



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 11:31 PM GMT

PDB ID : 2OIP
Title : Crystal Structure of the S290G Active Site Mutant of TS-DHFR from *Cryptosporidium hominis*
Authors : Martucci, W.E.; Vargo, M.A.
Deposited on : 2007-01-11
Resolution : 2.80 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>

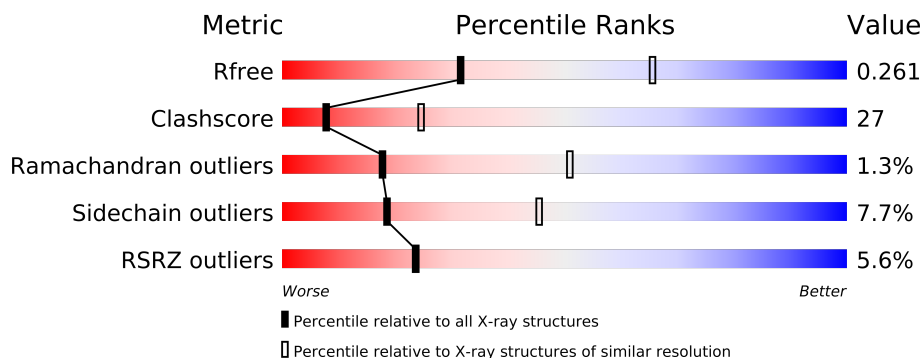
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.80 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	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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	519	
1	B	519	
1	C	519	
1	D	519	
1	E	519	

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	CB3	A	604	-	X
3	CB3	D	616	-	X
3	CB3	E	620	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21931 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.

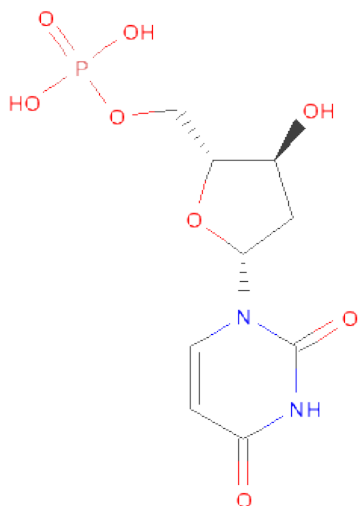
- Molecule 1 is a protein called Chain A, crystal structure of Dhfr.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	516	Total	C	N	O	S	0	0	0
			4182	2669	706	784	23			
1	B	516	Total	C	N	O	S	0	0	0
			4189	2674	707	786	22			
1	C	514	Total	C	N	O	S	0	0	0
			4164	2660	703	779	22			
1	D	515	Total	C	N	O	S	0	0	0
			4167	2662	702	781	22			
1	E	511	Total	C	N	O	S	0	0	0
			4145	2648	697	778	22			

There are 5 discrepancies between the modelled and reference sequences:

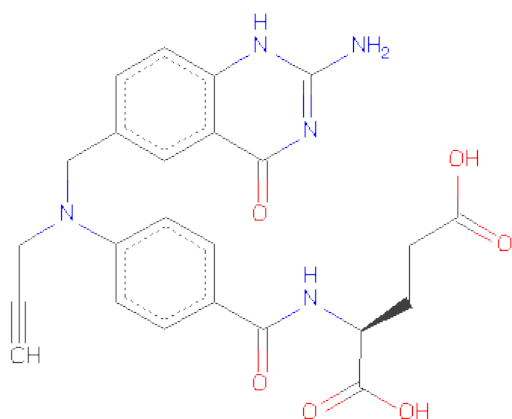
Chain	Residue	Modelled	Actual	Comment	Reference
A	290	GLY	SER	ENGINEERED	UNP Q5CGA3
B	290	GLY	SER	ENGINEERED	UNP Q5CGA3
C	290	GLY	SER	ENGINEERED	UNP Q5CGA3
D	290	GLY	SER	ENGINEERED	UNP Q5CGA3
E	290	GLY	SER	ENGINEERED	UNP Q5CGA3

- Molecule 2 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (three-letter code: UMP) (formula: $C_9H_{13}N_2O_8P$).



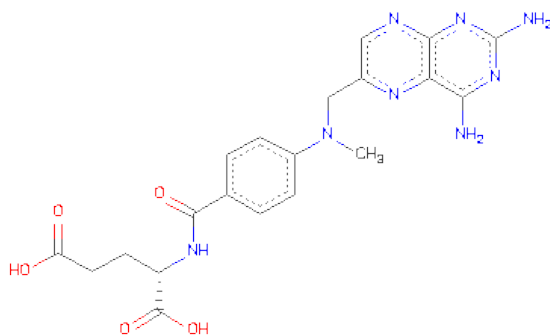
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	C	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	D	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	E	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

- Molecule 3 is 10-PROPARGYL-5,8-DIDEAZAFOLICACID (three-letter code: CB3) (formula: C₂₄H₂₃N₅O₆).



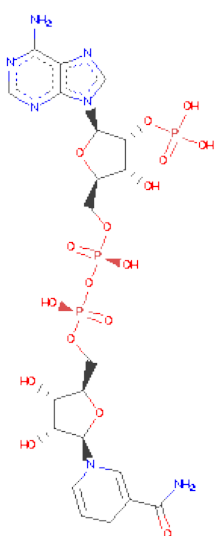
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			35	24	5	6		
3	B	1	Total	C	N	O	0	0
			35	24	5	6		
3	C	1	Total	C	N	O	0	0
			35	24	5	6		
3	D	1	Total	C	N	O	0	0
			35	24	5	6		
3	E	1	Total	C	N	O	0	0
			35	24	5	6		

- Molecule 4 is METHOTREXATE (three-letter code: MTX) (formula: $C_{20}H_{22}N_8O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			33	20	8	5		
4	B	1	Total	C	N	O	0	0
			33	20	8	5		
4	C	1	Total	C	N	O	0	0
			33	20	8	5		
4	D	1	Total	C	N	O	0	0
			33	20	8	5		
4	E	1	Total	C	N	O	0	0
			33	20	8	5		

- Molecule 5 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDEPHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
5	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
5	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
5	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
5	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 6 is water.

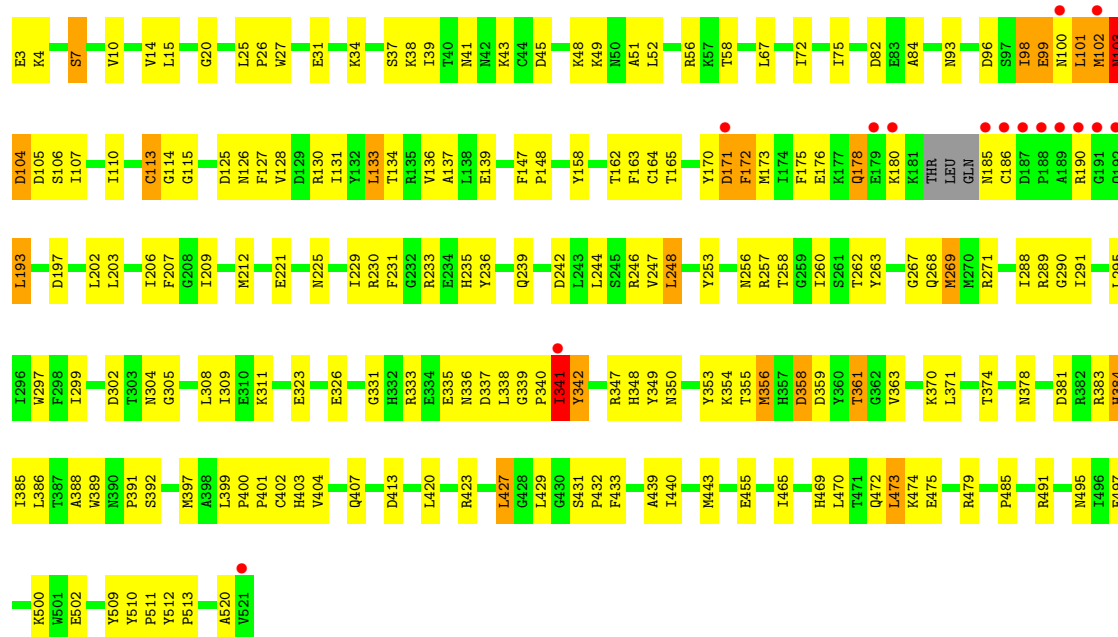
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	113	Total 113	O 113	0	0
6	B	143	Total 143	O 143	0	0
6	C	68	Total 68	O 68	0	0
6	D	61	Total 61	O 61	0	0
6	E	19	Total 19	O 19	0	0

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.

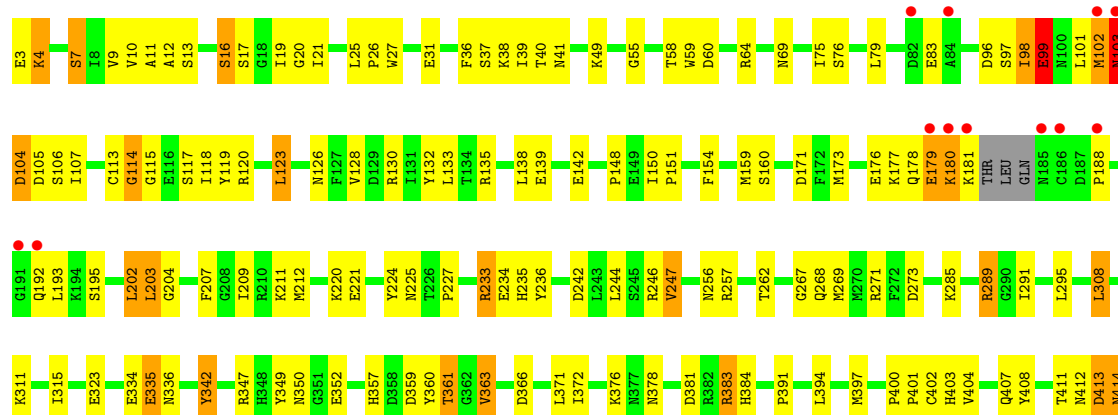
- Molecule 1: Chain A, crystal structure of Dhfr

Chain A: 



- Molecule 1: Chain A, crystal structure of Dhfr

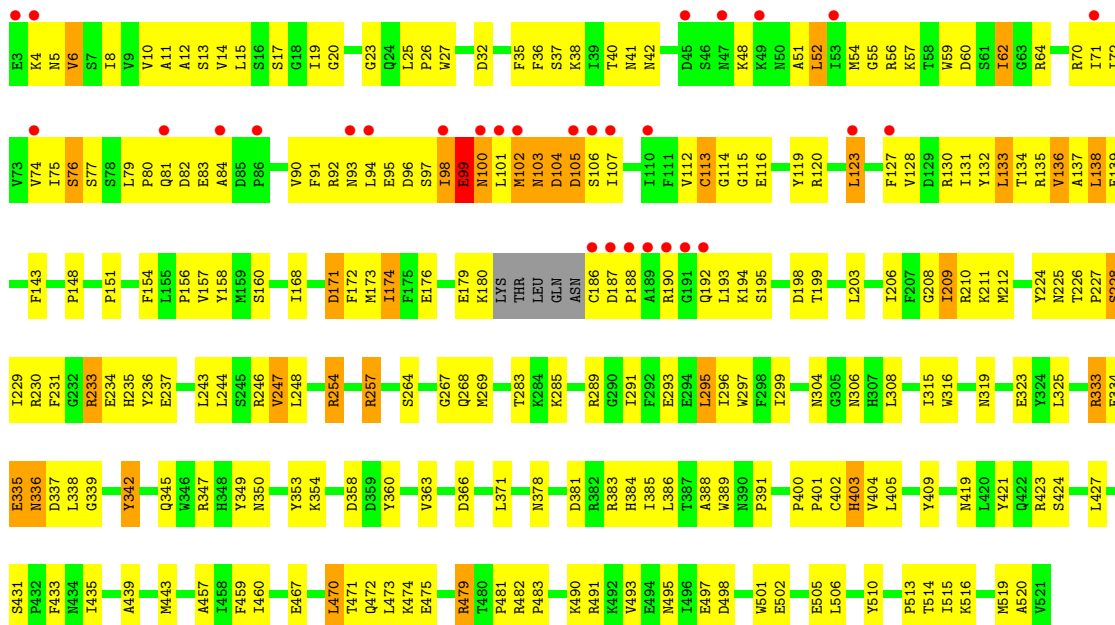
Chain B: 





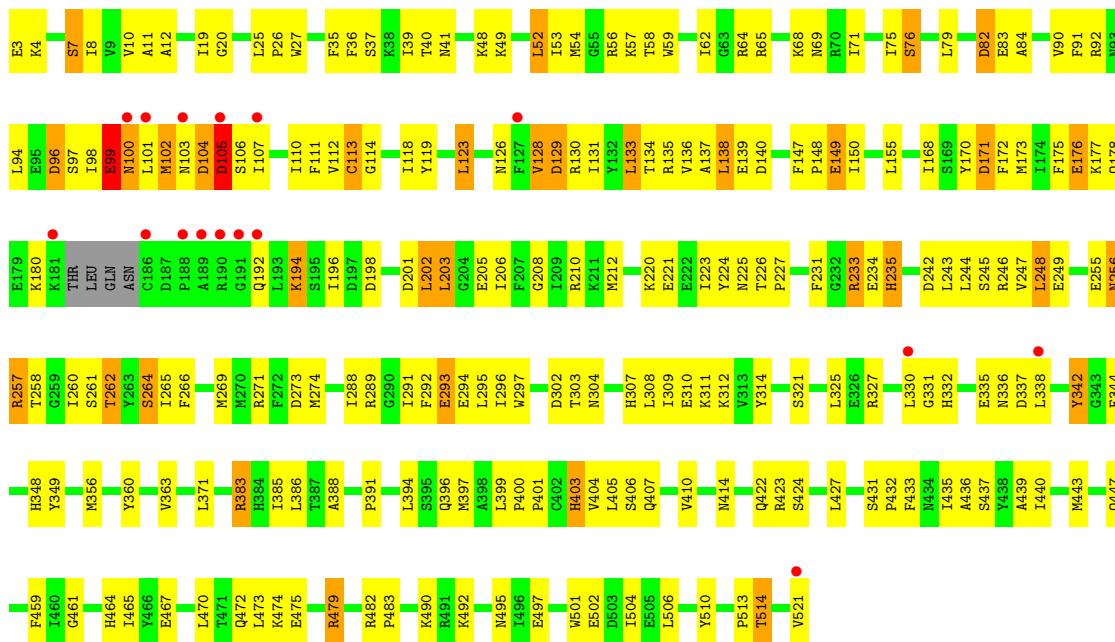
• Molecule 1: Chain A, crystal structure of Dhfr

Chain C:



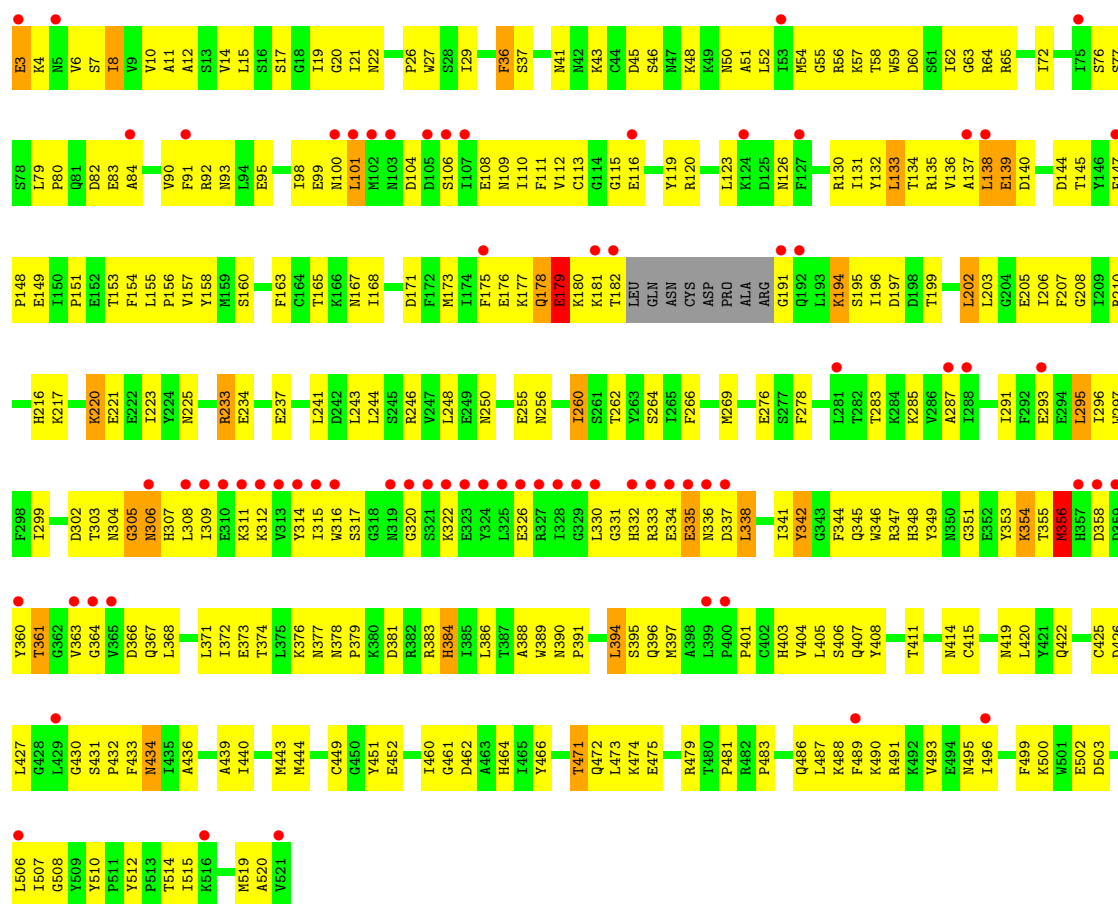
• Molecule 1: Chain A, crystal structure of Dhfr

Chain D:



• Molecule 1: Chain A, crystal structure of Dhfr

Chain E:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	215.03Å 116.20Å 216.60Å 90.00° 94.27° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 49.74 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-2.80) 99.3 (49.74-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.20 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.222 , 0.259 0.224 , 0.261	Depositor DCC
R_{free} test set	6550 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	57.9	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	1 of 130114 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	21931	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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: CB3, MTX, UMP, NDP

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	0.40	0/4278	0.66	0/5782
1	B	0.43	0/4285	0.68	2/5790 (0.0%)
1	C	0.37	0/4260	0.61	0/5758
1	D	0.36	0/4263	0.62	0/5763
1	E	0.35	0/4240	0.63	0/5730
All	All	0.38	0/21326	0.64	2/28823 (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	5
1	B	0	4
1	C	0	6
1	D	0	3
1	E	0	5
All	All	0	23

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	104	ASP	CB-CG-OD2	-5.36	113.48	118.30
1	B	104	ASP	CB-CG-OD1	5.20	122.98	118.30

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	CYS	Peptide
1	A	114	GLY	Peptide
1	A	171	ASP	Peptide
1	A	340	PRO	Peptide
1	A	341	ILE	Peptide
1	B	102	MET	Peptide
1	B	113	CYS	Peptide
1	B	114	GLY	Peptide
1	B	99	GLU	Peptide
1	C	104	ASP	Peptide
1	C	112	VAL	Peptide
1	C	113	CYS	Peptide
1	C	136	VAL	Peptide
1	C	254	ARG	Sidechain
1	C	403	HIS	Peptide
1	D	113	CYS	Peptide
1	D	403	HIS	Peptide
1	D	99	GLU	Peptide
1	E	179	GLU	Peptide
1	E	180	LYS	Peptide
1	E	305	GLY	Peptide
1	E	351	GLY	Peptide
1	E	356	MET	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	4182	0	4100	201	0
1	B	4189	0	4112	159	0
1	C	4164	0	4085	266	0
1	D	4167	0	4082	226	0
1	E	4145	0	4064	291	1
2	A	20	0	11	3	0
2	B	20	0	11	2	0
2	C	20	0	11	5	0
2	D	20	0	11	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	20	0	11	8	0
3	A	35	0	21	2	0
3	B	35	0	21	7	0
3	C	35	0	20	9	0
3	D	35	0	21	4	0
3	E	35	0	21	17	0
4	A	33	0	19	6	0
4	B	33	0	19	8	0
4	C	33	0	20	6	0
4	D	33	0	20	7	0
4	E	33	0	20	10	0
5	A	48	0	26	5	0
5	B	48	0	26	8	0
5	C	48	0	26	12	0
5	D	48	0	26	7	0
5	E	48	0	26	12	0
6	A	113	0	0	12	0
6	B	143	0	0	6	0
6	C	68	0	0	9	0
6	D	61	0	0	9	0
6	E	19	0	0	3	0
All	All	21931	0	20830	1148	1

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 27.

