



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 04:39 PM GMT

PDB ID : 3PVM
Title : Structure of Complement C5 in Complex with CVF
Authors : Laursen, N.S.; Andersen, K.R.; Braren, I.; Sottrup-Jensen, L.; Spillner, E.;
Andersen, G.R.
Deposited on : 2010-12-07
Resolution : 4.30 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>

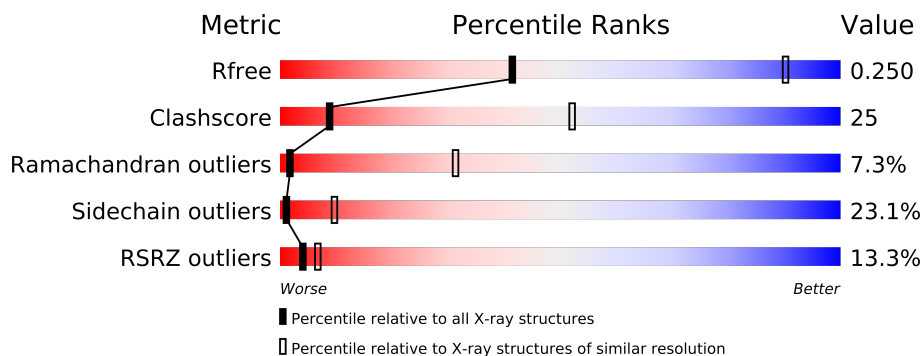
The following versions of software and data (see [references](#)) were used in the production of this report:

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 4.30 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	1016 (5.08-3.50)
Clashscore	79885	1280 (5.08-3.50)
Ramachandran outliers	78287	1210 (5.08-3.50)
Sidechain outliers	78261	1192 (5.08-3.50)
RSRZ outliers	66119	1016 (5.08-3.50)

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	C	1676	
2	B	1642	
2	D	1642	

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

Mol	Type	Chain	Res	Geometry	Electron density
3	NAG	B	2002	-	X
3	NAG	C	2003	-	X

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 45268 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.

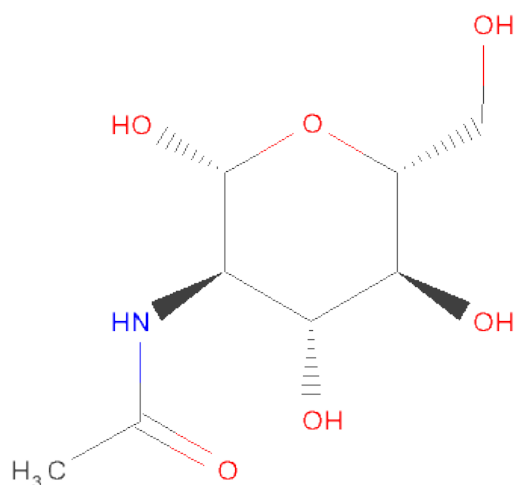
- Molecule 1 is a protein called Complement C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1627	Total	C	N	O	S	0	0	0
			12881	8246	2114	2469	52			
1	C	1627	Total	C	N	O	S	0	0	0
			12881	8246	2114	2469	52			

- Molecule 2 is a protein called Cobra venom factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1225	Total	C	N	O	S	0	0	0
			9711	6187	1633	1851	40			
2	D	1225	Total	C	N	O	S	0	0	0
			9711	6187	1633	1851	40			

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

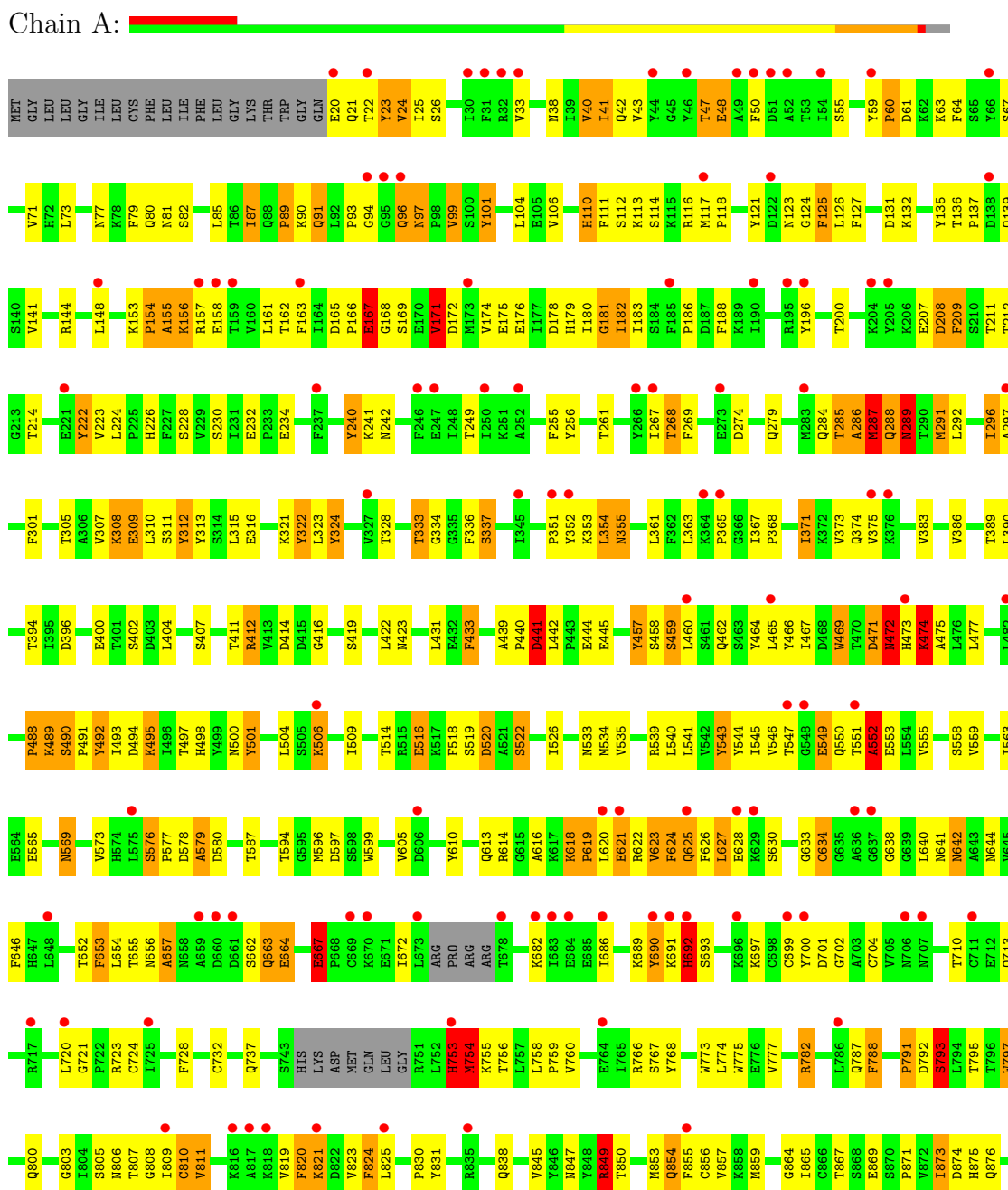


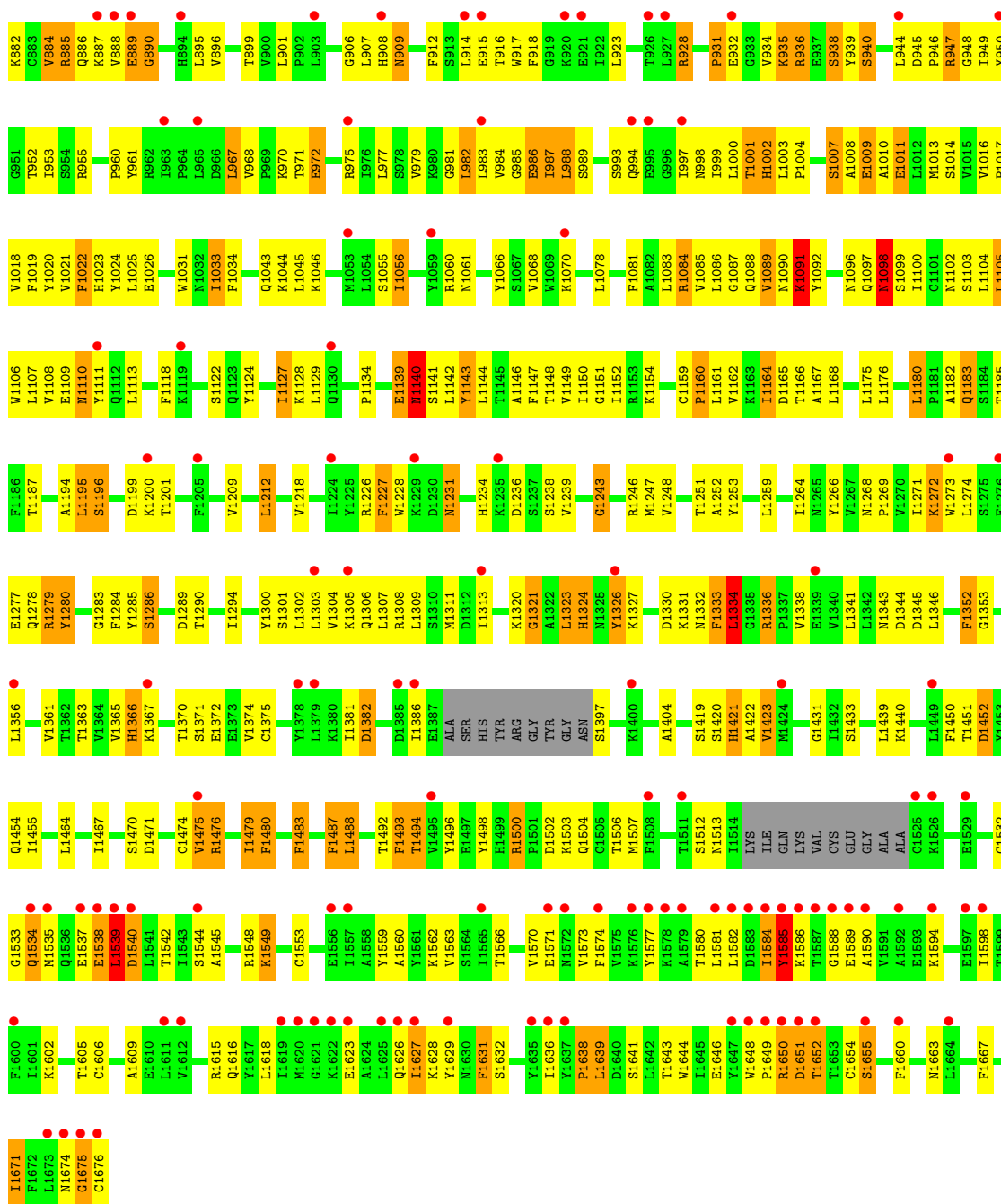
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	B	1	Total 14	C 8	N 1	O 5	0	0
3	B	1	Total 14	C 8	N 1	O 5	0	0
3	C	1	Total 14	C 8	N 1	O 5	0	0
3	D	1	Total 14	C 8	N 1	O 5	0	0
3	D	1	Total 14	C 8	N 1	O 5	0	0

3 Residue-property plots

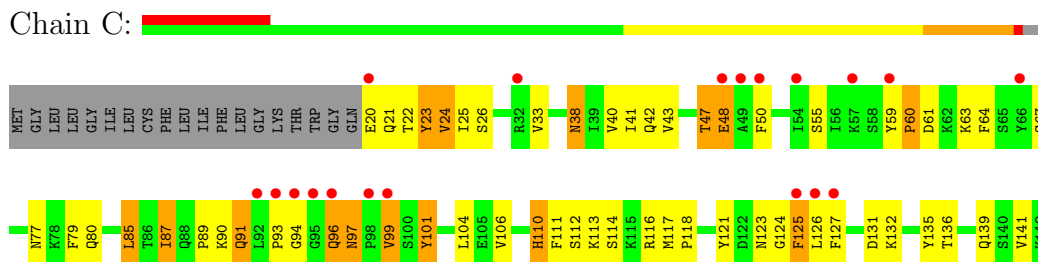
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

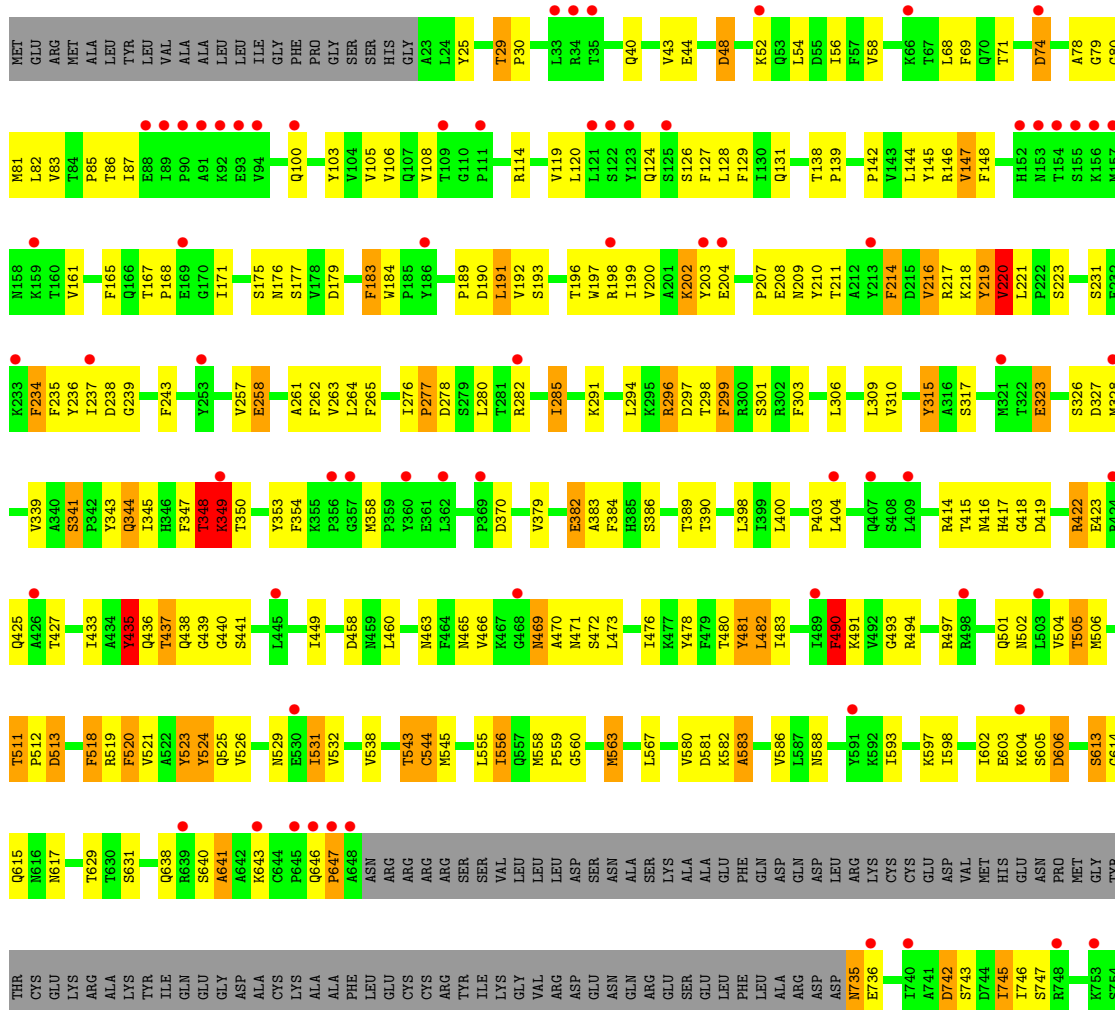




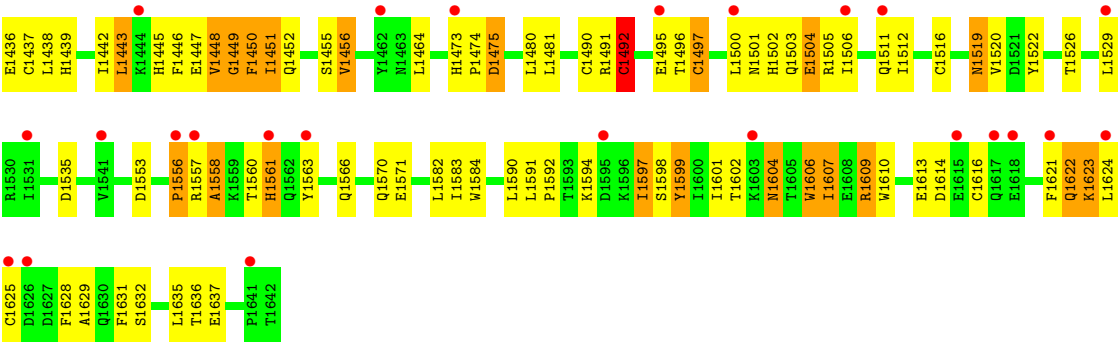
• Molecule 1: Complement C5



W1273	Q1183	H1102	M1013	D945	T867	L774	S693	V623	Y544	Y464	A297	Y222	W149
S1184	S1184	S1103	S1014	P946	S868	W775	V694	F624	I545	L465	Q298	V223	D150
T1185	T1185	L1104	V1015	R947	S869	E776	V695	F625	V546	Y466	F301	L224	D151
F1186	F1186	L1105	V1016	G948	S870	V777	K696	F626	T547	Y467		P225	L152
K1279	T1187	L1106	P1017	I949	P871		G697	K627	G548	D468	T305	H226	K153
L1280	L1107	L1107	V1018	Y950	V872	R782	C698	E628	E549	V469	A306	F227	P154
	L1108	V1108	F1019	G951	I873		C699	K629	Q550	T470	V307	S228	A155
	E1109	E1109	F1020	T952	D874		Y700	D630	T551	D471	K308	V229	K156
	M1110	V1021	V1021	N953	H875	Q787	D701	S631	A552	K472	E309	S230	L157
	L1111	G954	F1022	R954	Q876	F788	G702	L632	E553	H473	L310	E232	T158
	Q1112	R955	H1023	R955	G877	A769	A703	G633	L554	K474	L310	E232	T159
	L1113		V1024	P960	T878	L790	C704	C634	V555	A475	S311	P233	V160
			L1025	P961	K879	P791	V705			L476	Y312	E234	L161
			E1026	Y961		D792	W706			L477	Y313		T162
				R962	K882	S793	W707				S314		F163
					C883	L794	D708			P488	V397		L164
				L965	V884	T795	E709			K489	E316		D165
				L966	R885	T796				S490	Q399		P166
				L967	Q886	W797	T710			P491	L318		E167
				V968	K887		Q713			Y492			G168
						Q800				L493	K321		S169
						G803	L720			D494	Y322		E170
						I804	G721			K495	L323		V171
						S805	P722			S407	Y324		D172
						N806	R723			T497	T325		M173
						T807	C724			H498	A326		V174
						G808				N500	V327		E175
						I809	F728			Y501	T328		T177
						C810	C732						I177
						W811				L504	E331		D178
							T742			S805	S332		H179
						V819	S743			K506	T333		I180
						F820	HIS				G334		G181
						K821	LVS				G335		I182
						D822	ASP				F336		I183
						R823	NET				S337		
						F824	GLN				A340		P186
						L825	LEU						
						P830	GLY				S350		F194
						Y831	R751				P351		R195
							L752				Y352		G197
							H753				K353		M198
							K754				L354		V199
							W755				N355		T200
							T756						
							L757				L361		K204
							P758				E281		Y205
							W760				L362		K206
											K364		E207
											T285		D208
											A286		F209
											I367		S210
											P368		T211
													T212
													G213
													T214
													K220
													E221







4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	176.52Å 179.20Å 389.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.47 – 4.30 49.47 – 4.30	Depositor EDS
% Data completeness (in resolution range)	94.2 (49.47-4.30) 90.4 (49.47-4.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 4.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.233 , 0.262 0.225 , 0.250	Depositor DCC
R_{free} test set	1732 reflections (2.17%)	DCC
Wilson B-factor (Å ²)	135.2	Xtriage
Anisotropy	0.503	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 132.6	EDS
Estimated twinning fraction	0.026 for k,h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 79835 reflections	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	45268	wwPDB-VP
Average B, all atoms (Å ²)	192.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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	0.57	1/13158 (0.0%)	0.77	6/17851 (0.0%)
1	C	0.58	0/13158	0.76	5/17851 (0.0%)
2	B	0.55	0/9912	0.74	1/13454 (0.0%)
2	D	0.55	0/9912	0.74	2/13454 (0.0%)
All	All	0.57	1/46140 (0.0%)	0.75	14/62610 (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	3
1	C	0	3
2	B	0	1
2	D	0	1
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	810	CYS	CB-SG	-5.27	1.73	1.81

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1539	LEU	CA-CB-CG	6.88	131.12	115.30
1	A	1539	LEU	CA-CB-CG	6.87	131.10	115.30
1	A	1195	LEU	CA-CB-CG	-6.42	100.53	115.30
1	C	1195	LEU	CA-CB-CG	-6.27	100.87	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1346	ASN	CA-CB-CG	5.54	125.58	113.40
2	D	1346	ASN	CA-CB-CG	5.53	125.56	113.40
1	A	1000	LEU	CA-CB-CG	-5.35	102.99	115.30
1	A	181	GLY	N-CA-C	5.32	126.40	113.10
1	A	1105	LEU	CA-CB-CG	-5.28	103.16	115.30
2	D	1492	CYS	CA-CB-SG	-5.22	104.59	114.00
1	C	982	LEU	CA-CB-CG	-5.19	103.36	115.30
1	C	1000	LEU	CA-CB-CG	-5.19	103.37	115.30
1	A	982	LEU	CA-CB-CG	-5.17	103.40	115.30
1	C	181	GLY	N-CA-C	5.09	125.83	113.10

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	472	ASN	Peptide
1	A	552	ALA	Peptide
1	A	667	GLU	Peptide
2	B	1351	ASN	Peptide
1	C	472	ASN	Peptide
1	C	552	ALA	Peptide
1	C	667	GLU	Peptide
2	D	1351	ASN	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	12881	0	0	380	0
1	C	12881	0	0	384	0
2	B	9711	0	0	204	0
2	D	9711	0	0	199	0
3	A	14	0	0	0	0
3	B	28	0	0	1	0
3	C	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	28	0	0	1	0
All	All	45268	0	0	1154	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 25.

