE:CD2	1:B:1285:TYR:CD1	3.08	0.41
1:A:1497:GLU:O	1:A:1498:TYR:C	2.58	0.41
1:B:193:ASN:OD1	1:B:1070:LYS:CE	2.69	0.41
1:A:121:TYR:O	1:A:210:SER:N	2.53	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:257:ASN:CG	1:B:257:ASN:O	2.59	0.41
1:A:614:ARG:O	1:A:615:GLY:C	2.59	0.41
1:A:438:ASP:C	1:A:439:ALA:O	2.58	0.41
1:A:149:ASN:O	1:A:150:ASP:C	2.58	0.41
1:B:1443:VAL:CG2	1:B:1444:GLU:N	2.84	0.41
1:B:897:THR:O	1:B:898:PHE:CD2	2.74	0.41
1:B:153:LYS:CB	1:B:154:PRO:CD	2.99	0.41
1:A:1173:ASN:O	1:A:1174:PHE:C	2.59	0.41
1:B:497:THR:CG2	1:B:498:HIS:N	2.84	0.41
1:A:934:VAL:CG2	1:A:1366:HIS:CD2	3.04	0.41
1:A:709:GLU:CA	1:A:713:GLN:OE1	2.69	0.41
1:A:355:ASN:O	1:A:356:LEU:C	2.58	0.41
1:B:185:PHE:CB	1:B:186:PRO:CD	2.98	0.41
1:B:240:TYR:CE1	1:B:443:PRO:CG	3.04	0.41
1:B:614:ARG:O	1:B:615:GLY:C	2.59	0.41
1:B:935:LYS:O	1:B:1365:VAL:O	2.39	0.41
1:B:409:SER:OG	1:B:410:VAL:N	2.53	0.41
1:B:1475:VAL:CG2	1:B:1476:ARG:N	2.84	0.41
1:B:1280:TYR:OH	1:B:1337:PRO:CG	2.69	0.40
1:A:1443:VAL:CG2	1:A:1444:GLU:N	2.82	0.40
1:A:1008:ALA:O	1:A:1011:GLU:N	2.54	0.40
1:A:518:PHE:O	1:A:519:SER:C	2.60	0.40
1:A:101:TYR:CE1	1:A:116:ARG:CZ	3.05	0.40
1:B:494:ASP:O	1:B:496:ILE:CD1	2.69	0.40
1:A:1054:LEU:O	1:A:1057:MET:N	2.54	0.40
1:B:170:GLU:O	1:B:171:VAL:CG2	2.68	0.40
1:A:1180:LEU:CD1	1:A:1204:GLN:NE2	2.84	0.40
1:B:1295:GLU:O	1:B:1296:GLY:O	2.40	0.40
1:B:1452:ASP:O	1:B:1463:GLN:N	2.54	0.40
1:B:569:ASN:OD1	1:B:596:MET:CB	2.69	0.40
1:A:991:VAL:O	1:A:991:VAL:CG1	2.69	0.40
1:A:1280:TYR:CD2	1:A:1281:GLY:N	2.89	0.40
1:B:1019:PHE:CE2	1:B:1020:TYR:CD1	3.08	0.40
1:A:357:VAL:O	1:A:358:ALA:C	2.59	0.40
1:B:833:VAL:O	1:B:930:VAL:N	2.55	0.40
1:A:1323:LEU:CG	1:A:1324:HIS:N	2.84	0.40
1:A:342:ILE:O	1:A:343:PRO:C	2.60	0.40
1:B:1364:VAL:CG1	1:B:1365:VAL:N	2.84	0.40
1:A:1323:LEU:CD1	1:A:1324:HIS:N	2.85	0.40
1:B:604:ALA:N	1:B:773:TRP:O	2.55	0.40
1:A:1037:ASP:OD1	1:A:1038:PRO:N	2.54	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	1449/1676 (86%)	1039 (72%)	255 (18%)	155 (11%)	1	17
1	B	1449/1676 (86%)	1026 (71%)	274 (19%)	149 (10%)	1	19
2	X	100/103 (97%)	86 (86%)	9 (9%)	5 (5%)	3	43
2	Y	100/103 (97%)	84 (84%)	11 (11%)	5 (5%)	3	43
All	All	3098/3558 (87%)	2235 (72%)	549 (18%)	314 (10%)	1	20