All (1148) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:100:ASN:CA	1:C:103:ASN:HB2	1.03	1.50
1:C:100:ASN:HA	1:C:103:ASN:CB	0.91	1.36
1:A:43:LYS:HE3	1:A:48:LYS:O	1.36	1.23
1:C:100:ASN:C	1:C:103:ASN:HB2	1.64	1.16
1:C:99:GLU:CD	1:C:103:ASN:HD21	1.49	1.16
1:A:4:LYS:HG2	1:A:101:LEU:HD23	1.15	1.15
1:C:100:ASN:HA	1:C:103:ASN:CG	1.67	1.12
1:C:96:ASP:O	1:C:99:GLU:HG2	1.47	1.12
1:C:99:GLU:C	1:C:103:ASN:HD22	1.52	1.11
1:B:411:THR:HG22	1:B:413:ASP:H	1.07	1.08
1:A:341:ILE:HA	1:A:397:MET:CE	1.82	1.08
1:C:104:ASP:OD2	1:C:106:SER:N	1.88	1.05
1:A:186:CYS:HA	1:A:230:ARG:HD2	1.40	1.03
1:A:258:THR:HG22	1:A:260:ILE:H	1.20	1.02

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:337:ASP:HB2	1:E:356:MET:SD	1.99	1.01
1:B:4:LYS:HB3	1:B:101:LEU:CD2	1.90	1.01
1:A:341:ILE:HA	1:A:397:MET:HE2	1.02	0.99
1:D:102:MET:HA	1:D:102:MET:HE3	1.40	0.99
1:B:103:ASN:ND2	1:B:104:ASP:H	1.59	0.99
1:E:100:ASN:O	1:E:104:ASP:HB3	1.63	0.98
1:C:100:ASN:HA	1:C:103:ASN:HB3	1.43	0.98
1:E:426:ASP:HB2	2:E:619:UMP:H2''	1.44	0.98
1:C:99:GLU:C	1:C:103:ASN:ND2	2.16	0.97
1:C:391:PRO:HD2	1:D:349:TYR:CE2	1.98	0.96
1:D:56:ARG:HB2	1:D:76:SER:OG	1.65	0.96
1:C:335:GLU:O	1:C:336:ASN:HB2	1.63	0.96
1:A:4:LYS:HG2	1:A:101:LEU:CD2	1.95	0.95
1:E:8:ILE:HG12	1:E:112:VAL:HB	1.49	0.94
1:C:100:ASN:CA	1:C:103:ASN:CB	1.85	0.94
1:A:4:LYS:H	1:A:101:LEU:HD22	1.32	0.94
1:C:138:LEU:CD2	1:C:138:LEU:H	1.79	0.94
1:D:4:LYS:HE2	1:D:101:LEU:HA	1.50	0.94
1:E:191:GLY:HA2	1:E:197:ASP:OD2	1.69	0.92
1:A:304:ASN:HA	1:A:356:MET:HE3	1.49	0.92
1:B:179:GLU:O	1:B:180:LYS:HG3	1.71	0.91
3:D:616:CB3:O	3:D:616:CB3:HB1	1.68	0.91
1:D:102:MET:HA	1:D:102:MET:CE	1.97	0.91
1:C:137:ALA:O	1:C:510:TYR:HE2	1.53	0.90
2:E:619:UMP:H1'	3:E:620:CB3:C2	2.02	0.89
1:D:96:ASP:O	1:D:99:GLU:HG2	1.73	0.89
1:A:341:ILE:CA	1:A:397:MET:HE2	1.98	0.89
1:A:4:LYS:H	1:A:101:LEU:CD2	1.85	0.88
1:D:337:ASP:HA	1:D:356:MET:HE3	1.55	0.88
1:B:180:LYS:HD3	1:B:181:LYS:N	1.88	0.88
1:D:54:MET:HA	1:D:114:GLY:HA2	1.55	0.88
1:B:209:ILE:H	1:B:209:ILE:HD12	1.34	0.88
1:D:399:LEU:HD12	1:D:400:PRO:HD2	1.56	0.88
1:C:190:ARG:HB3	1:C:190:ARG:HH11	1.39	0.88
1:B:103:ASN:CG	1:B:104:ASP:H	1.76	0.88
4:E:621:MTX:HG1	4:E:621:MTX:O1	1.74	0.87
1:A:271:ARG:NH2	1:B:267:GLY:O	2.09	0.86
1:E:304:ASN:CG	1:E:356:MET:HE2	1.95	0.86
1:D:220:LYS:HD3	1:D:249:GLU:OE1	1.75	0.86
1:A:104:ASP:HB3	1:A:107:ILE:HG12	1.56	0.85
1:A:326:GLU:HA	6:A:609:HOH:O	1.76	0.85
1:E:37:SER:HB2	4:E:621:MTX:HG2	1.58	0.85