All (1154) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:492:TYR:CD2	1:C:493:ILE:N	2.27	1.03
1:A:492:TYR:CD2	1:A:493:ILE:N	2.27	1.03
1:A:490:SER:N	1:A:491:PRO:CD	2.36	0.88
1:C:490:SER:N	1:C:491:PRO:CD	2.38	0.86
1:A:1278:GLN:OE1	1:A:1283:GLY:CA	2.25	0.85
2:D:1450:PHE:CD1	2:D:1451:ILE:N	2.45	0.84
2:B:1450:PHE:CD1	2:B:1451:ILE:N	2.47	0.82
1:C:1278:GLN:OE1	1:C:1283:GLY:CA	2.28	0.81
2:D:435:TYR:CD1	2:D:436:GLN:N	2.49	0.80
1:A:23:TYR:CD1	1:A:23:TYR:N	2.46	0.80
1:C:500:ASN:CB	1:C:543:TYR:CE1	2.65	0.80
1:A:500:ASN:CB	1:A:543:TYR:CE1	2.65	0.79
1:A:492:TYR:CG	1:A:493:ILE:N	2.50	0.79
2:B:435:TYR:CD1	2:B:436:GLN:N	2.50	0.79
1:C:492:TYR:CG	1:C:493:ILE:N	2.50	0.76
1:C:620:LEU:O	1:C:622:ARG:N	2.21	0.74
1:A:322:TYR:CD2	1:A:322:TYR:N	2.55	0.74
1:C:23:TYR:N	1:C:23:TYR:CD1	2.54	0.74
2:B:952:ASP:N	2:B:952:ASP:OD1	2.21	0.73
1:C:154:PRO:O	1:C:155:ALA:CB	2.37	0.73
1:A:1090:ASN:O	1:A:1092:TYR:N	2.22	0.72
1:A:620:LEU:O	1:A:622:ARG:N	2.23	0.72
1:A:653:PHE:O	1:A:653:PHE:CD1	2.43	0.72
1:C:1228:TRP:N	1:C:1251:THR:CG2	2.54	0.71
2:B:481:TYR:O	2:B:481:TYR:CD2	2.42	0.71
1:C:322:TYR:N	1:C:322:TYR:CD2	2.59	0.71
1:C:180:ILE:O	1:C:182:ILE:N	2.24	0.70
2:D:1284:ARG:CG	2:D:1285:GLU:N	2.55	0.70
1:C:1090:ASN:O	1:C:1092:TYR:N	2.25	0.69
1:A:154:PRO:O	1:A:155:ALA:CB	2.40	0.69
2:D:1475:ASP:N	2:D:1475:ASP:OD1	2.25	0.69
2:B:603:GLU:O	2:B:605:SER:N	2.25	0.69
1:C:906:GLY:O	1:C:908:HIS:CE1	2.46	0.69
2:D:603:GLU:O	2:D:605:SER:N	2.26	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:513:ASP:N	2:D:513:ASP:OD2	2.25	0.68
1:C:1644:TRP:NE1	1:C:1646:GLU:OE1	2.26	0.68
2:D:481:TYR:CD2	2:D:481:TYR:O	2.45	0.68
1:C:1487:PHE:CD2	1:C:1487:PHE:N	2.61	0.68
1:C:222:TYR:CD2	1:C:223:VAL:N	2.62	0.68
2:B:513:ASP:OD2	2:B:513:ASP:N	2.26	0.68
1:A:1019:PHE:CD2	1:A:1019:PHE:C	2.67	0.68
2:B:128:LEU:O	2:B:129:PHE:CD1	2.47	0.68
2:B:1475:ASP:N	2:B:1475:ASP:OD1	2.27	0.68
1:A:906:GLY:O	1:A:908:HIS:CE1	2.47	0.67
1:A:1227:PHE:C	1:A:1227:PHE:CD1	2.67	0.67
2:D:214:PHE:O	2:D:214:PHE:CD1	2.47	0.67
1:C:653:PHE:O	1:C:653:PHE:CD1	2.48	0.67
1:A:222:TYR:CD2	1:A:223:VAL:N	2.63	0.67
2:B:1607:ILE:CD1	2:B:1607:ILE:N	2.57	0.67
1:C:489:LYS:CG	1:C:490:SER:N	2.58	0.67
2:B:1284:ARG:CG	2:B:1285:GLU:N	2.58	0.67
1:C:489:LYS:C	1:C:491:PRO:CD	2.63	0.67
1:A:1228:TRP:N	1:A:1251:THR:CG2	2.57	0.67
1:C:90:LYS:O	1:C:91:GLN:NE2	2.28	0.67
2:D:183:PHE:CD2	2:D:183:PHE:N	2.62	0.67
1:C:473:HIS:CE1	2:D:455:LYS:NZ	2.63	0.66
1:C:1227:PHE:C	1:C:1227:PHE:CD1	2.68	0.66
1:C:1127:ILE:CG1	1:C:1143:TYR:CE2	2.79	0.66
2:D:1284:ARG:CD	2:D:1285:GLU:N	2.58	0.66
2:B:183:PHE:CD2	2:B:183:PHE:N	2.63	0.66
2:D:347:PHE:O	2:D:349:LYS:N	2.29	0.66
1:A:90:LYS:O	1:A:91:GLN:NE2	2.29	0.66
1:A:489:LYS:C	1:A:491:PRO:CD	2.63	0.66
2:D:417:HIS:O	2:D:419:ASP:N	2.28	0.65
1:C:123:ASN:C	1:C:123:ASN:OD1	2.33	0.65
2:B:785:THR:OG1	2:B:786:THR:N	2.29	0.65
1:C:1180:LEU:O	1:C:1182:ALA:N	2.30	0.65
1:A:180:ILE:O	1:A:182:ILE:N	2.30	0.65
2:D:476:ILE:CG2	2:D:476:ILE:O	2.44	0.65
1:C:1016:VAL:N	1:C:1017:PRO:CD	2.60	0.65
1:C:1024:TYR:CD2	1:C:1025:LEU:N	2.64	0.65
1:C:1226:ARG:CZ	1:C:1266:TYR:CE1	2.80	0.65
2:B:417:HIS:O	2:B:419:ASP:N	2.30	0.65
1:A:123:ASN:OD1	1:A:123:ASN:C	2.35	0.65
2:D:1607:ILE:N	2:D:1607:ILE:CD1	2.59	0.65
1:A:1487:PHE:N	1:A:1487:PHE:CD2	2.64	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:489:LYS:CG	1:A:490:SER:N	2.61	0.64
2:B:1284:ARG:CD	2:B:1285:GLU:N	2.60	0.64
1:C:1019:PHE:C	1:C:1019:PHE:CD2	2.70	0.64
1:A:1127:ILE:CG1	1:A:1143:TYR:CE2	2.81	0.64
1:A:702:GLY:CA	1:A:728:PHE:CE1	2.80	0.64
2:B:476:ILE:O	2:B:476:ILE:CG2	2.46	0.64
1:C:979:VAL:CG2	1:C:1326:TYR:CE1	2.81	0.63
1:A:1644:TRP:NE1	1:A:1646:GLU:OE1	2.31	0.63
1:A:1627:ILE:O	1:A:1627:ILE:CG1	2.45	0.63
1:C:753:HIS:O	1:C:754:MET:CB	2.46	0.63
1:A:1431:GLY:CA	1:A:1483:PHE:CE1	2.81	0.63
2:D:1609:ARG:CG	2:D:1609:ARG:NH1	2.61	0.63
1:C:932:GLU:OE1	1:C:932:GLU:N	2.32	0.63
2:D:216:VAL:CG1	2:D:216:VAL:O	2.46	0.63
1:A:1226:ARG:CZ	1:A:1266:TYR:CE1	2.82	0.62
2:D:128:LEU:O	2:D:129:PHE:CD1	2.52	0.62
1:A:1159:CYS:O	1:A:1161:LEU:N	2.32	0.62
1:A:1180:LEU:O	1:A:1182:ALA:N	2.32	0.62
1:A:1097:GLN:O	1:A:1098:ASN:C	2.37	0.62
1:A:371:ILE:CD1	1:A:433:PHE:CE2	2.83	0.62
1:C:623:VAL:O	1:C:624:PHE:C	2.38	0.62
1:C:371:ILE:CD1	1:C:433:PHE:CE2	2.82	0.62
1:A:1008:ALA:O	1:A:1009:GLU:C	2.38	0.62
2:D:131:GLN:OE1	2:D:146:ARG:NH1	2.32	0.62
1:A:1024:TYR:CD2	1:A:1025:LEU:N	2.67	0.62
2:B:239:GLY:N	2:B:296:ARG:NH2	2.48	0.62
1:A:59:TYR:CE2	1:A:99:VAL:CG2	2.82	0.62
1:C:132:LYS:O	1:C:135:TYR:CE2	2.53	0.62
1:C:1431:GLY:CA	1:C:1483:PHE:CE1	2.82	0.62
1:A:788:PHE:N	1:A:788:PHE:CD2	2.67	0.62
1:A:1199:ASP:CG	1:A:1199:ASP:O	2.37	0.62
1:A:961:TYR:OH	1:A:1343:ASN:CG	2.37	0.62
1:C:1199:ASP:O	1:C:1199:ASP:CG	2.37	0.62
1:A:754:MET:SD	1:A:755:LYS:N	2.73	0.61
2:B:214:PHE:CD1	2:B:214:PHE:O	2.53	0.61
1:A:551:THR:O	1:A:552:ALA:CB	2.47	0.61
2:D:239:GLY:N	2:D:296:ARG:NH2	2.48	0.61
1:A:87:ILE:N	1:A:87:ILE:CD1	2.63	0.61
2:D:1606:TRP:C	2:D:1606:TRP:CD1	2.73	0.61
2:D:423:GLU:OE2	2:D:423:GLU:N	2.33	0.61
1:C:386:VAL:N	1:C:411:THR:CG2	2.62	0.61
1:C:1451:THR:O	1:C:1452:ASP:CB	2.49	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:754:MET:SD	1:C:755:LYS:N	2.74	0.61
1:C:949:ILE:O	1:C:950:TYR:CD1	2.54	0.61
1:A:655:THR:O	1:A:657:ALA:N	2.33	0.61
1:C:87:ILE:CD1	1:C:87:ILE:N	2.64	0.61
1:A:932:GLU:OE1	1:A:932:GLU:N	2.34	0.61
1:A:311:SER:O	1:A:313:TYR:N	2.33	0.61
1:C:551:THR:O	1:C:552:ALA:CB	2.48	0.61
1:C:830:PRO:CG	1:C:1483:PHE:CZ	2.84	0.61
1:A:623:VAL:CG1	1:A:624:PHE:N	2.61	0.61
2:B:423:GLU:N	2:B:423:GLU:OE2	2.33	0.61
2:B:481:TYR:CE1	2:B:506:MET:SD	2.94	0.61
1:A:753:HIS:O	1:A:754:MET:CB	2.49	0.60
2:B:1609:ARG:CG	2:B:1609:ARG:NH1	2.63	0.60
1:A:1016:VAL:N	1:A:1017:PRO:CD	2.64	0.60
1:C:539:ARG:NH2	1:C:634:CYS:N	2.49	0.60
1:C:24:VAL:CA	1:C:655:THR:CG2	2.80	0.60
2:D:197:TRP:CB	2:D:214:PHE:CE1	2.85	0.60
1:C:623:VAL:CG1	1:C:624:PHE:N	2.61	0.60
1:A:386:VAL:N	1:A:411:THR:CG2	2.64	0.60
1:A:979:VAL:CG2	1:A:1326:TYR:CE1	2.85	0.60
1:C:311:SER:O	1:C:313:TYR:N	2.34	0.60
1:C:961:TYR:OH	1:C:1343:ASN:CG	2.40	0.60
1:C:788:PHE:N	1:C:788:PHE:CD2	2.68	0.60
1:C:655:THR:O	1:C:657:ALA:N	2.35	0.60
1:A:884:VAL:O	1:A:885:ARG:CB	2.49	0.60
2:D:785:THR:OG1	2:D:786:THR:N	2.34	0.60
1:C:934:VAL:CG2	1:C:1366:HIS:CD2	2.85	0.60
1:C:549:GLU:N	1:C:549:GLU:CD	2.56	0.60
2:B:1331:ALA:O	2:B:1332:GLN:CB	2.49	0.59
2:B:478:TYR:CD1	2:B:478:TYR:O	2.55	0.59
2:B:315:TYR:CD1	2:B:315:TYR:O	2.55	0.59
2:D:257:VAL:CG1	2:D:258:GLU:N	2.65	0.59
1:C:1008:ALA:O	1:C:1009:GLU:C	2.41	0.59
2:B:529:ASN:OD1	2:B:529:ASN:O	2.21	0.59
2:D:1331:ALA:O	2:D:1332:GLN:CB	2.49	0.59
2:B:234:PHE:CD1	2:B:234:PHE:C	2.76	0.59
1:A:773:TRP:CZ3	1:A:788:PHE:CE1	2.90	0.59
1:C:1627:ILE:CG1	1:C:1627:ILE:O	2.50	0.59
2:B:347:PHE:O	2:B:349:LYS:N	2.36	0.59
1:A:1421:HIS:C	1:A:1421:HIS:CD2	2.75	0.59
1:A:1451:THR:O	1:A:1452:ASP:CB	2.51	0.59
2:B:285:ILE:N	2:B:285:ILE:CD1	2.66	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:745:ILE:CG2	2:D:745:ILE:O	2.51	0.58
1:A:623:VAL:O	1:A:624:PHE:C	2.39	0.58
2:D:478:TYR:O	2:D:478:TYR:CD1	2.56	0.58
1:A:549:GLU:CD	1:A:549:GLU:N	2.57	0.58
1:A:830:PRO:CG	1:A:1483:PHE:CZ	2.86	0.58
2:B:953:ARG:CG	2:B:954:VAL:N	2.67	0.58
2:B:606:ASP:O	2:B:606:ASP:OD1	2.21	0.58
1:A:60:PRO:CD	1:A:61:ASP:N	2.66	0.58
2:B:315:TYR:CD1	2:B:315:TYR:C	2.77	0.58
1:C:884:VAL:O	1:C:885:ARG:CB	2.51	0.58
2:B:1606:TRP:CD1	2:B:1606:TRP:C	2.76	0.58
1:C:628:GLU:C	1:C:630:SER:N	2.56	0.58
1:A:24:VAL:CA	1:A:655:THR:CG2	2.82	0.58
1:A:985:GLY:O	1:A:986:GLU:C	2.42	0.58
1:C:1033:ILE:CG2	1:C:1034:PHE:CD1	2.87	0.58
1:C:773:TRP:CZ3	1:C:788:PHE:CE1	2.92	0.57
1:C:111:PHE:CE2	1:C:113:LYS:CB	2.87	0.57
2:D:861:THR:O	2:D:863:GLY:N	2.37	0.57
1:C:1097:GLN:O	1:C:1098:ASN:C	2.41	0.57
1:A:457:TYR:C	1:A:457:TYR:CD2	2.78	0.57
2:D:234:PHE:CD1	2:D:234:PHE:C	2.77	0.57
1:A:101:TYR:CE1	1:A:116:ARG:NH2	2.73	0.57
1:C:469:TRP:CE3	1:C:469:TRP:N	2.72	0.57
1:C:60:PRO:CD	1:C:61:ASP:N	2.68	0.57
2:D:481:TYR:CE1	2:D:506:MET:SD	2.98	0.57
2:B:1426:TYR:N	2:B:1426:TYR:CD2	2.72	0.57
2:D:315:TYR:CD1	2:D:315:TYR:O	2.58	0.57
1:A:1421:HIS:CD2	1:A:1422:ALA:N	2.72	0.57
2:D:953:ARG:CG	2:D:954:VAL:N	2.68	0.57
2:B:257:VAL:CG1	2:B:258:GLU:N	2.67	0.57
1:A:628:GLU:C	1:A:630:SER:N	2.57	0.57
1:C:1333:PHE:O	1:C:1334:LEU:CB	2.52	0.57
1:C:1352:PHE:CD2	1:C:1353:GLY:N	2.73	0.57
1:A:539:ARG:NH2	1:A:634:CYS:N	2.52	0.57
1:C:516:GLU:OE1	1:C:516:GLU:N	2.38	0.57
1:A:469:TRP:CE3	1:A:469:TRP:N	2.73	0.57
1:C:985:GLY:O	1:C:986:GLU:C	2.42	0.57
1:A:934:VAL:CG2	1:A:1366:HIS:CD2	2.88	0.56
2:D:348:THR:O	2:D:348:THR:OG1	2.23	0.56
1:A:949:ILE:O	1:A:950:TYR:CD1	2.58	0.56
1:A:1081:PHE:O	1:A:1084:ARG:N	2.38	0.56
1:A:269:PHE:CG	1:A:301:PHE:CE1	2.92	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:1426:TYR:CD2	2:D:1426:TYR:N	2.73	0.56
2:B:745:ILE:O	2:B:745:ILE:CG2	2.53	0.56
1:C:654:LEU:O	1:C:655:THR:CG2	2.53	0.56
1:A:1227:PHE:CD2	1:A:1273:TRP:CE2	2.93	0.56
1:A:1333:PHE:O	1:A:1334:LEU:CB	2.52	0.56
1:C:1420:SER:O	1:C:1421:HIS:C	2.44	0.56
1:A:165:ASP:C	1:A:165:ASP:OD2	2.44	0.56
2:D:523:TYR:C	2:D:523:TYR:CD1	2.79	0.56
1:A:518:PHE:O	1:A:520:ASP:N	2.39	0.56
1:C:1164:ILE:O	1:C:1165:ASP:C	2.41	0.56
1:C:803:GLY:O	1:C:810:CYS:CB	2.53	0.56
1:A:1549:LYS:NZ	1:A:1667:PHE:CB	2.67	0.56
1:A:1533:GLY:O	1:A:1534:GLN:CB	2.54	0.56
2:D:582:LYS:O	2:D:583:ALA:O	2.23	0.56
2:D:236:TYR:O	2:D:238:ASP:N	2.38	0.56
1:A:831:TYR:O	1:A:928:ARG:CD	2.54	0.56
1:A:653:PHE:C	1:A:653:PHE:CD1	2.79	0.56
2:B:235:PHE:CE2	2:B:299:PHE:CE2	2.93	0.56
1:C:702:GLY:CA	1:C:728:PHE:CE1	2.88	0.56
2:D:285:ILE:N	2:D:285:ILE:CD1	2.69	0.56
1:A:1139:GLU:OE2	1:A:1187:THR:OG1	2.24	0.56
2:B:861:THR:O	2:B:863:GLY:N	2.38	0.56
1:C:459:SER:O	1:C:462:GLN:N	2.38	0.56
1:A:132:LYS:O	1:A:135:TYR:CE2	2.59	0.56
1:A:1139:GLU:O	1:A:1142:LEU:N	2.38	0.56
1:A:654:LEU:O	1:A:655:THR:CG2	2.53	0.56
1:C:59:TYR:CE2	1:C:99:VAL:CG2	2.89	0.56
1:A:889:GLU:O	1:A:890:GLY:O	2.24	0.56
2:B:236:TYR:O	2:B:238:ASP:N	2.39	0.56
1:C:906:GLY:O	1:C:908:HIS:NE2	2.39	0.55
2:B:825:VAL:N	2:B:828:GLU:OE1	2.39	0.55
1:C:91:GLN:CA	1:C:91:GLN:OE1	2.54	0.55
1:A:113:LYS:CG	1:A:114:SER:N	2.69	0.55
2:D:1443:LEU:N	2:D:1443:LEU:CD1	2.69	0.55
1:C:1139:GLU:O	1:C:1142:LEU:N	2.40	0.55
2:D:315:TYR:C	2:D:315:TYR:CD1	2.78	0.55
1:A:309:GLU:O	1:A:312:TYR:N	2.39	0.55
1:C:457:TYR:C	1:C:457:TYR:CD2	2.79	0.55
1:C:1584:ILE:CG2	1:C:1585:TYR:N	2.70	0.55
2:B:469:ASN:ND2	2:B:469:ASN:C	2.57	0.55
2:D:529:ASN:O	2:D:529:ASN:OD1	2.24	0.55
1:C:653:PHE:CD1	1:C:653:PHE:C	2.80	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:938:SER:C	1:A:940:SER:N	2.57	0.55
2:B:918:GLU:OE2	2:B:918:GLU:N	2.39	0.55
2:D:825:VAL:N	2:D:828:GLU:OE1	2.39	0.55
1:C:938:SER:C	1:C:940:SER:N	2.60	0.55
1:A:1019:PHE:CD2	1:A:1020:TYR:N	2.75	0.55
1:C:1008:ALA:O	1:C:1011:GLU:N	2.40	0.55
2:B:481:TYR:CE2	2:B:493:GLY:CA	2.89	0.55
1:A:1420:SER:O	1:A:1421:HIS:C	2.45	0.55
2:B:1473:HIS:CD2	2:B:1474:PRO:CD	2.90	0.55
2:B:216:VAL:CG1	2:B:216:VAL:O	2.54	0.55
1:C:1421:HIS:C	1:C:1421:HIS:CD2	2.78	0.55
2:D:850:LEU:CG	2:D:851:LEU:N	2.69	0.55
2:D:235:PHE:CE2	2:D:299:PHE:CE2	2.94	0.55
1:A:803:GLY:O	1:A:810:CYS:CB	2.55	0.55
2:D:582:LYS:O	2:D:583:ALA:C	2.45	0.55
2:B:138:THR:O	2:B:139:PRO:C	2.44	0.55
1:A:1252:ALA:O	1:A:1253:TYR:C	2.46	0.55
1:C:1268:ASN:N	1:C:1269:PRO:CD	2.70	0.55
1:C:1164:ILE:O	1:C:1167:ALA:N	2.40	0.54
1:A:1008:ALA:O	1:A:1011:GLU:N	2.40	0.54
1:A:805:SER:O	1:A:807:THR:N	2.40	0.54
1:A:1304:VAL:CG1	1:A:1305:LYS:N	2.70	0.54
1:A:1560:ALA:O	1:A:1585:TYR:CD2	2.61	0.54
1:A:1045:LEU:O	1:A:1046:LYS:C	2.45	0.54
1:A:970:LYS:O	1:A:971:THR:CG2	2.56	0.54
2:D:481:TYR:CE2	2:D:493:GLY:CA	2.90	0.54
1:C:1421:HIS:CD2	1:C:1422:ALA:N	2.76	0.54
1:C:286:ALA:O	1:C:287:MET:C	2.46	0.54
1:C:831:TYR:O	1:C:928:ARG:CD	2.56	0.54
1:A:1139:GLU:O	1:A:1140:ASN:C	2.45	0.54
1:C:1549:LYS:NZ	1:C:1667:PHE:CB	2.70	0.54
2:B:800:ILE:CG2	2:B:801:CYS:N	2.69	0.54
1:A:1033:ILE:CG2	1:A:1034:PHE:CD1	2.91	0.54
2:D:519:ARG:NH1	2:D:606:ASP:OD2	2.40	0.54
1:C:1139:GLU:OE2	1:C:1187:THR:OG1	2.26	0.54
1:A:934:VAL:CG1	1:A:935:LYS:N	2.71	0.54
1:A:1066:TYR:N	1:A:1066:TYR:CD1	2.74	0.54
1:C:1493:PHE:C	1:C:1493:PHE:CD1	2.79	0.54
1:A:1164:ILE:O	1:A:1167:ALA:N	2.41	0.54
2:D:1623:LYS:CB	2:D:1623:LYS:NZ	2.71	0.54
1:C:42:GLN:CG	1:C:43:VAL:N	2.71	0.53
2:D:138:THR:O	2:D:139:PRO:C	2.43	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1493:PHE:C	1:A:1493:PHE:CD1	2.79	0.53
1:A:931:PRO:CB	1:A:1366:HIS:CD2	2.91	0.53
1:A:111:PHE:CD2	1:A:112:SER:N	2.76	0.53
1:C:309:GLU:O	1:C:312:TYR:N	2.41	0.53
1:A:1268:ASN:N	1:A:1269:PRO:CD	2.71	0.53
2:D:866:TYR:CD2	2:D:866:TYR:C	2.82	0.53
1:C:875:HIS:CB	2:D:901:GLN:NE2	2.72	0.53
1:A:1110:ASN:O	1:A:1111:TYR:CG	2.62	0.53
1:A:1352:PHE:CD2	1:A:1353:GLY:N	2.76	0.53
2:D:830:VAL:CG2	2:D:831:GLU:N	2.71	0.53
2:B:806:TYR:C	2:B:806:TYR:CD1	2.81	0.53
1:C:1475:VAL:CG2	1:C:1476:ARG:N	2.71	0.53
2:B:850:LEU:CG	2:B:851:LEU:N	2.70	0.53
2:B:853:ASN:OD1	2:B:855:ALA:N	2.41	0.53
1:A:906:GLY:O	1:A:908:HIS:NE2	2.41	0.53
1:A:433:PHE:CD1	1:A:433:PHE:N	2.75	0.53
1:C:889:GLU:O	1:C:890:GLY:O	2.27	0.53
1:A:459:SER:O	1:A:462:GLN:N	2.41	0.53
2:B:348:THR:OG1	2:B:348:THR:O	2.27	0.53
1:C:111:PHE:CD2	1:C:112:SER:N	2.76	0.53
1:A:1584:ILE:CG2	1:A:1585:TYR:N	2.72	0.53
1:C:1304:VAL:CG1	1:C:1305:LYS:N	2.71	0.53
1:C:1533:GLY:O	1:C:1534:GLN:CB	2.56	0.53
1:C:1081:PHE:O	1:C:1084:ARG:N	2.42	0.53
2:B:1330:ASN:N	2:B:1330:ASN:ND2	2.56	0.53
1:C:982:LEU:N	1:C:982:LEU:CD1	2.72	0.53
2:B:1443:LEU:CD1	2:B:1443:LEU:N	2.72	0.53
1:C:1279:ARG:NH1	1:C:1280:TYR:CE2	2.77	0.53
2:B:1621:PHE:O	2:B:1622:GLN:C	2.47	0.53
1:C:1300:TYR:CD2	1:C:1300:TYR:C	2.82	0.53
2:B:415:THR:O	2:B:425:GLN:NE2	2.42	0.53
2:D:841:ASN:O	2:D:842:GLU:C	2.47	0.53
1:A:618:LYS:N	1:A:619:PRO:CD	2.72	0.53
2:D:463:ASN:OD1	2:D:505:THR:OG1	2.27	0.53
1:C:433:PHE:N	1:C:433:PHE:CD1	2.77	0.53
1:A:520:ASP:N	1:A:520:ASP:OD1	2.41	0.53
2:D:1473:HIS:CD2	2:D:1474:PRO:CD	2.92	0.53
1:C:1159:CYS:O	1:C:1161:LEU:N	2.42	0.53
1:C:855:PHE:CD1	1:C:855:PHE:C	2.83	0.53
2:B:131:GLN:OE1	2:B:146:ARG:NH1	2.41	0.52
1:C:1066:TYR:CD1	1:C:1066:TYR:N	2.75	0.52
1:A:516:GLU:OE1	1:A:516:GLU:N	2.42	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1159:CYS:N	1:A:1160:PRO:CD	2.73	0.52
1:A:1022:PHE:O	1:A:1024:TYR:N	2.42	0.52
1:C:1493:PHE:CD1	1:C:1494:THR:N	2.76	0.52
1:C:1571:GLU:O	1:C:1574:PHE:CD2	2.62	0.52
1:C:970:LYS:O	1:C:971:THR:CG2	2.57	0.52
1:A:491:PRO:CG	1:A:494:ASP:CB	2.88	0.52
1:A:938:SER:O	1:A:940:SER:N	2.43	0.52
1:C:307:VAL:O	1:C:308:LYS:O	2.27	0.52
2:B:1590:LEU:CD2	2:B:1591:LEU:N	2.72	0.52
2:B:841:ASN:O	2:B:842:GLU:C	2.48	0.52
1:C:165:ASP:OD2	1:C:165:ASP:C	2.47	0.52
2:B:582:LYS:O	2:B:583:ALA:C	2.46	0.52
1:A:702:GLY:CA	1:A:728:PHE:CD1	2.93	0.52
1:C:269:PHE:CG	1:C:301:PHE:CE1	2.97	0.52
2:B:881:PRO:O	2:B:882:PHE:CD2	2.63	0.52
2:B:1445:HIS:CG	2:B:1446:PHE:N	2.77	0.52
2:B:518:PHE:CD2	2:B:518:PHE:C	2.83	0.52
2:D:344:GLN:NE2	2:D:344:GLN:CA	2.72	0.52
1:C:491:PRO:CG	1:C:494:ASP:CB	2.88	0.52
2:D:415:THR:O	2:D:425:GLN:NE2	2.43	0.52
1:C:365:PRO:CG	1:C:464:TYR:CE2	2.91	0.52
2:D:806:TYR:C	2:D:806:TYR:CD1	2.83	0.52
2:B:209:ASN:CG	3:B:2001:NAG:C7	2.78	0.52
1:A:1300:TYR:CD2	1:A:1300:TYR:C	2.83	0.52
2:D:1504:GLU:OE2	2:D:1505:ARG:N	2.43	0.52
2:D:860:SER:OG	2:D:866:TYR:N	2.42	0.52
1:C:576:SER:CB	1:C:577:PRO:CD	2.87	0.52
1:A:1475:VAL:CG2	1:A:1476:ARG:N	2.72	0.52
1:C:500:ASN:CB	1:C:543:TYR:CD1	2.93	0.52
2:D:952:ASP:N	2:D:952:ASP:OD1	2.43	0.52
1:A:101:TYR:CE1	1:A:116:ARG:CZ	2.93	0.52
1:A:111:PHE:CE2	1:A:113:LYS:CB	2.92	0.52
2:D:1621:PHE:O	2:D:1622:GLN:C	2.48	0.52
2:D:1556:PRO:O	2:D:1558:ALA:N	2.43	0.52
1:C:1560:ALA:O	1:C:1585:TYR:CD2	2.63	0.52
1:C:101:TYR:CE1	1:C:116:ARG:NH2	2.78	0.52
1:C:947:ARG:NH1	1:C:1352:PHE:CE2	2.78	0.52
2:B:1556:PRO:O	2:B:1558:ALA:N	2.43	0.52
2:D:853:ASN:OD1	2:D:855:ALA:N	2.43	0.51
1:C:518:PHE:O	1:C:520:ASP:N	2.43	0.51
1:A:1227:PHE:CD2	1:A:1273:TRP:NE1	2.78	0.51
1:A:307:VAL:O	1:A:308:LYS:O	2.27	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:618:LYS:N	1:C:619:PRO:CD	2.73	0.51
2:B:640:SER:O	2:B:641:ALA:CB	2.57	0.51
1:C:1176:LEU:CD2	1:C:1176:LEU:N	2.73	0.51
1:C:178:ASP:OD2	1:C:179:HIS:N	2.43	0.51
2:D:918:GLU:N	2:D:918:GLU:OE2	2.43	0.51
1:A:982:LEU:N	1:A:982:LEU:CD1	2.73	0.51
2:D:1330:ASN:ND2	2:D:1330:ASN:N	2.59	0.51
1:C:1024:TYR:C	1:C:1024:TYR:CD2	2.83	0.51
1:A:165:ASP:O	1:A:165:ASP:OD2	2.28	0.51
1:C:641:ASN:O	1:C:642:ASN:C	2.49	0.51
2:D:1445:HIS:CG	2:D:1446:PHE:N	2.79	0.51
2:D:1624:LEU:O	2:D:1625:CYS:C	2.49	0.51
1:C:25:ILE:N	1:C:655:THR:CG2	2.73	0.51
1:C:874:ASP:O	1:C:875:HIS:CG	2.63	0.51
1:C:1110:ASN:N	1:C:1110:ASN:OD1	2.44	0.51
1:A:682:LYS:NZ	1:A:686:ILE:CD1	2.74	0.51
2:B:1623:LYS:CB	2:B:1623:LYS:NZ	2.74	0.51