All (314) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	TYR
1	A	86	THR
1	A	97	ASN
1	A	99	VAL
1	A	170	GLU
1	A	174	VAL
1	A	207	GLU
1	A	209	PHE
1	A	282	MET
1	A	289	ASN
1	A	291	MET
1	A	305	THR
1	A	316	GLU
1	A	317	ASP
1	A	318	LEU
1	A	426	SER
1	A	457	TYR
1	A	477	LEU
1	A	480	GLU
1	A	489	LYS
1	A	490	SER
1	A	519	SER
1	A	520	ASP
1	A	522	SER

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Mol	Chain	Res	Type
1	A	609	VAL
1	A	610	TYR
1	A	638	GLY
1	A	657	ALA
1	A	662	SER
1	A	700	TYR
1	A	704	CYS
1	A	720	LEU
1	A	863	GLU
1	A	1231	ASN
1	A	1264	ILE
1	A	1275	SER
1	A	1284	PHE
1	A	1286	SER
1	A	1297	LEU
1	A	1304	VAL
1	A	1311	MET
1	A	1335	GLY
1	A	1342	LEU
1	A	1373	GLU
1	A	1433	SER
2	X	185	LYS
1	B	59	TYR
1	B	97	ASN
1	B	99	VAL
1	B	133	PRO
1	B	174	VAL
1	B	207	GLU
1	B	209	PHE
1	B	282	MET
1	B	289	ASN
1	B	305	THR
1	B	426	SER
1	B	457	TYR
1	B	490	SER
1	B	520	ASP
1	B	522	SER
1	B	609	VAL
1	B	610	TYR
1	B	638	GLY
1	B	657	ALA
1	B	661	ASP

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Mol	Chain	Res	Type
1	B	700	TYR
1	B	704	CYS
1	B	720	LEU
1	B	863	GLU
1	B	949	ILE
1	B	1068	VAL
1	B	1097	GLN
1	B	1231	ASN
1	B	1264	ILE
1	B	1284	PHE
1	B	1311	MET
1	B	1335	GLY
1	B	1342	LEU
1	B	1373	GLU
1	B	1433	SER
2	Y	185	LYS
1	A	90	LYS
1	A	101	TYR
1	A	150	ASP
1	A	302	ASP
1	A	304	GLU
1	A	306	ALA
1	A	307	VAL
1	A	308	LYS
1	A	523	TYR
1	A	615	GLY
1	A	619	PRO
1	A	661	ASP
1	A	669	CYS
1	A	705	VAL
1	A	814	THR
1	A	817	ALA
1	A	909	ASN
1	A	931	PRO
1	A	996	GLY
1	A	1007	SER
1	A	1029	ASN
1	A	1055	SER
1	A	1097	GLN
1	A	1166	THR
1	A	1216	ALA
1	A	1296	GLY

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Mol	Chain	Res	Type
1	A	1312	ASP
1	A	1321	GLY
1	A	1352	PHE
1	A	1457	ASP
1	A	1486	GLY
2	X	144	GLY
1	B	28	PRO
1	B	86	THR
1	B	90	LYS
1	B	101	TYR
1	B	170	GLU
1	B	291	MET
1	B	302	ASP
1	B	304	GLU
1	B	307	VAL
1	B	308	LYS
1	B	378	SER
1	B	388	VAL
1	B	480	GLU
1	B	489	LYS
1	B	495	LYS
1	B	607	SER
1	B	612	VAL
1	B	619	PRO
1	B	662	SER
1	B	669	CYS
1	B	710	THR
1	B	814	THR
1	B	817	ALA
1	B	909	ASN
1	B	931	PRO
1	B	948	GLY
1	B	996	GLY
1	B	1029	ASN
1	B	1098	ASN
1	B	1162	VAL
1	B	1177	GLU
1	B	1216	ALA
1	B	1286	SER
1	B	1296	GLY
1	B	1297	LEU
1	B	1304	VAL

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Mol	Chain	Res	Type
1	B	1310	SER
2	Y	144	GLY
2	Y	195	ASP
1	A	85	LEU
1	A	133	PRO
1	A	173	MET
1	A	231	ILE
1	A	272	ARG
1	A	356	LEU
1	A	388	VAL
1	A	491	PRO
1	A	612	VAL
1	A	625	GLN
1	A	648	LEU
1	A	660	ASP
1	A	663	GLN
1	A	691	LYS
1	A	793	SER
1	A	1240	PRO
1	A	1247	MET
1	A	1263	ASP
1	A	1308	ARG
1	A	1310	SER
2	X	195	ASP
1	B	36	SER
1	B	150	ASP
1	B	186	PRO
1	B	240	TYR
1	B	306	ALA
1	B	356	LEU
1	B	445	GLU
1	B	491	PRO
1	B	519	SER
1	B	617	LYS
1	B	627	LEU
1	B	660	ASP
1	B	663	GLN
1	B	666	ASP
1	B	691	LYS
1	B	793	SER
1	B	856	CYS
1	B	1105	LEU