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:196:ILE:HG22	1:E:197:ASP:N	1.93	0.84
1:D:75:ILE:O	5:D:618:NDP:H1B	1.77	0.84
1:E:304:ASN:HA	1:E:356:MET:HE3	1.59	0.84
1:A:333:ARG:HG2	1:A:337:ASP:HB3	1.58	0.84
1:E:336:ASN:O	1:E:338:LEU:HD23	1.78	0.83
1:D:82:ASP:OD1	1:D:84:ALA:HB3	1.77	0.83
1:C:99:GLU:CD	1:C:103:ASN:ND2	2.31	0.83
1:E:79:LEU:HD23	1:E:80:PRO:HD2	1.59	0.83
3:D:616:CB3:H13	3:D:616:CB3:CP2	2.09	0.82
1:B:411:THR:HG22	1:B:413:ASP:N	1.93	0.82
1:B:411:THR:CG2	1:B:413:ASP:HB2	2.10	0.81
1:B:4:LYS:HB3	1:B:101:LEU:HD22	1.60	0.81
1:C:319:ASN:ND2	3:C:612:CB3:H8	1.94	0.81
1:C:102:MET:O	1:C:103:ASN:O	1.97	0.81
1:C:360:TYR:O	1:C:363:VAL:HG12	1.81	0.81
1:E:334:GLU:HG3	1:E:335:GLU:H	1.44	0.81
1:A:103:ASN:C	1:A:103:ASN:HD22	1.84	0.81
1:C:100:ASN:N	1:C:103:ASN:ND2	2.28	0.80
1:E:338:LEU:HD23	1:E:338:LEU:N	1.97	0.80
4:D:617:MTX:O1	4:D:617:MTX:HG2	1.79	0.80
1:A:349:TYR:CE2	1:B:391:PRO:HD2	2.16	0.80
2:E:619:UMP:O2	2:E:619:UMP:H2'	1.80	0.80
1:E:151:PRO:HG2	1:E:154:PHE:HD2	1.47	0.80
1:E:302:ASP:OD2	1:E:307:HIS:CD2	2.35	0.80
1:E:422:GLN:HG2	1:E:425:CYS:HB2	1.63	0.80
1:E:207:PHE:HB3	1:E:210:ARG:HB2	1.63	0.80
1:C:190:ARG:HB3	1:C:190:ARG:NH1	1.96	0.80
1:C:62:ILE:HD13	1:C:62:ILE:O	1.81	0.80
1:B:103:ASN:ND2	1:B:104:ASP:N	2.29	0.79
2:E:619:UMP:H1'	3:E:620:CB3:N3	1.96	0.79
1:C:158:TYR:HB3	1:C:174:ILE:HG23	1.64	0.79
1:C:349:TYR:CE2	1:D:391:PRO:HD2	2.17	0.79
1:E:306:ASN:O	1:E:309:ILE:HB	1.83	0.79
1:D:4:LYS:CB	1:D:101:LEU:HD23	2.12	0.78
4:E:621:MTX:CG	4:E:621:MTX:O1	2.30	0.78
1:B:285:LYS:HB3	1:B:514:THR:HG22	1.65	0.78
1:C:138:LEU:HD22	1:C:138:LEU:H	1.48	0.78
1:D:25:LEU:HD11	4:D:617:MTX:H7	1.64	0.78
1:C:333:ARG:HG3	1:C:337:ASP:HB3	1.66	0.78
1:C:151:PRO:HG2	1:C:154:PHE:HD2	1.49	0.78
1:B:411:THR:HG21	1:B:413:ASP:HB2	1.66	0.78
1:E:196:ILE:O	1:E:197:ASP:HB2	1.84	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:123:LEU:HD12	1:C:128:VAL:HG11	1.66	0.78
1:E:378:ASN:ND2	1:E:381:ASP:HB2	1.99	0.78
1:A:38:LYS:HB3	1:B:202:LEU:HG	1.66	0.77
1:A:14:VAL:HG23	1:A:136:VAL:O	1.83	0.77
1:C:55:GLY:HA3	5:C:614:NDP:O2A	1.84	0.77
1:A:258:THR:HG21	1:A:520:ALA:HB1	1.66	0.77
1:D:82:ASP:OD1	1:D:84:ALA:CB	2.32	0.77
3:B:608:CB3:O1	3:B:608:CB3:HG2	1.85	0.77
1:E:314:TYR:HB3	1:E:317:SER:HB2	1.67	0.77
1:C:79:LEU:HD23	1:C:80:PRO:HD2	1.65	0.77
1:A:163:PHE:HB2	1:A:170:TYR:CE2	2.19	0.76
1:E:58:THR:CG2	4:E:621:MTX:HM2	2.15	0.76
1:A:43:LYS:CE	1:A:48:LYS:O	2.26	0.76
1:A:103:ASN:ND2	1:A:103:ASN:C	2.37	0.76
1:C:171:ASP:OD2	1:C:483:PRO:HG3	1.86	0.76
1:C:26:PRO:HB2	1:C:27:TRP:CE3	2.21	0.76
1:E:196:ILE:CG2	1:E:197:ASP:N	2.49	0.75
1:B:103:ASN:O	1:B:104:ASP:C	2.24	0.75
1:C:79:LEU:HD23	1:C:80:PRO:CD	2.16	0.75
1:E:391:PRO:O	1:E:394:LEU:HD11	1.87	0.75
1:C:138:LEU:H	1:C:138:LEU:HD23	1.52	0.75
1:A:82:ASP:OD2	1:A:84:ALA:HB3	1.86	0.75
1:D:304:ASN:HA	1:D:356:MET:HE2	1.67	0.74
1:E:389:TRP:HB2	1:E:404:VAL:HG13	1.68	0.74
2:D:615:UMP:H5	6:D:667:HOH:O	1.69	0.74
1:C:19:ILE:O	5:C:614:NDP:H2N	1.87	0.74
1:E:243:LEU:HA	1:E:246:ARG:NH1	2.03	0.74
1:A:258:THR:CG2	1:A:520:ALA:HB1	2.18	0.74
1:D:342:TYR:CE1	1:D:403:HIS:CE1	2.76	0.74
1:E:264:SER:HB3	1:E:464:HIS:HB3	1.67	0.74
1:E:56:ARG:HD3	5:E:622:NDP:O1X	1.88	0.73
1:E:304:ASN:HA	1:E:356:MET:CE	2.18	0.73
1:A:258:THR:HG22	1:A:260:ILE:N	2.01	0.73
1:C:209:ILE:H	1:C:209:ILE:HD13	1.53	0.73
1:A:374:THR:HG22	1:A:384:HIS:CE1	2.23	0.73
1:C:4:LYS:H	1:C:101:LEU:HD22	1.54	0.73
1:A:102:MET:O	1:A:103:ASN:HB3	1.86	0.73
1:E:76:SER:HA	5:E:622:NDP:O2X	1.89	0.73
1:E:56:ARG:HH21	1:E:57:LYS:HG2	1.53	0.73
1:C:333:ARG:HG2	1:C:333:ARG:HH11	1.53	0.73
1:E:302:ASP:OD2	1:E:307:HIS:HD2	1.72	0.73
1:D:100:ASN:HB2	1:D:110:ILE:HD11	1.69	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:225:ASN:O	1:B:233:ARG:NH2	2.22	0.73
1:E:153:THR:O	1:E:177:LYS:HD2	1.88	0.73
1:D:135:ARG:NH2	1:D:482:ARG:HA	2.04	0.72
1:C:138:LEU:CD2	1:C:138:LEU:N	2.50	0.72
1:E:342:TYR:O	1:E:345:GLN:HB2	1.88	0.72
1:D:289:ARG:HG3	1:D:501:TRP:CE2	2.24	0.72
1:E:337:ASP:HB2	1:E:356:MET:CG	2.19	0.72
1:C:135:ARG:NH2	1:C:482:ARG:HA	2.04	0.72
1:E:79:LEU:HD23	1:E:80:PRO:CD	2.19	0.72
1:D:62:ILE:HD11	4:D:617:MTX:C14	2.20	0.72
1:D:26:PRO:HB2	1:D:27:TRP:CE3	2.23	0.72
1:D:137:ALA:O	1:D:510:TYR:HE2	1.73	0.71
1:C:225:ASN:O	1:C:233:ARG:NH2	2.22	0.71
1:E:115:GLY:HA3	5:E:622:NDP:O1A	1.91	0.71
1:C:419:ASN:ND2	1:C:457:ALA:HB3	2.05	0.71
1:B:102:MET:O	1:B:103:ASN:HB3	1.91	0.71
1:C:254:ARG:NH2	1:D:410:VAL:O	2.23	0.71
1:E:336:ASN:O	1:E:338:LEU:CD2	2.38	0.71
1:A:500:LYS:HE3	6:A:714:HOH:O	1.90	0.71
1:D:337:ASP:CA	1:D:356:MET:HE3	2.20	0.71
1:D:224:TYR:O	1:D:227:PRO:HG3	1.90	0.70
1:D:514:THR:HG22	6:D:622:HOH:O	1.91	0.70
1:A:172:PHE:N	1:A:172:PHE:CD1	2.59	0.70
3:D:616:CB3:O	3:D:616:CB3:CB	2.38	0.70
1:D:126:ASN:CG	1:D:177:LYS:HZ1	1.93	0.70
1:A:102:MET:O	1:A:103:ASN:CB	2.38	0.70
1:C:52:LEU:HD11	1:C:70:ARG:HD2	1.71	0.70
1:E:337:ASP:HB2	1:E:356:MET:HG2	1.74	0.70
1:E:363:VAL:HG13	1:E:364:GLY:H	1.54	0.70
1:D:257:ARG:HH11	2:D:615:UMP:P	2.15	0.70
1:E:179:GLU:HG2	6:E:635:HOH:O	1.92	0.70
1:E:430:GLY:HA2	3:E:620:CB3:CP3	2.22	0.69
1:A:374:THR:HG22	1:A:384:HIS:HE1	1.56	0.69
4:D:617:MTX:CG	4:D:617:MTX:O1	2.40	0.69
1:E:374:THR:HG22	1:E:384:HIS:CE1	2.26	0.69
1:E:283:THR:O	1:E:512:TYR:HB2	1.93	0.69
4:B:609:MTX:O1	4:B:609:MTX:CG	2.39	0.69
1:C:114:GLY:HA2	1:C:119:TYR:CZ	2.28	0.69
1:E:430:GLY:HA2	3:E:620:CB3:HP3	1.75	0.69
1:D:225:ASN:O	1:D:233:ARG:NH2	2.24	0.69
1:E:296:ILE:HD12	1:E:297:TRP:N	2.07	0.69
1:D:97:SER:O	1:D:99:GLU:HG3	1.93	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:360:TYR:O	1:B:363:VAL:HG13	1.92	0.68
1:B:103:ASN:CG	1:B:104:ASP:N	2.46	0.68
1:A:389:TRP:HB2	1:A:404:VAL:HG13	1.73	0.68
1:D:255:GLU:CD	1:D:255:GLU:H	1.96	0.68
1:E:507:ILE:HD12	1:E:507:ILE:N	2.08	0.68
1:A:7:SER:HB3	1:A:130:ARG:HB3	1.75	0.68
1:C:226:THR:HG22	1:C:226:THR:O	1.93	0.68
1:A:289:ARG:NH2	1:A:311:LYS:O	2.27	0.68
1:A:130:ARG:NH1	1:A:176:GLU:OE2	2.27	0.68
1:D:130:ARG:HG3	1:D:176:GLU:OE1	1.94	0.68
1:C:335:GLU:O	1:C:336:ASN:CB	2.42	0.67
1:B:209:ILE:H	1:B:209:ILE:CD1	2.07	0.67
1:C:104:ASP:CG	1:C:106:SER:H	1.98	0.67
1:E:256:ASN:HD21	1:E:262:THR:HG23	1.60	0.67
1:D:257:ARG:NH1	2:D:615:UMP:O5'	2.28	0.67
1:D:490:LYS:HD2	1:D:502:GLU:O	1.94	0.67
1:E:439:ALA:O	1:E:443:MET:HG3	1.94	0.67
1:E:135:ARG:HD3	1:E:171:ASP:HB2	1.75	0.67
5:E:622:NDP:O2X	5:E:622:NDP:H1B	1.95	0.67
1:A:48:LYS:HB3	1:A:106:SER:O	1.95	0.67
1:D:94:LEU:O	1:D:98:ILE:HG12	1.94	0.67
1:E:363:VAL:HG13	1:E:364:GLY:N	2.09	0.67
1:A:399:LEU:HD12	1:A:400:PRO:HD2	1.76	0.67
1:E:56:ARG:O	1:E:59:TRP:HB3	1.95	0.66
1:E:160:SER:HA	1:E:234:GLU:HB3	1.77	0.66
1:E:135:ARG:CD	1:E:171:ASP:HB2	2.24	0.66
1:C:156:PRO:O	1:C:228:SER:HB2	1.95	0.66
1:C:319:ASN:HD21	3:C:612:CB3:H8	1.58	0.66
1:C:160:SER:HA	1:C:234:GLU:HB3	1.77	0.66
1:C:100:ASN:CA	1:C:103:ASN:CG	2.44	0.66
3:B:608:CB3:H15	3:B:608:CB3:C6	2.24	0.66
1:E:391:PRO:HA	1:E:394:LEU:HD21	1.76	0.66
1:E:394:LEU:HD12	1:E:395:SER:H	1.61	0.66
1:D:467:GLU:HA	1:D:470:LEU:CD2	2.26	0.66
1:B:470:LEU:O	1:B:474:LYS:HG2	1.96	0.66
3:C:612:CB3:O	3:C:612:CB3:CB	2.42	0.66
1:A:56:ARG:NH1	5:A:606:NDP:O2X	2.29	0.66
1:C:285:LYS:HB3	1:C:514:THR:CG2	2.26	0.66
1:E:20:GLY:HA2	1:E:26:PRO:HD3	1.77	0.66
1:B:209:ILE:N	1:B:209:ILE:HD12	2.10	0.66
1:C:389:TRP:HE3	1:C:401:PRO:HG2	1.60	0.66
1:C:10:VAL:HG22	1:C:11:ALA:N	2.11	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:51:ALA:C	1:C:52:LEU:HD23	2.16	0.66
1:D:98:ILE:O	1:D:99:GLU:HB3	1.97	0.65
1:E:260:ILE:HD13	1:E:466:TYR:HD1	1.62	0.65
1:E:194:LYS:HD3	1:E:195:SER:H	1.60	0.65
1:C:37:SER:O	1:C:41:ASN:HB2	1.97	0.65
1:D:360:TYR:O	1:D:363:VAL:HG12	1.97	0.65
1:B:20:GLY:HA2	1:B:26:PRO:HD3	1.79	0.65
1:B:247:VAL:HG22	1:B:465:ILE:HD12	1.79	0.65
1:C:99:GLU:CG	1:C:103:ASN:HD21	2.09	0.65
2:C:611:UMP:OP1	1:D:383:ARG:NH1	2.26	0.65
1:D:155:LEU:HB2	1:D:178:GLN:NE2	2.12	0.65
1:E:374:THR:HG22	1:E:384:HIS:HE1	1.60	0.64
1:C:54:MET:HE3	1:C:72:ILE:HD13	1.78	0.64
1:D:4:LYS:HB3	1:D:101:LEU:HD23	1.79	0.64
1:E:55:GLY:HA3	5:E:622:NDP:O1A	1.97	0.64
1:A:162:THR:HA	1:A:171:ASP:OD1	1.96	0.64
1:E:479:ARG:HG2	1:E:512:TYR:CD2	2.32	0.64
1:E:444:MET:HG2	1:E:489:PHE:CZ	2.32	0.64
1:A:190:ARG:NH1	1:A:190:ARG:HB3	2.13	0.64
3:E:620:CB3:C15	3:E:620:CB3:C5	2.76	0.64
1:A:58:THR:CG2	4:A:605:MTX:HM2	2.28	0.64
3:E:620:CB3:C14	3:E:620:CB3:H5	2.27	0.64
1:E:79:LEU:CD2	1:E:80:PRO:HD2	2.27	0.64
1:D:20:GLY:HA2	1:D:26:PRO:HD3	1.80	0.64
1:A:348:HIS:HB3	1:A:363:VAL:O	1.98	0.64
1:A:4:LYS:HE3	1:A:101:LEU:HA	1.80	0.64
1:B:180:LYS:HD3	1:B:181:LYS:CB	2.27	0.64
1:D:123:LEU:HD12	1:D:128:VAL:HG11	1.78	0.64
1:C:38:LYS:HB3	1:D:202:LEU:HG	1.80	0.64
1:E:330:LEU:O	1:E:332:HIS:N	2.30	0.64
1:C:105:ASP:N	1:C:105:ASP:OD1	2.30	0.64
1:E:334:GLU:HG3	1:E:335:GLU:N	2.13	0.64
3:B:608:CB3:C15	3:B:608:CB3:C6	2.74	0.64
1:C:206:ILE:HD11	1:D:35:PHE:HA	1.80	0.63
1:D:342:TYR:CZ	1:D:403:HIS:NE2	2.66	0.63
1:E:167:ASN:HD21	1:E:488:LYS:HG3	1.63	0.63
1:D:248:LEU:HD13	1:D:465:ILE:HD12	1.79	0.63
1:E:149:GLU:HG3	6:E:631:HOH:O	1.98	0.63
1:A:99:GLU:O	1:A:103:ASN:ND2	2.31	0.63
1:C:104:ASP:OD2	1:C:106:SER:HB3	1.98	0.63
1:C:285:LYS:HB3	1:C:514:THR:HG22	1.81	0.63
1:C:389:TRP:CE3	1:C:401:PRO:HG2	2.33	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:260:ILE:HD12	1:E:260:ILE:H	1.63	0.63
1:D:65:ARG:HD3	6:D:643:HOH:O	1.99	0.63
1:E:426:ASP:HB2	2:E:619:UMP:C2'	2.26	0.63
1:D:123:LEU:HD12	1:D:128:VAL:CG1	2.29	0.63
1:C:82:ASP:OD2	1:C:84:ALA:HB2	1.98	0.63
1:B:479:ARG:HG2	1:B:512:TYR:CD2	2.33	0.63
1:E:225:ASN:ND2	1:E:241:LEU:HD13	2.12	0.63
1:A:133:LEU:C	1:A:133:LEU:HD22	2.19	0.63
1:E:295:LEU:O	1:E:299:ILE:HG12	1.99	0.63
1:D:467:GLU:HA	1:D:470:LEU:HD23	1.79	0.63
1:A:288:ILE:HD11	1:A:440:ILE:HD11	1.80	0.63
1:E:14:VAL:HG23	1:E:15:LEU:HG	1.79	0.63
1:E:519:MET:HG2	1:E:520:ALA:N	2.13	0.63
1:C:99:GLU:O	1:C:103:ASN:N	2.25	0.62
1:C:19:ILE:HB	5:C:614:NDP:N7N	2.14	0.62
1:E:131:ILE:HB	1:E:175:PHE:HB2	1.79	0.62
1:D:293:GLU:HA	1:D:296:ILE:HD11	1.81	0.62
1:C:104:ASP:HB3	1:C:107:ILE:HG13	1.81	0.62
1:E:431:SER:HB3	1:E:432:PRO:HD3	1.81	0.62
1:A:212:MET:SD	1:B:273:ASP:HB2	2.39	0.62
1:C:4:LYS:NZ	1:C:100:ASN:O	2.33	0.62
1:E:344:PHE:O	1:E:348:HIS:O	2.17	0.62
1:E:217:LYS:HZ1	1:E:220:LYS:HE3	1.65	0.62
1:B:64:ARG:NH2	1:B:79:LEU:HD21	2.14	0.62
1:D:56:ARG:CB	1:D:76:SER:OG	2.45	0.61
1:E:305:GLY:HA3	1:E:336:ASN:O	1.99	0.61
1:E:338:LEU:CD2	1:E:338:LEU:N	2.62	0.61
1:B:257:ARG:HD3	2:B:607:UMP:OP2	2.00	0.61
1:C:74:VAL:O	1:C:75:ILE:HD12	2.00	0.61
1:B:25:LEU:HD11	4:B:609:MTX:H7	1.83	0.61
1:B:58:THR:CG2	4:B:609:MTX:HM2	2.30	0.61
1:C:35:PHE:HA	1:D:206:ILE:HD11	1.82	0.61
1:B:180:LYS:CD	1:B:181:LYS:N	2.62	0.61
1:B:335:GLU:O	1:B:336:ASN:HB2	1.99	0.61
1:B:413:ASP:O	1:B:414:ASN:CB	2.48	0.61
1:C:333:ARG:HG2	1:C:333:ARG:NH1	2.15	0.61
1:C:342:TYR:CZ	1:C:403:HIS:NE2	2.68	0.61
1:D:260:ILE:N	1:D:260:ILE:HD12	2.15	0.61
1:A:341:ILE:CA	1:A:397:MET:CE	2.69	0.61
1:A:4:LYS:N	1:A:101:LEU:HD22	2.11	0.61
4:B:609:MTX:O1	4:B:609:MTX:HG2	2.00	0.61
1:B:178:GLN:HB2	6:B:742:HOH:O	2.00	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:433:PHE:CZ	3:E:620:CB3:H12	2.36	0.61
1:C:334:GLU:O	1:C:336:ASN:N	2.34	0.61
1:B:224:TYR:O	1:B:227:PRO:HD3	2.01	0.61
1:B:342:TYR:CZ	1:B:403:HIS:NE2	2.69	0.61
1:E:333:ARG:HH22	1:E:396:GLN:HB3	1.66	0.60
1:B:378:ASN:ND2	1:B:381:ASP:HB2	2.16	0.60
1:C:19:ILE:HB	5:C:614:NDP:H71N	1.65	0.60
1:E:14:VAL:HG13	1:E:136:VAL:O	2.00	0.60
1:C:13:SER:HB2	1:C:139:GLU:OE1	2.01	0.60
1:C:269:MET:HE2	1:D:269:MET:CE	2.31	0.60
3:C:612:CB3:HG2	3:C:612:CB3:O1	2.00	0.60
1:C:133:LEU:HD22	1:C:134:THR:N	2.17	0.60
1:B:160:SER:HA	1:B:234:GLU:HB3	1.84	0.60
1:A:52:LEU:HB3	1:A:113:CYS:SG	2.41	0.60
1:D:114:GLY:HA3	1:D:118:ILE:HB	1.84	0.60
1:A:495:ASN:OD1	1:A:497:GLU:HG3	2.01	0.60
1:E:260:ILE:HD13	1:E:466:TYR:CD1	2.37	0.60
2:E:619:UMP:C2'	2:E:619:UMP:O2	2.50	0.60
1:E:191:GLY:HA2	1:E:197:ASP:CG	2.22	0.60
1:D:133:LEU:HD13	1:D:135:ARG:HG3	1.84	0.60
1:D:247:VAL:HG21	1:D:465:ILE:HG13	1.83	0.60
1:C:100:ASN:OD1	1:C:100:ASN:N	2.30	0.60
1:D:296:ILE:HD12	1:D:297:TRP:N	2.17	0.60
1:E:157:VAL:HG11	1:E:176:GLU:HG3	1.82	0.60
2:A:603:UMP:P	1:B:383:ARG:HH11	2.25	0.59
1:A:101:LEU:O	1:A:103:ASN:N	2.35	0.59
2:A:603:UMP:P	1:B:383:ARG:NH1	2.74	0.59
1:B:104:ASP:OD2	1:B:106:SER:OG	2.20	0.59
1:C:137:ALA:O	1:C:510:TYR:CE2	2.44	0.59
1:D:58:THR:HG23	4:D:617:MTX:HM2	1.83	0.59
1:C:4:LYS:H	1:C:101:LEU:CD2	2.14	0.59
1:A:225:ASN:O	1:A:233:ARG:NH2	2.36	0.59
1:B:99:GLU:O	1:B:103:ASN:ND2	2.35	0.59
1:E:138:LEU:HD11	1:E:168:ILE:HD13	1.85	0.59
1:D:262:THR:HG23	1:D:464:HIS:HB2	1.84	0.59
1:A:4:LYS:CG	1:A:101:LEU:HD23	2.10	0.59
3:B:608:CB3:C5	3:B:608:CB3:C14	2.76	0.59
1:E:52:LEU:HB3	1:E:113:CYS:SG	2.42	0.59
1:D:292:PHE:CD1	1:D:504:ILE:HD11	2.37	0.59
1:E:305:GLY:H	1:E:356:MET:HE3	1.67	0.59
1:A:304:ASN:CA	1:A:356:MET:HE3	2.29	0.59
1:E:386:LEU:HB3	1:E:406:SER:HB2	1.83	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:291:ILE:HG12	1:C:433:PHE:CD2	2.37	0.59
1:C:138:LEU:HD13	1:C:168:ILE:HD13	1.85	0.59
1:E:126:ASN:HD22	1:E:177:LYS:NZ	2.00	0.59
1:C:75:ILE:O	5:C:614:NDP:H1B	2.02	0.59
1:E:217:LYS:NZ	1:E:220:LYS:HE3	2.16	0.59
1:C:439:ALA:O	1:C:443:MET:HG3	2.02	0.59
1:E:264:SER:CB	1:E:464:HIS:HB3	2.32	0.59
1:C:208:GLY:C	1:C:210:ARG:H	2.06	0.59
1:A:341:ILE:O	1:A:397:MET:HE3	2.03	0.58
1:D:7:SER:HB3	1:D:130:ARG:HB3	1.83	0.58
1:E:225:ASN:O	1:E:233:ARG:NH2	2.29	0.58
1:D:342:TYR:CD1	1:D:403:HIS:CE1	2.90	0.58
1:E:394:LEU:HD12	1:E:395:SER:N	2.17	0.58
1:D:439:ALA:O	1:D:443:MET:HG3	2.04	0.58
1:E:303:THR:HG21	1:E:344:PHE:HB2	1.85	0.58
1:B:7:SER:HB3	1:B:130:ARG:HB3	1.84	0.58
1:E:126:ASN:HD22	1:E:177:LYS:HZ2	1.50	0.58
1:C:403:HIS:HD2	2:C:611:UMP:O4	1.87	0.58
1:E:116:GLU:HB2	1:E:145:THR:HG23	1.85	0.58
1:E:430:GLY:CA	3:E:620:CB3:HP3	2.33	0.58
1:E:123:LEU:HD12	1:E:151:PRO:HG3	1.85	0.58
1:A:10:VAL:HG13	1:A:133:LEU:HD23	1.85	0.58
1:D:147:PHE:CD2	1:D:148:PRO:HD2	2.38	0.58
1:C:104:ASP:OD2	1:C:106:SER:CB	2.52	0.58
3:E:620:CB3:C6	3:E:620:CB3:H15	2.33	0.57
1:C:37:SER:HB2	4:C:613:MTX:HG2	1.86	0.57
1:C:15:LEU:HB2	1:C:139:GLU:HG2	1.86	0.57
1:A:193:LEU:HD23	6:A:607:HOH:O	2.02	0.57
1:E:151:PRO:HG2	1:E:154:PHE:CD2	2.33	0.57
1:C:360:TYR:HB3	1:C:363:VAL:CG1	2.34	0.57
1:E:4:LYS:HG2	1:E:101:LEU:CD2	2.34	0.57
1:C:136:VAL:HG12	1:C:138:LEU:HD22	1.87	0.57
1:A:75:ILE:O	5:A:606:NDP:H1B	2.04	0.57
1:C:342:TYR:CE1	1:C:403:HIS:CE1	2.92	0.57
1:A:233:ARG:HH12	1:A:242:ASP:CG	2.07	0.57
2:E:619:UMP:C1'	3:E:620:CB3:C2	2.79	0.57
1:E:56:ARG:NH2	1:E:57:LYS:HG2	2.19	0.57
4:A:605:MTX:O1	4:A:605:MTX:HG2	2.04	0.57
1:D:257:ARG:NH1	2:D:615:UMP:P	2.77	0.57
1:C:495:ASN:HB2	1:C:498:ASP:OD1	2.05	0.57
1:E:341:ILE:HA	1:E:397:MET:CE	2.35	0.57
1:D:247:VAL:HG12	1:D:265:ILE:HG12	1.87	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:C:649:HOH:O	1:D:262:THR:HG21	2.04	0.57
1:C:74:VAL:C	1:C:75:ILE:HD12	2.26	0.56
1:B:21:ILE:HD13	1:B:142:GLU:HB3	1.86	0.56
1:A:178:GLN:HE21	1:A:178:GLN:N	2.02	0.56
1:B:211:LYS:HE3	6:B:699:HOH:O	2.05	0.56
1:D:194:LYS:HE3	1:D:198:ASP:OD1	2.03	0.56
1:E:440:ILE:HG12	1:E:487:LEU:CD2	2.35	0.56
1:A:342:TYR:CE2	1:A:403:HIS:CE1	2.94	0.56
1:E:58:THR:HG23	4:E:621:MTX:HM2	1.86	0.56
1:D:226:THR:HG22	1:D:226:THR:O	2.05	0.56
1:E:360:TYR:O	1:E:363:VAL:HG12	2.05	0.56
1:E:179:GLU:OE1	1:E:179:GLU:N	2.37	0.56
1:D:244:LEU:CD1	1:D:427:LEU:HB3	2.34	0.56
1:D:495:ASN:HB2	6:D:670:HOH:O	2.06	0.56
1:B:411:THR:HG22	1:B:413:ASP:HB2	1.86	0.56
1:E:297:TRP:CD2	1:E:308:LEU:HD21	2.41	0.56
1:D:103:ASN:O	1:D:104:ASP:C	2.44	0.56
1:B:37:SER:O	1:B:41:ASN:HB2	2.05	0.56
1:B:99:GLU:CA	1:B:99:GLU:OE1	2.53	0.56
1:C:114:GLY:HA2	1:C:119:TYR:CE1	2.40	0.56
1:A:331:GLY:N	6:A:609:HOH:O	2.38	0.56
1:E:444:MET:HG2	1:E:489:PHE:HZ	1.70	0.56
1:E:19:ILE:HB	5:E:622:NDP:N7N	2.21	0.56
1:D:82:ASP:OD2	1:D:82:ASP:C	2.43	0.56
1:E:283:THR:HA	1:E:512:TYR:HD1	1.70	0.56
1:C:350:ASN:HA	6:C:642:HOH:O	2.06	0.56
1:B:423:ARG:HG3	1:B:424:SER:N	2.19	0.56