1:A:500:ASN:CB	1:A:543:TYR:CD1	2.94	0.51
2:B:415:THR:O	2:B:425:GLN:CD	2.49	0.51
1:C:1007:SER:OG	1:C:1008:ALA:N	2.40	0.51
2:D:44:GLU:OE2	2:D:523:TYR:OH	2.28	0.51
2:D:881:PRO:O	2:D:882:PHE:CD2	2.64	0.51
2:B:518:PHE:O	2:B:518:PHE:CD2	2.63	0.51
1:A:96:GLN:O	1:A:97:ASN:O	2.29	0.51
1:C:1045:LEU:O	1:C:1046:LYS:C	2.47	0.51
2:D:210:TYR:CG	2:D:211:THR:N	2.79	0.51
2:B:353:TYR:CD2	2:B:614:GLY:O	2.64	0.51
1:A:1279:ARG:NH1	1:A:1280:TYR:CE2	2.79	0.51
1:A:286:ALA:O	1:A:287:MET:C	2.48	0.51
2:D:800:ILE:CG2	2:D:801:CYS:N	2.72	0.51
1:C:961:TYR:O	1:C:961:TYR:CD1	2.64	0.51
1:C:113:LYS:CG	1:C:114:SER:N	2.74	0.51
1:A:1110:ASN:N	1:A:1110:ASN:OD1	2.43	0.51
2:B:842:GLU:O	2:B:843:ASP:C	2.48	0.51
2:D:347:PHE:O	2:D:348:THR:C	2.49	0.51
1:A:91:GLN:CA	1:A:91:GLN:OE1	2.58	0.51
1:C:947:ARG:O	1:C:949:ILE:N	2.44	0.51
2:B:866:TYR:C	2:B:866:TYR:CD2	2.84	0.51
1:A:1421:HIS:CE1	1:A:1498:TYR:CD1	2.98	0.51
1:C:1616:GLN:NE2	1:C:1648:TRP:CZ3	2.79	0.51
2:B:523:TYR:C	2:B:523:TYR:CD1	2.83	0.51
1:C:1279:ARG:NH1	1:C:1280:TYR:CD2	2.79	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:820:PHE:CG	1:C:821:LYS:N	2.79	0.51
1:A:1176:LEU:CD2	1:A:1176:LEU:N	2.74	0.51
2:B:1424:ILE:CD1	2:B:1424:ILE:N	2.74	0.51
1:C:1139:GLU:O	1:C:1140:ASN:C	2.49	0.50
1:C:1019:PHE:CD2	1:C:1020:TYR:N	2.78	0.50
2:B:1624:LEU:O	2:B:1625:CYS:C	2.49	0.50
1:C:1068:VAL:CG2	1:C:1124:TYR:CD1	2.94	0.50
1:A:1007:SER:OG	1:A:1008:ALA:N	2.39	0.50
1:C:1110:ASN:O	1:C:1111:TYR:CG	2.63	0.50
2:B:189:PRO:C	2:B:191:LEU:N	2.65	0.50
1:C:931:PRO:CB	1:C:1366:HIS:CD2	2.95	0.50
1:C:819:VAL:O	1:C:820:PHE:O	2.29	0.50
1:C:488:PRO:O	1:C:489:LYS:O	2.29	0.50
1:A:42:GLN:CG	1:A:43:VAL:N	2.75	0.50
1:A:1421:HIS:NE2	1:A:1498:TYR:CD1	2.80	0.50
1:A:820:PHE:CG	1:A:821:LYS:N	2.79	0.50
1:A:855:PHE:C	1:A:855:PHE:CD1	2.84	0.50
1:C:1365:VAL:CG2	1:C:1366:HIS:N	2.75	0.50
2:B:347:PHE:O	2:B:348:THR:C	2.49	0.50
1:A:947:ARG:O	1:A:949:ILE:N	2.45	0.50
1:A:178:ASP:OD2	1:A:179:HIS:N	2.45	0.50
1:C:792:ASP:OD1	1:C:792:ASP:N	2.45	0.50
2:D:103:TYR:N	2:D:103:TYR:CD2	2.77	0.50
2:B:481:TYR:CD2	2:B:493:GLY:O	2.64	0.50
1:C:1266:TYR:CD1	1:C:1266:TYR:O	2.64	0.50
2:B:582:LYS:O	2:B:583:ALA:O	2.30	0.50
2:D:778:PHE:CD2	2:D:778:PHE:N	2.80	0.50
1:C:96:GLN:O	1:C:97:ASN:O	2.30	0.50
1:A:1571:GLU:O	1:A:1574:PHE:CD2	2.64	0.50
1:C:934:VAL:CG1	1:C:935:LYS:N	2.74	0.50
1:A:1493:PHE:CD1	1:A:1494:THR:N	2.79	0.50
1:A:1279:ARG:NH1	1:A:1280:TYR:CD2	2.80	0.50
2:D:469:ASN:C	2:D:469:ASN:ND2	2.65	0.50
1:C:1227:PHE:CD2	1:C:1273:TRP:CE2	3.00	0.50
1:A:1068:VAL:CG2	1:A:1124:TYR:CD1	2.95	0.50
2:B:344:GLN:CA	2:B:344:GLN:NE2	2.74	0.50
1:C:1421:HIS:CE1	1:C:1498:TYR:CD1	2.99	0.49
1:A:1024:TYR:CD2	1:A:1024:TYR:C	2.84	0.49
2:B:519:ARG:NH1	2:B:606:ASP:OD2	2.45	0.49
1:A:809:ILE:CG1	1:A:810:CYS:N	2.75	0.49
1:C:805:SER:O	1:C:807:THR:N	2.45	0.49
2:B:463:ASN:OD1	2:B:505:THR:OG1	2.29	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:576:SER:CB	1:A:577:PRO:CD	2.89	0.49
2:D:209:ASN:CG	3:D:2001:NAG:C7	2.80	0.49
1:C:1562:LYS:O	1:C:1563:VAL:CG1	2.60	0.49
1:C:50:PHE:C	1:C:50:PHE:CD1	2.85	0.49
1:A:854:GLN:OE1	1:A:854:GLN:O	2.30	0.49
1:A:500:ASN:OD1	1:A:514:THR:CG2	2.61	0.49
2:B:481:TYR:CB	2:B:520:PHE:CE1	2.95	0.49
2:D:415:THR:O	2:D:425:GLN:CD	2.51	0.49
1:A:884:VAL:CG1	1:A:886:GLN:CG	2.90	0.49
1:A:1164:ILE:O	1:A:1165:ASP:C	2.47	0.49
2:D:563:MET:CB	2:D:778:PHE:CE2	2.94	0.49
1:C:989:SER:O	1:C:993:SER:CB	2.60	0.49
1:A:50:PHE:C	1:A:50:PHE:CD1	2.86	0.49
2:B:417:HIS:N	2:B:425:GLN:OE1	2.45	0.49
1:C:820:PHE:O	1:C:821:LYS:CG	2.60	0.49
1:A:1487:PHE:O	1:A:1488:LEU:C	2.50	0.49
1:C:1056:ILE:C	1:C:1056:ILE:CD1	2.80	0.49
1:C:792:ASP:O	1:C:793:SER:CB	2.60	0.49
2:B:482:LEU:N	2:B:482:LEU:CD1	2.76	0.49
1:C:1227:PHE:CD2	1:C:1273:TRP:NE1	2.80	0.49
1:C:702:GLY:CA	1:C:728:PHE:CD1	2.95	0.49
2:B:778:PHE:N	2:B:778:PHE:CD2	2.81	0.49
2:D:145:TYR:C	2:D:145:TYR:CD1	2.86	0.49
2:B:806:TYR:CE1	2:B:807:GLU:O	2.66	0.49
2:B:581:ASP:O	2:B:582:LYS:C	2.51	0.49
1:C:682:LYS:NZ	1:C:686:ILE:CD1	2.75	0.49
2:B:25:TYR:O	2:B:631:SER:N	2.46	0.49
1:C:1252:ALA:O	1:C:1253:TYR:C	2.50	0.49
2:D:353:TYR:CD2	2:D:614:GLY:O	2.66	0.49
1:C:207:GLU:O	1:C:209:PHE:N	2.45	0.49
2:D:482:LEU:CD1	2:D:482:LEU:N	2.75	0.49
2:D:69:PHE:CD2	2:D:69:PHE:C	2.86	0.49
1:A:874:ASP:O	1:A:875:HIS:CG	2.66	0.49
2:B:481:TYR:C	2:B:481:TYR:CD2	2.85	0.49
1:C:1008:ALA:O	1:C:1010:ALA:N	2.45	0.49
1:C:111:PHE:CG	1:C:112:SER:N	2.81	0.49
2:B:1385:SER:OG	2:B:1455:SER:N	2.46	0.49
2:D:1424:ILE:N	2:D:1424:ILE:CD1	2.76	0.49
1:C:20:GLU:O	1:C:20:GLU:CG	2.61	0.49
1:A:1088:GLN:O	1:A:1090:ASN:N	2.46	0.49
1:C:222:TYR:CE1	1:C:768:TYR:CB	2.96	0.49
1:C:1024:TYR:O	1:C:1025:LEU:C	2.51	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:618:LYS:O	1:A:619:PRO:O	2.31	0.49
1:C:1324:HIS:CD2	1:C:1336:ARG:NH2	2.81	0.49
2:B:103:TYR:CD2	2:B:103:TYR:N	2.79	0.49
2:B:481:TYR:CE2	2:B:493:GLY:C	2.86	0.48
1:C:1480:PHE:CD1	1:C:1480:PHE:N	2.81	0.48
1:A:1024:TYR:O	1:A:1025:LEU:C	2.51	0.48
1:C:773:TRP:CZ2	1:C:797:TRP:CD1	3.02	0.48
1:A:819:VAL:O	1:A:820:PHE:O	2.30	0.48
1:C:288:GLN:N	1:C:288:GLN:OE1	2.46	0.48
2:B:742:ASP:OD1	2:B:742:ASP:C	2.52	0.48
1:C:309:GLU:N	1:C:309:GLU:OE1	2.46	0.48
2:B:44:GLU:OE2	2:B:523:TYR:OH	2.30	0.48
2:D:265:PHE:CD2	2:D:294:LEU:CB	2.97	0.48
1:C:1623:GLU:CB	1:C:1638:PRO:CG	2.91	0.48
1:A:471:ASP:OD2	1:A:474:LYS:CB	2.62	0.48
2:D:1613:GLU:O	2:D:1616:CYS:CB	2.61	0.48
1:C:1381:ILE:O	1:C:1382:ASP:CB	2.59	0.48
1:C:494:ASP:CG	1:C:494:ASP:O	2.52	0.48
1:C:1022:PHE:O	1:C:1024:TYR:N	2.47	0.48
1:A:1008:ALA:O	1:A:1010:ALA:N	2.46	0.48
1:A:961:TYR:CD1	1:A:961:TYR:O	2.66	0.48
1:C:1320:LYS:CD	1:C:1321:GLY:N	2.77	0.48
1:A:1562:LYS:O	1:A:1563:VAL:CG1	2.62	0.48
2:D:543:THR:OG1	2:D:544:CYS:N	2.43	0.48
2:B:830:VAL:CG2	2:B:831:GLU:N	2.72	0.48
2:D:742:ASP:C	2:D:742:ASP:OD1	2.52	0.48
2:B:69:PHE:C	2:B:69:PHE:CD2	2.87	0.48
1:C:809:ILE:CG1	1:C:810:CYS:N	2.76	0.48
1:A:1320:LYS:CD	1:A:1321:GLY:N	2.77	0.48
1:C:1675:GLY:O	1:C:1676:CYS:OXT	2.32	0.48
1:A:1102:ASN:ND2	1:C:1162:VAL:N	2.61	0.48
2:D:640:SER:O	2:D:641:ALA:CB	2.61	0.48
2:D:214:PHE:C	2:D:214:PHE:CD1	2.86	0.48
1:A:1143:TYR:O	1:A:1144:LEU:C	2.52	0.48
1:C:618:LYS:O	1:C:619:PRO:O	2.32	0.48
2:B:860:SER:OG	2:B:866:TYR:N	2.46	0.48
2:D:189:PRO:C	2:D:191:LEU:N	2.67	0.48
1:A:423:ASN:CB	2:B:501:GLN:NE2	2.77	0.48
2:B:1522:TYR:OH	2:B:1563:TYR:OH	2.31	0.48
1:A:641:ASN:O	1:A:642:ASN:C	2.50	0.48
1:A:1118:PHE:CD2	1:A:1148:THR:OG1	2.67	0.48
2:B:276:ILE:O	2:B:277:PRO:C	2.52	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:236:TYR:C	2:D:238:ASP:N	2.67	0.48
2:D:353:TYR:CD2	2:D:614:GLY:C	2.87	0.48
1:A:792:ASP:N	1:A:792:ASP:OD1	2.47	0.48
1:A:1381:ILE:O	1:A:1382:ASP:CB	2.62	0.48
1:C:439:ALA:O	1:C:441:ASP:N	2.47	0.48
1:C:471:ASP:OD2	1:C:474:LYS:CB	2.62	0.48
2:B:1601:ILE:CD1	2:B:1601:ILE:N	2.77	0.48
1:A:494:ASP:CG	1:A:494:ASP:O	2.52	0.47
1:C:1143:TYR:O	1:C:1146:ALA:N	2.47	0.47
1:A:1143:TYR:O	1:A:1146:ALA:N	2.47	0.47
1:A:1532:CYS:SG	1:A:1533:GLY:N	2.87	0.47
2:D:1385:SER:OG	2:D:1455:SER:N	2.47	0.47
1:C:854:GLN:OE1	1:C:854:GLN:O	2.32	0.47
2:B:145:TYR:CD1	2:B:145:TYR:C	2.88	0.47
1:A:811:VAL:O	1:A:811:VAL:CG1	2.62	0.47
2:D:842:GLU:O	2:D:843:ASP:C	2.53	0.47
1:C:101:TYR:CE1	1:C:116:ARG:CZ	2.97	0.47
1:C:289:ASN:OD1	1:C:289:ASN:N	2.46	0.47
2:D:581:ASP:O	2:D:582:LYS:C	2.50	0.47
1:A:1271:ILE:CD1	1:A:1300:TYR:CZ	2.97	0.47
2:D:126:SER:OG	2:D:127:PHE:N	2.47	0.47
1:C:333:THR:OG1	1:C:334:GLY:N	2.48	0.47
1:C:1344:ASP:OD1	1:C:1345:ASP:N	2.47	0.47
2:D:1628:PHE:O	2:D:1629:ALA:C	2.52	0.47
1:C:849:ARG:CG	1:C:849:ARG:NH1	2.75	0.47
2:D:556:ILE:N	2:D:556:ILE:CD1	2.77	0.47
2:D:481:TYR:CD2	2:D:493:GLY:O	2.67	0.47
1:C:1487:PHE:O	1:C:1488:LEU:C	2.53	0.47
2:D:417:HIS:N	2:D:425:GLN:OE1	2.48	0.47
1:A:1022:PHE:O	1:A:1023:HIS:C	2.51	0.47
1:A:111:PHE:CG	1:A:112:SER:N	2.82	0.47
1:C:520:ASP:N	1:C:520:ASP:OD1	2.47	0.47
1:A:820:PHE:CE2	1:A:821:LYS:O	2.67	0.47
1:A:374:GLN:CA	1:A:416:GLY:O	2.62	0.47
1:A:23:TYR:C	1:A:23:TYR:CD1	2.88	0.47
1:C:153:LYS:O	1:C:154:PRO:C	2.53	0.47
1:A:908:HIS:O	1:A:909:ASN:CB	2.61	0.47
1:A:59:TYR:CD1	1:A:60:PRO:CD	2.97	0.47
2:D:203:TYR:O	2:D:204:GLU:C	2.53	0.47
1:C:196:TYR:CD2	1:C:196:TYR:N	2.82	0.47
1:C:1085:VAL:O	1:C:1089:VAL:CG2	2.63	0.47
1:C:495:LYS:CA	1:C:495:LYS:CE	2.92	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:436:GLN:O	2:B:437:THR:C	2.53	0.47
1:C:59:TYR:CD1	1:C:60:PRO:CD	2.97	0.47
1:A:365:PRO:CG	1:A:464:TYR:CE2	2.97	0.47
1:C:174:VAL:CG2	1:C:175:GLU:N	2.77	0.47
2:D:481:TYR:C	2:D:481:TYR:CD2	2.87	0.47
1:A:222:TYR:CE1	1:A:768:TYR:CB	2.98	0.47
1:C:624:PHE:CD1	1:C:625:GLN:N	2.83	0.47
2:B:197:TRP:CB	2:B:214:PHE:CE1	2.98	0.47
1:A:25:ILE:N	1:A:655:THR:CG2	2.77	0.47
1:A:1365:VAL:CG2	1:A:1366:HIS:N	2.77	0.47
1:C:1421:HIS:NE2	1:C:1498:TYR:CD1	2.82	0.47
2:B:236:TYR:C	2:B:238:ASP:N	2.68	0.47
1:A:820:PHE:O	1:A:821:LYS:CG	2.62	0.47
1:A:853:MET:O	1:A:888:VAL:CG1	2.63	0.47
1:A:824:PHE:CD2	1:A:824:PHE:N	2.82	0.47
2:D:916:VAL:CG2	2:D:917:PRO:N	2.78	0.47
2:D:1296:ASN:O	2:D:1297:ALA:C	2.53	0.47
2:B:1270:HIS:CG	2:B:1270:HIS:O	2.68	0.47
1:A:135:TYR:CZ	1:A:141:VAL:CG1	2.98	0.47
1:C:1159:CYS:N	1:C:1160:PRO:CD	2.77	0.47
2:D:853:ASN:C	2:D:853:ASN:OD1	2.53	0.47
2:D:48:ASP:OD2	2:D:52:LYS:NZ	2.48	0.47
1:C:165:ASP:OD2	1:C:165:ASP:O	2.32	0.47
2:D:1522:TYR:OH	2:D:1563:TYR:OH	2.33	0.47
1:A:1344:ASP:OD1	1:A:1345:ASP:N	2.47	0.47
2:D:518:PHE:CD2	2:D:518:PHE:C	2.88	0.47
2:D:422:ARG:N	2:D:422:ARG:CD	2.78	0.47
2:B:556:ILE:N	2:B:556:ILE:CD1	2.78	0.47
1:A:495:LYS:CA	1:A:495:LYS:CE	2.92	0.47
1:C:1146:ALA:O	1:C:1147:PHE:C	2.53	0.46
1:C:985:GLY:O	1:C:987:ILE:N	2.48	0.46
1:C:938:SER:O	1:C:940:SER:N	2.48	0.46
1:A:174:VAL:CG2	1:A:175:GLU:N	2.77	0.46
1:A:1480:PHE:CD1	1:A:1480:PHE:N	2.83	0.46
1:C:623:VAL:O	1:C:625:GLN:N	2.49	0.46
2:D:1590:LEU:CD2	2:D:1591:LEU:N	2.78	0.46
2:B:1635:LEU:O	2:B:1637:GLU:N	2.48	0.46
1:C:692:HIS:O	1:C:692:HIS:CD2	2.68	0.46
2:D:162:ILE:CG2	2:D:162:ILE:O	2.63	0.46
2:B:214:PHE:CD1	2:B:214:PHE:C	2.88	0.46
1:A:792:ASP:O	1:A:793:SER:CB	2.63	0.46
2:B:1635:LEU:O	2:B:1636:THR:C	2.53	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:1613:GLU:O	2:B:1616:CYS:CB	2.63	0.46
1:C:853:MET:O	1:C:888:VAL:CG1	2.64	0.46
1:C:1615:ARG:NH2	1:C:1650:ARG:NH2	2.63	0.46
2:B:1296:ASN:O	2:B:1297:ALA:C	2.53	0.46
1:C:1290:THR:O	1:C:1294:ILE:CG1	2.63	0.46
1:C:1271:ILE:CD1	1:C:1300:TYR:CZ	2.98	0.46
2:D:806:TYR:CE1	2:D:807:GLU:O	2.68	0.46
1:A:1623:GLU:CB	1:A:1638:PRO:CG	2.93	0.46
1:C:700:TYR:CD2	1:C:701:ASP:N	2.83	0.46
2:D:25:TYR:O	2:D:631:SER:N	2.48	0.46
1:A:20:GLU:CG	1:A:20:GLU:O	2.63	0.46
1:A:1479:ILE:CD1	1:A:1479:ILE:N	2.78	0.46
1:A:488:PRO:O	1:A:489:LYS:O	2.33	0.46
1:A:1266:TYR:CD1	1:A:1266:TYR:O	2.69	0.46
2:B:853:ASN:C	2:B:853:ASN:OD1	2.54	0.46
2:D:1591:LEU:CD2	2:D:1591:LEU:C	2.84	0.46
1:A:288:GLN:O	1:A:289:ASN:C	2.54	0.46
1:C:267:ILE:CG2	1:C:268:THR:N	2.78	0.46
1:A:849:ARG:CG	1:A:849:ARG:NH1	2.76	0.46
1:A:165:ASP:O	1:A:167:GLU:N	2.48	0.46
1:A:1549:LYS:NZ	1:A:1667:PHE:CD1	2.84	0.46
1:C:286:ALA:O	1:C:287:MET:O	2.33	0.46
1:C:308:LYS:CG	1:C:309:GLU:N	2.78	0.46
1:C:820:PHE:CE2	1:C:821:LYS:O	2.69	0.46
1:C:1320:LYS:CG	1:C:1321:GLY:N	2.79	0.46
2:B:210:TYR:CG	2:B:211:THR:N	2.83	0.46
1:A:1616:GLN:NE2	1:A:1648:TRP:CZ3	2.84	0.46
2:D:1635:LEU:O	2:D:1636:THR:C	2.53	0.46
2:B:165:PHE:CZ	2:B:199:ILE:CD1	2.98	0.46
2:D:531:ILE:O	2:D:617:ASN:ND2	2.48	0.46
2:D:481:TYR:CE2	2:D:493:GLY:C	2.88	0.46
1:C:135:TYR:CZ	1:C:141:VAL:CG1	2.98	0.46
2:B:1591:LEU:C	2:B:1591:LEU:CD2	2.84	0.46
2:D:1274:ASN:ND2	2:D:1293:ASN:CB	2.79	0.46
2:B:48:ASP:OD2	2:B:52:LYS:NZ	2.49	0.46
1:A:501:TYR:C	1:A:501:TYR:CD1	2.89	0.46
2:B:1500:LEU:C	2:B:1500:LEU:CD1	2.84	0.46
1:A:985:GLY:O	1:A:987:ILE:N	2.49	0.46
1:A:1323:LEU:O	1:A:1324:HIS:O	2.33	0.46
1:A:1675:GLY:O	1:A:1676:CYS:OXT	2.34	0.46
1:A:692:HIS:O	1:A:692:HIS:CD2	2.69	0.46
1:C:1631:PHE:CD2	1:C:1631:PHE:N	2.82	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:42:GLN:OE1	1:A:500:ASN:ND2	2.49	0.46
1:A:625:GLN:CG	1:A:626:PHE:N	2.79	0.46
1:C:884:VAL:CG1	1:C:886:GLN:CG	2.93	0.46
1:A:1056:ILE:CD1	1:A:1066:TYR:CE2	2.99	0.46
2:B:851:LEU:CD2	2:B:852:TYR:N	2.79	0.46
1:C:691:LYS:O	1:C:693:SER:N	2.49	0.46
1:C:85:LEU:CD2	1:C:85:LEU:N	2.79	0.46
1:A:1631:PHE:N	1:A:1631:PHE:CD2	2.80	0.46
1:A:153:LYS:O	1:A:154:PRO:C	2.54	0.46
1:A:1320:LYS:CG	1:A:1321:GLY:N	2.79	0.46
1:C:869:GLU:C	1:C:871:PRO:CD	2.84	0.46
2:B:1628:PHE:O	2:B:1629:ALA:C	2.54	0.46
2:B:1448:VAL:O	2:B:1449:GLY:O	2.34	0.46
1:A:1103:SER:O	1:A:1106:TRP:N	2.48	0.46
2:B:1599:TYR:N	2:B:1599:TYR:CD1	2.84	0.46
1:C:1532:CYS:SG	1:C:1533:GLY:N	2.89	0.45
1:A:700:TYR:CD2	1:A:701:ASP:N	2.83	0.45
1:A:439:ALA:O	1:A:441:ASP:N	2.48	0.45
1:C:1419:SER:OG	1:C:1467:ILE:N	2.49	0.45
1:C:1151:GLY:O	1:C:1152:ILE:C	2.54	0.45
1:A:1274:LEU:O	1:A:1277:GLU:N	2.49	0.45
1:A:309:GLU:OE1	1:A:309:GLU:N	2.50	0.45
2:B:884:ILE:CG1	2:B:885:VAL:N	2.79	0.45
2:B:1602:THR:C	2:B:1604:ASN:N	2.69	0.45
2:B:543:THR:OG1	2:B:544:CYS:N	2.42	0.45
1:C:1088:GLN:O	1:C:1090:ASN:N	2.49	0.45
2:D:147:VAL:N	2:D:183:PHE:CZ	2.85	0.45
2:B:353:TYR:CD2	2:B:614:GLY:C	2.89	0.45
1:A:333:THR:OG1	1:A:334:GLY:N	2.49	0.45
2:B:1504:GLU:OE2	2:B:1505:ARG:N	2.49	0.45
1:C:811:VAL:CG1	1:C:811:VAL:O	2.64	0.45
2:B:490:PHE:CG	2:B:491:LYS:N	2.83	0.45
1:A:1088:GLN:C	1:A:1090:ASN:N	2.69	0.45
1:C:516:GLU:N	1:C:516:GLU:CD	2.70	0.45
2:D:1506:ILE:CD1	2:D:1628:PHE:CD1	2.99	0.45
1:A:989:SER:O	1:A:993:SER:CB	2.64	0.45
1:A:267:ILE:CG2	1:A:268:THR:N	2.79	0.45
1:A:1099:SER:O	1:A:1100:ILE:C	2.55	0.45
2:B:203:TYR:O	2:B:204:GLU:C	2.55	0.45
1:C:296:ILE:CG2	1:C:297:ALA:N	2.78	0.45
1:A:226:HIS:ND1	1:A:336:PHE:CE2	2.85	0.45
1:A:869:GLU:C	1:A:871:PRO:CD	2.84	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:908:HIS:O	1:C:909:ASN:CB	2.64	0.45
1:A:773:TRP:CZ2	1:A:797:TRP:CD1	3.04	0.45
1:C:773:TRP:NE1	1:C:797:TRP:NE1	2.64	0.45
1:A:947:ARG:NH1	1:A:1352:PHE:CE2	2.84	0.45
1:C:917:TRP:O	2:D:813:VAL:CG2	2.65	0.45
2:D:1448:VAL:O	2:D:1449:GLY:O	2.34	0.45
1:A:691:LYS:O	1:A:693:SER:N	2.50	0.45
2:B:415:THR:OG1	2:B:415:THR:O	2.35	0.45
1:A:1627:ILE:O	1:A:1629:TYR:N	2.50	0.45
1:C:625:GLN:CG	1:C:626:PHE:N	2.80	0.45
1:C:1627:ILE:O	1:C:1629:TYR:N	2.50	0.45
1:A:1056:ILE:C	1:A:1056:ILE:CD1	2.84	0.45
1:A:1404:ALA:CB	1:A:1493:PHE:CE2	2.99	0.45
2:D:1270:HIS:O	2:D:1270:HIS:CG	2.70	0.45
1:C:1103:SER:O	1:C:1106:TRP:N	2.50	0.45
1:A:1020:TYR:O	1:A:1021:VAL:C	2.54	0.45
2:D:825:VAL:O	2:D:826:LYS:C	2.55	0.45
2:B:78:ALA:O	2:B:80:GLY:N	2.49	0.45
1:A:1290:THR:O	1:A:1294:ILE:CG1	2.65	0.45
2:B:323:GLU:C	2:B:323:GLU:OE1	2.55	0.45
2:B:422:ARG:N	2:B:422:ARG:CD	2.80	0.45
1:C:1323:LEU:O	1:C:1324:HIS:O	2.35	0.45
2:B:883:VAL:N	2:B:1452:GLN:OE1	2.50	0.45
1:C:1190:ILE:O	1:C:1191:SER:C	2.55	0.45
2:D:370:ASP:OD1	2:D:370:ASP:N	2.50	0.45
1:C:412:ARG:NH2	1:C:472:ASN:ND2	2.65	0.45
2:D:518:PHE:CD2	2:D:518:PHE:O	2.69	0.45
1:A:501:TYR:O	1:A:501:TYR:CD1	2.69	0.45
1:A:1324:HIS:CD2	1:A:1336:ARG:NH2	2.85	0.45
1:A:1289:ASP:O	1:A:1290:THR:C	2.55	0.45
1:C:683:ILE:O	1:C:687:ALA:CB	2.65	0.45
1:C:374:GLN:CA	1:C:416:GLY:O	2.65	0.45
2:D:309:LEU:O	2:D:310:VAL:C	2.54	0.45
1:A:163:PHE:CE1	1:A:188:PHE:CG	3.04	0.45
1:C:916:THR:O	1:C:918:PHE:N	2.50	0.45
2:B:192:VAL:CG2	2:B:193:SER:N	2.79	0.45
1:C:23:TYR:C	1:C:23:TYR:CD1	2.90	0.45
1:A:624:PHE:CD1	1:A:625:GLN:N	2.85	0.45
2:B:563:MET:CB	2:B:778:PHE:CE2	3.00	0.45
2:D:490:PHE:CG	2:D:491:LYS:N	2.85	0.45
1:C:1243:GLY:O	1:C:1285:TYR:CE2	2.69	0.45
1:C:506:LYS:CE	1:C:533:ASN:O	2.65	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:180:ILE:CG2	1:C:599:TRP:CE3	3.00	0.44
1:A:1226:ARG:NH1	1:A:1266:TYR:CE1	2.85	0.44
1:C:1549:LYS:NZ	1:C:1667:PHE:CD1	2.85	0.44
1:C:701:ASP:N	1:C:701:ASP:OD1	2.50	0.44
2:D:382:GLU:C	2:D:384:PHE:N	2.71	0.44
1:A:1641:SER:C	1:A:1643:THR:N	2.71	0.44
2:D:884:ILE:CG1	2:D:885:VAL:N	2.79	0.44
1:A:351:PRO:CG	1:A:352:TYR:CD2	3.00	0.44
1:C:1088:GLN:C	1:C:1090:ASN:N	2.71	0.44
1:C:1366:HIS:N	1:C:1366:HIS:ND1	2.66	0.44
1:C:916:THR:C	1:C:918:PHE:N	2.71	0.44
1:A:1231:ASN:O	1:A:1234:HIS:O	2.35	0.44
1:C:1118:PHE:CD2	1:C:1148:THR:OG1	2.71	0.44
1:C:1559:TYR:CE1	1:C:1586:LYS:O	2.70	0.44
1:A:361:LEU:N	1:A:361:LEU:CD1	2.79	0.44
2:D:1601:ILE:N	2:D:1601:ILE:CD1	2.81	0.44
1:C:371:ILE:O	1:C:371:ILE:CG2	2.66	0.44
1:A:623:VAL:O	1:A:625:GLN:N	2.51	0.44
1:A:970:LYS:C	1:A:971:THR:CG2	2.86	0.44
1:C:1562:LYS:C	1:C:1563:VAL:CG1	2.85	0.44
1:C:1327:LYS:O	1:C:1332:ASN:ND2	2.50	0.44
2:D:219:TYR:CD1	2:D:220:VAL:N	2.86	0.44
1:C:171:VAL:CG1	1:C:172:ASP:N	2.80	0.44
1:A:207:GLU:O	1:A:209:PHE:N	2.50	0.44
1:A:1366:HIS:ND1	1:A:1366:HIS:N	2.65	0.44
2:B:518:PHE:CE2	2:B:538:VAL:CB	3.00	0.44
2:B:126:SER:OG	2:B:127:PHE:N	2.49	0.44
1:C:1099:SER:O	1:C:1100:ILE:C	2.53	0.44