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Mol	Chain	Res	Type
1	B	1240	PRO
1	B	1269	PRO
1	B	1280	TYR
1	B	1308	ARG
1	B	1312	ASP
1	B	1341	LEU
1	B	1352	PHE
1	B	1457	ASP
1	A	62	LYS
1	A	129	HIS
1	A	141	VAL
1	A	166	PRO
1	A	186	PRO
1	A	425	PRO
1	A	492	TYR
1	A	495	LYS
1	A	607	SER
1	A	627	LEU
1	A	717	ARG
1	A	815	VAL
1	A	856	CYS
1	A	993	SER
1	A	1016	VAL
1	A	1101	CYS
1	A	1113	LEU
1	A	1114	ASP
1	A	1153	ARG
1	A	1177	GLU
1	A	1280	TYR
1	A	1341	LEU
1	A	1349	SER
1	A	1444	GLU
1	A	1468	PRO
1	B	62	LYS
1	B	166	PRO
1	B	173	MET
1	B	398	ASN
1	B	425	PRO
1	B	492	TYR
1	B	625	GLN
1	B	759	PRO
1	B	952	THR

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Mol	Chain	Res	Type
1	B	982	LEU
1	B	1007	SER
1	B	1055	SER
1	B	1057	MET
1	B	1084	ARG
1	B	1153	ARG
1	B	1444	GLU
1	A	497	THR
1	A	536	PRO
1	A	666	ASP
1	A	710	THR
1	A	759	PRO
1	A	892	SER
1	A	969	PRO
1	A	1122	SER
1	A	1481	GLU
1	A	1501	PRO
1	B	78	LYS
1	B	85	LEU
1	B	312	TYR
1	B	320	ASN
1	B	536	PRO
1	B	664	GLU
1	B	667	GLU
1	B	892	SER
1	B	993	SER
1	B	1126	PRO
1	B	1218	VAL
1	B	1239	VAL
1	B	1468	PRO
1	B	1501	PRO
1	A	299	VAL
1	A	617	LYS
1	A	667	GLU
1	A	760	VAL
1	A	1036	SER
1	A	1126	PRO
1	A	1181	PRO
1	A	1432	ILE
1	B	111	PHE
1	B	343	PRO
1	B	565	GLU

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Mol	Chain	Res	Type
1	B	760	VAL
1	B	815	VAL
1	B	1009	GLU
1	B	1263	ASP
1	B	1486	GLY
1	A	686	ILE
1	A	1269	PRO
2	X	178	GLY
1	A	1108	VAL
2	X	196	GLY
1	B	705	VAL
1	B	1016	VAL
1	B	1268	ASN
1	B	1347	ILE
2	Y	196	GLY
1	A	92	LEU
1	A	765	ILE
1	A	1135	VAL
1	A	1218	VAL
1	A	1239	VAL
1	B	92	LEU
1	B	231	ILE
1	B	615	GLY
1	B	1038	PRO
1	B	1432	ILE
1	A	28	PRO
1	A	296	ILE
1	A	510	ILE
1	A	1162	VAL
1	B	171	VAL
1	B	345	ILE
1	B	686	ILE
2	Y	178	GLY
1	A	238	ILE
1	A	668	PRO
1	A	1038	PRO
1	A	1068	VAL
1	B	668	PRO

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	1296/1484 (87%)	1061 (82%)	235 (18%)	2	19
1	B	1296/1484 (87%)	1051 (81%)	245 (19%)	2	17
2	X	93/94 (99%)	87 (94%)	6 (6%)	24	72
2	Y	93/94 (99%)	86 (92%)	7 (8%)	19	66
All	All	2778/3156 (88%)	2285 (82%)	493 (18%)	3	20