1:C:90:VAL:HG12	1:C:91:PHE:N	2.21	0.56
1:B:289:ARG:NH2	1:B:311:LYS:O	2.39	0.56
1:C:104:ASP:OD1	1:C:106:SER:OG	2.20	0.56
4:E:621:MTX:N5	5:E:622:NDP:H42N	2.21	0.56
4:D:617:MTX:N5	5:D:618:NDP:H42N	2.21	0.56
1:E:138:LEU:CD1	1:E:168:ILE:HD13	2.36	0.56
1:C:26:PRO:HB2	1:C:27:TRP:HE3	1.70	0.55
1:E:391:PRO:HA	1:E:394:LEU:CD2	2.36	0.55
1:C:135:ARG:HH21	1:C:482:ARG:HA	1.70	0.55
1:D:396:GLN:HG3	6:D:644:HOH:O	2.05	0.55
1:A:186:CYS:HA	1:A:230:ARG:CD	2.26	0.55
1:D:4:LYS:HB2	1:D:101:LEU:HD23	1.87	0.55
1:E:244:LEU:CD1	1:E:427:LEU:HB3	2.35	0.55
1:E:135:ARG:HD2	1:E:173:MET:HG3	1.89	0.55
1:D:99:GLU:OE2	1:D:99:GLU:C	2.45	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:342:TYR:CE1	1:D:403:HIS:NE2	2.75	0.55
1:B:58:THR:HG23	4:B:609:MTX:HM2	1.87	0.55
1:B:402:CYS:SG	2:B:607:UMP:C6	3.00	0.55
1:B:4:LYS:CB	1:B:101:LEU:CD2	2.76	0.55
1:C:360:TYR:HD1	1:C:363:VAL:HG11	1.71	0.55
4:B:609:MTX:N5	5:B:610:NDP:H42N	2.21	0.55
1:C:32:ASP:O	1:C:35:PHE:HB3	2.06	0.55
1:E:120:ARG:HG2	1:E:120:ARG:HH11	1.72	0.55
1:E:337:ASP:CB	1:E:356:MET:SD	2.85	0.55
1:C:133:LEU:HD11	1:C:135:ARG:HG3	1.89	0.55
1:D:104:ASP:C	1:D:106:SER:H	2.08	0.55
1:C:12:ALA:HB1	1:C:17:SER:HA	1.89	0.55
1:B:188:PRO:O	1:B:192:GLN:NE2	2.40	0.55
1:B:502:GLU:CD	1:B:502:GLU:H	2.10	0.55
1:C:409:TYR:HH	1:D:264:SER:HG	1.53	0.55
1:B:411:THR:HG22	1:B:412:ASN:N	2.20	0.55
1:C:138:LEU:N	1:C:138:LEU:HD23	2.18	0.55
4:C:613:MTX:O1	4:C:613:MTX:HG1	2.07	0.55
1:E:304:ASN:ND2	1:E:356:MET:HE2	2.22	0.55
1:E:179:GLU:CD	1:E:179:GLU:N	2.60	0.55
1:B:76:SER:OG	5:B:610:NDP:O3X	2.22	0.55
1:C:99:GLU:CG	1:C:103:ASN:ND2	2.70	0.55
1:A:341:ILE:HG13	1:A:342:TYR:O	2.07	0.55
1:E:304:ASN:OD1	1:E:306:ASN:HB2	2.07	0.55
3:B:608:CB3:C15	3:B:608:CB3:C5	2.85	0.55
1:A:99:GLU:C	1:A:99:GLU:OE1	2.45	0.54
1:C:81:GLN:HB2	1:C:92:ARG:HH21	1.72	0.54
1:D:171:ASP:HB2	1:D:483:PRO:HG3	1.88	0.54
1:E:43:LYS:NZ	1:E:46:SER:HA	2.22	0.54
1:E:347:ARG:HD3	1:E:368:LEU:HD23	1.89	0.54
1:B:334:GLU:OE2	1:B:357:HIS:NE2	2.32	0.54
1:E:119:TYR:HB3	1:E:148:PRO:HG3	1.88	0.54
1:C:97:SER:O	1:C:100:ASN:OD1	2.25	0.54
1:C:52:LEU:HB3	1:C:113:CYS:SG	2.48	0.54
1:A:391:PRO:HD2	1:B:349:TYR:CE2	2.42	0.54
1:A:104:ASP:O	1:A:107:ILE:N	2.21	0.54
1:B:413:ASP:O	1:B:414:ASN:HB2	2.07	0.54
1:E:296:ILE:HA	1:E:299:ILE:CG1	2.38	0.54
1:A:470:LEU:O	1:A:474:LYS:HG3	2.07	0.54
1:A:185:ASN:O	1:A:230:ARG:NH1	2.39	0.54
1:A:139:GLU:HB2	1:A:510:TYR:CE1	2.42	0.54
1:D:104:ASP:OD2	1:D:106:SER:OG	2.25	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:83:GLU:HA	1:B:83:GLU:OE2	2.06	0.54
1:E:389:TRP:CZ3	1:E:401:PRO:HD2	2.41	0.54
1:A:335:GLU:O	1:A:336:ASN:HB2	2.08	0.54
1:A:403:HIS:CD2	1:A:403:HIS:H	2.26	0.54
1:B:36:PHE:O	1:B:39:ILE:HG22	2.07	0.54
1:C:360:TYR:HB3	1:C:363:VAL:HG12	1.88	0.54
1:D:330:LEU:O	1:D:332:HIS:N	2.41	0.54
1:C:57:LYS:HA	1:C:60:ASP:OD2	2.07	0.54
1:A:342:TYR:CZ	1:A:403:HIS:NE2	2.76	0.54
1:D:100:ASN:HB2	1:D:110:ILE:CD1	2.36	0.54
1:C:133:LEU:CD1	1:C:135:ARG:HG3	2.38	0.54
1:D:123:LEU:CD1	1:D:128:VAL:HG11	2.38	0.54
1:E:440:ILE:HG12	1:E:487:LEU:HD21	1.89	0.54
1:E:335:GLU:OE1	1:E:335:GLU:O	2.26	0.54
1:C:123:LEU:CD1	1:C:128:VAL:HG11	2.35	0.54
1:E:296:ILE:HA	1:E:299:ILE:HG12	1.90	0.54
1:A:186:CYS:HB2	6:A:613:HOH:O	2.08	0.53
1:E:287:ALA:O	1:E:291:ILE:HG13	2.08	0.53
1:C:186:CYS:HA	1:C:230:ARG:HE	1.72	0.53
1:A:331:GLY:C	1:A:333:ARG:H	2.09	0.53
1:C:97:SER:O	1:C:99:GLU:HG3	2.08	0.53
1:D:337:ASP:CG	1:D:356:MET:HG2	2.28	0.53
1:C:114:GLY:CA	1:C:119:TYR:CZ	2.91	0.53
1:E:471:THR:HA	1:E:474:LYS:HE3	1.90	0.53
1:E:407:GLN:HB3	1:E:419:ASN:HB2	1.90	0.53
1:E:347:ARG:O	1:E:366:ASP:HA	2.09	0.53
1:A:34:LYS:O	1:A:38:LYS:HG2	2.07	0.53
1:C:490:LYS:HD3	1:C:502:GLU:O	2.09	0.53
1:E:21:ILE:HD12	1:E:144:ASP:OD2	2.08	0.53
1:E:171:ASP:OD2	1:E:483:PRO:HB3	2.09	0.53
1:E:512:TYR:HA	6:E:639:HOH:O	2.09	0.53
1:C:388:ALA:O	1:C:401:PRO:HG3	2.09	0.53
1:E:472:GLN:O	1:E:475:GLU:HB3	2.09	0.53
1:E:354:LYS:O	1:E:355:THR:HG23	2.09	0.53
1:D:470:LEU:O	1:D:474:LYS:HD3	2.09	0.53
1:C:400:PRO:HD2	1:D:383:ARG:NH1	2.24	0.53
1:C:98:ILE:O	1:C:99:GLU:HB3	2.09	0.52
1:E:3:GLU:O	1:E:4:LYS:HB3	2.09	0.52
1:E:196:ILE:CG2	1:E:197:ASP:H	2.20	0.52
1:A:14:VAL:HG23	1:A:137:ALA:HA	1.89	0.52
1:D:171:ASP:OD2	1:D:483:PRO:HG3	2.09	0.52
1:C:350:ASN:N	6:C:642:HOH:O	2.38	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:496:ILE:O	1:E:499:PHE:HD1	1.92	0.52
1:E:82:ASP:C	1:E:84:ALA:H	2.12	0.52
1:A:131:ILE:HB	1:A:175:PHE:HB2	1.91	0.52
1:E:304:ASN:CG	1:E:356:MET:CE	2.75	0.52
3:C:612:CB3:O1	3:C:612:CB3:CG	2.46	0.52
1:C:56:ARG:HB3	5:C:614:NDP:O3B	2.09	0.52
1:E:507:ILE:HD12	1:E:507:ILE:H	1.72	0.52
1:C:342:TYR:CD1	1:C:403:HIS:CE1	2.96	0.52
1:E:330:LEU:C	1:E:332:HIS:H	2.13	0.52
1:C:472:GLN:HB3	1:C:515:ILE:HG21	1.91	0.52
1:D:37:SER:O	1:D:41:ASN:HB2	2.09	0.52
1:C:102:MET:C	1:C:103:ASN:O	2.48	0.52
1:C:59:TRP:O	1:C:62:ILE:HG22	2.09	0.52
1:C:209:ILE:N	1:C:209:ILE:HD13	2.24	0.52
1:E:167:ASN:ND2	1:E:488:LYS:HG3	2.25	0.52
1:E:77:SER:O	1:E:92:ARG:NH1	2.43	0.52
1:E:320:GLY:O	1:E:335:GLU:O	2.27	0.52
1:D:467:GLU:O	1:D:470:LEU:HD23	2.10	0.52
1:E:10:VAL:HG22	1:E:11:ALA:N	2.24	0.52
1:A:388:ALA:O	1:A:401:PRO:HG2	2.10	0.52
1:C:99:GLU:OE2	1:C:103:ASN:ND2	2.34	0.52
1:A:3:GLU:HA	1:A:101:LEU:HD22	1.91	0.52
1:D:102:MET:CE	1:D:102:MET:CA	2.76	0.52
1:D:262:THR:CG2	1:D:464:HIS:HB2	2.38	0.52
1:D:201:ASP:O	1:D:205:GLU:HG3	2.09	0.52
1:D:321:SER:O	1:D:325:LEU:HD13	2.09	0.52
1:A:45:ASP:OD2	1:A:48:LYS:HE3	2.10	0.52
1:A:99:GLU:CA	6:A:674:HOH:O	2.56	0.52
1:B:411:THR:HG23	6:B:632:HOH:O	2.10	0.52
1:E:304:ASN:CA	1:E:356:MET:CE	2.87	0.52
1:B:115:GLY:HA2	5:B:610:NDP:O5D	2.10	0.52
1:A:512:TYR:HB3	1:A:513:PRO:HD2	1.92	0.52
1:C:192:GLN:HG3	1:D:231:PHE:CD2	2.44	0.52
2:E:619:UMP:H1'	3:E:620:CB3:C4	2.39	0.52
1:E:19:ILE:HB	5:E:622:NDP:H71N	1.75	0.52
1:D:137:ALA:O	1:D:510:TYR:CE2	2.57	0.52
1:E:303:THR:CG2	1:E:344:PHE:HB2	2.40	0.52
1:D:155:LEU:HB2	1:D:178:GLN:HE21	1.74	0.52
1:B:291:ILE:HG12	1:B:433:PHE:CD2	2.45	0.52
1:B:204:GLY:O	1:B:207:PHE:O	2.28	0.52
1:A:37:SER:O	1:A:41:ASN:HB2	2.10	0.52
1:E:425:CYS:SG	1:E:431:SER:HB2	2.50	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:447:GLN:NE2	1:D:492:LYS:HA	2.25	0.52
1:C:381:ASP:HB3	1:C:384:HIS:CE1	2.45	0.52
1:C:6:VAL:HG11	1:C:127:PHE:O	2.10	0.52
1:C:231:PHE:CE2	1:D:192:GLN:HG3	2.45	0.51
1:B:16:SER:O	1:B:17:SER:HB2	2.10	0.51
1:E:342:TYR:O	1:E:345:GLN:N	2.43	0.51
4:A:605:MTX:N5	5:A:606:NDP:H42N	2.24	0.51
1:E:403:HIS:H	1:E:403:HIS:CD2	2.27	0.51
1:A:104:ASP:C	1:A:106:SER:N	2.64	0.51
1:A:342:TYR:CD1	1:A:342:TYR:N	2.78	0.51
1:E:178:GLN:CD	1:E:178:GLN:H	2.05	0.51
1:D:139:GLU:O	1:D:140:ASP:HB2	2.10	0.51
1:A:4:LYS:N	1:A:101:LEU:CD2	2.67	0.51
1:D:102:MET:CA	1:D:102:MET:HE3	2.28	0.51
1:E:178:GLN:HA	1:E:179:GLU:OE1	2.10	0.51
1:C:350:ASN:CA	6:C:642:HOH:O	2.57	0.51
1:D:288:ILE:HG23	1:D:501:TRP:HH2	1.76	0.51
1:B:342:TYR:CE1	1:B:403:HIS:NE2	2.79	0.51
1:C:243:LEU:O	1:C:247:VAL:HG13	2.11	0.51
1:A:385:ILE:CG2	1:A:386:LEU:N	2.73	0.51
1:D:82:ASP:CG	1:D:84:ALA:H	2.13	0.51
1:D:135:ARG:O	1:D:170:TYR:HA	2.11	0.51
1:C:98:ILE:O	1:C:99:GLU:CB	2.59	0.51
1:D:126:ASN:ND2	1:D:177:LYS:HZ1	2.09	0.51
1:E:178:GLN:N	1:E:178:GLN:OE1	2.32	0.51
1:C:194:LYS:HE3	1:C:198:ASP:OD1	2.10	0.51
1:C:104:ASP:CB	1:C:107:ILE:HG13	2.41	0.51
1:A:297:TRP:CD1	1:A:302:ASP:HB3	2.45	0.51
1:E:372:ILE:O	1:E:376:LYS:HG2	2.10	0.51
1:E:50:ASN:OD1	1:E:109:ASN:HB2	2.11	0.51
1:B:447:GLN:HG3	6:B:751:HOH:O	2.10	0.51
1:C:211:LYS:NZ	1:D:234:GLU:OE1	2.44	0.51
1:E:322:LYS:O	1:E:326:GLU:HB2	2.11	0.51
1:C:138:LEU:N	1:C:138:LEU:HD22	2.20	0.51
1:E:79:LEU:HD22	1:E:90:VAL:HG21	1.93	0.51
1:B:39:ILE:HG23	1:B:40:THR:N	2.26	0.51
1:E:21:ILE:HA	1:E:144:ASP:OD2	2.11	0.51
1:E:7:SER:O	1:E:111:PHE:HA	2.11	0.51
4:C:613:MTX:O1	4:C:613:MTX:CG	2.59	0.50
1:A:51:ALA:C	1:A:52:LEU:HD23	2.30	0.50
3:A:604:CB3:H13	3:A:604:CB3:CP2	2.25	0.50
1:A:93:ASN:ND2	1:A:96:ASP:H	2.10	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:243:LEU:HA	1:E:246:ARG:HH12	1.74	0.50
1:A:115:GLY:HA3	5:A:606:NDP:O1A	2.11	0.50
1:C:100:ASN:N	1:C:103:ASN:CG	2.62	0.50
1:B:411:THR:CG2	1:B:412:ASN:N	2.74	0.50
1:A:25:LEU:HD11	4:A:605:MTX:H7	1.93	0.50
1:B:342:TYR:CD1	1:B:403:HIS:CE1	2.99	0.50
1:C:231:PHE:CD2	1:D:192:GLN:HG3	2.45	0.50
1:C:48:LYS:HA	1:C:106:SER:O	2.10	0.50
1:D:62:ILE:HD11	4:D:617:MTX:C15	2.42	0.50
1:E:153:THR:OG1	1:E:177:LYS:HE3	2.11	0.50
1:E:237:GLU:O	1:E:241:LEU:HG	2.11	0.50
1:B:10:VAL:HG22	1:B:11:ALA:N	2.26	0.50
1:E:216:HIS:HA	1:E:250:ASN:ND2	2.26	0.50
1:B:128:VAL:HG22	1:B:154:PHE:HZ	1.76	0.50
3:E:620:CB3:C14	3:E:620:CB3:C5	2.87	0.50
4:E:621:MTX:H92	5:E:622:NDP:H42N	1.93	0.50
1:C:10:VAL:CG2	1:C:11:ALA:N	2.74	0.50
1:C:237:GLU:OE2	1:C:283:THR:HG23	2.12	0.50
1:C:404:VAL:HG11	1:D:405:LEU:HD11	1.93	0.50
1:D:405:LEU:C	1:D:405:LEU:HD23	2.31	0.50
1:B:431:SER:O	1:B:435:ILE:HG13	2.11	0.50
1:A:469:HIS:HB3	1:A:473:LEU:HD22	1.92	0.50
1:B:415:CYS:HA	1:B:452:GLU:O	2.12	0.50
1:B:407:GLN:HG2	1:B:408:TYR:N	2.26	0.50
1:C:56:ARG:NH1	5:C:614:NDP:O2X	2.43	0.50
4:C:613:MTX:N5	5:C:614:NDP:H42N	2.26	0.50
1:D:134:THR:HA	1:D:171:ASP:O	2.11	0.50
1:C:419:ASN:HD22	1:C:457:ALA:HB3	1.74	0.50
1:E:181:LYS:O	1:E:182:THR:CB	2.60	0.50
5:D:618:NDP:O1A	5:D:618:NDP:O2N	2.30	0.50
1:A:349:TYR:O	1:A:350:ASN:HB2	2.12	0.50
1:E:297:TRP:CG	1:E:308:LEU:HD21	2.47	0.50
1:E:355:THR:OG1	1:E:358:ASP:OD1	2.30	0.50
1:C:475:GLU:OE2	1:C:479:ARG:HD3	2.12	0.50
1:A:14:VAL:CG2	1:A:137:ALA:HA	2.42	0.50
1:E:299:ILE:HG23	1:E:368:LEU:HD21	1.93	0.50
1:A:291:ILE:HG12	1:A:433:PHE:CD2	2.46	0.50
1:B:59:TRP:NE1	1:B:64:ARG:HG2	2.27	0.50
1:A:233:ARG:NH1	1:A:242:ASP:OD2	2.45	0.50
1:C:10:VAL:HG22	1:C:11:ALA:H	1.76	0.49
1:C:48:LYS:HG2	1:C:106:SER:HA	1.94	0.49
1:A:339:GLY:O	1:A:341:ILE:HG23	2.11	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:172:PHE:CD2	1:D:203:LEU:HD21	2.47	0.49
1:B:372:ILE:HG22	1:B:376:LYS:HE2	1.94	0.49
1:B:98:ILE:O	1:B:98:ILE:HG23	2.11	0.49
3:D:616:CB3:C13	3:D:616:CB3:CP2	2.77	0.49
1:D:337:ASP:OD1	1:D:356:MET:HG2	2.12	0.49
1:E:126:ASN:ND2	1:E:177:LYS:NZ	2.60	0.49
1:A:358:ASP:OD1	1:A:358:ASP:N	2.45	0.49
1:A:333:ARG:CG	1:A:337:ASP:HB3	2.39	0.49
1:C:342:TYR:CE1	1:C:403:HIS:NE2	2.81	0.49
1:E:147:PHE:CD2	1:E:148:PRO:HD2	2.48	0.49
1:E:495:ASN:ND2	1:E:496:ILE:H	2.10	0.49
1:E:486:GLN:O	1:E:506:LEU:HD23	2.12	0.49
1:C:203:LEU:HD11	1:D:172:PHE:CE2	2.47	0.49
1:B:403:HIS:H	1:B:403:HIS:CD2	2.28	0.49
1:E:311:LYS:O	1:E:312:LYS:HB2	2.12	0.49
1:C:208:GLY:C	1:C:210:ARG:N	2.65	0.49
1:A:231:PHE:CD2	1:B:192:GLN:HG2	2.48	0.49
1:A:359:ASP:OD1	1:A:361:THR:HG22	2.12	0.49
1:C:212:MET:SD	1:D:273:ASP:HB2	2.52	0.49
1:D:242:ASP:O	1:D:246:ARG:HB2	2.13	0.49
1:A:58:THR:HG23	4:A:605:MTX:HM2	1.94	0.49
1:C:199:THR:O	1:C:203:LEU:HB2	2.12	0.49
1:D:149:GLU:HG2	6:D:632:HOH:O	2.13	0.49
1:E:305:GLY:N	1:E:356:MET:HE3	2.28	0.49
1:B:99:GLU:HA	1:B:99:GLU:OE1	2.13	0.49
1:A:269:MET:HE1	1:B:269:MET:HG2	1.95	0.49
1:E:264:SER:HB2	1:E:462:ASP:OD2	2.12	0.48
1:D:330:LEU:C	1:D:332:HIS:H	2.16	0.48
1:A:323:GLU:OE1	1:A:323:GLU:N	2.44	0.48
1:D:385:ILE:CG2	1:D:386:LEU:N	2.76	0.48
1:A:256:ASN:OD1	1:A:258:THR:HB	2.12	0.48
1:C:378:ASN:O	1:C:384:HIS:CE1	2.66	0.48
1:E:60:ASP:OD1	1:E:64:ARG:NH1	2.46	0.48
1:A:455:GLU:HG3	6:A:657:HOH:O	2.13	0.48
1:B:359:ASP:OD2	1:B:361:THR:HG23	2.13	0.48
1:D:138:LEU:HD21	1:D:168:ILE:HD13	1.95	0.48
1:D:62:ILE:O	1:D:62:ILE:CG2	2.62	0.48
1:E:241:LEU:HD11	1:E:481:PRO:HG3	1.95	0.48
1:C:103:ASN:O	1:C:104:ASP:C	2.52	0.48
1:D:266:PHE:HA	1:D:461:GLY:O	2.13	0.48
1:C:100:ASN:CB	1:C:103:ASN:CB	2.82	0.48
1:E:434:ASN:HD22	1:E:434:ASN:N	2.12	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:37:SER:CB	4:E:621:MTX:HG2	2.38	0.48
1:B:60:ASP:OD1	1:B:64:ARG:NH1	2.47	0.48
1:A:231:PHE:CE2	1:B:192:GLN:HG2	2.49	0.48
1:C:203:LEU:HD11	1:D:172:PHE:CD2	2.48	0.48
1:A:439:ALA:O	1:A:443:MET:HG3	2.14	0.48
1:E:12:ALA:HB1	1:E:17:SER:C	2.34	0.48
1:D:39:ILE:CG2	1:D:40:THR:N	2.76	0.48
1:A:99:GLU:HA	6:A:674:HOH:O	2.14	0.48
1:E:37:SER:O	1:E:41:ASN:ND2	2.46	0.48
1:C:55:GLY:CA	5:C:614:NDP:O2A	2.59	0.48
1:B:19:ILE:O	5:B:610:NDP:H2N	2.14	0.48
1:E:449:CYS:HB3	1:E:451:TYR:CE1	2.48	0.48
1:A:98:ILE:CG2	1:A:98:ILE:O	2.61	0.48
1:B:102:MET:O	1:B:103:ASN:CB	2.60	0.48
1:C:72:ILE:HG13	6:C:676:HOH:O	2.14	0.48
1:D:131:ILE:HB	1:D:175:PHE:HB2	1.95	0.48
1:D:388:ALA:O	1:D:401:PRO:HG2	2.14	0.48
1:A:402:CYS:O	1:A:404:VAL:HG23	2.14	0.48
1:B:342:TYR:CZ	1:B:403:HIS:CD2	3.02	0.48
1:B:130:ARG:HG3	1:B:130:ARG:HH11	1.79	0.48
1:E:373:GLU:O	1:E:377:ASN:HB2	2.14	0.48
1:A:52:LEU:N	1:A:52:LEU:HD23	2.29	0.48
1:E:493:VAL:HG21	1:E:499:PHE:CE1	2.49	0.48
1:D:405:LEU:HD23	1:D:406:SER:N	2.29	0.48
1:B:55:GLY:N	1:B:118:ILE:HG13	2.29	0.48
1:D:100:ASN:CB	1:D:110:ILE:HD11	2.39	0.47
1:A:137:ALA:O	1:A:510:TYR:HE2	1.97	0.47
4:A:605:MTX:CG	4:A:605:MTX:O1	2.61	0.47
1:A:190:ARG:HA	1:A:197:ASP:OD1	2.14	0.47
1:E:15:LEU:HD12	1:E:139:GLU:HG2	1.94	0.47
1:A:407:GLN:HB3	1:B:421:TYR:OH	2.13	0.47
1:E:407:GLN:HG3	1:E:408:TYR:N	2.29	0.47
1:E:60:ASP:O	1:E:63:GLY:N	2.43	0.47
1:C:289:ARG:HG3	1:C:501:TRP:CE2	2.49	0.47
1:E:36:PHE:C	1:E:36:PHE:CD1	2.87	0.47
2:D:615:UMP:C5	6:D:667:HOH:O	2.56	0.47
1:B:384:HIS:O	1:B:407:GLN:HA	2.14	0.47
1:B:323:GLU:H	1:B:323:GLU:CD	2.17	0.47
1:C:23:GLY:HA2	5:C:614:NDP:O3D	2.15	0.47
1:D:135:ARG:HD2	1:D:173:MET:SD	2.54	0.47
1:E:217:LYS:HB3	1:E:217:LYS:NZ	2.30	0.47
1:E:21:ILE:HG13	1:E:22:ASN:ND2	2.29	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:354:LYS:HE2	1:C:358:ASP:OD2	2.14	0.47
1:E:93:ASN:ND2	1:E:95:GLU:HB3	2.29	0.47
1:D:291:ILE:HD13	1:D:436:ALA:HB3	1.97	0.47
1:D:436:ALA:O	1:D:440:ILE:HG13	2.14	0.47
1:E:98:ILE:O	1:E:98:ILE:HG22	2.14	0.47
1:C:151:PRO:HG2	1:C:154:PHE:CD2	2.39	0.47
1:C:209:ILE:CD1	1:C:209:ILE:H	2.24	0.47
1:B:359:ASP:OD1	1:B:361:THR:HG22	2.14	0.47
1:B:135:ARG:HB2	1:B:171:ASP:HB2	1.97	0.47
1:E:223:ILE:HD12	1:E:248:LEU:HB3	1.97	0.47
1:E:244:LEU:HD21	1:E:473:LEU:HD22	1.96	0.47
1:E:341:ILE:HA	1:E:397:MET:HE2	1.96	0.47
1:B:308:LEU:HD12	1:B:308:LEU:HA	1.76	0.47
1:B:103:ASN:N	1:B:103:ASN:HD22	2.13	0.47
1:A:333:ARG:HD3	1:A:337:ASP:O	2.14	0.47
1:D:348:HIS:HB3	1:D:363:VAL:O	2.15	0.47
1:A:248:LEU:HD13	1:A:465:ILE:HD12	1.97	0.47
1:D:135:ARG:HD3	1:D:171:ASP:HB3	1.97	0.47
1:E:278:PHE:CZ	1:E:487:LEU:HD22	2.50	0.47
1:C:244:LEU:HD21	1:C:473:LEU:HD22	1.97	0.47
1:D:223:ILE:O	1:D:245:SER:HB2	2.14	0.47
1:C:323:GLU:OE2	1:C:323:GLU:N	2.37	0.47
1:B:3:GLU:O	1:B:4:LYS:CB	2.62	0.47
1:E:210:ARG:HG3	1:E:210:ARG:HH11	1.79	0.47
1:E:390:ASN:O	1:E:394:LEU:HG	2.15	0.47
1:B:130:ARG:HD2	1:B:132:TYR:CE1	2.50	0.47
1:E:43:LYS:HB3	1:E:50:ASN:HD21	1.80	0.47
1:B:171:ASP:OD2	1:B:483:PRO:HG3	2.15	0.47
1:D:309:ILE:HG23	1:D:314:TYR:CE1	2.50	0.47
1:C:99:GLU:CB	1:C:103:ASN:ND2	2.78	0.47
1:D:423:ARG:HG3	1:D:424:SER:N	2.29	0.47
1:C:472:GLN:HB3	1:C:515:ILE:CG2	2.45	0.47
1:E:490:LYS:HD3	1:E:502:GLU:O	2.15	0.47
1:A:479:ARG:HG2	1:A:512:TYR:CD2	2.51	0.46
1:A:267:GLY:O	1:B:271:ARG:NH2	2.48	0.46
1:D:180:LYS:CB	6:D:629:HOH:O	2.62	0.46
1:D:327:ARG:HH11	1:D:327:ARG:HB2	1.79	0.46
1:D:248:LEU:HD12	1:D:248:LEU:HA	1.76	0.46
1:D:335:GLU:O	1:D:336:ASN:HB2	2.14	0.46
1:E:208:GLY:C	1:E:210:ARG:H	2.18	0.46
1:E:158:TYR:O	1:E:173:MET:HA	2.14	0.46
1:B:257:ARG:NH2	1:B:521:VAL:OXT	2.48	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:120:ARG:HG2	1:E:120:ARG:NH1	2.31	0.46
1:B:114:GLY:HA2	1:B:119:TYR:CZ	2.50	0.46
1:D:475:GLU:OE2	1:D:479:ARG:HD3	2.15	0.46
1:C:36:PHE:CE1	1:C:40:THR:HG21	2.51	0.46
1:D:126:ASN:ND2	1:D:177:LYS:NZ	2.64	0.46
1:D:255:GLU:N	1:D:255:GLU:OE1	2.37	0.46
1:A:202:LEU:HG	1:B:38:LYS:HB3	1.96	0.46
1:E:291:ILE:HG12	1:E:433:PHE:CD2	2.51	0.46
1:C:138:LEU:O	1:C:138:LEU:HD23	2.16	0.46
3:B:608:CB3:H5	3:B:608:CB3:C14	2.46	0.46
1:D:244:LEU:HD21	1:D:473:LEU:HD22	1.98	0.46
1:C:267:GLY:O	1:D:271:ARG:NH2	2.49	0.46
1:A:509:TYR:CE1	1:A:511:PRO:HG3	2.51	0.46
1:A:67:LEU:HD12	1:A:72:ILE:HD11	1.98	0.46