2:D:481:TYR:CB	2:D:520:PHE:CE1	3.01	0.44
2:D:951:ASP:C	2:D:953:ARG:N	2.68	0.44
1:A:286:ALA:O	1:A:287:MET:O	2.35	0.44
2:B:1274:ASN:ND2	2:B:1293:ASN:CB	2.81	0.44
1:C:500:ASN:ND2	1:C:543:TYR:CE1	2.86	0.44
1:C:1127:ILE:CD1	1:C:1127:ILE:N	2.80	0.44
2:D:415:THR:OG1	2:D:415:THR:O	2.34	0.44
2:D:476:ILE:CG1	2:D:524:TYR:CD2	3.01	0.44
2:B:951:ASP:C	2:B:953:ARG:N	2.68	0.44
1:A:171:VAL:CG1	1:A:172:ASP:N	2.81	0.44
1:C:226:HIS:ND1	1:C:336:PHE:CE2	2.86	0.44
2:D:1602:THR:C	2:D:1604:ASN:N	2.70	0.44
2:D:850:LEU:CB	2:D:882:PHE:CE1	3.01	0.44
1:C:165:ASP:O	1:C:167:GLU:N	2.50	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:1381:ILE:CG1	1:C:1382:ASP:N	2.81	0.44
1:A:226:HIS:ND1	1:A:336:PHE:CD2	2.85	0.44
2:B:219:TYR:CD1	2:B:220:VAL:N	2.86	0.44
2:B:309:LEU:O	2:B:310:VAL:C	2.57	0.44
1:A:1151:GLY:O	1:A:1152:ILE:C	2.53	0.44
1:A:1247:MET:O	1:A:1248:VAL:C	2.56	0.44
1:A:721:GLY:O	1:A:724:CYS:N	2.51	0.44
1:A:1559:TYR:CE1	1:A:1586:LYS:O	2.70	0.44
1:A:1285:TYR:O	1:A:1286:SER:O	2.36	0.44
1:A:85:LEU:N	1:A:85:LEU:CD2	2.81	0.44
1:A:324:TYR:CD2	1:A:324:TYR:C	2.91	0.44
2:D:1599:TYR:CD1	2:D:1599:TYR:N	2.86	0.44
1:A:1183:GLN:O	1:A:1183:GLN:NE2	2.50	0.44
1:A:110:HIS:N	1:A:110:HIS:ND1	2.65	0.44
2:B:147:VAL:N	2:B:183:PHE:CZ	2.86	0.43
2:D:916:VAL:CG2	2:D:917:PRO:CD	2.95	0.43
1:A:284:GLN:O	1:A:285:THR:CB	2.66	0.43
1:C:504:LEU:N	1:C:504:LEU:CD1	2.80	0.43
2:B:354:PHE:C	2:B:354:PHE:CD1	2.91	0.43
1:C:494:ASP:OD1	1:C:494:ASP:C	2.57	0.43
1:A:1142:LEU:O	1:A:1143:TYR:O	2.36	0.43
1:A:805:SER:O	1:A:808:GLY:N	2.51	0.43
1:C:1279:ARG:C	1:C:1279:ARG:CD	2.87	0.43
1:A:516:GLU:CD	1:A:516:GLU:N	2.71	0.43
1:A:642:ASN:ND2	1:A:646:PHE:CD1	2.86	0.43
1:A:701:ASP:N	1:A:701:ASP:OD1	2.51	0.43
2:B:531:ILE:O	2:B:617:ASN:ND2	2.51	0.43
1:C:1439:LEU:O	1:C:1440:LYS:C	2.57	0.43
2:D:883:VAL:N	2:D:1452:GLN:OE1	2.51	0.43
1:A:578:ASP:O	1:A:579:ALA:O	2.35	0.43
2:B:382:GLU:C	2:B:384:PHE:N	2.72	0.43
1:A:127:PHE:N	1:A:127:PHE:CD1	2.84	0.43
1:C:1226:ARG:NH1	1:C:1266:TYR:CE1	2.86	0.43
1:A:1146:ALA:O	1:A:1147:PHE:C	2.57	0.43
1:A:1562:LYS:C	1:A:1563:VAL:CG1	2.86	0.43
2:D:518:PHE:CE2	2:D:538:VAL:CB	3.01	0.43
1:C:1231:ASN:O	1:C:1234:HIS:O	2.37	0.43
1:A:47:THR:O	1:A:48:GLU:CB	2.66	0.43
1:A:1239:VAL:CG1	1:A:1239:VAL:O	2.66	0.43
2:B:919:GLY:CA	2:B:1331:ALA:O	2.66	0.43
1:C:135:TYR:CE1	1:C:141:VAL:CA	3.01	0.43
1:C:949:ILE:O	1:C:949:ILE:CG2	2.67	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:238:ASP:O	2:B:238:ASP:OD1	2.36	0.43
1:C:1279:ARG:O	1:C:1280:TYR:C	2.57	0.43
1:C:1315:VAL:CG1	1:C:1324:HIS:O	2.67	0.43
1:A:642:ASN:ND2	1:A:642:ASN:C	2.72	0.43
1:A:444:GLU:O	1:A:445:GLU:C	2.57	0.43
1:C:1500:ARG:C	1:C:1502:ASP:N	2.72	0.43
1:A:1582:LEU:O	1:A:1594:LYS:NZ	2.52	0.43
2:D:735:ASN:OD1	2:D:735:ASN:N	2.52	0.43
1:C:610:TYR:N	1:C:610:TYR:CD1	2.86	0.43
2:D:436:GLN:O	2:D:437:THR:C	2.56	0.43
1:C:1584:ILE:O	1:C:1585:TYR:CB	2.65	0.43
1:C:1601:ILE:O	1:C:1638:PRO:O	2.36	0.43
1:A:1615:ARG:NH2	1:A:1650:ARG:NH2	2.66	0.43
1:A:506:LYS:CE	1:A:533:ASN:O	2.66	0.43
1:C:873:ILE:O	1:C:873:ILE:CD1	2.66	0.43
1:C:1239:VAL:CG1	1:C:1239:VAL:O	2.67	0.43
1:C:1644:TRP:CD1	1:C:1646:GLU:OE1	2.71	0.43
1:C:1585:TYR:CD1	1:C:1671:ILE:CG1	3.02	0.43
1:C:689:LYS:O	1:C:691:LYS:N	2.52	0.43
1:C:1243:GLY:O	1:C:1285:TYR:CZ	2.71	0.43
1:C:226:HIS:ND1	1:C:336:PHE:CD2	2.87	0.43
1:A:1151:GLY:O	1:A:1154:LYS:N	2.52	0.43
1:C:33:VAL:CG2	1:C:121:TYR:CD1	3.02	0.43
1:C:975:ARG:NH1	1:C:1340:VAL:CG1	2.82	0.43
1:C:38:ASN:ND2	1:C:509:ILE:O	2.51	0.43
2:B:735:ASN:N	2:B:735:ASN:OD1	2.51	0.43
1:A:967:LEU:CD1	1:A:968:VAL:N	2.81	0.43
2:D:866:TYR:OH	2:D:1388:THR:CG2	2.67	0.43
1:C:970:LYS:C	1:C:971:THR:CG2	2.87	0.43
1:A:464:TYR:O	1:A:544:TYR:OH	2.36	0.43
1:A:1243:GLY:O	1:A:1285:TYR:CE2	2.72	0.43
1:A:412:ARG:CD	2:B:458:ASP:OD1	2.66	0.43
1:A:81:ASN:CG	1:A:82:SER:N	2.72	0.43
1:C:824:PHE:N	1:C:824:PHE:CD2	2.85	0.43
1:A:494:ASP:C	1:A:494:ASP:OD1	2.57	0.43
1:C:1142:LEU:O	1:C:1143:TYR:O	2.37	0.43
2:D:261:ALA:N	2:D:285:ILE:CD1	2.82	0.43
1:A:689:LYS:O	1:A:691:LYS:N	2.52	0.43
1:A:163:PHE:CE1	1:A:188:PHE:CD1	3.06	0.43
1:C:1120:GLU:OE2	1:C:1121:ASN:N	2.52	0.43
2:B:341:SER:OG	2:B:343:TYR:O	2.37	0.43
1:A:367:ILE:O	1:A:368:PRO:C	2.57	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:338:ILE:C	2:D:339:VAL:CG1	2.87	0.43
2:B:762:LEU:N	2:B:762:LEU:CD1	2.82	0.43
1:C:1090:ASN:C	1:C:1092:TYR:N	2.71	0.43
2:B:511:THR:O	2:B:513:ASP:N	2.52	0.43
1:C:1022:PHE:O	1:C:1023:HIS:C	2.57	0.43
1:C:552:ALA:O	1:C:658:ASN:ND2	2.52	0.43
1:C:971:THR:O	1:C:972:GLU:C	2.57	0.43
2:B:1556:PRO:C	2:B:1558:ALA:N	2.72	0.43
2:B:755:TRP:O	2:B:756:LEU:CB	2.66	0.43
1:A:1148:THR:O	1:A:1149:VAL:C	2.57	0.43
2:D:1561:HIS:CE1	2:D:1597:ILE:CD1	3.02	0.43
2:B:847:ARG:CZ	2:B:867:ARG:NH1	2.82	0.43
2:B:646:GLN:O	2:B:647:PRO:C	2.57	0.43
2:B:265:PHE:CD2	2:B:294:LEU:CB	3.02	0.43
2:D:276:ILE:O	2:D:277:PRO:C	2.57	0.43
1:A:355:ASN:ND2	1:A:355:ASN:N	2.66	0.43
1:C:156:LYS:C	1:C:156:LYS:CD	2.87	0.43
1:A:936:ARG:CG	1:A:936:ARG:NH1	2.81	0.43
1:A:1159:CYS:SG	1:A:1161:LEU:CD2	3.07	0.43
1:A:101:TYR:N	1:A:101:TYR:CD2	2.87	0.43
1:C:101:TYR:CD2	1:C:101:TYR:N	2.87	0.43
2:D:202:LYS:CG	2:D:203:TYR:N	2.82	0.43
2:D:74:ASP:OD1	2:D:74:ASP:N	2.52	0.43
1:C:1455:ILE:CD1	1:C:1455:ILE:N	2.82	0.43
1:C:1298:THR:O	1:C:1301:SER:N	2.52	0.43
2:B:1491:ARG:CG	2:B:1492:CYS:N	2.82	0.43
1:A:1090:ASN:C	1:A:1092:TYR:N	2.72	0.42
2:D:580:VAL:CG1	2:D:581:ASP:N	2.81	0.42
2:D:851:LEU:CD2	2:D:852:TYR:N	2.82	0.42
2:B:1505:ARG:NH1	2:B:1627:ASP:OD1	2.51	0.42
1:A:1327:LYS:O	1:A:1332:ASN:ND2	2.52	0.42
1:A:916:THR:O	1:A:918:PHE:N	2.52	0.42
1:A:196:TYR:CD2	1:A:196:TYR:N	2.85	0.42
2:B:370:ASP:N	2:B:370:ASP:OD1	2.52	0.42
1:A:489:LYS:NZ	2:B:502:ASN:N	2.67	0.42
1:A:153:LYS:O	1:A:154:PRO:O	2.37	0.42
1:C:1645:ILE:O	1:C:1646:GLU:CG	2.67	0.42
1:C:1143:TYR:O	1:C:1144:LEU:C	2.56	0.42
1:A:1022:PHE:O	1:A:1025:LEU:N	2.52	0.42
2:D:919:GLY:CA	2:D:1331:ALA:O	2.67	0.42
1:A:1279:ARG:O	1:A:1280:TYR:C	2.56	0.42
1:C:1324:HIS:CG	1:C:1336:ARG:NH2	2.87	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1060:ARG:CG	1:A:1061:ASN:N	2.82	0.42
1:A:594:THR:O	1:A:782:ARG:CD	2.67	0.42
1:C:110:HIS:ND1	1:C:110:HIS:N	2.66	0.42
1:C:355:ASN:ND2	1:C:355:ASN:N	2.67	0.42
1:A:1091:LYS:NZ	1:A:1092:TYR:CE2	2.87	0.42
1:A:847:ASN:ND2	1:A:853:MET:CB	2.83	0.42
1:A:1086:LEU:O	1:A:1087:GLY:C	2.57	0.42
1:A:1370:THR:O	1:A:1371:SER:C	2.56	0.42
2:B:480:THR:OG1	2:B:494:ARG:NE	2.51	0.42
1:C:1641:SER:C	1:C:1643:THR:N	2.73	0.42
1:A:1162:VAL:N	1:C:1102:ASN:ND2	2.67	0.42
1:A:626:PHE:O	1:A:628:GLU:N	2.52	0.42
1:A:308:LYS:CG	1:A:309:GLU:N	2.81	0.42
1:C:1280:TYR:O	1:C:1280:TYR:CG	2.72	0.42
1:C:642:ASN:ND2	1:C:642:ASN:C	2.73	0.42
1:C:1479:ILE:N	1:C:1479:ILE:CD1	2.83	0.42
1:A:132:LYS:NZ	1:A:139:GLN:NE2	2.67	0.42
1:C:1570:VAL:CA	1:C:1574:PHE:O	2.68	0.42
2:D:1635:LEU:O	2:D:1637:GLU:N	2.52	0.42
2:B:1506:ILE:CD1	2:B:1628:PHE:CD1	3.03	0.42
1:C:917:TRP:CB	2:D:558:MET:SD	3.07	0.42
1:C:461:SER:CB	1:C:553:GLU:OE2	2.68	0.42
2:D:1491:ARG:CG	2:D:1492:CYS:N	2.83	0.42
1:C:444:GLU:O	1:C:445:GLU:C	2.57	0.42
1:A:610:TYR:CD1	1:A:610:TYR:N	2.86	0.42
1:C:1183:GLN:O	1:C:1183:GLN:NE2	2.53	0.42
1:C:365:PRO:CD	1:C:464:TYR:CE2	3.03	0.42
1:C:1176:LEU:CD2	1:C:1195:LEU:CD2	2.98	0.42
1:C:849:ARG:NH2	2:D:556:ILE:O	2.52	0.42
2:B:490:PHE:C	2:B:490:PHE:CD1	2.91	0.42
2:B:1274:ASN:OD1	2:B:1291:ARG:NH1	2.53	0.42
2:D:218:LYS:CB	2:D:822:TYR:CD2	3.03	0.42
1:C:721:GLY:O	1:C:724:CYS:N	2.53	0.42
1:C:1056:ILE:CD1	1:C:1066:TYR:CE2	3.02	0.42
2:B:29:THR:CB	2:B:30:PRO:CD	2.97	0.42
1:A:1109:GLU:CG	1:C:1163:LYS:NZ	2.83	0.42
1:A:117:MET:CB	1:A:118:PRO:CD	2.98	0.42
1:C:1560:ALA:CB	1:C:1620:MET:CG	2.98	0.42
1:A:1585:TYR:CD1	1:A:1671:ILE:CG1	3.03	0.42
1:A:1671:ILE:CG1	1:A:1671:ILE:O	2.68	0.42
2:B:742:ASP:OD1	2:B:743:SER:N	2.53	0.42
1:C:1148:THR:O	1:C:1149:VAL:C	2.56	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:594:THR:OG1	1:A:782:ARG:CA	2.67	0.42
1:C:1043:GLN:O	1:C:1044:LYS:C	2.58	0.42
2:D:819:GLN:NE2	2:D:819:GLN:CA	2.82	0.42
1:A:873:ILE:CD1	1:A:873:ILE:O	2.67	0.42
2:B:350:THR:O	2:B:350:THR:CG2	2.68	0.42
1:C:1020:TYR:O	1:C:1021:VAL:C	2.59	0.42
1:A:1127:ILE:CD1	1:A:1127:ILE:N	2.82	0.42
2:B:476:ILE:CG1	2:B:524:TYR:CD2	3.03	0.42
2:D:296:ARG:NH1	2:D:296:ARG:CG	2.83	0.42
1:C:949:ILE:C	1:C:950:TYR:CG	2.93	0.42
1:A:831:TYR:O	1:A:928:ARG:CB	2.67	0.42
1:C:1279:ARG:CZ	1:C:1280:TYR:CD2	3.03	0.42
1:C:805:SER:O	1:C:808:GLY:N	2.53	0.42
1:A:1243:GLY:O	1:A:1285:TYR:CZ	2.73	0.42
2:D:262:PHE:CE1	2:D:282:ARG:CG	3.03	0.42
2:D:1289:ARG:O	2:D:1290:TYR:CD1	2.73	0.42
1:C:1060:ARG:CG	1:C:1061:ASN:N	2.83	0.42
2:B:262:PHE:CE1	2:B:282:ARG:CG	3.02	0.42
2:B:958:GLU:CA	2:B:958:GLU:OE1	2.68	0.42
1:C:1636:ILE:CG2	1:C:1636:ILE:O	2.68	0.42
2:D:646:GLN:O	2:D:647:PRO:C	2.59	0.42
1:C:1545:ALA:CB	1:C:1660:PHE:CE1	3.03	0.42
2:D:1378:THR:O	2:D:1379:MET:C	2.58	0.42
1:A:371:ILE:CG2	1:A:371:ILE:O	2.67	0.42
2:B:825:VAL:O	2:B:826:LYS:C	2.58	0.42
1:A:289:ASN:N	1:A:289:ASN:OD1	2.52	0.42
1:A:721:GLY:C	1:A:723:ARG:N	2.73	0.42
1:A:472:ASN:O	1:A:473:HIS:CB	2.67	0.42
1:A:296:ILE:CG2	1:A:297:ALA:N	2.82	0.42
2:D:621:PHE:N	2:D:621:PHE:CD2	2.86	0.42
1:A:222:TYR:C	1:A:222:TYR:CD2	2.94	0.41
2:D:756:LEU:CD2	2:D:778:PHE:CE1	3.03	0.41
1:A:412:ARG:NH2	1:A:472:ASN:ND2	2.68	0.41
2:B:83:VAL:C	2:B:85:PRO:CD	2.89	0.41
1:C:1026:GLU:OE1	1:C:1031:TRP:NE1	2.53	0.41
1:C:594:THR:OG1	1:C:782:ARG:CA	2.68	0.41
1:C:501:TYR:C	1:C:501:TYR:CD1	2.93	0.41
2:B:438:GLN:O	2:B:439:GLY:C	2.58	0.41
1:C:47:THR:O	1:C:48:GLU:CB	2.67	0.41
1:C:1435:ASN:O	1:C:1436:GLU:C	2.58	0.41
1:A:354:LEU:CD2	1:A:354:LEU:N	2.83	0.41
1:A:1584:ILE:O	1:A:1585:TYR:CB	2.68	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:971:THR:O	1:A:972:GLU:C	2.58	0.41
1:A:1271:ILE:O	1:A:1272:LYS:C	2.57	0.41
1:A:1118:PHE:CE2	1:A:1148:THR:OG1	2.73	0.41
1:A:1500:ARG:C	1:A:1502:ASP:N	2.73	0.41
1:A:465:LEU:CG	1:A:466:TYR:N	2.83	0.41
1:A:1545:ALA:CB	1:A:1660:PHE:CE1	3.03	0.41
2:D:1431:SER:N	2:D:1436:GLU:OE2	2.52	0.41
1:A:240:TYR:CD2	1:A:240:TYR:C	2.89	0.41
1:C:127:PHE:CD1	1:C:127:PHE:N	2.87	0.41
2:D:762:LEU:N	2:D:762:LEU:CD1	2.83	0.41
1:C:405:ASP:OD1	1:C:405:ASP:N	2.52	0.41
2:B:1498:SER:O	2:B:1573:LEU:CD2	2.68	0.41
1:C:132:LYS:NZ	1:C:139:GLN:NE2	2.67	0.41
1:C:546:VAL:O	1:C:553:GLU:CB	2.67	0.41
2:D:1407:TYR:CD2	2:D:1407:TYR:C	2.92	0.41
1:A:791:PRO:CG	1:A:797:TRP:NE1	2.83	0.41
1:A:655:THR:OG1	1:A:655:THR:O	2.37	0.41
2:D:1610:TRP:CG	2:D:1628:PHE:CD2	3.07	0.41
2:B:494:ARG:NH1	2:B:494:ARG:CG	2.82	0.41
2:B:148:PHE:CZ	2:B:792:VAL:CG1	3.04	0.41
1:A:124:GLY:C	1:A:125:PHE:CG	2.93	0.41
1:A:864:GLY:CA	1:A:907:LEU:CD2	2.98	0.41
1:C:1083:LEU:CD2	1:C:1104:LEU:CD2	2.98	0.41
2:D:341:SER:OG	2:D:343:TYR:O	2.38	0.41
2:D:165:PHE:CZ	2:D:199:ILE:CD1	3.03	0.41
2:B:299:PHE:CE1	2:B:303:PHE:CD2	3.08	0.41
2:D:1556:PRO:C	2:D:1558:ALA:N	2.73	0.41
1:A:1570:VAL:CA	1:A:1574:PHE:O	2.69	0.41
1:C:288:GLN:O	1:C:289:ASN:C	2.57	0.41
2:D:1610:TRP:CA	2:D:1628:PHE:CE2	3.04	0.41
1:C:501:TYR:O	1:C:501:TYR:CD1	2.73	0.41
2:D:1456:VAL:CG1	2:D:1456:VAL:O	2.63	0.41
1:C:361:LEU:CD1	1:C:361:LEU:N	2.83	0.41
2:D:466:VAL:CG1	2:D:524:TYR:CE2	3.04	0.41
1:A:59:TYR:N	1:A:60:PRO:CD	2.84	0.41
1:A:24:VAL:CG1	1:A:24:VAL:O	2.69	0.41
2:B:1606:TRP:CD1	2:B:1606:TRP:O	2.74	0.41
1:C:938:SER:OG	1:C:1284:PHE:CZ	2.74	0.41
1:C:1616:GLN:CD	1:C:1648:TRP:CZ3	2.94	0.41
2:B:756:LEU:CD2	2:B:778:PHE:CE1	3.03	0.41
1:C:501:TYR:CE1	1:C:512:PHE:C	2.94	0.41
1:A:1419:SER:OG	1:A:1467:ILE:N	2.54	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1085:VAL:O	1:A:1089:VAL:CG2	2.68	0.41
2:D:78:ALA:O	2:D:80:GLY:N	2.53	0.41
1:A:1026:GLU:OE1	1:A:1031:TRP:NE1	2.53	0.41
2:D:1512:ILE:CG2	2:D:1631:PHE:CD1	3.03	0.41
1:A:775:TRP:O	1:A:775:TRP:CD1	2.74	0.41
1:A:1455:ILE:N	1:A:1455:ILE:CD1	2.84	0.41
1:A:42:GLN:CB	1:A:80:GLN:NE2	2.84	0.41
2:B:952:ASP:O	2:B:1331:ALA:CA	2.68	0.41
2:D:603:GLU:C	2:D:605:SER:N	2.74	0.41
1:A:1212:LEU:CD1	1:A:1228:TRP:NE1	2.83	0.41
1:C:594:THR:O	1:C:782:ARG:CD	2.69	0.41
1:C:1582:LEU:O	1:C:1594:LYS:NZ	2.54	0.41
2:B:1387:LEU:CD2	2:B:1472:TYR:CE1	3.04	0.41
2:D:323:GLU:OE1	2:D:323:GLU:C	2.59	0.41
1:C:42:GLN:OE1	1:C:500:ASN:ND2	2.53	0.41
1:C:1022:PHE:O	1:C:1025:LEU:N	2.54	0.41
2:D:952:ASP:O	2:D:1331:ALA:CA	2.69	0.41
1:A:1667:PHE:CD2	1:A:1667:PHE:N	2.88	0.41
1:A:1176:LEU:CD2	1:A:1195:LEU:CD2	2.99	0.41
2:D:383:ALA:C	2:D:384:PHE:CD2	2.94	0.41
1:A:77:ASN:C	1:A:79:PHE:N	2.73	0.41
1:A:1423:VAL:CG1	1:A:1496:TYR:CZ	3.04	0.41
1:A:1537:GLU:O	1:A:1539:LEU:N	2.54	0.41
1:A:917:TRP:O	2:B:813:VAL:CG2	2.69	0.41
2:D:438:GLN:O	2:D:439:GLY:C	2.59	0.41
1:A:690:TYR:CG	1:A:690:TYR:O	2.73	0.41
2:B:819:GLN:CA	2:B:819:GLN:NE2	2.84	0.41
2:B:603:GLU:C	2:B:605:SER:N	2.73	0.41
2:B:168:PRO:CD	2:B:197:TRP:CD1	3.04	0.41
1:C:791:PRO:CG	1:C:797:TRP:NE1	2.84	0.41
2:B:261:ALA:N	2:B:285:ILE:CD1	2.84	0.41
2:D:238:ASP:O	2:D:238:ASP:OD1	2.39	0.41
1:A:1279:ARG:CZ	1:A:1280:TYR:CD2	3.04	0.41
1:A:1280:TYR:CG	1:A:1280:TYR:O	2.74	0.41
2:B:866:TYR:OH	2:B:1388:THR:CG2	2.69	0.41
2:D:1632:SER:O	2:D:1636:THR:CB	2.68	0.41
2:B:1610:TRP:CG	2:B:1628:PHE:CD2	3.08	0.41
2:B:383:ALA:C	2:B:384:PHE:CD2	2.94	0.41
1:C:721:GLY:C	1:C:723:ARG:N	2.73	0.41
1:C:781:PRO:O	1:C:782:ARG:CB	2.69	0.41
2:B:1561:HIS:CE1	2:B:1597:ILE:CD1	3.04	0.41
1:C:124:GLY:C	1:C:125:PHE:CG	2.94	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:350:THR:O	2:D:350:THR:CG2	2.69	0.41
2:B:200:VAL:CG2	2:B:200:VAL:O	2.68	0.41
2:B:74:ASP:OD1	2:B:74:ASP:N	2.54	0.41
1:C:1213:LYS:C	1:C:1215:GLU:N	2.73	0.41
1:C:465:LEU:CG	1:C:466:TYR:N	2.83	0.41
2:B:440:GLY:O	2:B:441:SER:C	2.60	0.41
1:C:351:PRO:CG	1:C:352:TYR:CD2	3.04	0.41
1:C:1277:GLU:O	1:C:1278:GLN:C	2.58	0.41
2:D:147:VAL:O	2:D:147:VAL:CG1	2.68	0.41
2:D:860:SER:OG	2:D:866:TYR:CB	2.69	0.41
1:C:1159:CYS:SG	1:C:1161:LEU:CD2	3.09	0.41
1:A:1538:GLU:O	1:A:1539:LEU:C	2.59	0.41
1:C:77:ASN:C	1:C:79:PHE:N	2.73	0.41
2:D:1519:ASN:O	2:D:1520:VAL:CG2	2.69	0.41
1:C:367:ILE:O	1:C:368:PRO:C	2.58	0.41
2:B:1575:LEU:CD2	2:B:1575:LEU:N	2.84	0.41
2:B:1407:TYR:CD2	2:B:1407:TYR:C	2.94	0.41
1:C:316:GLU:N	1:C:316:GLU:OE1	2.54	0.41
2:B:184:TRP:CD2	2:B:184:TRP:N	2.89	0.41
1:C:1483:PHE:CD1	1:C:1483:PHE:O	2.74	0.40
1:A:949:ILE:CG2	1:A:949:ILE:O	2.69	0.40
1:A:1162:VAL:CG2	1:C:1102:ASN:ND2	2.83	0.40
2:D:1289:ARG:C	2:D:1290:TYR:CD1	2.94	0.40
1:A:1539:LEU:O	1:A:1540:ASP:CB	2.69	0.40
2:B:1414:ASP:O	2:B:1415:ASN:C	2.58	0.40
1:A:33:VAL:CG2	1:A:121:TYR:CD1	3.04	0.40
1:A:546:VAL:O	1:A:553:GLU:CB	2.68	0.40
1:A:40:VAL:CG2	1:A:41:ILE:N	2.84	0.40
1:A:662:SER:OG	1:A:663:GLN:N	2.54	0.40
2:D:1369:THR:OG1	2:D:1370:ARG:N	2.54	0.40
1:A:1277:GLU:O	1:A:1278:GLN:C	2.58	0.40
2:D:511:THR:O	2:D:513:ASP:N	2.54	0.40
1:C:1226:ARG:NE	1:C:1266:TYR:CE1	2.89	0.40
1:C:196:TYR:CE1	1:C:221:GLU:CB	3.03	0.40
1:A:691:LYS:C	1:A:693:SER:N	2.75	0.40
1:C:1285:TYR:O	1:C:1286:SER:O	2.39	0.40
1:A:1439:LEU:O	1:A:1440:LYS:C	2.60	0.40
1:C:967:LEU:CD1	1:C:968:VAL:N	2.84	0.40
1:A:1083:LEU:CD2	1:A:1104:LEU:CD2	2.99	0.40
2:D:354:PHE:CD1	2:D:354:PHE:C	2.93	0.40
2:B:1285:GLU:O	2:B:1287:PRO:CD	2.69	0.40
1:C:1560:ALA:O	1:C:1561:TYR:CB	2.69	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:580:VAL:CG1	2:B:581:ASP:N	2.84	0.40
2:D:742:ASP:OD1	2:D:743:SER:N	2.55	0.40
1:C:1289:ASP:O	1:C:1290:THR:C	2.60	0.40
1:C:350:SER:OG	1:C:352:TYR:O	2.40	0.40
2:B:218:LYS:CB	2:B:822:TYR:CD2	3.05	0.40
1:C:632:LEU:CD2	1:C:632:LEU:N	2.82	0.40
1:A:1043:GLN:O	1:A:1044:LYS:C	2.59	0.40
1:C:42:GLN:CB	1:C:80:GLN:NE2	2.85	0.40
2:B:296:ARG:NH1	2:B:296:ARG:CG	2.85	0.40
1:C:1033:ILE:CG2	1:C:1034:PHE:N	2.80	0.40
2:D:1506:ILE:CD1	2:D:1628:PHE:CE1	3.05	0.40
2:B:202:LYS:CG	2:B:203:TYR:N	2.84	0.40
1:C:398:ASN:O	1:C:399:GLN:CB	2.69	0.40
1:C:117:MET:CB	1:C:118:PRO:CD	2.99	0.40
1:C:1423:VAL:CG1	1:C:1496:TYR:CZ	3.05	0.40
2:B:1327:THR:CG2	2:B:1328:PHE:N	2.84	0.40
2:B:1569:CYS:O	2:B:1570:GLN:C	2.59	0.40
1:A:156:LYS:C	1:A:156:LYS:CD	2.89	0.40
1:C:775:TRP:CD1	1:C:775:TRP:O	2.75	0.40
1:C:23:TYR:CE1	1:C:655:THR:CB	3.05	0.40
1:C:626:PHE:O	1:C:628:GLU:N	2.54	0.40
1:A:1324:HIS:CG	1:A:1336:ARG:NH2	2.89	0.40
1:C:1538:GLU:O	1:C:1539:LEU:C	2.60	0.40
1:A:316:GLU:N	1:A:316:GLU:OE1	2.55	0.40
1:C:324:TYR:CD2	1:C:324:TYR:C	2.95	0.40
2:D:405:ASN:OD1	2:D:405:ASN:N	2.54	0.40
1:C:240:TYR:C	1:C:240:TYR:CD2	2.92	0.40
1:A:945:ASP:OD1	1:A:945:ASP:C	2.59	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	1617/1676 (96%)	1173 (72%)	292 (18%)	152 (9%)	1 23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	1617/1676 (96%)	1179 (73%)	288 (18%)	150 (9%)	1	23
2	B	1215/1642 (74%)	998 (82%)	161 (13%)	56 (5%)	4	45
2	D	1215/1642 (74%)	995 (82%)	162 (13%)	58 (5%)	4	44
All	All	5664/6636 (85%)	4345 (77%)	903 (16%)	416 (7%)	2	31