All (493) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	THR
1	A	23	TYR
1	A	41	ILE
1	A	42	GLN
1	A	51	ASP
1	A	56	ILE
1	A	64	PHE
1	A	73	LEU
1	A	81	ASN
1	A	88	GLN
1	A	100	SER
1	A	109	LYS
1	A	112	SER
1	A	114	SER
1	A	116	ARG
1	A	119	ILE
1	A	123	ASN
1	A	125	PHE
1	A	126	LEU
1	A	128	ILE
1	A	130	THR
1	A	131	ASP
1	A	140	SER
1	A	143	VAL
1	A	144	ARG
1	A	151	ASP

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Mol	Chain	Res	Type
1	A	161	LEU
1	A	162	THR
1	A	163	PHE
1	A	169	SER
1	A	175	GLU
1	A	176	GLU
1	A	177	ILE
1	A	180	ILE
1	A	184	SER
1	A	192	SER
1	A	195	ARG
1	A	224	LEU
1	A	231	ILE
1	A	232	GLU
1	A	235	TYR
1	A	242	ASN
1	A	249	THR
1	A	264	ASP
1	A	273	GLU
1	A	280	LYS
1	A	296	ILE
1	A	299	VAL
1	A	312	TYR
1	A	313	TYR
1	A	324	TYR
1	A	333	THR
1	A	349	LEU
1	A	354	LEU
1	A	363	LEU
1	A	364	LYS
1	A	373	VAL
1	A	378	SER
1	A	381	GLN
1	A	383	VAL
1	A	386	VAL
1	A	389	THR
1	A	393	GLN
1	A	394	THR
1	A	403	ASP
1	A	411	THR
1	A	419	SER
1	A	421	VAL

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Mol	Chain	Res	Type
1	A	422	LEU
1	A	423	ASN
1	A	431	LEU
1	A	433	PHE
1	A	436	LYS
1	A	441	ASP
1	A	457	TYR
1	A	461	SER
1	A	466	TYR
1	A	469	TRP
1	A	473	HIS
1	A	476	LEU
1	A	482	LEU
1	A	484	ILE
1	A	492	TYR
1	A	493	ILE
1	A	495	LYS
1	A	497	THR
1	A	504	LEU
1	A	518	PHE
1	A	528	ILE
1	A	535	VAL
1	A	539	ARG
1	A	540	LEU
1	A	541	LEU
1	A	544	TYR
1	A	556	SER
1	A	563	ILE
1	A	570	GLN
1	A	573	VAL
1	A	588	VAL
1	A	589	SER
1	A	594	THR
1	A	624	PHE
1	A	631	ASP
1	A	640	LEU
1	A	641	ASN
1	A	644	ASN
1	A	648	LEU
1	A	652	THR
1	A	653	PHE
1	A	667	GLU

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Mol	Chain	Res	Type
1	A	673	LEU
1	A	680	GLN
1	A	705	VAL
1	A	710	THR
1	A	711	CYS
1	A	712	GLU
1	A	724	CYS
1	A	729	THR
1	A	753	HIS
1	A	758	LEU
1	A	767	SER
1	A	786	LEU
1	A	790	LEU
1	A	799	ILE
1	A	800	GLN
1	A	802	ILE
1	A	804	ILE
1	A	809	ILE
1	A	814	THR
1	A	840	GLN
1	A	866	CYS
1	A	867	THR
1	A	886	GLN
1	A	887	LYS
1	A	891	SER
1	A	894	HIS
1	A	895	LEU
1	A	897	THR
1	A	900	VAL
1	A	901	LEU
1	A	903	LEU
1	A	908	HIS
1	A	921	GLU
1	A	924	VAL
1	A	926	THR
1	A	927	LEU
1	A	935	LYS
1	A	936	ARG
1	A	942	VAL
1	A	949	ILE
1	A	952	THR
1	A	957	LYS

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Mol	Chain	Res	Type
1	A	961	TYR
1	A	962	ARG
1	A	973	ILE
1	A	979	VAL
1	A	980	LYS
1	A	982	LEU
1	A	983	LEU
1	A	986	GLU
1	A	995	GLU
1	A	998	ASN
1	A	1001	THR
1	A	1003	LEU
1	A	1015	VAL
1	A	1024	TYR
1	A	1027	THR
1	A	1029	ASN
1	A	1033	ILE
1	A	1039	LEU
1	A	1040	ILE
1	A	1053	MET
1	A	1056	ILE
1	A	1076	THR
1	A	1084	ARG
1	A	1096	ASN
1	A	1101	CYS
1	A	1115	ASN
1	A	1127	ILE
1	A	1128	LYS
1	A	1132	THR
1	A	1140	ASN
1	A	1147	PHE
1	A	1148	THR
1	A	1158	ILE
1	A	1161	LEU
1	A	1164	ILE
1	A	1168	LEU
1	A	1200	LYS
1	A	1208	ILE
1	A	1210	SER
1	A	1217	LEU
1	A	1218	VAL
1	A	1228	TRP