1:D:256:ASN:O	1:D:257:ARG:C	2.53	0.46
1:E:337:ASP:CB	1:E:356:MET:HG2	2.45	0.46
1:A:212:MET:HB3	1:B:236:TYR:OH	2.15	0.46
1:C:96:ASP:O	1:C:99:GLU:CG	2.40	0.46
1:E:304:ASN:HB3	1:E:307:HIS:NE2	2.31	0.46
1:A:163:PHE:HB2	1:A:170:TYR:CZ	2.50	0.46
1:B:12:ALA:HB1	1:B:17:SER:HA	1.98	0.46
1:A:402:CYS:SG	2:A:603:UMP:C6	3.09	0.46
1:E:29:ILE:HG23	1:E:165:THR:HG21	1.97	0.46
1:B:103:ASN:O	1:B:105:ASP:N	2.49	0.46
1:D:12:ALA:HB2	1:D:19:ILE:HG22	1.98	0.46
1:E:378:ASN:O	1:E:384:HIS:CE1	2.69	0.46
1:E:51:ALA:C	1:E:52:LEU:HD23	2.37	0.46
1:E:490:LYS:HG3	1:E:503:ASP:O	2.15	0.46
1:B:139:GLU:HB2	1:B:510:TYR:CE1	2.50	0.46
1:E:405:LEU:O	1:E:420:LEU:HD12	2.16	0.46
1:A:236:TYR:CE2	1:B:212:MET:HE1	2.51	0.46
1:E:3:GLU:CA	1:E:3:GLU:OE2	2.63	0.45
1:C:135:ARG:HD2	1:C:173:MET:SD	2.55	0.45
1:D:514:THR:HG21	6:D:633:HOH:O	2.17	0.45
1:C:10:VAL:CG2	1:C:11:ALA:H	2.29	0.45
1:B:394:LEU:HA	1:B:397:MET:HE3	1.98	0.45
1:E:338:LEU:H	1:E:338:LEU:HD23	1.79	0.45
1:B:180:LYS:HE2	1:B:180:LYS:HB2	1.76	0.45
1:E:26:PRO:HB2	1:E:27:TRP:CE3	2.52	0.45
1:A:98:ILE:C	1:A:100:ASN:H	2.19	0.45
1:E:299:ILE:HD13	1:E:346:TRP:HZ3	1.82	0.45
1:C:193:LEU:HG	1:C:195:SER:OG	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:260:ILE:HD12	1:E:260:ILE:N	2.31	0.45
1:A:158:TYR:O	1:A:173:MET:HB2	2.16	0.45
1:A:163:PHE:CB	1:A:170:TYR:CZ	2.99	0.45
1:A:133:LEU:HD22	1:A:134:THR:N	2.31	0.45
1:A:207:PHE:CE1	1:B:31:GLU:HG2	2.52	0.45
3:E:620:CB3:C15	3:E:620:CB3:H5	2.46	0.45
1:D:19:ILE:HB	5:D:618:NDP:N7N	2.32	0.45
1:A:172:PHE:HD1	1:A:172:PHE:N	2.14	0.45
1:D:394:LEU:HD23	1:D:397:MET:HE1	1.99	0.45
1:C:459:PHE:CD2	1:D:459:PHE:CD2	3.05	0.45
1:A:337:ASP:OD2	1:A:353:TYR:OH	2.29	0.45
1:D:171:ASP:CG	1:D:483:PRO:HG3	2.37	0.45
1:C:402:CYS:SG	2:C:611:UMP:C6	3.10	0.45
1:A:246:ARG:HG2	6:A:632:HOH:O	2.16	0.45
1:E:367:GLN:O	1:E:371:LEU:N	2.49	0.45
1:A:26:PRO:HB2	1:A:27:TRP:CE3	2.51	0.45
3:E:620:CB3:H15	3:E:620:CB3:C5	2.46	0.45
3:C:612:CB3:O	3:C:612:CB3:HB2	2.16	0.45
1:C:59:TRP:C	1:C:62:ILE:HG22	2.37	0.45
1:C:74:VAL:HG12	1:C:75:ILE:N	2.31	0.45
1:C:56:ARG:CG	1:C:76:SER:OG	2.65	0.45
1:D:289:ARG:NH2	1:D:311:LYS:O	2.50	0.45
1:E:225:ASN:CG	1:E:241:LEU:HD13	2.36	0.45
1:E:48:LYS:HB3	1:E:106:SER:O	2.17	0.45
1:A:392:SER:CB	1:B:350:ASN:HD22	2.29	0.45
1:C:431:SER:O	1:C:435:ILE:HG13	2.15	0.45
1:C:4:LYS:HD3	1:C:101:LEU:HA	1.99	0.45
1:A:100:ASN:HB2	1:A:110:ILE:HD11	1.98	0.45
1:E:304:ASN:CA	1:E:356:MET:HE3	2.39	0.45
1:E:422:GLN:HB3	1:E:460:ILE:HD13	1.98	0.45
1:C:59:TRP:CD1	1:C:64:ARG:HG2	2.52	0.45
1:C:79:LEU:H	1:C:92:ARG:HH12	1.65	0.45
1:B:192:GLN:HA	1:B:192:GLN:OE1	2.16	0.45
1:C:502:GLU:CD	1:C:502:GLU:H	2.20	0.45
1:C:315:ILE:HG13	1:C:316:TRP:CD1	2.52	0.45
1:C:333:ARG:HH22	1:C:339:GLY:HA3	1.81	0.45
1:A:134:THR:HG23	1:A:171:ASP:O	2.16	0.45
1:A:178:GLN:HE21	1:A:178:GLN:CA	2.28	0.45
1:C:130:ARG:HD2	1:C:132:TYR:CE1	2.52	0.45
1:A:383:ARG:HD3	1:B:400:PRO:HG2	1.98	0.45
1:B:120:ARG:HG3	1:B:148:PRO:HG3	1.99	0.45
1:A:257:ARG:HE	1:B:383:ARG:HH12	1.65	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:258:THR:HG23	1:A:520:ALA:HB1	1.97	0.45
1:B:4:LYS:HG2	1:B:101:LEU:HD23	1.99	0.45
1:E:381:ASP:HB3	1:E:384:HIS:NE2	2.32	0.45
1:C:400:PRO:HG2	1:D:383:ARG:CZ	2.47	0.45
1:A:246:ARG:NH1	1:A:268:GLN:OE1	2.43	0.45
1:A:253:TYR:HD2	1:A:263:TYR:CZ	2.34	0.45
1:E:163:PHE:HA	1:E:276:GLU:HB3	1.98	0.45
1:C:71:ILE:HD12	1:C:71:ILE:N	2.32	0.45
1:A:256:ASN:HD21	1:A:262:THR:HG23	1.82	0.44
1:A:260:ILE:HD12	1:A:260:ILE:N	2.32	0.44
1:B:180:LYS:HD3	1:B:181:LYS:CA	2.47	0.44
1:E:427:LEU:HD23	1:E:464:HIS:O	2.17	0.44
1:E:305:GLY:N	1:E:356:MET:CE	2.80	0.44
1:C:20:GLY:HA2	1:C:26:PRO:HD3	1.99	0.44
1:A:209:ILE:HG12	1:A:209:ILE:O	2.18	0.44
1:C:100:ASN:C	1:C:103:ASN:CB	2.56	0.44
1:C:94:LEU:HA	1:C:97:SER:OG	2.18	0.44
1:A:104:ASP:C	1:A:106:SER:H	2.20	0.44
1:A:96:ASP:O	1:A:99:GLU:HG3	2.18	0.44
1:C:193:LEU:HD21	1:D:176:GLU:OE2	2.16	0.44
1:A:331:GLY:C	1:A:333:ARG:N	2.70	0.44
1:A:15:LEU:HD12	1:A:139:GLU:HG3	1.99	0.44
1:E:293:GLU:O	1:E:297:TRP:HB2	2.17	0.44
1:D:261:SER:HB2	1:D:467:GLU:OE2	2.17	0.44
1:B:26:PRO:HB2	1:B:27:TRP:CE3	2.53	0.44
1:A:509:TYR:CZ	1:A:511:PRO:HB3	2.52	0.44
1:D:10:VAL:HG22	1:D:11:ALA:N	2.32	0.44
1:E:202:LEU:HA	1:E:205:GLU:OE1	2.18	0.44
1:C:423:ARG:HA	1:D:407:GLN:OE1	2.18	0.44
1:C:293:GLU:OE2	1:C:296:ILE:HD11	2.18	0.44
1:C:233:ARG:HG3	6:C:626:HOH:O	2.17	0.44
1:B:115:GLY:HA3	5:B:610:NDP:PA	2.58	0.44
1:C:421:TYR:OH	1:D:407:GLN:HB3	2.17	0.44
1:E:137:ALA:O	1:E:510:TYR:CE2	2.70	0.44
1:E:285:LYS:HE2	1:E:514:THR:OG1	2.17	0.44
1:A:389:TRP:HB2	1:A:404:VAL:CG1	2.44	0.44
1:E:337:ASP:OD2	1:E:353:TYR:OH	2.33	0.44
1:B:117:SER:OG	5:B:610:NDP:H8A	2.17	0.44
1:D:48:LYS:HB3	1:D:106:SER:O	2.17	0.44
1:D:330:LEU:C	1:D:332:HIS:N	2.69	0.44
1:D:431:SER:O	1:D:435:ILE:HG13	2.18	0.44
1:C:471:THR:HG23	6:C:659:HOH:O	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:100:ASN:OD1	1:E:101:LEU:N	2.51	0.44
1:C:345:GLN:O	1:C:349:TYR:HB2	2.18	0.44
1:B:479:ARG:NH2	1:B:513:PRO:O	2.50	0.44
1:A:20:GLY:HA2	1:A:26:PRO:HD3	1.99	0.44
1:C:519:MET:HG2	1:C:520:ALA:N	2.31	0.44
1:C:246:ARG:NH1	1:C:268:GLN:OE1	2.50	0.44
1:B:96:ASP:O	1:B:99:GLU:HB2	2.18	0.44
1:D:171:ASP:CB	1:D:483:PRO:HG3	2.48	0.44
1:A:178:GLN:NE2	1:A:178:GLN:CA	2.81	0.44
1:E:63:GLY:O	1:E:65:ARG:HG3	2.18	0.44
1:C:104:ASP:OD2	1:C:106:SER:CA	2.66	0.44
1:E:58:THR:O	1:E:62:ILE:HG12	2.17	0.44
5:E:622:NDP:C5D	5:E:622:NDP:O2A	2.65	0.44
1:A:239:GLN:HG3	1:A:271:ARG:O	2.18	0.44
1:C:131:ILE:O	1:C:174:ILE:HA	2.18	0.44
1:D:27:TRP:CE2	1:D:136:VAL:HG21	2.53	0.44
1:B:342:TYR:CE1	1:B:403:HIS:CE1	3.05	0.44
1:C:14:VAL:HG13	1:C:15:LEU:N	2.32	0.44
1:C:405:LEU:HD23	1:C:405:LEU:C	2.38	0.44
1:D:303:THR:HG21	1:D:344:PHE:HB2	2.00	0.44
1:D:129:ASP:N	1:D:129:ASP:OD2	2.50	0.44
3:C:612:CB3:H12	3:C:612:CB3:HN	1.41	0.43
1:C:36:PHE:HE2	4:C:613:MTX:NA4	2.16	0.43
1:E:283:THR:HA	1:E:512:TYR:CD1	2.51	0.43
1:D:233:ARG:NH1	1:D:242:ASP:OD1	2.51	0.43
1:A:512:TYR:HB3	1:A:513:PRO:CD	2.48	0.43
1:A:31:GLU:HG2	1:B:207:PHE:CE1	2.53	0.43
1:C:479:ARG:NH2	1:C:513:PRO:O	2.50	0.43
1:D:208:GLY:C	1:D:210:ARG:N	2.71	0.43
1:E:422:GLN:HB3	1:E:460:ILE:CD1	2.48	0.43
1:D:311:LYS:O	1:D:312:LYS:HB2	2.17	0.43
1:E:304:ASN:ND2	1:E:356:MET:HB2	2.34	0.43
1:D:100:ASN:HB3	1:D:107:ILE:HG21	2.00	0.43
1:E:244:LEU:HD12	1:E:427:LEU:HB3	1.99	0.43
1:C:224:TYR:CZ	1:C:233:ARG:NH1	2.86	0.43
1:E:295:LEU:CD2	1:E:299:ILE:HD11	2.48	0.43
1:A:233:ARG:NH1	1:A:242:ASP:CG	2.72	0.43
1:D:147:PHE:HE1	1:D:150:ILE:HD11	1.83	0.43
1:E:278:PHE:CE1	1:E:487:LEU:HD22	2.52	0.43
1:C:467:GLU:HA	1:C:470:LEU:HD22	2.00	0.43
1:C:133:LEU:HD22	1:C:133:LEU:C	2.38	0.43
1:C:285:LYS:HB3	1:C:514:THR:HG23	1.99	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:305:GLY:O	1:A:309:ILE:HG13	2.19	0.43
1:B:262:THR:HG22	1:B:466:TYR:HA	2.01	0.43
1:B:246:ARG:NE	1:B:268:GLN:OE1	2.49	0.43
1:A:472:GLN:N	1:A:472:GLN:OE1	2.49	0.43
1:B:193:LEU:CD2	1:B:195:SER:OG	2.66	0.43
1:E:8:ILE:HD12	1:E:123:LEU:HD21	2.01	0.43
1:D:98:ILE:O	1:D:99:GLU:CB	2.62	0.43
1:D:58:THR:OG1	5:D:618:NDP:H6N	2.19	0.43
1:C:423:ARG:HG3	1:C:424:SER:N	2.33	0.43
1:C:98:ILE:C	1:C:99:GLU:CG	2.86	0.43
1:A:381:ASP:HB3	1:A:384:HIS:CE1	2.53	0.43
1:C:402:CYS:SG	2:C:611:UMP:H2'	2.58	0.43
1:A:502:GLU:H	1:A:502:GLU:CD	2.22	0.43
1:D:4:LYS:HD2	1:D:107:ILE:O	2.19	0.43
1:D:248:LEU:CD1	1:D:465:ILE:HD12	2.47	0.43
1:A:288:ILE:O	1:A:291:ILE:HB	2.18	0.43
1:A:472:GLN:O	1:A:475:GLU:HB3	2.19	0.43
1:C:48:LYS:CA	1:C:106:SER:O	2.66	0.43
1:B:4:LYS:HE3	1:B:101:LEU:HA	1.99	0.43
1:A:400:PRO:HG2	1:A:423:ARG:NH2	2.34	0.43
1:A:125:ASP:HB2	1:A:127:PHE:CE1	2.53	0.43
1:E:315:ILE:HG13	1:E:316:TRP:CD1	2.54	0.43
1:E:130:ARG:HD2	1:E:132:TYR:CZ	2.53	0.43
1:C:56:ARG:HB2	1:C:76:SER:OG	2.19	0.43
1:A:98:ILE:HG22	1:A:98:ILE:O	2.19	0.42
1:E:434:ASN:ND2	3:E:620:CB3:CP3	2.82	0.42
1:B:115:GLY:HA3	5:B:610:NDP:O2A	2.18	0.42
1:B:335:GLU:O	1:B:336:ASN:CB	2.67	0.42
1:B:359:ASP:OD2	1:B:361:THR:CG2	2.67	0.42
1:D:472:GLN:O	1:D:475:GLU:HB3	2.18	0.42
1:C:304:ASN:OD1	1:C:306:ASN:HB2	2.19	0.42
1:E:411:THR:OG1	1:E:415:CYS:HB2	2.20	0.42
4:E:621:MTX:C6	5:E:622:NDP:H42N	2.49	0.42
1:E:378:ASN:HD21	1:E:381:ASP:HB2	1.82	0.42
1:D:342:TYR:CZ	1:D:403:HIS:CD2	3.06	0.42
1:C:254:ARG:HD2	1:C:264:SER:HB3	2.02	0.42
1:C:38:LYS:O	1:C:42:ASN:HB2	2.19	0.42
1:A:236:TYR:CE2	1:B:212:MET:CE	3.02	0.42
1:C:187:ASP:HA	1:C:188:PRO:HD3	1.91	0.42
1:A:258:THR:HG21	1:A:520:ALA:CB	2.41	0.42
1:C:339:GLY:HA2	1:C:353:TYR:CE2	2.54	0.42
1:C:123:LEU:HD12	1:C:128:VAL:CG1	2.40	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:133:LEU:HD22	1:D:134:THR:N	2.35	0.42
1:C:226:THR:N	1:C:227:PRO:HD3	2.34	0.42
1:A:115:GLY:HA3	5:A:606:NDP:PA	2.60	0.42
1:E:54:MET:CE	1:E:72:ILE:HG23	2.50	0.42
1:D:36:PHE:C	1:D:36:PHE:CD1	2.93	0.42
1:E:361:THR:O	1:E:361:THR:HG23	2.18	0.42
1:D:52:LEU:N	1:D:52:LEU:HD23	2.34	0.42
1:E:3:GLU:HA	1:E:3:GLU:OE2	2.19	0.42
1:E:208:GLY:C	1:E:210:ARG:N	2.71	0.42
1:C:158:TYR:HB3	1:C:174:ILE:CG2	2.42	0.42
1:D:59:TRP:CD1	1:D:64:ARG:HG2	2.55	0.42
1:E:6:VAL:HG22	1:E:110:ILE:HB	2.02	0.42
1:B:315:ILE:HB	3:B:608:CB3:C15	2.50	0.42
1:C:135:ARG:NH2	1:C:481:PRO:O	2.51	0.42
1:C:226:THR:HG22	1:C:229:ILE:HG13	2.01	0.42
1:A:206:ILE:HG13	1:B:38:LYS:NZ	2.35	0.42
1:E:8:ILE:CG1	1:E:112:VAL:HB	2.36	0.42
1:E:363:VAL:CG1	1:E:364:GLY:N	2.79	0.42
1:D:291:ILE:HG12	1:D:433:PHE:CD2	2.54	0.42
1:D:8:ILE:HG12	1:D:112:VAL:HB	2.02	0.42
1:B:150:ILE:HA	1:B:151:PRO:HD3	1.86	0.42
1:A:49:LYS:O	1:A:107:ILE:HA	2.19	0.42
1:E:56:ARG:HG3	1:E:79:LEU:HD12	2.01	0.42
1:E:43:LYS:HZ2	1:E:46:SER:HA	1.82	0.42
1:D:208:GLY:C	1:D:210:ARG:H	2.23	0.42
1:A:290:GLY:HA3	6:A:718:HOH:O	2.19	0.42
1:C:190:ARG:HH11	1:C:190:ARG:CB	2.20	0.42
1:D:226:THR:N	1:D:227:PRO:HD3	2.34	0.42
1:D:243:LEU:HA	1:D:246:ARG:NH1	2.35	0.42
1:E:472:GLN:HB3	1:E:515:ILE:CG2	2.50	0.42
1:E:223:ILE:HB	1:E:248:LEU:HD23	2.01	0.42
1:D:49:LYS:HD2	1:D:71:ILE:HD11	2.01	0.42
1:C:179:GLU:HA	6:C:651:HOH:O	2.20	0.42
1:D:258:THR:HG22	1:D:521:VAL:O	2.20	0.42
1:C:391:PRO:HD2	1:D:349:TYR:CD2	2.52	0.42
1:B:347:ARG:O	1:B:366:ASP:HA	2.20	0.42
1:B:123:LEU:HA	1:B:123:LEU:HD12	1.87	0.42
1:E:452:GLU:HA	1:E:452:GLU:OE2	2.20	0.42
3:C:612:CB3:HP12	3:C:612:CB3:H13	1.63	0.42
3:C:612:CB3:HB1	3:C:612:CB3:O	2.14	0.42
1:C:26:PRO:HG2	1:C:143:PHE:HE1	1.85	0.42
1:E:246:ARG:HH11	1:E:246:ARG:HB2	1.85	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:501:TRP:CE3	1:D:501:TRP:HA	2.55	0.42
1:B:400:PRO:HA	1:B:401:PRO:HD3	1.91	0.42
1:C:347:ARG:O	1:C:366:ASP:HA	2.20	0.42
1:A:427:LEU:HD12	1:A:427:LEU:HA	1.85	0.42
1:B:426:ASP:OD2	1:B:426:ASP:C	2.58	0.42
1:E:348:HIS:CE1	1:E:360:TYR:O	2.73	0.41
1:E:43:LYS:HB2	1:E:108:GLU:OE1	2.20	0.41
1:B:39:ILE:CG2	1:B:40:THR:N	2.81	0.41
1:D:302:ASP:OD2	1:D:307:HIS:ND1	2.53	0.41
1:E:133:LEU:HD23	1:E:134:THR:N	2.35	0.41
1:B:49:LYS:O	1:B:107:ILE:HA	2.20	0.41
1:D:53:ILE:HG23	1:D:75:ILE:HD13	2.03	0.41
1:C:257:ARG:NH1	2:C:611:UMP:O5'	2.53	0.41
1:D:103:ASN:O	1:D:105:ASP:N	2.53	0.41
1:E:155:LEU:HA	1:E:156:PRO:HD3	1.57	0.41
1:C:295:LEU:HD22	1:C:299:ILE:HD11	2.01	0.41
1:E:266:PHE:HA	1:E:461:GLY:O	2.20	0.41
1:C:157:VAL:HG23	1:D:196:ILE:HD11	2.01	0.41
1:D:400:PRO:HG2	1:D:423:ARG:NH2	2.35	0.41
1:E:90:VAL:HG12	1:E:91:PHE:N	2.34	0.41
1:C:360:TYR:CD1	1:C:363:VAL:HG11	2.53	0.41
1:E:389:TRP:HB2	1:E:404:VAL:CG1	2.44	0.41
1:C:419:ASN:HD22	1:C:419:ASN:HA	1.58	0.41
4:B:609:MTX:O1	4:B:609:MTX:HG1	2.19	0.41
1:E:171:ASP:OD2	1:E:483:PRO:HD3	2.20	0.41
1:C:381:ASP:HB3	1:C:384:HIS:NE2	2.35	0.41
1:C:267:GLY:HA2	1:C:460:ILE:O	2.20	0.41
1:C:180:LYS:CB	6:C:650:HOH:O	2.68	0.41
1:A:48:LYS:CB	1:A:106:SER:O	2.67	0.41
1:A:102:MET:O	1:A:103:ASN:CG	2.59	0.41
1:E:76:SER:CA	5:E:622:NDP:O2X	2.64	0.41
5:C:614:NDP:O2X	5:C:614:NDP:O3B	2.30	0.41
1:A:163:PHE:CB	1:A:170:TYR:CE2	2.97	0.41
1:B:75:ILE:O	5:B:610:NDP:H1B	2.20	0.41
1:D:7:SER:O	1:D:111:PHE:HA	2.21	0.41
1:D:104:ASP:C	1:D:106:SER:N	2.73	0.41
3:A:604:CB3:C15	3:A:604:CB3:C6	2.98	0.41
1:A:323:GLU:H	1:A:323:GLU:CD	2.22	0.41
1:A:164:CYS:SG	6:A:667:HOH:O	2.63	0.41
1:C:236:TYR:OH	1:D:212:MET:HB3	2.21	0.41
1:D:90:VAL:HG12	1:D:91:PHE:N	2.36	0.41
1:B:203:LEU:HA	1:B:203:LEU:HD12	1.95	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:433:PHE:CE2	3:E:620:CB3:H12	2.56	0.41
1:C:79:LEU:HD23	1:C:80:PRO:CG	2.49	0.41
1:A:171:ASP:C	1:A:172:PHE:CD1	2.94	0.41
1:C:403:HIS:H	1:C:403:HIS:CD2	2.37	0.41
1:A:248:LEU:HD13	1:A:465:ILE:CD1	2.51	0.41
1:B:193:LEU:HD23	1:B:195:SER:H	1.86	0.41
1:D:506:LEU:HA	1:D:506:LEU:HD23	1.90	0.41
1:E:4:LYS:HG2	1:E:101:LEU:HD23	2.00	0.41
1:E:436:ALA:O	1:E:439:ALA:HB3	2.21	0.41
1:E:135:ARG:HD3	1:E:171:ASP:OD2	2.20	0.41
1:D:360:TYR:HB3	1:D:363:VAL:CG1	2.51	0.41
1:C:291:ILE:HG12	1:C:433:PHE:CE2	2.55	0.41
1:E:371:LEU:HD13	1:E:371:LEU:C	2.41	0.41
1:D:68:LYS:HE2	1:D:69:ASN:OD1	2.21	0.41
1:C:248:LEU:HA	1:C:248:LEU:HD12	1.86	0.41
1:C:115:GLY:O	1:C:116:GLU:C	2.59	0.41
1:D:92:ARG:O	5:D:618:NDP:C2A	2.67	0.41
1:E:388:ALA:O	1:E:401:PRO:HG2	2.20	0.41
1:E:199:THR:O	1:E:203:LEU:HB2	2.21	0.41
1:D:3:GLU:OE2	1:D:3:GLU:HA	2.21	0.41
1:A:147:PHE:CD2	1:A:148:PRO:HD2	2.55	0.41
1:C:77:SER:H	5:C:614:NDP:P2B	2.43	0.41
1:B:9:VAL:O	4:B:609:MTX:NA4	2.47	0.41
1:E:135:ARG:CG	1:E:171:ASP:HB2	2.50	0.41
1:D:294:GLU:O	1:D:297:TRP:HB3	2.21	0.41
1:D:10:VAL:HB	1:D:119:TYR:CZ	2.56	0.41
1:D:431:SER:HB3	1:D:432:PRO:HD3	2.03	0.41
1:A:403:HIS:HB2	1:A:420:LEU:HD11	2.02	0.41
1:E:337:ASP:OD2	1:E:337:ASP:C	2.59	0.41
1:C:391:PRO:HD2	1:D:349:TYR:HE2	1.71	0.41
1:E:59:TRP:O	1:E:62:ILE:HB	2.20	0.41
1:D:12:ALA:HB2	1:D:19:ILE:CG2	2.51	0.41
1:D:62:ILE:O	1:D:62:ILE:HG23	2.21	0.41
1:A:165:THR:N	1:A:170:TYR:HE1	2.19	0.41
1:E:347:ARG:HA	1:E:366:ASP:OD2	2.21	0.41
1:C:269:MET:HE2	1:D:269:MET:HE2	2.03	0.41
1:E:341:ILE:HA	1:E:397:MET:HE3	2.03	0.41
1:D:495:ASN:OD1	1:D:497:GLU:HG3	2.21	0.41
1:A:180:LYS:N	6:A:614:HOH:O	2.54	0.41
1:A:431:SER:HB3	1:A:432:PRO:HD3	2.02	0.41
1:A:299:ILE:O	1:A:347:ARG:NH1	2.51	0.41
1:D:235:HIS:C	1:D:235:HIS:ND1	2.74	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:100:ASN:O	1:C:103:ASN:HB2	2.14	0.41
1:A:258:THR:CG2	1:A:260:ILE:HB	2.51	0.41
1:E:100:ASN:HA	1:E:104:ASP:CB	2.50	0.41
1:C:8:ILE:HD11	1:C:123:LEU:HD13	2.03	0.41
1:B:233:ARG:NH1	1:B:242:ASP:OD1	2.54	0.41
1:E:14:VAL:HG13	1:E:136:VAL:C	2.41	0.41
1:D:297:TRP:HH2	1:D:338:LEU:HD12	1.86	0.41
1:C:405:LEU:HD11	1:D:404:VAL:HG11	2.02	0.41
1:A:98:ILE:CG2	1:A:101:LEU:HD12	2.51	0.40
1:D:470:LEU:HD13	1:D:470:LEU:HA	1.95	0.40
1:C:491:ARG:CZ	1:C:493:VAL:HG12	2.51	0.40
1:C:385:ILE:CG2	1:C:386:LEU:N	2.84	0.40
1:C:297:TRP:HH2	1:C:338:LEU:HD12	1.85	0.40
1:D:97:SER:C	1:D:99:GLU:HG3	2.40	0.40
1:B:285:LYS:HD3	1:B:514:THR:HG22	2.02	0.40
1:A:229:ILE:HG22	1:A:233:ARG:HG2	2.03	0.40
1:D:274:MET:SD	1:D:439:ALA:HA	2.61	0.40
1:B:256:ASN:HB3	6:B:748:HOH:O	2.21	0.40
1:E:255:GLU:CD	1:E:255:GLU:H	2.25	0.40
1:E:206:ILE:HG22	1:E:207:PHE:N	2.36	0.40
1:A:297:TRP:CE3	1:A:308:LEU:HD11	2.56	0.40
1:A:297:TRP:HH2	1:A:338:LEU:HD12	1.86	0.40
1:E:508:GLY:O	1:E:510:TYR:CD2	2.74	0.40
1:B:193:LEU:HD21	6:B:660:HOH:O	2.21	0.40
1:D:49:LYS:HD2	1:D:71:ILE:CD1	2.51	0.40
1:C:120:ARG:NH1	1:C:148:PRO:HB3	2.36	0.40
1:B:97:SER:C	1:B:99:GLU:H	2.25	0.40
1:E:434:ASN:HD21	3:E:620:CB3:CP3	2.34	0.40
1:E:62:ILE:HD11	4:E:621:MTX:C13	2.51	0.40
1:A:333:ARG:CD	1:A:337:ASP:O	2.70	0.40
1:C:25:LEU:HD11	4:C:613:MTX:H7	2.04	0.40
1:D:135:ARG:HH22	1:D:482:ARG:HA	1.82	0.40
1:C:4:LYS:HB2	1:C:101:LEU:HD23	2.03	0.40
1:A:258:THR:HG21	1:A:260:ILE:HB	2.03	0.40
1:D:57:LYS:HB2	5:D:618:NDP:O3	2.22	0.40
1:E:299:ILE:O	1:E:347:ARG:HD3	2.21	0.40
1:B:291:ILE:HD13	1:B:436:ALA:HB3	2.02	0.40
1:D:479:ARG:NH2	1:D:513:PRO:O	2.55	0.40
1:A:485:PRO:HB3	1:A:509:TYR:HA	2.03	0.40
1:B:159:MET:HE2	1:B:173:MET:SD	2.62	0.40
1:C:93:ASN:OD1	1:C:95:GLU:HB3	2.22	0.40
1:A:39:ILE:HD13	1:A:39:ILE:HA	1.86	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:349:TYR:OH	1:E:349:TYR:OH[2_457]	1.93	0.27