All (416) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	GLU
1	A	60	PRO
1	A	89	PRO
1	A	96	GLN
1	A	97	ASN
1	A	154	PRO
1	A	155	ALA
1	A	181	GLY
1	A	208	ASP
1	A	255	PHE
1	A	285	THR
1	A	287	MET
1	A	308	LYS
1	A	309	GLU
1	A	312	TYR
1	A	489	LYS
1	A	490	SER
1	A	519	SER
1	A	522	SER
1	A	579	ALA
1	A	619	PRO
1	A	621	GLU
1	A	656	ASN
1	A	692	HIS
1	A	754	MET
1	A	759	PRO
1	A	793	SER
1	A	873	ILE
1	A	884	VAL
1	A	885	ARG
1	A	931	PRO
1	A	946	PRO
1	A	948	GLY

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Mol	Chain	Res	Type
1	A	960	PRO
1	A	1091	LYS
1	A	1143	TYR
1	A	1284	PHE
1	A	1286	SER
1	A	1352	PHE
1	A	1386	ILE
1	A	1452	ASP
1	A	1534	GLN
1	A	1584	ILE
1	A	1585	TYR
1	A	1589	GLU
1	A	1628	LYS
1	A	1638	PRO
1	A	1639	LEU
1	A	1651	ASP
1	A	1654	CYS
1	A	1674	ASN
2	B	48	ASP
2	B	207	PRO
2	B	220	VAL
2	B	349	LYS
2	B	418	GLY
2	B	490	PHE
2	B	545	MET
2	B	583	ALA
2	B	641	ALA
2	B	643	LYS
2	B	647	PRO
2	B	736	GLU
2	B	937	VAL
2	B	1297	ALA
2	B	1449	GLY
2	B	1529	LEU
2	B	1597	ILE
1	C	48	GLU
1	C	60	PRO
1	C	89	PRO
1	C	96	GLN
1	C	97	ASN
1	C	154	PRO
1	C	155	ALA