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Mol	Chain	Res	Type
1	A	1229	LYS
1	A	1232	LEU
1	A	1251	THR
1	A	1257	THR
1	A	1274	LEU
1	A	1278	GLN
1	A	1291	ILE
1	A	1297	LEU
1	A	1301	SER
1	A	1307	LEU
1	A	1311	MET
1	A	1313	ILE
1	A	1316	SER
1	A	1318	LYS
1	A	1325	ASN
1	A	1332	ASN
1	A	1334	LEU
1	A	1336	ARG
1	A	1342	LEU
1	A	1343	ASN
1	A	1345	ASP
1	A	1347	ILE
1	A	1365	VAL
1	A	1376	SER
1	A	1383	THR
1	A	1401	ARG
1	A	1437	GLU
1	A	1443	VAL
1	A	1464	LEU
1	A	1465	ASN
1	A	1476	ARG
1	A	1480	PHE
1	A	1483	PHE
1	A	1487	PHE
1	A	1488	LEU
1	A	1496	TYR
1	A	1500	ARG
1	A	1503	LYS
1	A	1507	MET
1	A	1509	TYR
1	A	1511	THR
2	X	134	THR

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Mol	Chain	Res	Type
2	X	136	LEU
2	X	146	LEU
2	X	150	ILE
2	X	166	ASP
2	X	184	THR
1	B	23	TYR
1	B	24	VAL
1	B	26	SER
1	B	41	ILE
1	B	42	GLN
1	B	51	ASP
1	B	56	ILE
1	B	59	TYR
1	B	64	PHE
1	B	73	LEU
1	B	81	ASN
1	B	88	GLN
1	B	100	SER
1	B	109	LYS
1	B	112	SER
1	B	114	SER
1	B	116	ARG
1	B	119	ILE
1	B	123	ASN
1	B	125	PHE
1	B	126	LEU
1	B	128	ILE
1	B	130	THR
1	B	131	ASP
1	B	148	LEU
1	B	151	ASP
1	B	160	VAL
1	B	161	LEU
1	B	162	THR
1	B	163	PHE
1	B	175	GLU
1	B	176	GLU
1	B	177	ILE
1	B	180	ILE
1	B	184	SER
1	B	188	PHE
1	B	189	LYS

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Mol	Chain	Res	Type
1	B	194	PRO
1	B	195	ARG
1	B	212	THR
1	B	224	LEU
1	B	231	ILE
1	B	232	GLU
1	B	235	TYR
1	B	242	ASN
1	B	249	THR
1	B	253	ARG
1	B	257	ASN
1	B	264	ASP
1	B	273	GLU
1	B	280	LYS
1	B	290	THR
1	B	296	ILE
1	B	299	VAL
1	B	312	TYR
1	B	317	ASP
1	B	318	LEU
1	B	324	TYR
1	B	333	THR
1	B	349	LEU
1	B	354	LEU
1	B	363	LEU
1	B	364	LYS
1	B	373	VAL
1	B	378	SER
1	B	379	LEU
1	B	383	VAL
1	B	386	VAL
1	B	389	THR
1	B	393	GLN
1	B	394	THR
1	B	403	ASP
1	B	411	THR
1	B	421	VAL
1	B	422	LEU
1	B	423	ASN
1	B	431	LEU
1	B	433	PHE
1	B	436	LYS

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Mol	Chain	Res	Type
1	B	441	ASP
1	B	457	TYR
1	B	461	SER
1	B	463	SER
1	B	466	TYR
1	B	469	TRP
1	B	473	HIS
1	B	476	LEU
1	B	484	ILE
1	B	492	TYR
1	B	493	ILE
1	B	495	LYS
1	B	497	THR
1	B	500	ASN
1	B	502	LEU
1	B	509	ILE
1	B	517	LYS
1	B	528	ILE
1	B	535	VAL
1	B	539	ARG
1	B	540	LEU
1	B	541	LEU
1	B	544	TYR
1	B	553	GLU
1	B	556	SER
1	B	563	ILE
1	B	570	GLN
1	B	573	VAL
1	B	588	VAL
1	B	589	SER
1	B	594	THR
1	B	624	PHE
1	B	640	LEU
1	B	641	ASN
1	B	644	ASN
1	B	648	LEU
1	B	652	THR
1	B	653	PHE
1	B	667	GLU
1	B	669	CYS
1	B	673	LEU
1	B	680	GLN