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	512/519 (99%)	481 (94%)	24 (5%)	7 (1%)	16	49
1	B	512/519 (99%)	482 (94%)	25 (5%)	5 (1%)	22	60
1	C	510/519 (98%)	468 (92%)	37 (7%)	5 (1%)	22	60
1	D	511/519 (98%)	464 (91%)	38 (7%)	9 (2%)	13	39
1	E	507/519 (98%)	458 (90%)	42 (8%)	7 (1%)	16	49
All	All	2552/2595 (98%)	2353 (92%)	166 (6%)	33 (1%)	18	51

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	MET
1	A	103	ASN
1	B	103	ASN
1	B	342	TYR
1	C	103	ASN
1	C	335	GLU
1	C	336	ASN
1	C	342	TYR
1	D	99	GLU
1	D	257	ARG
1	D	342	TYR
1	E	331	GLY
1	E	342	TYR
1	A	105	ASP
1	B	414	ASN
1	C	99	GLU

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Mol	Chain	Res	Type
1	D	105	ASP
1	B	69	ASN
1	D	102	MET
1	D	194	LYS
1	D	331	GLY
1	E	83	GLU
1	A	384	HIS
1	E	140	ASP
1	E	361	THR
1	E	379	PRO
1	E	384	HIS
1	A	98	ILE
1	A	101	LEU
1	B	4	LYS
1	D	100	ASN
1	D	104	ASP
1	A	341	ILE

5.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	460/467 (98%)	427 (93%)	33 (7%)	21	50
1	B	461/467 (99%)	423 (92%)	38 (8%)	17	43
1	C	457/467 (98%)	420 (92%)	37 (8%)	17	43
1	D	457/467 (98%)	419 (92%)	38 (8%)	16	42
1	E	456/467 (98%)	425 (93%)	31 (7%)	22	54
All	All	2291/2335 (98%)	2114 (92%)	177 (8%)	18	45

All (177) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	99	GLU
1	A	103	ASN
1	A	104	ASP

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Mol	Chain	Res	Type
1	A	126	ASN
1	A	128	VAL
1	A	133	LEU
1	A	172	PHE
1	A	178	GLN
1	A	193	LEU
1	A	203	LEU
1	A	221	GLU
1	A	235	HIS
1	A	244	LEU
1	A	247	VAL
1	A	248	LEU
1	A	269	MET
1	A	295	LEU
1	A	341	ILE
1	A	342	TYR
1	A	354	LYS
1	A	355	THR
1	A	356	MET
1	A	358	ASP
1	A	361	THR
1	A	370	LYS
1	A	371	LEU
1	A	378	ASN
1	A	413	ASP
1	A	427	LEU
1	A	429	LEU
1	A	473	LEU
1	A	491	ARG
1	B	7	SER
1	B	13	SER
1	B	16	SER
1	B	98	ILE
1	B	99	GLU
1	B	103	ASN
1	B	123	LEU
1	B	126	ASN
1	B	133	LEU
1	B	138	LEU
1	B	176	GLU
1	B	177	LYS
1	B	179	GLU