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Mol	Chain	Res	Type
1	C	181	GLY
1	C	208	ASP
1	C	255	PHE
1	C	285	THR
1	C	287	MET
1	C	308	LYS
1	C	309	GLU
1	C	312	TYR
1	C	489	LYS
1	C	490	SER
1	C	522	SER
1	C	616	ALA
1	C	621	GLU
1	C	656	ASN
1	C	692	HIS
1	C	754	MET
1	C	759	PRO
1	C	793	SER
1	C	820	PHE
1	C	873	ILE
1	C	884	VAL
1	C	885	ARG
1	C	931	PRO
1	C	946	PRO
1	C	948	GLY
1	C	960	PRO
1	C	1091	LYS
1	C	1143	TYR
1	C	1284	PHE
1	C	1286	SER
1	C	1352	PHE
1	C	1386	ILE
1	C	1452	ASP
1	C	1534	GLN
1	C	1584	ILE
1	C	1585	TYR
1	C	1589	GLU
1	C	1628	LYS
1	C	1638	PRO
1	C	1639	LEU
1	C	1651	ASP
1	C	1654	CYS

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Mol	Chain	Res	Type
1	C	1674	ASN
2	D	48	ASP
2	D	220	VAL
2	D	348	THR
2	D	349	LYS
2	D	418	GLY
2	D	490	PHE
2	D	545	MET
2	D	583	ALA
2	D	641	ALA
2	D	643	LYS
2	D	647	PRO
2	D	736	GLU
2	D	937	VAL
2	D	1297	ALA
2	D	1449	GLY
2	D	1529	LEU
2	D	1597	ILE
1	A	459	SER
1	A	474	LYS
1	A	475	ALA
1	A	552	ALA
1	A	569	ASN
1	A	616	ALA
1	A	623	VAL
1	A	627	LEU
1	A	638	GLY
1	A	664	GLU
1	A	806	ASN
1	A	820	PHE
1	A	889	GLU
1	A	890	GLY
1	A	939	TYR
1	A	981	GLY
1	A	998	ASN
1	A	1001	THR
1	A	1004	PRO
1	A	1009	GLU
1	A	1096	ASN
1	A	1122	SER
1	A	1140	ASN
1	A	1238	SER

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Mol	Chain	Res	Type
1	A	1321	GLY
1	A	1324	HIS
1	A	1334	LEU
1	A	1382	ASP
1	A	1421	HIS
1	A	1471	ASP
1	A	1538	GLU
1	A	1590	ALA
2	B	237	ILE
2	B	348	THR
2	B	604	LYS
2	B	842	GLU
2	B	862	LYS
2	B	873	LYS
2	B	1319	GLY
2	B	1379	MET
2	B	1503	GLN
2	B	1558	ALA
2	B	1570	GLN
1	C	305	THR
1	C	459	SER
1	C	474	LYS
1	C	519	SER
1	C	552	ALA
1	C	569	ASN
1	C	579	ALA
1	C	619	PRO
1	C	623	VAL
1	C	627	LEU
1	C	634	CYS
1	C	638	GLY
1	C	664	GLU
1	C	889	GLU
1	C	890	GLY
1	C	981	GLY
1	C	994	GLN
1	C	998	ASN
1	C	1001	THR
1	C	1004	PRO
1	C	1009	GLU
1	C	1096	ASN
1	C	1140	ASN

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Mol	Chain	Res	Type
1	C	1238	SER
1	C	1321	GLY
1	C	1324	HIS
1	C	1334	LEU
1	C	1382	ASP
1	C	1421	HIS
1	C	1471	ASP
1	C	1538	GLU
1	C	1590	ALA
1	C	1609	ALA
2	D	142	PRO
2	D	207	PRO
2	D	237	ILE
2	D	470	ALA
2	D	604	LYS
2	D	842	GLU
2	D	873	LYS
2	D	1319	GLY
2	D	1379	MET
2	D	1503	GLN
2	D	1558	ALA
2	D	1570	GLN
1	A	209	PHE
1	A	286	ALA
1	A	289	ASN
1	A	305	THR
1	A	440	PRO
1	A	441	ASP
1	A	472	ASN
1	A	624	PHE
1	A	634	CYS
1	A	657	ALA
1	A	791	PRO
1	A	821	LYS
1	A	823	VAL
1	A	849	ARG
1	A	938	SER
1	A	994	GLN
1	A	1194	ALA
1	A	1196	SER
1	A	1539	LEU
1	A	1588	GLY

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Mol	Chain	Res	Type
1	A	1609	ALA
1	A	1632	SER
1	A	1652	THR
2	B	142	PRO
2	B	435	TYR
2	B	470	ALA
2	B	613	SER
2	B	780	LEU
2	B	1340	CYS
2	B	1497	CYS
2	B	1557	ARG
1	C	167	GLU
1	C	440	PRO
1	C	441	ASP
1	C	472	ASN
1	C	475	ALA
1	C	488	PRO
1	C	520	ASP
1	C	624	PHE
1	C	657	ALA
1	C	760	VAL
1	C	791	PRO
1	C	806	ASN
1	C	821	LYS
1	C	823	VAL
1	C	849	ARG
1	C	938	SER
1	C	939	TYR
1	C	1122	SER
1	C	1194	ALA
1	C	1196	SER
1	C	1539	LEU
1	C	1632	SER
1	C	1652	THR
2	D	326	SER
2	D	435	TYR
2	D	613	SER
2	D	780	LEU
2	D	862	LYS
2	D	1340	CYS
2	D	1497	CYS
2	D	1557	ARG

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Mol	Chain	Res	Type
1	A	234	GLU
1	A	256	TYR
1	A	520	ASP
1	A	667	GLU
1	A	690	TYR
1	A	760	VAL
1	A	882	LYS
1	A	909	ASN
1	A	988	LEU
1	A	1139	GLU
1	A	1150	ILE
1	A	1513	ASN
1	A	1540	ASP
1	A	1573	VAL
1	A	1655	SER
2	B	81	MET
2	B	277	PRO
2	B	326	SER
2	B	959	ILE
2	B	1447	GLU
2	B	1501	ASN
1	C	94	GLY
1	C	256	TYR
1	C	286	ALA
1	C	289	ASN
1	C	337	SER
1	C	667	GLU
1	C	690	TYR
1	C	909	ASN
1	C	987	ILE
1	C	988	LEU
1	C	997	ILE
1	C	1098	ASN
1	C	1139	GLU
1	C	1540	ASP
1	C	1573	VAL
1	C	1588	GLY
1	C	1655	SER
2	D	81	MET
2	D	277	PRO
2	D	471	ASN
2	D	821	PRO

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Mol	Chain	Res	Type
2	D	959	ILE
2	D	1298	LEU
2	D	1332	GLN
2	D	1447	GLU
2	D	1501	ASN
2	D	1553	ASP
2	D	1560	THR
1	A	94	GLY
1	A	101	TYR
1	A	167	GLU
1	A	186	PRO
1	A	274	ASP
1	A	291	MET
1	A	337	SER
1	A	488	PRO
1	A	576	SER
1	A	737	GLN
1	A	753	HIS
1	A	987	ILE
1	A	997	ILE
1	A	1098	ASN
1	A	1134	PRO
1	A	1160	PRO
1	A	1272	LYS
1	A	1675	GLY
2	B	471	ASN
2	B	950	LEU
2	B	1332	GLN
2	B	1556	PRO
2	B	1639	GLY
1	C	101	TYR
1	C	186	PRO
1	C	234	GLU
1	C	291	MET
1	C	576	SER
1	C	753	HIS
1	C	882	LYS
1	C	1023	HIS
1	C	1134	PRO
1	C	1150	ILE
1	C	1513	ASN
1	C	1675	GLY

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Mol	Chain	Res	Type
2	D	1556	PRO
2	D	1592	PRO
1	A	633	GLY
1	A	986	GLU
1	A	1002	HIS
1	A	1022	PHE
1	A	1243	GLY
2	B	560	GLY
2	B	1514	LYS
2	B	1592	PRO
1	C	274	ASP
1	C	970	LYS
1	C	1272	LYS
2	D	49	SER
2	D	950	LEU
2	B	821	PRO
1	C	633	GLY
1	C	1160	PRO
1	C	1243	GLY
1	C	1649	PRO
2	D	560	GLY
1	A	166	PRO
1	A	1649	PRO
2	B	339	VAL
1	C	510	ILE
1	C	1671	ILE
2	D	339	VAL
2	D	403	PRO
1	A	93	PRO
1	A	171	VAL
1	A	999	ILE
1	A	1671	ILE
2	B	79	GLY
2	B	403	PRO
2	B	512	PRO
2	B	559	PRO
1	C	93	PRO
1	C	166	PRO
1	C	171	VAL
2	D	79	GLY
2	D	512	PRO
2	D	584	VAL

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Mol	Chain	Res	Type
1	A	137	PRO
1	A	168	GLY
1	C	168	GLY
1	C	999	ILE
1	C	1239	VAL

5.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1446/1484 (97%)	1108 (77%)	338 (23%)	1	9
1	C	1446/1484 (97%)	1109 (77%)	337 (23%)	1	9
2	B	1093/1435 (76%)	845 (77%)	248 (23%)	1	10
2	D	1093/1435 (76%)	845 (77%)	248 (23%)	1	10
All	All	5078/5838 (87%)	3907 (77%)	1171 (23%)	1	10

All (1171) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	22	THR
1	A	23	TYR
1	A	24	VAL
1	A	26	SER
1	A	38	ASN
1	A	40	VAL
1	A	41	ILE
1	A	47	THR
1	A	55	SER
1	A	63	LYS
1	A	64	PHE
1	A	67	SER
1	A	71	VAL
1	A	73	LEU
1	A	87	ILE
1	A	89	PRO

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Mol	Chain	Res	Type
1	A	91	GLN
1	A	99	VAL
1	A	104	LEU
1	A	106	VAL
1	A	110	HIS
1	A	125	PHE
1	A	126	LEU
1	A	131	ASP
1	A	136	THR
1	A	144	ARG
1	A	148	LEU
1	A	156	LYS
1	A	157	ARG
1	A	158	GLU
1	A	161	LEU
1	A	162	THR
1	A	167	GLU
1	A	169	SER
1	A	171	VAL
1	A	176	GLU
1	A	182	ILE
1	A	183	ILE
1	A	200	THR
1	A	208	ASP
1	A	211	THR
1	A	212	THR
1	A	214	THR
1	A	222	TYR
1	A	224	LEU
1	A	228	SER
1	A	230	SER
1	A	232	GLU
1	A	240	TYR
1	A	241	LYS
1	A	242	ASN
1	A	249	THR
1	A	261	THR
1	A	268	THR
1	A	279	GLN
1	A	287	MET
1	A	288	GLN
1	A	289	ASN

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Mol	Chain	Res	Type
1	A	291	MET
1	A	292	LEU
1	A	296	ILE
1	A	310	LEU
1	A	315	LEU
1	A	321	LYS
1	A	322	TYR
1	A	323	LEU
1	A	324	TYR
1	A	328	THR
1	A	333	THR
1	A	337	SER
1	A	353	LYS
1	A	354	LEU
1	A	355	ASN
1	A	363	LEU
1	A	371	ILE
1	A	373	VAL
1	A	375	VAL
1	A	383	VAL
1	A	389	THR
1	A	390	LEU
1	A	394	THR
1	A	396	ASP
1	A	400	GLU
1	A	402	SER
1	A	404	LEU
1	A	407	SER
1	A	412	ARG
1	A	414	ASP
1	A	419	SER
1	A	422	LEU
1	A	431	LEU
1	A	433	PHE
1	A	441	ASP
1	A	442	LEU
1	A	457	TYR
1	A	458	SER
1	A	460	LEU
1	A	467	ILE
1	A	469	TRP
1	A	471	ASP

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Mol	Chain	Res	Type
1	A	474	LYS
1	A	477	LEU
1	A	492	TYR
1	A	495	LYS
1	A	497	THR
1	A	498	HIS
1	A	501	TYR
1	A	504	LEU
1	A	506	LYS
1	A	509	ILE
1	A	516	GLU
1	A	522	SER
1	A	526	ILE
1	A	534	MET
1	A	535	VAL
1	A	540	LEU
1	A	541	LEU
1	A	543	TYR
1	A	545	ILE
1	A	547	THR
1	A	549	GLU
1	A	550	GLN
1	A	555	VAL
1	A	558	SER
1	A	559	VAL
1	A	563	ILE
1	A	565	GLU
1	A	569	ASN
1	A	573	VAL
1	A	580	ASP
1	A	587	THR
1	A	596	MET
1	A	597	ASP
1	A	599	TRP
1	A	605	VAL
1	A	613	GLN
1	A	614	ARG
1	A	618	LYS
1	A	621	GLU
1	A	625	GLN
1	A	627	LEU
1	A	640	LEU

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Mol	Chain	Res	Type
1	A	642	ASN
1	A	644	ASN
1	A	652	THR
1	A	653	PHE
1	A	663	GLN
1	A	664	GLU
1	A	667	GLU
1	A	672	ILE
1	A	692	HIS
1	A	697	LYS
1	A	699	CYS
1	A	704	CYS
1	A	710	THR
1	A	713	GLN
1	A	720	LEU
1	A	732	CYS
1	A	753	HIS
1	A	754	MET
1	A	756	THR
1	A	758	LEU
1	A	766	ARG
1	A	767	SER
1	A	774	LEU
1	A	777	VAL
1	A	782	ARG
1	A	787	GLN
1	A	788	PHE
1	A	793	SER
1	A	795	THR
1	A	797	TRP
1	A	800	GLN
1	A	811	VAL
1	A	824	PHE
1	A	825	LEU
1	A	838	GLN
1	A	845	VAL
1	A	849	ARG
1	A	850	THR
1	A	854	GLN
1	A	856	CYS
1	A	857	VAL
1	A	859	MET

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Mol	Chain	Res	Type
1	A	865	ILE
1	A	867	THR
1	A	876	GLN
1	A	887	LYS
1	A	895	LEU
1	A	896	VAL
1	A	899	THR
1	A	901	LEU
1	A	912	PHE
1	A	914	LEU
1	A	915	GLU
1	A	923	LEU
1	A	928	ARG
1	A	935	LYS
1	A	936	ARG
1	A	940	SER
1	A	944	LEU
1	A	947	ARG
1	A	952	THR
1	A	953	ILE
1	A	955	ARG
1	A	967	LEU
1	A	972	GLU
1	A	975	ARG
1	A	977	LEU
1	A	983	LEU
1	A	984	VAL
1	A	988	LEU
1	A	1001	THR
1	A	1002	HIS
1	A	1003	LEU
1	A	1007	SER
1	A	1011	GLU
1	A	1013	MET
1	A	1014	SER
1	A	1018	VAL
1	A	1033	ILE
1	A	1055	SER
1	A	1056	ILE
1	A	1070	LYS
1	A	1078	LEU
1	A	1084	ARG

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Mol	Chain	Res	Type
1	A	1089	VAL
1	A	1091	LYS
1	A	1098	ASN
1	A	1105	LEU
1	A	1107	LEU
1	A	1108	VAL
1	A	1110	ASN
1	A	1113	LEU
1	A	1127	ILE
1	A	1128	LYS
1	A	1129	LEU
1	A	1140	ASN
1	A	1141	SER
1	A	1164	ILE
1	A	1166	THR
1	A	1168	LEU
1	A	1175	LEU
1	A	1180	LEU
1	A	1183	GLN
1	A	1185	THR
1	A	1196	SER
1	A	1200	LYS
1	A	1201	THR
1	A	1209	VAL
1	A	1212	LEU
1	A	1218	VAL
1	A	1227	PHE
1	A	1231	ASN
1	A	1236	ASP
1	A	1246	ARG
1	A	1259	LEU
1	A	1264	ILE
1	A	1279	ARG
1	A	1280	TYR
1	A	1301	SER
1	A	1302	LEU
1	A	1303	LEU
1	A	1306	GLN
1	A	1307	LEU
1	A	1308	ARG
1	A	1309	LEU
1	A	1311	MET

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Mol	Chain	Res	Type
1	A	1313	ILE
1	A	1323	LEU
1	A	1326	TYR
1	A	1330	ASP
1	A	1331	LYS
1	A	1333	PHE
1	A	1334	LEU
1	A	1336	ARG
1	A	1338	VAL
1	A	1341	LEU
1	A	1346	LEU
1	A	1356	LEU
1	A	1361	VAL
1	A	1363	THR
1	A	1366	HIS
1	A	1367	LYS
1	A	1372	GLU
1	A	1374	VAL
1	A	1375	CYS
1	A	1397	SER
1	A	1423	VAL
1	A	1433	SER
1	A	1450	PHE
1	A	1454	GLN
1	A	1464	LEU
1	A	1470	SER
1	A	1474	CYS
1	A	1475	VAL
1	A	1476	ARG
1	A	1479	ILE
1	A	1480	PHE
1	A	1483	PHE
1	A	1487	PHE
1	A	1488	LEU
1	A	1492	THR
1	A	1493	PHE
1	A	1494	THR
1	A	1500	ARG
1	A	1503	LYS
1	A	1504	GLN
1	A	1506	THR
1	A	1507	MET

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Mol	Chain	Res	Type
1	A	1512	SER
1	A	1535	MET
1	A	1542	THR
1	A	1544	SER
1	A	1548	ARG
1	A	1549	LYS
1	A	1553	CYS
1	A	1566	THR
1	A	1577	TYR
1	A	1580	THR
1	A	1581	LEU
1	A	1585	TYR
1	A	1598	ILE
1	A	1602	LYS
1	A	1605	THR
1	A	1606	CYS
1	A	1618	LEU
1	A	1626	GLN
1	A	1627	ILE
1	A	1631	PHE
1	A	1636	ILE
1	A	1639	LEU
1	A	1650	ARG
1	A	1651	ASP
1	A	1652	THR
1	A	1655	SER
1	A	1663	ASN
2	B	29	THR
2	B	40	GLN
2	B	43	VAL
2	B	54	LEU
2	B	56	ILE
2	B	58	VAL
2	B	68	LEU
2	B	71	THR
2	B	74	ASP
2	B	82	LEU
2	B	86	THR
2	B	87	ILE
2	B	100	GLN
2	B	105	VAL
2	B	106	VAL

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Mol	Chain	Res	Type
2	B	108	VAL
2	B	114	ARG
2	B	119	VAL
2	B	120	LEU
2	B	124	GLN
2	B	144	LEU
2	B	147	VAL
2	B	161	VAL
2	B	167	THR
2	B	171	ILE
2	B	175	SER
2	B	176	ASN
2	B	177	SER
2	B	179	ASP
2	B	183	PHE
2	B	190	ASP
2	B	191	LEU
2	B	196	THR
2	B	198	ARG
2	B	202	LYS
2	B	208	GLU
2	B	214	PHE
2	B	216	VAL
2	B	217	ARG
2	B	219	TYR
2	B	220	VAL
2	B	221	LEU
2	B	223	SER
2	B	231	SER
2	B	234	PHE
2	B	243	PHE
2	B	258	GLU
2	B	263	VAL
2	B	264	LEU
2	B	278	ASP
2	B	280	LEU
2	B	285	ILE
2	B	291	LYS
2	B	296	ARG
2	B	297	ASP
2	B	298	THR
2	B	299	PHE

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Mol	Chain	Res	Type
2	B	301	SER
2	B	306	LEU
2	B	315	TYR
2	B	317	SER
2	B	323	GLU
2	B	327	ASP
2	B	328	MET
2	B	341	SER
2	B	344	GLN
2	B	345	ILE
2	B	348	THR
2	B	349	LYS
2	B	358	MET
2	B	379	VAL
2	B	382	GLU
2	B	386	SER
2	B	389	THR
2	B	390	THR
2	B	398	LEU
2	B	400	LEU
2	B	404	LEU
2	B	414	ARG
2	B	416	ASN
2	B	422	ARG
2	B	427	THR
2	B	433	ILE
2	B	435	TYR
2	B	437	THR
2	B	449	ILE
2	B	460	LEU
2	B	465	ASN
2	B	466	VAL
2	B	469	ASN
2	B	472	SER
2	B	473	LEU
2	B	481	TYR
2	B	482	LEU
2	B	483	ILE
2	B	490	PHE
2	B	497	ARG
2	B	504	VAL
2	B	505	THR

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Mol	Chain	Res	Type
2	B	511	THR
2	B	513	ASP
2	B	518	PHE
2	B	520	PHE
2	B	521	VAL
2	B	523	TYR
2	B	524	TYR
2	B	525	GLN
2	B	526	VAL
2	B	531	ILE
2	B	532	VAL
2	B	543	THR
2	B	544	CYS
2	B	555	LEU
2	B	556	ILE
2	B	558	MET
2	B	563	MET
2	B	567	LEU
2	B	586	VAL
2	B	588	ASN
2	B	593	ILE
2	B	597	LYS
2	B	598	ILE
2	B	602	ILE
2	B	606	ASP
2	B	613	SER
2	B	615	GLN
2	B	629	THR
2	B	638	GLN
2	B	735	ASN
2	B	742	ASP
2	B	745	ILE
2	B	746	ILE
2	B	747	SER
2	B	764	GLU
2	B	769	GLN
2	B	773	SER
2	B	778	PHE
2	B	780	LEU
2	B	784	ILE
2	B	789	VAL
2	B	800	ILE