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Mol	Chain	Res	Type
1	B	699	CYS
1	B	704	CYS
1	B	705	VAL
1	B	707	ASN
1	B	711	CYS
1	B	729	THR
1	B	753	HIS
1	B	758	LEU
1	B	767	SER
1	B	786	LEU
1	B	790	LEU
1	B	795	THR
1	B	799	ILE
1	B	802	ILE
1	B	804	ILE
1	B	809	ILE
1	B	814	THR
1	B	840	GLN
1	B	866	CYS
1	B	867	THR
1	B	886	GLN
1	B	887	LYS
1	B	891	SER
1	B	894	HIS
1	B	895	LEU
1	B	897	THR
1	B	900	VAL
1	B	901	LEU
1	B	903	LEU
1	B	908	HIS
1	B	924	VAL
1	B	926	THR
1	B	927	LEU
1	B	932	GLU
1	B	935	LYS
1	B	936	ARG
1	B	952	THR
1	B	961	TYR
1	B	962	ARG
1	B	972	GLU
1	B	973	ILE
1	B	975	ARG

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Mol	Chain	Res	Type
1	B	976	ILE
1	B	980	LYS
1	B	982	LEU
1	B	983	LEU
1	B	986	GLU
1	B	995	GLU
1	B	998	ASN
1	B	1001	THR
1	B	1003	LEU
1	B	1015	VAL
1	B	1024	TYR
1	B	1027	THR
1	B	1029	ASN
1	B	1040	ILE
1	B	1053	MET
1	B	1056	ILE
1	B	1069	TRP
1	B	1096	ASN
1	B	1108	VAL
1	B	1115	ASN
1	B	1127	ILE
1	B	1128	LYS
1	B	1132	THR
1	B	1140	ASN
1	B	1147	PHE
1	B	1148	THR
1	B	1158	ILE
1	B	1161	LEU
1	B	1164	ILE
1	B	1168	LEU
1	B	1200	LYS
1	B	1206	ARG
1	B	1208	ILE
1	B	1210	SER
1	B	1213	LYS
1	B	1217	LEU
1	B	1218	VAL
1	B	1226	ARG
1	B	1228	TRP
1	B	1232	LEU
1	B	1251	THR
1	B	1257	THR

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Mol	Chain	Res	Type
1	B	1269	PRO
1	B	1271	ILE
1	B	1278	GLN
1	B	1279	ARG
1	B	1280	TYR
1	B	1297	LEU
1	B	1301	SER
1	B	1307	LEU
1	B	1311	MET
1	B	1313	ILE
1	B	1316	SER
1	B	1318	LYS
1	B	1325	ASN
1	B	1332	ASN
1	B	1334	LEU
1	B	1336	ARG
1	B	1342	LEU
1	B	1343	ASN
1	B	1344	ASP
1	B	1345	ASP
1	B	1347	ILE
1	B	1358	THR
1	B	1376	SER
1	B	1383	THR
1	B	1401	ARG
1	B	1443	VAL
1	B	1464	LEU
1	B	1465	ASN
1	B	1474	CYS
1	B	1476	ARG
1	B	1480	PHE
1	B	1483	PHE
1	B	1487	PHE
1	B	1488	LEU
1	B	1496	TYR
1	B	1500	ARG
1	B	1502	ASP
1	B	1503	LYS
1	B	1507	MET
1	B	1509	TYR
2	Y	134	THR
2	Y	136	LEU

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Mol	Chain	Res	Type
2	Y	138	VAL
2	Y	146	LEU
2	Y	150	ILE
2	Y	184	THR
2	Y	210	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

4 carbohydrates 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	$\# Z > 2$
4	NAG	A	2001	1,4	12,14,15	0.62	1 (8%)	15,19,21	0.85	1 (6%)
4	NAG	A	2002	4	12,14,15	0.63	0	15,19,21	1.10	1 (6%)
4	NAG	B	2001	1,4	12,14,15	0.65	1 (8%)	15,19,21	1.06	1 (6%)
4	NAG	B	2002	4	12,14,15	0.64	0	15,19,21	1.10	1 (6%)