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Mol	Chain	Res	Type
1	B	180	LYS
1	B	202	LEU
1	B	203	LEU
1	B	220	LYS
1	B	221	GLU
1	B	233	ARG
1	B	235	HIS
1	B	244	LEU
1	B	247	VAL
1	B	289	ARG
1	B	295	LEU
1	B	308	LEU
1	B	335	GLU
1	B	352	GLU
1	B	361	THR
1	B	363	VAL
1	B	371	LEU
1	B	383	ARG
1	B	404	VAL
1	B	413	ASP
1	B	427	LEU
1	B	429	LEU
1	B	491	ARG
1	B	506	LEU
1	B	514	THR
1	C	5	ASN
1	C	6	VAL
1	C	52	LEU
1	C	62	ILE
1	C	76	SER
1	C	83	GLU
1	C	98	ILE
1	C	99	GLU
1	C	100	ASN
1	C	102	MET
1	C	105	ASP
1	C	123	LEU
1	C	133	LEU
1	C	138	LEU
1	C	171	ASP
1	C	174	ILE
1	C	176	GLU

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Mol	Chain	Res	Type
1	C	209	ILE
1	C	228	SER
1	C	233	ARG
1	C	235	HIS
1	C	247	VAL
1	C	257	ARG
1	C	295	LEU
1	C	308	LEU
1	C	325	LEU
1	C	333	ARG
1	C	371	LEU
1	C	383	ARG
1	C	427	LEU
1	C	470	LEU
1	C	474	LYS
1	C	479	ARG
1	C	497	GLU
1	C	505	GLU
1	C	506	LEU
1	C	516	LYS
1	D	7	SER
1	D	52	LEU
1	D	76	SER
1	D	79	LEU
1	D	82	ASP
1	D	83	GLU
1	D	96	ASP
1	D	99	GLU
1	D	105	ASP
1	D	113	CYS
1	D	123	LEU
1	D	128	VAL
1	D	129	ASP
1	D	133	LEU
1	D	138	LEU
1	D	149	GLU
1	D	171	ASP
1	D	176	GLU
1	D	202	LEU
1	D	203	LEU
1	D	221	GLU
1	D	233	ARG

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Mol	Chain	Res	Type
1	D	235	HIS
1	D	248	LEU
1	D	256	ASN
1	D	262	THR
1	D	264	SER
1	D	293	GLU
1	D	295	LEU
1	D	308	LEU
1	D	310	GLU
1	D	371	LEU
1	D	383	ARG
1	D	414	ASN
1	D	422	GLN
1	D	437	SER
1	D	479	ARG
1	D	514	THR
1	E	3	GLU
1	E	8	ILE
1	E	36	PHE
1	E	45	ASP
1	E	99	GLU
1	E	101	LEU
1	E	133	LEU
1	E	138	LEU
1	E	139	GLU
1	E	178	GLN
1	E	179	GLU
1	E	194	LYS
1	E	202	LEU
1	E	220	LYS
1	E	221	GLU
1	E	233	ARG
1	E	260	ILE
1	E	269	MET
1	E	295	LEU
1	E	306	ASN
1	E	335	GLU
1	E	338	LEU
1	E	354	LYS
1	E	356	MET
1	E	383	ARG
1	E	394	LEU

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Mol	Chain	Res	Type
1	E	414	ASN
1	E	434	ASN
1	E	471	THR
1	E	491	ARG
1	E	500	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	69	ASN
1	A	103	ASN
1	A	167	ASN
1	A	178	GLN
1	A	192	GLN
1	A	384	HIS
1	A	447	GLN
1	B	100	ASN
1	B	103	ASN
1	B	422	GLN
1	C	5	ASN
1	C	24	GLN
1	C	41	ASN
1	C	69	ASN
1	C	103	ASN
1	C	319	ASN
1	C	377	ASN
1	C	384	HIS
1	C	419	ASN
1	C	422	GLN
1	D	178	GLN
1	D	256	ASN
1	D	306	ASN
1	D	419	ASN
1	D	422	GLN
1	E	22	ASN
1	E	24	GLN
1	E	69	ASN
1	E	126	ASN
1	E	167	ASN
1	E	214	ASN
1	E	307	HIS

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Mol	Chain	Res	Type
1	E	377	ASN
1	E	378	ASN
1	E	384	HIS
1	E	396	GLN
1	E	403	HIS
1	E	434	ASN
1	E	495	ASN

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 ⓘ

20 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	UMP	A	603	1	21,21,21	3.16	4 (19%)	26,31,31	1.88	5 (19%)
3	CB3	A	604	-	37,37,37	2.37	16 (43%)	49,51,51	2.82	23 (46%)
4	MTX	A	605	-	35,35,35	1.34	2 (5%)	49,49,49	1.73	10 (20%)
5	NDP	A	606	-	52,52,52	1.51	5 (9%)	80,80,80	1.56	11 (13%)
2	UMP	B	607	-	21,21,21	3.18	5 (23%)	26,31,31	1.81	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CB3	B	608	-	37,37,37	3.27	27 (72%)	49,51,51	2.48	14 (28%)
4	MTX	B	609	-	35,35,35	1.34	2 (5%)	49,49,49	1.59	10 (20%)
5	NDP	B	610	-	52,52,52	1.54	5 (9%)	80,80,80	1.56	10 (12%)
2	UMP	C	611	-	21,21,21	3.17	5 (23%)	26,31,31	1.81	5 (19%)
3	CB3	C	612	-	37,37,37	2.53	21 (56%)	49,51,51	2.62	17 (34%)
4	MTX	C	613	-	35,35,35	1.28	2 (5%)	49,49,49	1.59	10 (20%)
5	NDP	C	614	-	52,52,52	1.34	5 (9%)	80,80,80	1.61	8 (10%)
2	UMP	D	615	1	21,21,21	3.17	5 (23%)	26,31,31	1.89	5 (19%)
3	CB3	D	616	-	37,37,37	2.19	18 (48%)	49,51,51	2.03	11 (22%)
4	MTX	D	617	-	35,35,35	1.31	2 (5%)	49,49,49	1.66	10 (20%)
5	NDP	D	618	-	52,52,52	1.49	5 (9%)	80,80,80	1.59	10 (12%)
2	UMP	E	619	-	21,21,21	3.23	5 (23%)	26,31,31	2.00	4 (15%)
3	CB3	E	620	-	37,37,37	1.52	3 (8%)	49,51,51	1.47	8 (16%)
4	MTX	E	621	-	35,35,35	1.26	2 (5%)	49,49,49	1.57	9 (18%)
5	NDP	E	622	-	52,52,52	1.42	5 (9%)	80,80,80	1.55	8 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UMP	A	603	1	-	0/7/22/22	0/2/2/2
3	CB3	A	604	-	-	0/27/28/28	0/1/3/3
4	MTX	A	605	-	-	0/25/25/25	0/1/3/3
5	NDP	A	606	-	-	0/35/77/77	0/3/5/5
2	UMP	B	607	-	-	0/7/22/22	0/2/2/2
3	CB3	B	608	-	-	0/27/28/28	0/1/3/3
4	MTX	B	609	-	-	0/25/25/25	0/1/3/3
5	NDP	B	610	-	-	0/35/77/77	0/3/5/5
2	UMP	C	611	-	-	0/7/22/22	0/2/2/2
3	CB3	C	612	-	1/1/5/6	0/27/28/28	0/1/3/3
4	MTX	C	613	-	-	0/25/25/25	0/1/3/3
5	NDP	C	614	-	-	0/35/77/77	0/3/5/5
2	UMP	D	615	1	-	0/7/22/22	0/2/2/2
3	CB3	D	616	-	-	0/27/28/28	0/1/3/3
4	MTX	D	617	-	-	0/25/25/25	0/1/3/3
5	NDP	D	618	-	-	0/35/77/77	0/3/5/5
2	UMP	E	619	-	-	0/7/22/22	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CB3	E	620	-	1/1/5/6	0/27/28/28	0/1/3/3
4	MTX	E	621	-	-	0/25/25/25	0/1/3/3
5	NDP	E	622	-	-	0/35/77/77	0/3/5/5

All (144) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	619	UMP	C6-C5	10.91	1.53	1.36
2	B	607	UMP	C6-C5	10.71	1.53	1.36
2	D	615	UMP	C6-C5	10.69	1.53	1.36
2	A	603	UMP	C6-C5	10.66	1.53	1.36
2	C	611	UMP	C6-C5	10.66	1.53	1.36
3	B	608	CB3	CP1-N10	-7.83	1.38	1.46
2	E	619	UMP	C6-N1	7.60	1.48	1.35
2	B	607	UMP	C6-N1	7.55	1.48	1.35
2	D	615	UMP	C6-N1	7.52	1.48	1.35
2	C	611	UMP	C6-N1	7.52	1.48	1.35
2	A	603	UMP	C6-N1	7.51	1.48	1.35
5	B	610	NDP	C4N-C3N	-6.43	1.37	1.50
5	D	618	NDP	C4N-C3N	-6.31	1.38	1.50
5	A	606	NDP	C4N-C3N	-6.25	1.38	1.50
5	E	622	NDP	C4N-C3N	-6.22	1.38	1.50
3	E	620	CB3	O4-C4	6.15	1.36	1.24
3	B	608	CB3	C2-N1	-5.73	1.27	1.36
5	C	614	NDP	C4N-C3N	-5.65	1.39	1.50
3	D	616	CB3	CP1-N10	-5.38	1.41	1.46
5	B	610	NDP	C4N-C5N	-5.03	1.38	1.49
5	A	606	NDP	C4N-C5N	-5.01	1.38	1.49
5	D	618	NDP	C4N-C5N	-4.97	1.38	1.49
4	E	621	MTX	O-C	4.80	1.32	1.23
5	E	622	NDP	C4N-C5N	-4.80	1.38	1.49
2	E	619	UMP	C5-C4	4.79	1.52	1.40
3	A	604	CB3	CP2-CP3	4.79	1.28	1.17
3	B	608	CB3	C12-C11	-4.79	1.30	1.39
2	D	615	UMP	C5-C4	4.77	1.52	1.40
2	B	607	UMP	C5-C4	4.76	1.52	1.40
3	B	608	CB3	C8A-N1	-4.75	1.29	1.38
4	C	613	MTX	O-C	4.75	1.32	1.23
2	A	603	UMP	C5-C4	4.75	1.52	1.40
2	C	611	UMP	C5-C4	4.72	1.52	1.40
4	D	617	MTX	O-C	4.68	1.32	1.23
4	B	609	MTX	O-C	4.65	1.32	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	612	CB3	C5-C4A	-4.62	1.32	1.42
4	A	605	MTX	O-C	4.57	1.32	1.23
3	E	620	CB3	CP2-CP3	4.57	1.28	1.17
5	C	614	NDP	C4N-C5N	-4.49	1.39	1.49
3	C	612	CB3	CP1-N10	-4.41	1.42	1.46
3	A	604	CB3	CP1-N10	-4.36	1.42	1.46
3	A	604	CB3	C2-N1	-4.24	1.29	1.36
3	B	608	CB3	C5-C4A	-4.19	1.33	1.42
3	B	608	CB3	C9-N10	-4.17	1.40	1.46
3	D	616	CB3	O4-C4	4.14	1.32	1.24
3	C	612	CB3	C4A-C8A	-4.12	1.32	1.41
3	B	608	CB3	O-C	-4.12	1.15	1.23
4	A	605	MTX	C-N	-4.10	1.25	1.34
4	B	609	MTX	C-N	-4.10	1.25	1.34
4	D	617	MTX	C-N	-4.03	1.25	1.34
3	B	608	CB3	C15-C14	-3.98	1.31	1.39
4	C	613	MTX	C-N	-3.92	1.25	1.34
3	C	612	CB3	C2-N1	-3.92	1.30	1.36
3	B	608	CB3	C2-N3	-3.91	1.28	1.33
3	B	608	CB3	C4A-C8A	-3.89	1.33	1.41
3	B	608	CB3	C-N	-3.87	1.25	1.34
3	A	604	CB3	C4-N3	-3.85	1.29	1.37
3	B	608	CB3	C4-N3	-3.84	1.29	1.37
4	E	621	MTX	C-N	-3.83	1.26	1.34
3	A	604	CB3	C15-C14	-3.75	1.31	1.39
3	C	612	CB3	CP1-CP2	-3.70	1.41	1.47
3	C	612	CB3	C4-N3	-3.66	1.30	1.37
5	B	610	NDP	C4A-N9A	-3.62	1.32	1.37
3	B	608	CB3	O4-C4	3.61	1.31	1.24
3	C	612	CB3	CB-CA	-3.59	1.45	1.53
3	B	608	CB3	C11-C	-3.50	1.42	1.50
3	A	604	CB3	C5-C4A	-3.49	1.35	1.42
5	A	606	NDP	C4A-N9A	-3.47	1.32	1.37
3	A	604	CB3	C8A-N1	-3.42	1.32	1.38
3	D	616	CB3	O-C	-3.36	1.16	1.23
3	C	612	CB3	O4-C4	3.33	1.31	1.24
3	C	612	CB3	C12-C11	-3.29	1.33	1.39
5	D	618	NDP	C4A-N9A	-3.28	1.33	1.37
3	A	604	CB3	C13-C14	-3.27	1.32	1.39
3	C	612	CB3	C8A-N1	-3.25	1.32	1.38
3	D	616	CB3	CP2-CP3	3.20	1.25	1.17
3	A	604	CB3	C4A-C8A	-3.16	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	608	CB3	C9-C6	-3.11	1.45	1.51
3	D	616	CB3	C-N	-3.06	1.27	1.34
3	B	608	CB3	O2-CT	-3.04	1.19	1.30
3	D	616	CB3	CP1-CP2	-3.02	1.42	1.47
3	A	604	CB3	C8-C8A	-2.99	1.34	1.40
5	C	614	NDP	C6N-C5N	2.92	1.39	1.33
3	A	604	CB3	O4-C4	2.86	1.30	1.24
3	B	608	CB3	CA-CT	-2.85	1.45	1.52
3	C	612	CB3	C-N	-2.84	1.28	1.34
3	C	612	CB3	O-C	-2.83	1.17	1.23
3	B	608	CB3	CP2-CP3	2.82	1.24	1.17
3	A	604	CB3	C2-N3	-2.80	1.30	1.33
3	D	616	CB3	C2-N1	-2.78	1.32	1.36
3	B	608	CB3	OE2-CD	-2.77	1.20	1.30
3	C	612	CB3	OE2-CD	-2.76	1.20	1.30
3	C	612	CB3	C11-C	-2.72	1.44	1.50
3	D	616	CB3	C5-C4A	-2.71	1.36	1.42
5	E	622	NDP	C4A-N9A	-2.70	1.33	1.37
5	E	622	NDP	C6N-C5N	2.67	1.38	1.33
3	D	616	CB3	C4A-C8A	-2.67	1.35	1.41
3	B	608	CB3	C7-C6	-2.67	1.32	1.38
3	C	612	CB3	CP2-CP3	2.63	1.23	1.17
3	A	604	CB3	O-C	-2.63	1.18	1.23
5	D	618	NDP	C6N-C5N	2.60	1.38	1.33
3	B	608	CB3	CP1-CP2	-2.57	1.43	1.47
3	D	616	CB3	C8A-N1	-2.56	1.33	1.38
3	C	612	CB3	C2-N3	-2.55	1.30	1.33
3	C	612	CB3	C9-C6	-2.54	1.46	1.51
3	D	616	CB3	C4-N3	-2.46	1.32	1.37
3	B	608	CB3	C16-C11	-2.46	1.35	1.39
2	E	619	UMP	C2-N1	2.46	1.41	1.38
3	B	608	CB3	C8-C8A	-2.45	1.35	1.40
3	B	608	CB3	C13-C12	-2.44	1.34	1.38
3	D	616	CB3	C12-C11	-2.43	1.35	1.39
5	C	614	NDP	C4A-N9A	-2.43	1.34	1.37
3	B	608	CB3	C13-C14	-2.41	1.34	1.39
3	A	604	CB3	OE2-CD	-2.39	1.21	1.30
3	B	608	CB3	C16-C15	-2.39	1.34	1.38
3	C	612	CB3	CA-CT	-2.39	1.46	1.52
5	B	610	NDP	C6N-C5N	2.39	1.38	1.33
5	C	614	NDP	C2N-C3N	2.37	1.39	1.34
3	D	616	CB3	C9-N10	-2.36	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	616	CB3	C11-C	-2.35	1.45	1.50
3	D	616	CB3	C16-C11	-2.34	1.35	1.39
3	B	608	CB3	C2-NA2	-2.33	1.28	1.32
5	A	606	NDP	C6N-C5N	2.27	1.38	1.33
3	E	620	CB3	C2-NA2	2.25	1.35	1.32
3	A	604	CB3	C16-C11	-2.24	1.35	1.39
5	A	606	NDP	C8A-N9A	-2.23	1.33	1.36
5	B	610	NDP	C8A-N9A	-2.22	1.33	1.36
2	C	611	UMP	C2-N1	2.21	1.40	1.38
3	A	604	CB3	C14-N10	-2.16	1.33	1.38
5	D	618	NDP	C8A-N9A	-2.15	1.33	1.36
3	D	616	CB3	O2-CT	-2.14	1.22	1.30
2	D	615	UMP	C2-N1	2.13	1.40	1.38
3	C	612	CB3	O2-CT	-2.13	1.22	1.30
3	C	612	CB3	C13-C14	-2.11	1.35	1.39
3	D	616	CB3	C8-C8A	-2.10	1.36	1.40
2	C	611	UMP	C4-N3	2.09	1.40	1.37
2	E	619	UMP	C4-N3	2.08	1.40	1.37
2	B	607	UMP	C4-N3	2.07	1.40	1.37
5	E	622	NDP	C2N-C3N	2.07	1.38	1.34
3	C	612	CB3	C9-N10	-2.06	1.43	1.46
2	A	603	UMP	C2-N1	2.06	1.40	1.38
2	B	607	UMP	C2-N1	2.05	1.40	1.38
3	D	616	CB3	C13-C14	-2.03	1.35	1.39
2	D	615	UMP	C4-N3	2.01	1.40	1.37