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Mol	Chain	Res	Type
2	B	813	VAL
2	B	816	ILE
2	B	817	ASP
2	B	819	GLN
2	B	829	GLN
2	B	830	VAL
2	B	836	LEU
2	B	840	VAL
2	B	851	LEU
2	B	857	CYS
2	B	868	GLN
2	B	870	PHE
2	B	872	ILE
2	B	873	LYS
2	B	884	ILE
2	B	887	LEU
2	B	889	GLN
2	B	891	LEU
2	B	918	GLU
2	B	920	VAL
2	B	925	VAL
2	B	926	THR
2	B	946	LYS
2	B	948	ARG
2	B	949	LYS
2	B	952	ASP
2	B	963	ILE
2	B	964	ILE
2	B	1273	LEU
2	B	1274	ASN
2	B	1278	THR
2	B	1279	ILE
2	B	1281	LEU
2	B	1291	ARG
2	B	1292	ILE
2	B	1301	ARG
2	B	1304	GLU
2	B	1305	THR
2	B	1308	ASN
2	B	1313	VAL
2	B	1322	THR
2	B	1324	THR

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Mol	Chain	Res	Type
2	B	1329	TYR
2	B	1330	ASN
2	B	1332	GLN
2	B	1344	HIS
2	B	1345	LEU
2	B	1346	ASN
2	B	1350	GLU
2	B	1351	ASN
2	B	1364	MET
2	B	1365	LEU
2	B	1372	LEU
2	B	1378	THR
2	B	1380	THR
2	B	1388	THR
2	B	1396	ASP
2	B	1398	THR
2	B	1401	SER
2	B	1406	ARG
2	B	1423	VAL
2	B	1424	ILE
2	B	1427	LEU
2	B	1429	LYS
2	B	1431	SER
2	B	1433	SER
2	B	1437	CYS
2	B	1438	LEU
2	B	1439	HIS
2	B	1442	ILE
2	B	1443	LEU
2	B	1448	VAL
2	B	1450	PHE
2	B	1451	ILE
2	B	1456	VAL
2	B	1464	LEU
2	B	1475	ASP
2	B	1480	LEU
2	B	1481	LEU
2	B	1490	CYS
2	B	1492	CYS
2	B	1495	GLU
2	B	1496	THR
2	B	1497	CYS

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Mol	Chain	Res	Type
2	B	1500	LEU
2	B	1502	HIS
2	B	1504	GLU
2	B	1511	GLN
2	B	1516	CYS
2	B	1519	ASN
2	B	1526	THR
2	B	1535	ASP
2	B	1561	HIS
2	B	1566	GLN
2	B	1571	GLU
2	B	1582	LEU
2	B	1583	ILE
2	B	1584	TRP
2	B	1594	LYS
2	B	1598	SER
2	B	1599	TYR
2	B	1604	ASN
2	B	1606	TRP
2	B	1607	ILE
2	B	1609	ARG
2	B	1622	GLN
2	B	1623	LYS
1	C	21	GLN
1	C	22	THR
1	C	23	TYR
1	C	24	VAL
1	C	26	SER
1	C	38	ASN
1	C	40	VAL
1	C	41	ILE
1	C	47	THR
1	C	55	SER
1	C	63	LYS
1	C	64	PHE
1	C	67	SER
1	C	71	VAL
1	C	73	LEU
1	C	85	LEU
1	C	87	ILE
1	C	91	GLN
1	C	99	VAL

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Mol	Chain	Res	Type
1	C	104	LEU
1	C	106	VAL
1	C	110	HIS
1	C	125	PHE
1	C	126	LEU
1	C	131	ASP
1	C	136	THR
1	C	143	VAL
1	C	144	ARG
1	C	148	LEU
1	C	156	LYS
1	C	157	ARG
1	C	158	GLU
1	C	161	LEU
1	C	162	THR
1	C	164	ILE
1	C	167	GLU
1	C	169	SER
1	C	176	GLU
1	C	182	ILE
1	C	183	ILE
1	C	200	THR
1	C	208	ASP
1	C	211	THR
1	C	212	THR
1	C	214	THR
1	C	222	TYR
1	C	224	LEU
1	C	228	SER
1	C	230	SER
1	C	232	GLU
1	C	240	TYR
1	C	241	LYS
1	C	242	ASN
1	C	249	THR
1	C	261	THR
1	C	268	THR
1	C	279	GLN
1	C	287	MET
1	C	288	GLN
1	C	289	ASN
1	C	291	MET

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Mol	Chain	Res	Type
1	C	292	LEU
1	C	296	ILE
1	C	310	LEU
1	C	315	LEU
1	C	322	TYR
1	C	323	LEU
1	C	324	TYR
1	C	328	THR
1	C	333	THR
1	C	337	SER
1	C	354	LEU
1	C	355	ASN
1	C	363	LEU
1	C	371	ILE
1	C	373	VAL
1	C	375	VAL
1	C	383	VAL
1	C	389	THR
1	C	390	LEU
1	C	394	THR
1	C	396	ASP
1	C	400	GLU
1	C	404	LEU
1	C	407	SER
1	C	412	ARG
1	C	414	ASP
1	C	419	SER
1	C	422	LEU
1	C	431	LEU
1	C	433	PHE
1	C	441	ASP
1	C	442	LEU
1	C	457	TYR
1	C	458	SER
1	C	460	LEU
1	C	467	ILE
1	C	469	TRP
1	C	471	ASP
1	C	474	LYS
1	C	477	LEU
1	C	492	TYR
1	C	495	LYS

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Mol	Chain	Res	Type
1	C	497	THR
1	C	498	HIS
1	C	501	TYR
1	C	504	LEU
1	C	506	LYS
1	C	509	ILE
1	C	516	GLU
1	C	522	SER
1	C	526	ILE
1	C	535	VAL
1	C	540	LEU
1	C	541	LEU
1	C	543	TYR
1	C	544	TYR
1	C	545	ILE
1	C	547	THR
1	C	549	GLU
1	C	550	GLN
1	C	555	VAL
1	C	558	SER
1	C	559	VAL
1	C	563	ILE
1	C	565	GLU
1	C	569	ASN
1	C	573	VAL
1	C	580	ASP
1	C	587	THR
1	C	596	MET
1	C	597	ASP
1	C	599	TRP
1	C	605	VAL
1	C	613	GLN
1	C	614	ARG
1	C	618	LYS
1	C	621	GLU
1	C	625	GLN
1	C	627	LEU
1	C	640	LEU
1	C	642	ASN
1	C	644	ASN
1	C	652	THR
1	C	653	PHE

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Mol	Chain	Res	Type
1	C	663	GLN
1	C	664	GLU
1	C	667	GLU
1	C	672	ILE
1	C	692	HIS
1	C	697	LYS
1	C	699	CYS
1	C	701	ASP
1	C	710	THR
1	C	713	GLN
1	C	720	LEU
1	C	732	CYS
1	C	753	HIS
1	C	754	MET
1	C	756	THR
1	C	758	LEU
1	C	766	ARG
1	C	767	SER
1	C	774	LEU
1	C	777	VAL
1	C	782	ARG
1	C	787	GLN
1	C	788	PHE
1	C	793	SER
1	C	795	THR
1	C	797	TRP
1	C	800	GLN
1	C	811	VAL
1	C	824	PHE
1	C	825	LEU
1	C	838	GLN
1	C	845	VAL
1	C	849	ARG
1	C	850	THR
1	C	854	GLN
1	C	856	CYS
1	C	857	VAL
1	C	859	MET
1	C	865	ILE
1	C	867	THR
1	C	876	GLN
1	C	887	LYS

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Mol	Chain	Res	Type
1	C	895	LEU
1	C	896	VAL
1	C	899	THR
1	C	901	LEU
1	C	912	PHE
1	C	914	LEU
1	C	915	GLU
1	C	923	LEU
1	C	928	ARG
1	C	935	LYS
1	C	936	ARG
1	C	940	SER
1	C	944	LEU
1	C	947	ARG
1	C	952	THR
1	C	953	ILE
1	C	955	ARG
1	C	967	LEU
1	C	972	GLU
1	C	975	ARG
1	C	977	LEU
1	C	983	LEU
1	C	984	VAL
1	C	988	LEU
1	C	1001	THR
1	C	1002	HIS
1	C	1003	LEU
1	C	1007	SER
1	C	1011	GLU
1	C	1013	MET
1	C	1014	SER
1	C	1033	ILE
1	C	1055	SER
1	C	1056	ILE
1	C	1070	LYS
1	C	1078	LEU
1	C	1084	ARG
1	C	1089	VAL
1	C	1091	LYS
1	C	1098	ASN
1	C	1105	LEU
1	C	1107	LEU

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Mol	Chain	Res	Type
1	C	1108	VAL
1	C	1110	ASN
1	C	1113	LEU
1	C	1127	ILE
1	C	1128	LYS
1	C	1129	LEU
1	C	1140	ASN
1	C	1141	SER
1	C	1164	ILE
1	C	1166	THR
1	C	1168	LEU
1	C	1175	LEU
1	C	1180	LEU
1	C	1183	GLN
1	C	1185	THR
1	C	1196	SER
1	C	1200	LYS
1	C	1201	THR
1	C	1209	VAL
1	C	1212	LEU
1	C	1218	VAL
1	C	1227	PHE
1	C	1231	ASN
1	C	1236	ASP
1	C	1246	ARG
1	C	1259	LEU
1	C	1264	ILE
1	C	1279	ARG
1	C	1280	TYR
1	C	1301	SER
1	C	1302	LEU
1	C	1303	LEU
1	C	1306	GLN
1	C	1307	LEU
1	C	1308	ARG
1	C	1309	LEU
1	C	1311	MET
1	C	1323	LEU
1	C	1326	TYR
1	C	1330	ASP
1	C	1331	LYS
1	C	1332	ASN

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Mol	Chain	Res	Type
1	C	1333	PHE
1	C	1334	LEU
1	C	1336	ARG
1	C	1338	VAL
1	C	1341	LEU
1	C	1346	LEU
1	C	1356	LEU
1	C	1358	THR
1	C	1361	VAL
1	C	1363	THR
1	C	1366	HIS
1	C	1367	LYS
1	C	1372	GLU
1	C	1374	VAL
1	C	1375	CYS
1	C	1397	SER
1	C	1423	VAL
1	C	1433	SER
1	C	1450	PHE
1	C	1454	GLN
1	C	1464	LEU
1	C	1470	SER
1	C	1474	CYS
1	C	1475	VAL
1	C	1476	ARG
1	C	1479	ILE
1	C	1480	PHE
1	C	1483	PHE
1	C	1487	PHE
1	C	1488	LEU
1	C	1492	THR
1	C	1493	PHE
1	C	1494	THR
1	C	1500	ARG
1	C	1503	LYS
1	C	1504	GLN
1	C	1506	THR
1	C	1507	MET
1	C	1512	SER
1	C	1535	MET
1	C	1542	THR
1	C	1544	SER

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Mol	Chain	Res	Type
1	C	1548	ARG
1	C	1549	LYS
1	C	1553	CYS
1	C	1566	THR
1	C	1577	TYR
1	C	1580	THR
1	C	1581	LEU
1	C	1585	TYR
1	C	1598	ILE
1	C	1602	LYS
1	C	1605	THR
1	C	1606	CYS
1	C	1616	GLN
1	C	1618	LEU
1	C	1626	GLN
1	C	1627	ILE
1	C	1631	PHE
1	C	1636	ILE
1	C	1639	LEU
1	C	1650	ARG
1	C	1651	ASP
1	C	1652	THR
1	C	1655	SER
1	C	1663	ASN
2	D	29	THR
2	D	40	GLN
2	D	43	VAL
2	D	54	LEU
2	D	56	ILE
2	D	58	VAL
2	D	68	LEU
2	D	71	THR
2	D	74	ASP
2	D	82	LEU
2	D	86	THR
2	D	87	ILE
2	D	100	GLN
2	D	105	VAL
2	D	106	VAL
2	D	108	VAL
2	D	114	ARG
2	D	119	VAL

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Mol	Chain	Res	Type
2	D	120	LEU
2	D	124	GLN
2	D	144	LEU
2	D	147	VAL
2	D	167	THR
2	D	171	ILE
2	D	175	SER
2	D	176	ASN
2	D	177	SER
2	D	179	ASP
2	D	183	PHE
2	D	190	ASP
2	D	191	LEU
2	D	196	THR
2	D	198	ARG
2	D	202	LYS
2	D	208	GLU
2	D	214	PHE
2	D	216	VAL
2	D	217	ARG
2	D	219	TYR
2	D	220	VAL
2	D	221	LEU
2	D	223	SER
2	D	226	VAL
2	D	231	SER
2	D	234	PHE
2	D	243	PHE
2	D	258	GLU
2	D	263	VAL
2	D	264	LEU
2	D	278	ASP
2	D	280	LEU
2	D	285	ILE
2	D	291	LYS
2	D	296	ARG
2	D	297	ASP
2	D	298	THR
2	D	299	PHE
2	D	301	SER
2	D	306	LEU
2	D	315	TYR

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Mol	Chain	Res	Type
2	D	317	SER
2	D	323	GLU
2	D	327	ASP
2	D	328	MET
2	D	344	GLN
2	D	345	ILE
2	D	348	THR
2	D	349	LYS
2	D	358	MET
2	D	368	ASN
2	D	379	VAL
2	D	382	GLU
2	D	386	SER
2	D	389	THR
2	D	390	THR
2	D	398	LEU
2	D	400	LEU
2	D	404	LEU
2	D	414	ARG
2	D	416	ASN
2	D	422	ARG
2	D	427	THR
2	D	433	ILE
2	D	435	TYR
2	D	437	THR
2	D	449	ILE
2	D	460	LEU
2	D	466	VAL
2	D	469	ASN
2	D	472	SER
2	D	473	LEU
2	D	481	TYR
2	D	482	LEU
2	D	483	ILE
2	D	490	PHE
2	D	497	ARG
2	D	504	VAL
2	D	505	THR
2	D	511	THR
2	D	513	ASP
2	D	518	PHE
2	D	520	PHE

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Mol	Chain	Res	Type
2	D	521	VAL
2	D	523	TYR
2	D	524	TYR
2	D	525	GLN
2	D	526	VAL
2	D	531	ILE
2	D	532	VAL
2	D	543	THR
2	D	544	CYS
2	D	555	LEU
2	D	556	ILE
2	D	558	MET
2	D	563	MET
2	D	567	LEU
2	D	586	VAL
2	D	588	ASN
2	D	593	ILE
2	D	597	LYS
2	D	598	ILE
2	D	602	ILE
2	D	613	SER
2	D	615	GLN
2	D	629	THR
2	D	638	GLN
2	D	735	ASN
2	D	742	ASP
2	D	745	ILE
2	D	746	ILE
2	D	747	SER
2	D	764	GLU
2	D	769	GLN
2	D	773	SER
2	D	778	PHE
2	D	780	LEU
2	D	784	ILE
2	D	789	VAL
2	D	800	ILE
2	D	812	LYS
2	D	813	VAL
2	D	816	ILE
2	D	817	ASP
2	D	819	GLN

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Mol	Chain	Res	Type
2	D	829	GLN
2	D	830	VAL
2	D	836	LEU
2	D	840	VAL
2	D	851	LEU
2	D	857	CYS
2	D	866	TYR
2	D	868	GLN
2	D	870	PHE
2	D	872	ILE
2	D	873	LYS
2	D	881	PRO
2	D	884	ILE
2	D	889	GLN
2	D	891	LEU
2	D	918	GLU
2	D	920	VAL
2	D	925	VAL
2	D	926	THR
2	D	946	LYS
2	D	948	ARG
2	D	949	LYS
2	D	952	ASP
2	D	963	ILE
2	D	964	ILE
2	D	1273	LEU
2	D	1274	ASN
2	D	1278	THR
2	D	1279	ILE
2	D	1281	LEU
2	D	1291	ARG
2	D	1292	ILE
2	D	1301	ARG
2	D	1304	GLU
2	D	1305	THR
2	D	1308	ASN
2	D	1313	VAL
2	D	1322	THR
2	D	1324	THR
2	D	1330	ASN
2	D	1332	GLN
2	D	1344	HIS

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Mol	Chain	Res	Type
2	D	1345	LEU
2	D	1346	ASN
2	D	1349	VAL
2	D	1350	GLU
2	D	1351	ASN
2	D	1365	LEU
2	D	1372	LEU
2	D	1378	THR
2	D	1380	THR
2	D	1388	THR
2	D	1396	ASP
2	D	1398	THR
2	D	1401	SER
2	D	1406	ARG
2	D	1423	VAL
2	D	1424	ILE
2	D	1427	LEU
2	D	1429	LYS
2	D	1431	SER
2	D	1433	SER
2	D	1437	CYS
2	D	1438	LEU
2	D	1439	HIS
2	D	1442	ILE
2	D	1443	LEU
2	D	1448	VAL
2	D	1450	PHE
2	D	1451	ILE
2	D	1456	VAL
2	D	1464	LEU
2	D	1475	ASP
2	D	1480	LEU
2	D	1481	LEU
2	D	1490	CYS
2	D	1492	CYS
2	D	1495	GLU
2	D	1496	THR
2	D	1497	CYS
2	D	1500	LEU
2	D	1502	HIS
2	D	1504	GLU
2	D	1511	GLN

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Mol	Chain	Res	Type
2	D	1516	CYS
2	D	1519	ASN
2	D	1526	THR
2	D	1535	ASP
2	D	1561	HIS
2	D	1566	GLN
2	D	1571	GLU
2	D	1582	LEU
2	D	1583	ILE
2	D	1584	TRP
2	D	1594	LYS
2	D	1598	SER
2	D	1599	TYR
2	D	1604	ASN
2	D	1606	TRP
2	D	1607	ILE
2	D	1609	ARG
2	D	1614	ASP
2	D	1622	GLN
2	D	1623	LYS

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 ⓘ

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	$\# Z > 2$
3	NAG	A	2003	1	12,14,15	0.68	0	15,19,21	1.47	3 (20%)
3	NAG	B	2001	2	12,14,15	0.66	0	15,19,21	1.38	4 (26%)
3	NAG	B	2002	2	12,14,15	0.85	0	15,19,21	0.96	1 (6%)
3	NAG	C	2003	1	12,14,15	0.67	0	15,19,21	1.49	3 (20%)
3	NAG	D	2001	2	12,14,15	0.58	0	15,19,21	1.44	3 (20%)
3	NAG	D	2002	2	12,14,15	0.86	0	15,19,21	0.96	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
3	NAG	A	2003	1	-	2/6/23/26	0/1/1/1
3	NAG	B	2001	2	-	0/6/23/26	0/1/1/1
3	NAG	B	2002	2	-	0/6/23/26	0/1/1/1
3	NAG	C	2003	1	-	2/6/23/26	0/1/1/1
3	NAG	D	2001	2	-	0/6/23/26	0/1/1/1
3	NAG	D	2002	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2001	NAG	O5-C5-C6	3.31	110.46	106.98
3	A	2003	NAG	C3-C4-C5	3.00	115.56	110.20
3	C	2003	NAG	C3-C4-C5	2.96	115.50	110.20
3	B	2001	NAG	O5-C5-C6	2.92	110.05	106.98
3	C	2003	NAG	C4-C3-C2	2.49	117.41	111.32
3	C	2003	NAG	O5-C5-C4	2.48	113.80	110.65
3	D	2002	NAG	C3-C2-N2	-2.48	107.99	111.76
3	B	2002	NAG	C3-C2-N2	-2.46	108.01	111.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2003	NAG	O5-C5-C4	2.44	113.75	110.65
3	A	2003	NAG	C4-C3-C2	2.42	117.23	111.32
3	D	2001	NAG	C2-N2-C7	-2.29	119.24	123.09
3	B	2001	NAG	O5-C5-C4	2.27	113.53	110.65
3	D	2001	NAG	O5-C5-C4	2.25	113.50	110.65
3	B	2001	NAG	C2-N2-C7	-2.13	119.52	123.09
3	B	2001	NAG	C3-C2-N2	2.02	114.84	111.76

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	2003	NAG	O7-C7-N2-C2
3	A	2003	NAG	O7-C7-N2-C2
3	A	2003	NAG	C8-C7-N2-C2
3	C	2003	NAG	C8-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, 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	1627/1676 (97%)	1.13	219 (13%) 4 6	90, 187, 312, 465	0
1	C	1627/1676 (97%)	1.12	242 (14%) 3 6	97, 186, 299, 486	0
2	B	1225/1642 (74%)	1.05	136 (11%) 6 9	107, 174, 261, 395	0
2	D	1225/1642 (74%)	1.07	159 (12%) 4 7	114, 181, 263, 371	0
All	All	5704/6636 (85%)	1.09	756 (13%) 4 7	90, 183, 291, 486	0

All (756) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1622	LYS	12.5
1	A	1585	TYR	10.3
1	C	1676	CYS	10.1
1	A	1676	CYS	9.9
2	D	1270	HIS	9.7
1	A	660	ASP	8.4
2	D	1271	LYS	8.1
2	B	123	TYR	8.0
1	A	1525	CYS	7.8
1	C	94	GLY	7.7
1	C	1550	GLN	7.7
1	A	1537	GLU	7.4
1	C	240	TYR	7.3
2	B	156	LYS	7.1
1	A	1592	ALA	6.6
1	A	661	ASP	6.2
1	A	1598	ILE	6.2
2	D	1360	LYS	6.2
1	A	1649	PRO	6.0
1	A	1534	GLN	5.8
1	A	1579	ALA	5.7

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Mol	Chain	Res	Type	RSRZ
1	A	1587	THR	5.7
1	A	997	ILE	5.4
1	A	1582	LEU	5.4
1	C	1611	LEU	5.4
2	D	648	ALA	5.4
1	A	1650	ARG	5.4
1	A	1557	ILE	5.3
2	B	1354	LEU	5.3
2	D	99	ARG	5.2
1	A	1623	GLU	5.2
2	B	1355	ASN	5.1
2	D	225	GLU	5.0
1	A	1540	ASP	4.9
1	A	95	GLY	4.9
2	D	152	HIS	4.9
1	C	93	PRO	4.8
1	C	473	HIS	4.8
1	C	95	GLY	4.8
1	A	678	THR	4.7
2	D	158	ASN	4.7
1	A	1539	LEU	4.7
2	B	155	SER	4.7
1	C	1551	THR	4.6
2	B	969	PRO	4.6
1	C	660	ASP	4.5
2	D	120	LEU	4.5
1	C	673	LEU	4.5
1	C	696	LYS	4.5
2	B	1353	HIS	4.5
1	C	271	ILE	4.4
1	C	1622	LYS	4.4
2	D	98	SER	4.4
2	B	1298	LEU	4.4
2	D	735	ASN	4.4
2	D	123	TYR	4.4
1	A	1556	GLU	4.3
1	C	1652	THR	4.3
2	D	642	ALA	4.3
1	C	695	VAL	4.3
1	C	1664	LEU	4.3
1	A	1586	LYS	4.3
2	D	153	ASN	4.3