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
4	NAG	A	2001	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	2002	4	-	0/6/23/26	0/1/1/1
4	NAG	B	2001	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	2002	4	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2001	NAG	O5-C5	-2.08	1.41	1.45
4	A	2001	NAG	O5-C5	-2.03	1.41	1.45

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2002	NAG	O5-C5-C6	3.50	110.65	106.98
4	A	2002	NAG	O5-C5-C6	3.30	110.45	106.98
4	A	2001	NAG	C3-C2-N2	-2.34	108.19	111.76
4	B	2001	NAG	C3-C2-N2	-2.21	108.40	111.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 5 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	1680	1	12,14,15	0.67	1 (8%)	15,19,21	1.49	2 (13%)
5	NAG	B	1679	1	12,14,15	0.72	1 (8%)	15,19,21	1.50	3 (20%)

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
5	NAG	A	1680	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1679	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1679	NAG	O5-C5	-2.18	1.41	1.45
5	A	1680	NAG	O5-C5	-2.03	1.41	1.45

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1680	NAG	O5-C5-C6	4.53	111.73	106.98
5	B	1679	NAG	O5-C5-C6	4.03	111.21	106.98
5	B	1679	NAG	C3-C2-N2	-2.75	107.57	111.76
5	A	1680	NAG	C3-C2-N2	-2.53	107.91	111.76
5	B	1679	NAG	O5-C5-C4	-2.13	107.95	110.65

There are no chirality outliers.

There are no torsion outliers.

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, 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	1459/1676 (87%)	0.56	71 (4%)	28 25	81, 190, 311, 455	0
1	B	1459/1676 (87%)	0.54	54 (3%)	39 33	85, 190, 308, 475	0
2	X	102/103 (99%)	1.06	21 (20%)	1 3	157, 292, 386, 530	0
2	Y	102/103 (99%)	1.02	19 (18%)	2 4	156, 292, 377, 494	0
All	All	3122/3558 (87%)	0.58	165 (5%)	25 23	81, 194, 328, 530	0