All (193) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	608	CB3	CP2-CP1-N10	-10.59	102.94	112.90
3	C	612	CB3	CT-CA-N	9.04	133.83	110.53
5	D	618	NDP	N3A-C2A-N1A	-8.97	121.21	128.71
5	E	622	NDP	N3A-C2A-N1A	-8.86	121.31	128.71
5	C	614	NDP	N3A-C2A-N1A	-8.75	121.39	128.71
5	A	606	NDP	N3A-C2A-N1A	-8.73	121.41	128.71
5	B	610	NDP	N3A-C2A-N1A	-8.53	121.58	128.71
2	E	619	UMP	N3-C2-N1	7.58	122.30	115.97
3	A	604	CB3	CP2-CP1-N10	-7.08	106.24	112.90
2	D	615	UMP	N3-C2-N1	6.84	121.68	115.97
2	A	603	UMP	N3-C2-N1	6.75	121.60	115.97
2	B	607	UMP	N3-C2-N1	6.60	121.48	115.97
3	D	616	CB3	C8-C8A-C4A	-6.54	117.73	121.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	611	UMP	N3-C2-N1	6.33	121.25	115.97
3	A	604	CB3	C5-C4A-C8A	5.82	122.47	118.25
3	A	604	CB3	CP1-N10-C14	-5.64	108.06	118.63
3	C	612	CB3	CB-CA-N	-5.61	100.14	110.83
3	D	616	CB3	CP2-CP1-N10	-5.13	108.08	112.90
3	B	608	CB3	C6-C9-N10	-5.12	106.81	114.44
3	A	604	CB3	C13-C14-N10	-5.12	114.06	121.37
3	C	612	CB3	CG-CB-CA	-5.11	102.96	112.99
3	A	604	CB3	C8-C8A-C4A	-4.91	118.73	121.72
3	A	604	CB3	C11-C-N	4.90	125.06	116.89
3	A	604	CB3	CP1-N10-C9	4.61	123.72	115.68
2	D	615	UMP	C5-C6-N1	-4.45	116.18	121.21
5	D	618	NDP	PN-O3-PA	-4.45	118.65	131.68
2	A	603	UMP	C5-C6-N1	-4.43	116.20	121.21
3	A	604	CB3	C4-N3-C2	4.39	121.66	116.91
3	D	616	CB3	C5-C4A-C8A	4.35	121.40	118.25
3	C	612	CB3	C9-N10-C14	4.33	128.32	120.71
4	B	609	MTX	N1-C2-N3	-4.30	120.75	127.54
4	A	605	MTX	C6-C9-N10	-4.28	106.32	113.79
3	A	604	CB3	C9-N10-C14	4.27	128.22	120.71
3	D	616	CB3	C4A-C4-N3	-4.27	118.73	123.72
4	E	621	MTX	N1-C2-N3	-4.25	120.82	127.54
4	A	605	MTX	N1-C2-N3	-4.24	120.85	127.54
4	D	617	MTX	C6-C9-N10	-4.22	106.41	113.79
5	E	622	NDP	N3A-C4A-N9A	4.20	133.02	125.43
5	C	614	NDP	N3A-C4A-N9A	4.15	132.93	125.43
3	C	612	CB3	C11-C-N	-4.15	109.98	116.89
2	E	619	UMP	C5-C6-N1	-4.14	116.53	121.21
4	D	617	MTX	N1-C2-N3	-4.13	121.02	127.54
3	C	612	CB3	C13-C14-N10	-4.07	115.56	121.37
2	C	611	UMP	C5-C6-N1	-4.07	116.61	121.21
2	B	607	UMP	C5-C6-N1	-4.07	116.61	121.21
3	B	608	CB3	C4A-C4-N3	-4.06	118.97	123.72
5	A	606	NDP	N3A-C4A-N9A	4.05	132.74	125.43
4	B	609	MTX	C6-C9-N10	-4.02	106.76	113.79
5	D	618	NDP	N3A-C4A-N9A	3.98	132.63	125.43
4	C	613	MTX	C6-C9-N10	-3.95	106.89	113.79
4	C	613	MTX	N1-C2-N3	-3.94	121.31	127.54
3	A	604	CB3	O-C-N	-3.83	115.53	122.44
4	D	617	MTX	CB-CA-N	-3.83	103.54	110.83
5	B	610	NDP	N3A-C4A-N9A	3.82	132.33	125.43
5	C	614	NDP	PN-O3-PA	-3.82	120.49	131.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	612	CB3	C15-C14-N10	3.80	126.80	121.37
3	C	612	CB3	C5-C4A-C8A	3.72	120.94	118.25
3	A	604	CB3	C16-C11-C12	-3.67	113.39	118.63
4	C	613	MTX	C2-N1-C8A	3.67	120.16	115.30
3	E	620	CB3	C4A-C4-N3	-3.64	119.46	123.72
5	E	622	NDP	PN-O3-PA	-3.64	121.01	131.68
3	B	608	CB3	C13-C12-C11	-3.61	116.44	120.76
4	D	617	MTX	C2-N1-C8A	3.61	120.08	115.30
3	A	604	CB3	C15-C14-N10	3.60	126.52	121.37
3	E	620	CB3	CP2-CP1-N10	-3.59	109.53	112.90
4	E	621	MTX	C2-N1-C8A	3.55	120.01	115.30
4	B	609	MTX	C2-N1-C8A	3.53	119.98	115.30
4	E	621	MTX	C6-C9-N10	-3.52	107.64	113.79
4	A	605	MTX	C2-N1-C8A	3.51	119.95	115.30
3	D	616	CB3	C9-N10-C14	3.50	126.86	120.71
3	C	612	CB3	CB-CA-CT	-3.46	103.26	110.71
3	B	608	CB3	CB-CA-N	-3.46	104.25	110.83
4	A	605	MTX	CB-CA-N	-3.43	104.29	110.83
3	E	620	CB3	C4-N3-C2	3.37	120.55	116.91
3	E	620	CB3	C6-C9-N10	-3.37	109.43	114.44
3	B	608	CB3	C8-C8A-C4A	3.31	123.73	121.72
3	D	616	CB3	C4-N3-C2	3.25	120.42	116.91
3	B	608	CB3	C7-C6-C5	3.22	123.44	118.98
3	B	608	CB3	C5-C4A-C8A	-3.20	115.93	118.25
3	D	616	CB3	O-C-N	-3.18	116.70	122.44
3	C	612	CB3	NA2-C2-N1	-3.16	114.38	117.86
3	D	616	CB3	C11-C-N	3.16	122.15	116.89
3	A	604	CB3	C4A-C4-N3	-3.15	120.04	123.72
3	C	612	CB3	C8-C8A-C4A	-3.14	119.81	121.72
3	B	608	CB3	C9-N10-C14	3.11	126.17	120.71
5	A	606	NDP	PN-O3-PA	-3.09	122.61	131.68
4	B	609	MTX	N8-C8A-N1	3.09	120.35	116.19
3	B	608	CB3	C12-C13-C14	3.08	124.59	120.44
4	A	605	MTX	N8-C8A-N1	3.07	120.34	116.19
3	E	620	CB3	CB-CA-N	-3.06	105.00	110.83
3	B	608	CB3	CG-CB-CA	3.05	118.96	112.99
4	C	613	MTX	N8-C8A-N1	3.03	120.28	116.19
3	A	604	CB3	O2-CT-CA	3.00	125.16	113.90
5	E	622	NDP	C5A-C4A-N3A	-2.99	119.19	125.70
4	D	617	MTX	N8-C8A-N1	2.96	120.19	116.19
3	A	604	CB3	CB-CG-CD	-2.96	105.71	112.88
3	C	612	CB3	C6-C9-N10	-2.94	110.06	114.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	605	MTX	C13-C14-N10	-2.94	117.56	121.61
5	B	610	NDP	O4B-C1B-N9A	2.93	111.17	108.44
5	C	614	NDP	C5A-C4A-N3A	-2.86	119.48	125.70
4	C	613	MTX	C6-C7-N8	-2.84	120.17	123.16
4	B	609	MTX	C4-C4A-C8A	2.82	119.22	116.87
4	D	617	MTX	C4-C4A-C8A	2.81	119.22	116.87
3	E	620	CB3	C8-C8A-C4A	-2.80	120.01	121.72
3	B	608	CB3	C8-C7-C6	-2.77	116.30	121.12
5	D	618	NDP	C5A-C4A-N3A	-2.76	119.70	125.70
5	A	606	NDP	C5A-C4A-N3A	-2.75	119.71	125.70
3	E	620	CB3	C5-C4A-C8A	2.74	120.23	118.25
5	B	610	NDP	C5A-C4A-N3A	-2.74	119.74	125.70
4	C	613	MTX	CB-CA-N	-2.72	105.65	110.83
3	C	612	CB3	CA-N-C	2.68	127.78	121.80
4	E	621	MTX	C6-C7-N8	-2.68	120.34	123.16
4	E	621	MTX	N8-C8A-N1	2.68	119.81	116.19
2	E	619	UMP	O5'-P-OP1	2.67	114.54	106.71
4	C	613	MTX	C4-C4A-C8A	2.67	119.10	116.87
5	B	610	NDP	PN-O3-PA	-2.67	123.86	131.68
2	A	603	UMP	C5-C4-N3	2.66	121.72	116.70
3	B	608	CB3	CB-CA-CT	-2.66	105.00	110.71
4	A	605	MTX	C4-C4A-C8A	2.65	119.08	116.87
2	C	611	UMP	C5-C4-N3	2.62	121.65	116.70
3	A	604	CB3	CB-CA-CT	-2.62	105.08	110.71
3	D	616	CB3	C13-C14-N10	-2.62	117.63	121.37
4	D	617	MTX	C13-C14-N10	-2.61	118.01	121.61
4	C	613	MTX	C7-N8-C8A	2.61	119.78	116.85
5	A	606	NDP	C2B-C1B-N9A	-2.60	103.87	113.74
4	E	621	MTX	C4-C4A-C8A	2.59	119.03	116.87
4	A	605	MTX	CM-N10-C9	2.57	120.96	114.12
4	B	609	MTX	CB-CA-N	-2.57	105.94	110.83
4	D	617	MTX	C6-C7-N8	-2.55	120.47	123.16
4	B	609	MTX	CM-N10-C9	2.55	120.90	114.12
2	A	603	UMP	C6-N1-C2	2.52	123.02	119.51
2	B	607	UMP	C5-C4-N3	2.50	121.41	116.70
3	A	604	CB3	CG-CB-CA	2.49	117.87	112.99
4	A	605	MTX	C7-N8-C8A	2.49	119.64	116.85
2	D	615	UMP	C5-C4-N3	2.49	121.39	116.70
3	E	620	CB3	CP1-N10-C9	2.48	120.00	115.68
4	E	621	MTX	C7-N8-C8A	2.47	119.63	116.85
5	C	614	NDP	C3D-C2D-C1D	2.47	106.25	101.35
5	B	610	NDP	C4A-C5A-N7A	-2.46	107.42	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	609	MTX	C6-C7-N8	-2.45	120.58	123.16
5	D	618	NDP	C4A-C5A-N7A	-2.44	107.43	109.52
4	A	605	MTX	C6-C7-N8	-2.44	120.59	123.16
4	B	609	MTX	C7-N8-C8A	2.43	119.58	116.85
3	A	604	CB3	C15-C16-C11	2.43	123.66	120.76
2	C	611	UMP	O5'-P-OP1	2.42	113.80	106.71
5	C	614	NDP	C4A-C5A-N7A	-2.41	107.46	109.52
3	A	604	CB3	C6-C9-N10	-2.41	110.86	114.44
5	A	606	NDP	C5N-C4N-C3N	2.40	119.09	112.60
2	B	607	UMP	O5'-P-OP1	2.39	113.72	106.71
4	E	621	MTX	CB-CA-N	-2.38	106.29	110.83
4	C	613	MTX	C13-C14-N10	-2.37	118.34	121.61
2	A	603	UMP	O5'-P-OP1	2.37	113.67	106.71
3	C	612	CB3	O2-CT-CA	2.37	122.79	113.90
3	C	612	CB3	O-C-C11	2.36	125.15	121.01
5	D	618	NDP	C2B-C1B-N9A	-2.36	104.79	113.74
2	D	615	UMP	C6-N1-C2	2.35	122.78	119.51
3	A	604	CB3	NA2-C2-N1	2.33	120.43	117.86
5	B	610	NDP	C2B-C1B-N9A	-2.32	104.94	113.74
5	E	622	NDP	C2A-N3A-C4A	2.30	120.56	114.01
2	E	619	UMP	C5-C4-N3	2.29	121.03	116.70
2	C	611	UMP	C6-N1-C2	2.28	122.69	119.51
3	A	604	CB3	CB-CA-N	2.27	115.16	110.83
4	D	617	MTX	C7-N8-C8A	2.26	119.39	116.85
5	A	606	NDP	C4N-C3N-C2N	-2.25	118.94	121.68
5	C	614	NDP	C5N-C4N-C3N	2.23	118.66	112.60
3	C	612	CB3	C12-C13-C14	2.23	123.44	120.44
5	E	622	NDP	C4A-C5A-N7A	-2.22	107.62	109.52
5	B	610	NDP	C5N-C4N-C3N	2.21	118.59	112.60
2	B	607	UMP	C6-N1-C2	2.20	122.58	119.51
5	D	618	NDP	C2A-N3A-C4A	2.20	120.28	114.01
5	C	614	NDP	C2A-N3A-C4A	2.18	120.22	114.01
5	A	606	NDP	O3X-P2B-O2X	2.17	116.06	107.61
5	D	618	NDP	C8A-N9A-C4A	2.17	108.56	106.90
4	C	613	MTX	CM-N10-C9	2.15	119.85	114.12
3	C	612	CB3	C8-C8A-N1	2.13	122.67	120.38
5	A	606	NDP	C2A-N3A-C4A	2.13	120.07	114.01
5	A	606	NDP	C4A-C5A-N7A	-2.12	107.71	109.52
5	D	618	NDP	C5N-C4N-C3N	2.12	118.34	112.60
5	E	622	NDP	C5N-C4N-C3N	2.10	118.29	112.60
5	A	606	NDP	C8A-N9A-C4A	2.09	108.50	106.90
5	B	610	NDP	C2A-N3A-C4A	2.09	119.96	114.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	604	CB3	C13-C12-C11	2.09	123.25	120.76
5	E	622	NDP	C2B-C1B-N9A	-2.08	105.84	113.74
4	E	621	MTX	C13-C14-N10	-2.06	118.77	121.61
4	D	617	MTX	CM-N10-C9	2.06	119.61	114.12
2	D	615	UMP	O5'-P-OP1	2.05	112.73	106.71
3	B	608	CB3	C4A-C8A-N1	-2.05	116.56	120.18
3	D	616	CB3	CB-CA-CT	2.04	115.11	110.71
3	D	616	CB3	O2-CT-O1	-2.02	119.50	124.07
4	B	609	MTX	C13-C14-N10	-2.02	118.83	121.61
5	D	618	NDP	O3X-P2B-O2X	2.01	115.45	107.61
3	A	604	CB3	O2-CT-O1	-2.01	119.52	124.07
5	B	610	NDP	O3X-P2B-O2X	2.00	115.41	107.61

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	612	CB3	CA
3	E	620	CB3	CA

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	516/519 (99%)	-0.03	15 (2%)	49	50	26, 45, 92, 140	0
1	B	516/519 (99%)	-0.17	12 (2%)	57	58	23, 39, 77, 139	0
1	C	514/519 (99%)	0.12	30 (5%)	22	22	34, 60, 111, 148	0
1	D	515/519 (99%)	0.11	16 (3%)	47	47	36, 60, 103, 136	0
1	E	511/519 (98%)	0.79	71 (13%)	4	3	65, 101, 146, 167	0
All	All	2572/2595 (99%)	0.16	144 (5%)	24	23	23, 58, 123, 167	0

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	186	CYS	8.3
1	E	103	ASN	7.4
1	D	103	ASN	6.6
1	D	191	GLY	6.4
1	D	186	CYS	6.3
1	C	186	CYS	6.3
1	B	185	ASN	6.2
1	A	186	CYS	6.2
1	E	364	GLY	6.1
1	D	192	GLN	5.6
1	E	327	ARG	5.6
1	D	190	ARG	5.5
1	E	320	GLY	5.4
1	E	137	ALA	5.3
1	A	185	ASN	4.9
1	E	314	TYR	4.9
1	C	189	ALA	4.9
1	A	191	GLY	4.8
1	E	335	GLU	4.7
1	E	521	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	102	MET	4.5
1	C	191	GLY	4.4
1	A	341	ILE	4.3
1	C	101	LEU	4.2
1	D	100	ASN	4.2
1	E	181	LYS	4.1
1	E	321	SER	4.0
1	E	287	ALA	4.0
1	A	192	GLN	3.9
1	E	323	GLU	3.9
1	D	188	PRO	3.8
1	E	333	ARG	3.8
1	E	326	GLU	3.7
1	E	107	ILE	3.7
1	E	328	ILE	3.7
1	C	107	ILE	3.6
1	E	182	THR	3.6
1	A	100	ASN	3.6
1	E	357	HIS	3.6
1	E	330	LEU	3.5
1	C	188	PRO	3.5
1	C	53	ILE	3.4
1	E	319	ASN	3.4
1	E	324	TYR	3.4
1	A	188	PRO	3.4
1	E	334	GLU	3.3
1	A	189	ALA	3.3
1	E	102	MET	3.3
1	E	313	VAL	3.3
1	E	53	ILE	3.3
1	E	316	TRP	3.3
1	A	521	VAL	3.2
1	E	127	PHE	3.2
1	E	191	GLY	3.2
1	C	102	MET	3.1
1	B	103	ASN	3.1
1	C	47	ASN	3.1
1	C	4	LYS	3.1
1	C	105	ASP	3.1
1	E	91	PHE	3.1
1	B	188	PRO	3.1
1	E	5	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	310	GLU	3.1
1	E	192	GLN	3.1
1	C	3	GLU	3.1
1	E	516	LYS	3.1
1	B	192	GLN	3.0
1	C	190	ARG	3.0
1	E	336	ASN	3.0
1	E	84	ALA	3.0
1	A	102	MET	3.0
1	D	107	ILE	2.9
1	E	325	LEU	2.9
1	E	101	LEU	2.8
1	C	98	ILE	2.8
1	E	329	GLY	2.8
1	C	192	GLN	2.8
1	E	489	PHE	2.8
1	E	309	ILE	2.8
1	E	322	LYS	2.7
1	C	84	ALA	2.7
1	C	94	LEU	2.7
1	D	101	LEU	2.7
1	E	306	ASN	2.7
1	E	399	LEU	2.7
1	C	100	ASN	2.7
1	A	171	ASP	2.7
1	E	360	TYR	2.7
1	C	110	ILE	2.7
1	D	330	LEU	2.7
1	E	100	ASN	2.6
1	C	187	ASP	2.6
1	D	105	ASP	2.6
1	E	124	LYS	2.6
1	B	180	LYS	2.6
1	B	84	ALA	2.6
1	C	45	ASP	2.6
1	E	358	ASP	2.5
1	B	179	GLU	2.5
1	E	288	ILE	2.5
1	D	181	LYS	2.5
1	C	93	ASN	2.5
1	A	179	GLU	2.5
1	D	189	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	281	LEU	2.4
1	E	363	VAL	2.4
1	C	86	PRO	2.4
1	E	496	ILE	2.4
1	D	338	LEU	2.4
1	A	180	LYS	2.4
1	E	400	PRO	2.4
1	C	71	ILE	2.4
1	C	74	VAL	2.4
1	E	308	LEU	2.4
1	C	49	LYS	2.4
1	D	127	PHE	2.4
1	E	75	ILE	2.3
1	A	190	ARG	2.3
1	A	187	ASP	2.3
1	E	116	GLU	2.3
1	E	147	PHE	2.3
1	C	123	LEU	2.3
1	D	521	VAL	2.2
1	E	138	LEU	2.2
1	E	106	SER	2.2
1	E	429	LEU	2.2
1	E	365	VAL	2.2
1	E	312	LYS	2.2
1	B	191	GLY	2.1
1	E	332	HIS	2.1
1	B	181	LYS	2.1
1	B	82	ASP	2.1
1	E	105	ASP	2.1
1	E	175	PHE	2.1
1	C	106	SER	2.1
1	E	506	LEU	2.1
1	C	81	GLN	2.0
1	E	337	ASP	2.0
1	E	359	ASP	2.0
1	E	3	GLU	2.0
1	E	293	GLU	2.0
1	C	127	PHE	2.0
1	E	315	ILE	2.0
1	E	311	LYS	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	CB3	D	616	35/35	0.32	3.12	107,110,114,115	0
3	CB3	A	604	35/35	0.29	2.76	68,77,89,90	0
3	CB3	E	620	35/35	0.51	2.17	131,134,135,135	0
3	CB3	C	612	35/35	0.23	1.86	59,71,80,82	0
4	MTX	C	613	33/33	0.27	1.86	75,83,87,87	0
3	CB3	B	608	35/35	0.20	1.56	44,52,63,66	0
4	MTX	E	621	33/33	0.24	1.31	96,102,103,104	0
4	MTX	D	617	33/33	0.20	1.24	61,68,71,71	0
4	MTX	B	609	33/33	0.18	0.96	44,50,51,54	0
4	MTX	A	605	33/33	0.18	0.86	42,48,50,52	0
5	NDP	C	614	48/48	0.23	0.43	92,96,111,112	0
2	UMP	B	607	20/20	0.17	0.09	37,43,46,50	0
2	UMP	C	611	20/20	0.18	0.08	44,62,68,70	0
2	UMP	D	615	20/20	0.17	-0.31	77,82,86,88	0
5	NDP	D	618	48/48	0.16	-0.49	49,64,75,75	0
5	NDP	E	622	48/48	0.17	-0.55	85,89,105,106	0
5	NDP	A	606	48/48	0.14	-0.69	41,46,50,50	0
2	UMP	E	619	20/20	0.18	-0.70	125,131,135,135	0
5	NDP	B	610	48/48	0.14	-0.83	33,41,45,46	0
2	UMP	A	603	20/20	0.16	-0.92	53,58,63,68	0

6.5 Other polymers ⓘ

There are no such residues in this entry.