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Mol	Chain	Res	Type	RSRZ
2	D	918	GLU	4.2
2	D	1298	LEU	4.2
1	C	48	GLU	4.2
1	C	682	LYS	4.2
1	A	691	LYS	4.2
1	A	1588	GLY	4.2
1	C	666	ASP	4.2
2	D	96	THR	4.2
2	B	153	ASN	4.1
1	C	1649	PRO	4.1
1	A	673	LEU	4.1
1	C	1593	GLU	4.1
2	D	1294	TYR	4.1
1	C	1537	GLU	4.1
1	A	975	ARG	4.1
2	B	1360	LYS	4.1
1	C	1579	ALA	4.1
1	C	20	GLU	4.1
2	B	648	ALA	4.1
1	A	283	MET	4.1
2	D	150	MET	4.1
1	C	720	LEU	4.0
1	C	150	ASP	4.0
2	B	34	ARG	4.0
2	B	1495	GLU	4.0
2	B	811	MET	3.9
1	C	1585	TYR	3.9
1	C	1581	LEU	3.9
1	A	1647	TYR	3.9
2	D	97	ASP	3.9
1	C	1620	MET	3.9
1	A	1626	GLN	3.9
1	C	1592	ALA	3.8
2	D	862	LYS	3.8
1	A	1577	TYR	3.8
1	A	94	GLY	3.8
2	D	236	TYR	3.8
2	D	343	TYR	3.8
1	C	278	ASP	3.8
2	D	1291	ARG	3.8
1	A	1583	ASP	3.8
1	C	324	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	1128	LYS	3.8
2	D	643	LYS	3.7
2	B	960	GLU	3.7
1	C	196	TYR	3.7
2	D	1355	ASN	3.7
1	A	1576	LYS	3.7
2	D	1618	GLU	3.7
2	D	445	LEU	3.6
1	C	1659	ALA	3.6
1	A	32	ARG	3.6
1	A	1611	LEU	3.6
2	B	1527	LYS	3.6
1	A	706	ASN	3.6
1	A	352	TYR	3.5
1	C	965	LEU	3.5
1	A	621	GLU	3.5
1	C	1041	GLU	3.5
2	B	203	TYR	3.5
2	B	645	PRO	3.5
1	C	1525	CYS	3.5
1	C	317	ASP	3.5
2	B	646	GLN	3.5
1	A	473	HIS	3.5
2	D	1617	GLN	3.5
1	C	283	MET	3.5
2	B	159	LYS	3.5
1	C	1306	GLN	3.5
2	B	503	LEU	3.5
1	C	1123	GLN	3.5
1	A	138	ASP	3.5
1	C	1553	CYS	3.4
2	B	1306	LYS	3.4
2	B	93	GLU	3.4
1	C	270	GLY	3.4
1	C	472	ASN	3.4
2	B	445	LEU	3.4
1	C	280	LYS	3.4
1	A	1378	TYR	3.4
1	C	92	LEU	3.4
1	C	354	LEU	3.4
1	A	547	THR	3.4
1	C	409	SER	3.4

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Mol	Chain	Res	Type	RSRZ
2	D	740	ILE	3.4
1	A	1200	LYS	3.4
1	C	489	LYS	3.4
1	C	1675	GLY	3.4
1	A	684	GLU	3.3
2	D	905	TRP	3.3
2	D	641	ALA	3.3
2	B	253	TYR	3.3
1	C	1556	GLU	3.3
1	C	1526	LYS	3.3
2	D	921	GLN	3.3
1	A	20	GLU	3.3
2	B	940	THR	3.3
1	A	1339	GLU	3.3
1	C	66	TYR	3.3
2	B	1550	GLN	3.3
1	A	1629	TYR	3.3
2	B	169	GLU	3.3
2	D	241	GLU	3.3
2	B	968	ASP	3.3
1	C	723	ARG	3.3
1	C	1667	PHE	3.3
1	A	1660	PHE	3.3
2	B	1542	MET	3.3
1	C	621	GLU	3.3
1	A	1621	GLY	3.2
1	C	272	ARG	3.2
1	A	575	LEU	3.2
2	D	253	TYR	3.2
2	B	941	GLN	3.2
1	C	260	VAL	3.2
1	A	717	ARG	3.2
1	C	1672	PHE	3.2
1	A	894	HIS	3.2
2	B	121	LEU	3.2
1	C	99	VAL	3.2
1	C	1549	LYS	3.2
1	C	238	ILE	3.2
2	D	1290	TYR	3.2
2	D	119	VAL	3.2
1	A	692	HIS	3.2
1	A	1651	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	532	GLN	3.2
1	C	127	PHE	3.1
1	C	1612	VAL	3.1
1	C	1479	ILE	3.1
1	A	816	LYS	3.1
2	D	115	LEU	3.1
2	D	156	LYS	3.1
2	D	547	THR	3.1
1	A	50	PHE	3.1
2	D	1615	GLU	3.1
2	D	205	HIS	3.1
1	A	66	TYR	3.1
2	D	558	MET	3.1
2	B	639	ARG	3.1
1	A	700	TYR	3.1
1	A	921	GLU	3.1
1	C	858	LYS	3.1
1	C	195	ARG	3.1
1	C	1308	ARG	3.1
1	A	1578	LYS	3.0
2	D	736	GLU	3.0
1	A	620	LEU	3.0
2	B	1545	LEU	3.0
1	C	1635	TYR	3.0
1	C	1636	ILE	3.0
2	B	959	ILE	3.0
2	D	960	GLU	3.0
1	A	273	GLU	3.0
2	B	88	GLU	3.0
2	D	1370	ARG	3.0
2	D	1349	VAL	3.0
1	C	693	SER	3.0
1	A	1635	TYR	3.0
1	C	707	ASN	3.0
1	A	1674	ASN	3.0
1	C	1229	LYS	3.0
1	A	1589	GLU	3.0
1	C	722	PRO	3.0
2	D	249	ALA	3.0
2	B	1466	GLU	3.0
2	B	1528	LEU	2.9
1	A	117	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	321	LYS	2.9
1	A	196	TYR	2.9
1	C	1673	LEU	2.9
2	B	647	PRO	2.9
1	C	273	GLU	2.9
2	D	235	PHE	2.9
2	D	545	MET	2.9
2	B	1373	GLY	2.9
1	A	944	LEU	2.9
2	D	460	LEU	2.9
2	D	219	TYR	2.9
1	A	252	ALA	2.9
2	B	213	TYR	2.9
1	C	603	ALA	2.9
1	C	944	LEU	2.9
1	A	1673	LEU	2.9
1	A	711	CYS	2.9
2	B	35	THR	2.9
1	A	887	LYS	2.8
1	A	764	GLU	2.8
1	A	994	GLN	2.8
1	C	1480	PHE	2.8
1	C	386	VAL	2.8
2	D	226	VAL	2.8
1	A	246	PHE	2.8
1	C	254	TYR	2.8
2	D	342	PRO	2.8
1	C	708	ASP	2.8
1	A	659	ALA	2.8
2	B	1532	GLU	2.8
2	D	38	GLU	2.8
2	D	1624	LEU	2.8
1	A	927	LEU	2.8
2	B	878	ARG	2.8
1	A	1597	GLU	2.8
1	C	627	LEU	2.8
2	B	357	GLY	2.8
1	A	49	ALA	2.8
2	D	424	ARG	2.8
2	D	39	GLU	2.8
2	B	157	MET	2.8
1	C	1527	CYS	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	1306	LYS	2.8
2	B	33	LEU	2.8
2	B	820	MET	2.8
2	D	872	ILE	2.8
1	C	857	VAL	2.8
1	A	1620	MET	2.8
1	A	52	ALA	2.8
1	A	351	PRO	2.8
2	B	1315	ALA	2.8
1	A	364	LYS	2.7
1	A	44	TYR	2.7
1	C	234	GLU	2.7
1	C	1236	ASP	2.7
2	B	74	ASP	2.7
2	D	1354	LEU	2.7
1	A	1619	ILE	2.7
1	A	1648	TRP	2.7
1	C	1373	GLU	2.7
1	C	874	ASP	2.7
2	D	910	ARG	2.7
2	D	1318	ASP	2.7
2	D	1625	CYS	2.7
1	A	696	LYS	2.7
1	C	1177	GLU	2.7
2	B	122	SER	2.7
2	B	836	LEU	2.7
2	D	75	MET	2.7
1	A	266	TYR	2.7
2	B	407	GLN	2.7
2	D	121	LEU	2.7
2	B	1292	ILE	2.7
1	C	246	PHE	2.7
1	A	926	THR	2.7
1	C	204	LYS	2.7
1	C	790	LEU	2.7
1	C	1356	LEU	2.7
1	A	648	LEU	2.7
1	C	220	LYS	2.7
1	C	1536	GLN	2.7
2	B	753	LYS	2.7
2	D	89	ILE	2.7
1	A	1574	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	699	CYS	2.7
1	C	59	TYR	2.7
2	B	1642	THR	2.7
1	C	1576	LYS	2.7
2	B	404	LEU	2.7
2	B	1451	ILE	2.7
1	C	1609	ALA	2.7
2	D	467	LYS	2.7
1	C	705	VAL	2.7
1	A	506	LYS	2.7
1	A	821	LYS	2.6
2	B	424	ARG	2.6
1	A	1379	LEU	2.6
1	C	1648	TRP	2.6
2	D	839	TYR	2.6
2	D	1462	TYR	2.6
1	A	888	VAL	2.6
2	B	1275	LEU	2.6
2	D	1317	GLY	2.6
1	C	667	GLU	2.6
1	C	877	GLY	2.6
1	C	1402	ILE	2.6
1	A	247	GLU	2.6
1	A	682	LYS	2.6
1	C	1562	LYS	2.6
2	D	634	LEU	2.6
1	C	490	SER	2.6
1	C	50	PHE	2.6
2	D	446	HIS	2.6
1	C	1399	TYR	2.6
2	B	839	TYR	2.6
1	C	1528	VAL	2.6
2	B	802	VAL	2.6
1	C	281	GLU	2.6
2	B	1371	TYR	2.6
1	C	661	ASP	2.6
1	A	1535	MET	2.6
2	B	198	ARG	2.6
2	D	1406	ARG	2.6
1	A	1572	ASN	2.6
1	C	1634	ARG	2.6
2	D	217	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	1509	TYR	2.6
2	B	1561	HIS	2.6
2	D	1557	ARG	2.6
2	B	94	VAL	2.6
1	A	1449	LEU	2.6
1	C	1670	ASP	2.6
2	B	356	PRO	2.6
1	A	965	LEU	2.6
1	C	450	GLU	2.6
1	A	1511	THR	2.5
1	C	1313	ILE	2.5
1	A	1625	LEU	2.5
1	C	269	PHE	2.5
2	D	1272	ASP	2.5
2	B	90	PRO	2.5
2	D	811	MET	2.5
1	A	1526	LYS	2.5
2	B	468	GLY	2.5
2	D	344	GLN	2.5
1	A	345	ILE	2.5
1	C	594	THR	2.5
1	C	804	ILE	2.5
1	C	1586	LYS	2.5
2	D	812	LYS	2.5
2	B	66	LYS	2.5
1	A	753	HIS	2.5
1	A	686	ILE	2.5
1	A	932	GLU	2.5
1	C	1477	PHE	2.5
2	D	165	PHE	2.5
1	A	1305	LYS	2.5
1	C	465	LEU	2.5
1	C	1307	LEU	2.5
2	D	256	GLU	2.5
2	D	191	LEU	2.5
2	B	498	ARG	2.5
2	D	568	GLU	2.5
1	A	920	LYS	2.5
1	A	1652	THR	2.5
1	A	707	ASN	2.5
1	C	205	TYR	2.5
2	D	356	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	628	GLU	2.5
1	A	460	LEU	2.5
1	A	725	ILE	2.5
1	A	1276	GLU	2.5
1	A	720	LEU	2.5
1	C	1124	TYR	2.5
1	A	817	ALA	2.5
2	B	643	LYS	2.5
1	A	190	ILE	2.5
1	C	233	PRO	2.5
1	A	1538	GLU	2.5
2	B	1544	VAL	2.5
2	D	262	PHE	2.5
2	B	111	PRO	2.5
1	A	375	VAL	2.5
1	C	323	LEU	2.5
1	C	1544	SER	2.5
2	D	969	PRO	2.5
1	C	1658	GLN	2.4
1	C	1339	GLU	2.4
1	A	1675	GLY	2.4
2	D	814	PHE	2.4
1	C	275	LEU	2.4
1	A	327	VAL	2.4
1	C	704	CYS	2.4
1	C	1554	LYS	2.4
1	C	975	ARG	2.4
2	D	257	VAL	2.4
1	A	670	LYS	2.4
1	C	1558	ALA	2.4
2	B	1611	PRO	2.4
1	A	889	GLU	2.4
1	C	879	LYS	2.4
2	B	810	VAL	2.4
2	B	1549	LYS	2.4
1	A	637	GLY	2.4
1	A	636	ALA	2.4
2	B	1301	ARG	2.4
1	C	1561	TYR	2.4
1	A	1070	LYS	2.4
1	C	326	ALA	2.4
1	A	1224	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	740	ILE	2.4
2	D	911	LYS	2.4
2	D	1511	GLN	2.4
1	A	250	ILE	2.4
2	D	935	LYS	2.4
1	C	315	LEU	2.4
1	C	511	HIS	2.4
1	C	1226	ARG	2.4
1	C	523	TYR	2.4
2	B	92	LYS	2.4
1	C	1626	GLN	2.4
2	D	104	VAL	2.4
2	B	1450	PHE	2.4
1	A	669	CYS	2.4
1	C	1305	LYS	2.4
1	C	1401	ARG	2.4
2	B	1481	LEU	2.4
2	D	365	TYR	2.4
2	B	1289	ARG	2.4
2	D	1307	LEU	2.4
1	C	1535	MET	2.4
1	C	809	ILE	2.4
1	A	59	TYR	2.4
1	A	1111	TYR	2.4
1	A	30	ILE	2.4
2	B	1583	ILE	2.4
2	D	1320	LYS	2.4
1	C	126	LEU	2.4
1	C	1650	ARG	2.4
2	B	426	ALA	2.4
1	A	1367	LYS	2.4
1	C	498	HIS	2.4
2	D	1506	ILE	2.4
1	A	33	VAL	2.4
2	D	1595	ASP	2.4
1	A	195	ARG	2.4
1	C	98	PRO	2.4
2	D	925	VAL	2.4
1	C	962	ARG	2.4
2	B	591	TYR	2.3
2	D	959	ILE	2.3
1	C	301	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	582	TYR	2.3
2	D	604	LYS	2.3
1	A	1565	ILE	2.3
2	B	1363	LEU	2.3
1	C	1548	ARG	2.3
1	C	618	LYS	2.3
2	D	154	THR	2.3
1	C	997	ILE	2.3
2	D	508	LEU	2.3
1	A	690	TYR	2.3
2	B	52	LYS	2.3
2	D	1444	LYS	2.3
2	B	800	ILE	2.3
2	D	1556	PRO	2.3
1	C	1597	GLU	2.3
2	D	349	LYS	2.3
1	A	1581	LEU	2.3
1	C	318	LEU	2.3
1	C	460	LEU	2.3
2	B	857	CYS	2.3
2	B	109	THR	2.3
1	C	772	SER	2.3
1	C	1432	ILE	2.3
1	C	1660	PHE	2.3
1	C	249	THR	2.3
2	D	865	ARG	2.3
1	A	1273	TRP	2.3
1	C	1644	TRP	2.3
1	A	855	PHE	2.3
1	C	1669	GLU	2.3
1	A	1130	GLN	2.3
2	B	967	GLY	2.3
2	D	185	PRO	2.3
2	B	328	MET	2.3
1	A	963	ILE	2.3
1	C	1629	TYR	2.3
2	B	237	ILE	2.3
2	D	164	GLU	2.3
2	D	819	GLN	2.3
1	C	765	ILE	2.3
1	C	1346	LEU	2.3
2	B	1480	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	482	LEU	2.3
1	A	914	LEU	2.3
1	C	248	ILE	2.3
1	A	950	TYR	2.3
2	D	611	ALA	2.3
1	C	686	ILE	2.3
1	A	1571	GLU	2.3
2	B	530	GLU	2.3
2	B	154	THR	2.3
2	B	837	HIS	2.3
1	A	629	LYS	2.3
1	A	1508	PHE	2.3
2	B	748	ARG	2.3
2	B	937	VAL	2.3
1	A	1386	ILE	2.3
1	A	1544	SER	2.3
1	C	1430	THR	2.3
2	B	186	TYR	2.3
2	D	157	MET	2.3
1	A	51	ASP	2.3
1	A	1235	LYS	2.3
1	C	49	ALA	2.3
1	C	1070	LYS	2.3
2	D	155	SER	2.3
2	D	466	VAL	2.3
1	A	1119	LYS	2.3
1	C	560	TRP	2.3
1	C	771	GLU	2.3
1	A	376	LYS	2.2
1	C	640	LEU	2.2
2	D	204	GLU	2.2
1	A	465	LEU	2.2
1	C	1235	LYS	2.2
1	C	1492	THR	2.2
1	A	1612	VAL	2.2
1	A	1053	MET	2.2
1	A	1600	PHE	2.2
2	B	125	SER	2.2
2	D	785	THR	2.2
2	D	1473	HIS	2.2
1	A	1529	GLU	2.2
2	B	409	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	1557	ARG	2.2
2	B	1582	LEU	2.2
2	D	224	PHE	2.2
1	C	1619	ILE	2.2
2	B	1539	ILE	2.2
2	B	850	LEU	2.2
2	D	1603	LYS	2.2
1	A	159	THR	2.2
1	C	54	ILE	2.2
1	C	766	ARG	2.2
1	A	1059	TYR	2.2
2	B	100	GLN	2.2
2	B	966	GLN	2.2
1	A	158	GLU	2.2
2	B	1467	LYS	2.2
1	A	205	TYR	2.2
2	B	1392	PRO	2.2
2	D	199	ILE	2.2
2	D	173	VAL	2.2
2	D	1541	VAL	2.2
1	C	194	PRO	2.2
1	A	1424	MET	2.2
1	A	31	PHE	2.2
1	A	551	THR	2.2
1	A	365	PRO	2.2
1	A	297	ALA	2.2
1	C	382	LEU	2.2
2	B	89	ILE	2.2
1	A	54	ILE	2.2
2	D	1342	LYS	2.2
1	A	267	ILE	2.2
1	C	208	ASP	2.2
2	D	88	GLU	2.2
2	D	329	VAL	2.2
1	A	96	GLN	2.2
2	D	1621	PHE	2.2
1	A	237	PHE	2.2
1	C	592	MET	2.2
1	C	1668	ALA	2.2
1	A	825	LEU	2.2
1	A	1303	LEU	2.2
1	A	1636	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	1290	TYR	2.2
1	C	32	ARG	2.2
2	D	80	GLY	2.2
2	D	1531	ILE	2.2
1	A	1356	LEU	2.2
1	C	152	LEU	2.2
1	C	982	LEU	2.2
2	D	1626	ASP	2.2
1	C	221	GLU	2.1
2	B	204	GLU	2.1
1	A	908	HIS	2.1
2	B	321	MET	2.1
2	D	228	LEU	2.1
2	D	321	MET	2.1
1	A	185	PHE	2.1
1	A	1590	ALA	2.1
1	A	22	THR	2.1
1	A	683	ILE	2.1
1	A	1664	LEU	2.1
1	C	1370	THR	2.1
2	D	924	ILE	2.1
2	D	1561	HIS	2.1
2	D	1641	PRO	2.1
1	A	606	ASP	2.1
2	B	349	LYS	2.1
2	D	968	ASP	2.1
1	C	1473	LEU	2.1
1	C	1482	LEU	2.1
2	B	362	LEU	2.1
2	B	1533	GLU	2.1
1	C	239	GLY	2.1
1	C	973	ILE	2.1
2	B	604	LYS	2.1
1	A	163	PHE	2.1
2	B	360	TYR	2.1
1	A	903	LEU	2.1
1	C	1568	ILE	2.1
1	C	1601	ILE	2.1
2	D	420	LEU	2.1
1	C	331	GLU	2.1
2	D	863	GLY	2.1
2	D	379	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	670	LYS	2.1
2	B	233	LYS	2.1
2	D	1529	LEU	2.1
1	A	46	TYR	2.1
1	A	173	MET	2.1
1	A	809	ILE	2.1
1	C	371	ILE	2.1
1	C	1326	TYR	2.1
2	D	345	ILE	2.1
1	A	1584	ILE	2.1
1	C	379	LEU	2.1
2	B	489	ILE	2.1
1	A	1655	SER	2.1
1	C	1237	SER	2.1
2	D	358	MET	2.1
1	A	122	ASP	2.1
1	C	936	ARG	2.1
1	C	1666	GLU	2.1
2	D	1495	GLU	2.1
1	A	1229	LYS	2.1
1	C	1011	GLU	2.1
2	B	842	GLU	2.1
2	B	1505	ARG	2.1
2	D	1361	GLY	2.1
1	C	96	GLN	2.1
1	C	856	CYS	2.1
1	A	157	ARG	2.1
1	A	835	ARG	2.1
1	C	680	GLN	2.1
2	D	889	GLN	2.1
1	A	1475	VAL	2.1
1	C	243	PHE	2.1
1	C	1671	ILE	2.1
2	D	81	MET	2.1
2	D	423	GLU	2.1
2	D	1289	ARG	2.1
2	D	570	ASP	2.1
1	C	759	PRO	2.1
1	C	1386	ILE	2.1
1	A	983	LEU	2.1
1	C	554	LEU	2.1
1	A	995	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1627	ILE	2.1
2	B	282	ARG	2.1
1	A	148	LEU	2.1
1	C	198	MET	2.1
1	C	1034	PHE	2.1
2	D	221	LEU	2.1
2	D	820	MET	2.1
2	D	843	ASP	2.1
1	A	1313	ILE	2.1
1	C	764	GLU	2.1
2	D	377	VAL	2.1
1	A	818	LYS	2.1
1	C	1059	TYR	2.1
2	B	965	ILE	2.1
2	D	1563	TYR	2.1
1	C	431	LEU	2.1
2	B	736	GLU	2.1
1	C	298	GLN	2.0
1	A	548	GLY	2.0
1	A	1637	TYR	2.0
1	C	1330	ASP	2.0
1	C	1674	ASN	2.0
2	B	875	LEU	2.0
2	B	1318	ASP	2.0
1	A	1400	LYS	2.0
1	C	340	ALA	2.0
1	C	1311	MET	2.0
2	D	114	ARG	2.0
1	A	915	GLU	2.0
1	C	912	PHE	2.0
2	B	889	GLN	2.0
2	D	428	LYS	2.0
1	A	786	LEU	2.0
1	A	1385	ASP	2.0
1	C	159	THR	2.0
1	C	274	ASP	2.0
1	C	378	SER	2.0
2	B	1462	TYR	2.0
2	D	1500	LEU	2.0
1	A	1594	LYS	2.0
1	C	57	LYS	2.0
2	D	118	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	551	THR	2.0
2	B	1538	ASP	2.0
1	C	1232	LEU	2.0
1	A	625	GLN	2.0
2	B	152	HIS	2.0
2	D	1344	HIS	2.0
1	C	742	ILE	2.0
1	C	1328	MET	2.0
1	A	1326	TYR	2.0
1	C	493	ILE	2.0
2	B	91	ALA	2.0
1	C	1433	SER	2.0
1	A	1205	PHE	2.0
2	D	929	LYS	2.0
1	C	449	ARG	2.0
2	B	369	PRO	2.0
2	B	851	LEU	2.0
1	A	204	LYS	2.0
1	A	1495	VAL	2.0
1	A	221	GLU	2.0
1	C	125	PHE	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 ⓘ

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, 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
3	NAG	B	2002	14/15	0.70	4.05	321,327,336,339	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	C	2003	14/15	0.55	1.78	260,272,284,287	0
3	NAG	D	2002	14/15	0.39	0.34	289,293,305,308	0
3	NAG	D	2001	14/15	0.38	-0.13	285,296,309,310	0
3	NAG	A	2003	14/15	0.41	-0.38	284,286,289,289	0
3	NAG	B	2001	14/15	0.27	-0.85	275,285,305,313	0

6.5 Other polymers ⓘ

There are no such residues in this entry.