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	X	193	LEU	9.2
2	Y	193	LEU	8.4
1	B	683	ILE	6.2
1	A	683	ILE	5.8
1	A	671	GLU	5.6
2	X	228	LEU	5.4
1	A	883	CYS	5.4
1	A	672	ILE	5.3
1	A	759	PRO	5.0
2	Y	159	GLU	4.9
1	B	671	GLU	4.8
1	B	252	ALA	4.8
2	Y	228	LEU	4.6
2	X	159	GLU	4.5
1	A	1511	THR	4.1
2	X	158	GLU	4.1
1	A	335	GLY	4.1
1	A	252	ALA	4.0
2	X	191	ILE	3.9
1	B	689	LYS	3.8
1	B	1511	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	672	ILE	3.8
2	Y	157	LYS	3.7
1	B	668	PRO	3.6
1	A	684	GLU	3.6
1	A	689	LYS	3.6
1	A	670	LYS	3.5
2	X	227	THR	3.5
1	B	117	MET	3.4
2	X	197	GLU	3.4
1	B	335	GLY	3.4
1	A	258	LYS	3.4
2	X	226	VAL	3.4
2	X	189	ILE	3.3
2	Y	189	ILE	3.3
2	Y	224	ILE	3.3
1	B	809	ILE	3.3
2	Y	191	ILE	3.2
2	X	157	LYS	3.2
1	B	258	LYS	3.2
1	A	117	MET	3.2
1	B	759	PRO	3.1
2	Y	158	GLU	3.1
1	A	1402	ILE	3.1
1	A	571	LEU	3.1
1	B	857	VAL	3.1
1	A	668	PRO	3.1
1	B	309	GLU	3.0
1	A	309	GLU	3.0
1	A	1428	LEU	2.9
2	Y	216	LEU	2.9
1	A	334	GLY	2.9
1	B	883	CYS	2.9
1	A	809	ILE	2.9
1	A	882	LYS	2.8
1	A	256	TYR	2.8
1	B	615	GLY	2.8
1	B	1473	LEU	2.8
1	B	1399	TYR	2.8
2	Y	192	ASN	2.8
1	A	831	TYR	2.7
1	B	720	LEU	2.7
1	A	667	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
2	Y	227	THR	2.7
1	B	731	CYS	2.7
1	A	467	ILE	2.7
1	B	571	LEU	2.6
1	A	857	VAL	2.6
1	B	684	GLU	2.6
1	B	670	LYS	2.6
2	Y	226	VAL	2.6
1	B	1356	LEU	2.6
1	B	666	ASP	2.6
2	Y	221	ILE	2.6
1	B	256	TYR	2.6
2	X	224	ILE	2.6
1	B	817	ALA	2.5
1	A	613	GLN	2.5
1	A	331	GLU	2.5
1	A	867	THR	2.5
1	A	866	CYS	2.5
2	X	216	LEU	2.5
1	B	882	LYS	2.5
1	A	841	LEU	2.5
1	A	902	PRO	2.5
2	X	230	GLN	2.5
1	B	331	GLU	2.5
1	A	352	TYR	2.4
1	A	86	THR	2.4
1	A	921	GLU	2.4
1	B	467	ILE	2.4
1	B	841	LEU	2.4
1	B	867	THR	2.4
1	B	329	VAL	2.4
2	X	192	ASN	2.4
2	Y	230	GLN	2.4
1	A	1356	LEU	2.4
1	B	334	GLY	2.4
1	B	47	THR	2.4
1	A	1473	LEU	2.4
1	A	180	ILE	2.4
1	A	85	LEU	2.4
1	A	757	LEU	2.4
1	B	694	VAL	2.3
1	A	47	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	336	PHE	2.3
1	B	85	LEU	2.3
2	X	221	ILE	2.3
1	A	1399	TYR	2.3
1	A	269	PHE	2.3
1	A	666	ASP	2.3
1	A	552	ALA	2.3
1	A	859	MET	2.3
1	A	760	VAL	2.3
1	B	866	CYS	2.3
2	X	207	LEU	2.3
2	X	212	MET	2.2
1	B	1324	HIS	2.2
1	B	180	ILE	2.2
1	A	104	LEU	2.2
1	A	903	LEU	2.2
1	A	87	ILE	2.2
2	Y	197	GLU	2.2
1	B	903	LEU	2.2
1	B	921	GLU	2.2
2	Y	207	LEU	2.2
2	X	162	LEU	2.2
1	A	373	VAL	2.2
1	A	570	GLN	2.2
1	A	182	ILE	2.2
2	Y	137	PHE	2.2
1	A	201	ILE	2.2
1	A	983	LEU	2.2
1	A	257	ASN	2.2
2	Y	212	MET	2.2
1	A	1480	PHE	2.2
1	B	201	ILE	2.2
2	X	214	ASP	2.1
1	A	817	ALA	2.1
1	A	691	LYS	2.1
1	B	691	LYS	2.1
1	B	1272	LYS	2.1
1	B	603	ALA	2.1
2	Y	150	ILE	2.1
2	X	203	LEU	2.1
1	B	858	LYS	2.1
1	B	667	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	859	MET	2.1
1	A	313	TYR	2.1
1	A	830	PRO	2.1
1	B	1323	LEU	2.1
1	A	1317	TYR	2.1
1	A	1323	LEU	2.1
2	X	225	GLU	2.1
1	B	613	GLN	2.0
1	A	88	GLN	2.0
1	B	251	LYS	2.0
1	B	86	THR	2.0
1	B	182	ILE	2.0
1	A	205	TYR	2.0
1	A	195	ARG	2.0
1	A	126	LEU	2.0
1	A	720	LEU	2.0
1	A	551	THR	2.0
1	A	424	LEU	2.0

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 ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	NAG	B	2001	14/15	0.24	0.05	280,280,280,280	0
4	NAG	A	2001	14/15	0.22	-0.24	293,293,293,293	0
4	NAG	B	2002	14/15	0.39	-	363,363,363,363	0
4	NAG	A	2002	14/15	0.39	-	343,343,343,343	0

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	NAG	A	1680	14/15	0.33	7.13	301,301,301,301	0
5	NAG	B	1679	14/15	0.30	5.18	290,290,290,290	0
3	CD	A	1678	1/1	0.36	-0.00	481,481,481,481	0
3	CD	B	1677	1/1	0.30	-0.60	466,466,466,466	0
3	CD	A	1679	1/1	0.12	-4.39	402,402,402,402	0
3	CD	B	1678	1/1	0.10	-4.78	397,397,397,397	0
3	CD	A	1677	1/1	0.10	-13.76	229,229,229,229	1

6.5 Other polymers ⓘ

There are no such residues in this entry.