



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:13 AM UTC

PDB ID : 3TAZ / pdb_00003taz
Title : Crystal structure of NurA bound to dAMP and manganese
Authors : Chae, J.; Kim, Y.C.; Cho, Y.
Deposited on : 2011-08-04
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

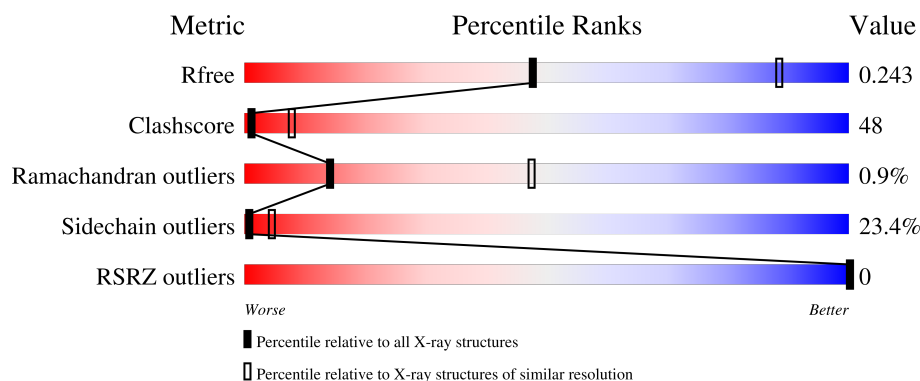
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	471	31% 45% 14% • 8%
1	B	471	30% 47% 14% • 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	D5M	B	453	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7020 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA double-strand break repair protein nurA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	432	Total	C	N	O	S	0	0	0
			3487	2235	597	648	7			
1	B	433	Total	C	N	O	S	0	0	0
			3494	2240	597	650	7			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q8U1N8
A	-18	GLY	-	expression tag	UNP Q8U1N8
A	-17	SER	-	expression tag	UNP Q8U1N8
A	-16	SER	-	expression tag	UNP Q8U1N8
A	-15	HIS	-	expression tag	UNP Q8U1N8
A	-14	HIS	-	expression tag	UNP Q8U1N8
A	-13	HIS	-	expression tag	UNP Q8U1N8
A	-12	HIS	-	expression tag	UNP Q8U1N8
A	-11	HIS	-	expression tag	UNP Q8U1N8
A	-10	HIS	-	expression tag	UNP Q8U1N8
A	-9	SER	-	expression tag	UNP Q8U1N8
A	-8	SER	-	expression tag	UNP Q8U1N8
A	-7	GLY	-	expression tag	UNP Q8U1N8
A	-6	LEU	-	expression tag	UNP Q8U1N8
A	-5	VAL	-	expression tag	UNP Q8U1N8
A	-4	PRO	-	expression tag	UNP Q8U1N8
A	-3	ARG	-	expression tag	UNP Q8U1N8
A	-2	GLY	-	expression tag	UNP Q8U1N8
A	-1	SER	-	expression tag	UNP Q8U1N8
A	0	HIS	-	expression tag	UNP Q8U1N8
B	-19	MET	-	expression tag	UNP Q8U1N8
B	-18	GLY	-	expression tag	UNP Q8U1N8
B	-17	SER	-	expression tag	UNP Q8U1N8
B	-16	SER	-	expression tag	UNP Q8U1N8
B	-15	HIS	-	expression tag	UNP Q8U1N8

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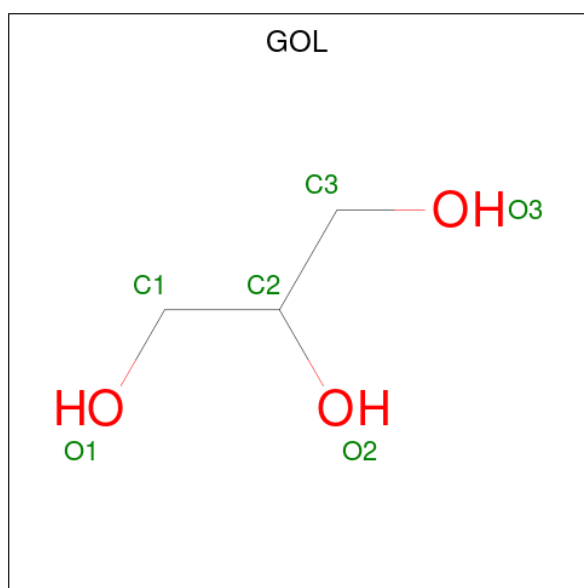
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP Q8U1N8
B	-13	HIS	-	expression tag	UNP Q8U1N8
B	-12	HIS	-	expression tag	UNP Q8U1N8
B	-11	HIS	-	expression tag	UNP Q8U1N8
B	-10	HIS	-	expression tag	UNP Q8U1N8
B	-9	SER	-	expression tag	UNP Q8U1N8
B	-8	SER	-	expression tag	UNP Q8U1N8
B	-7	GLY	-	expression tag	UNP Q8U1N8
B	-6	LEU	-	expression tag	UNP Q8U1N8
B	-5	VAL	-	expression tag	UNP Q8U1N8
B	-4	PRO	-	expression tag	UNP Q8U1N8
B	-3	ARG	-	expression tag	UNP Q8U1N8
B	-2	GLY	-	expression tag	UNP Q8U1N8
B	-1	SER	-	expression tag	UNP Q8U1N8
B	0	HIS	-	expression tag	UNP Q8U1N8

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

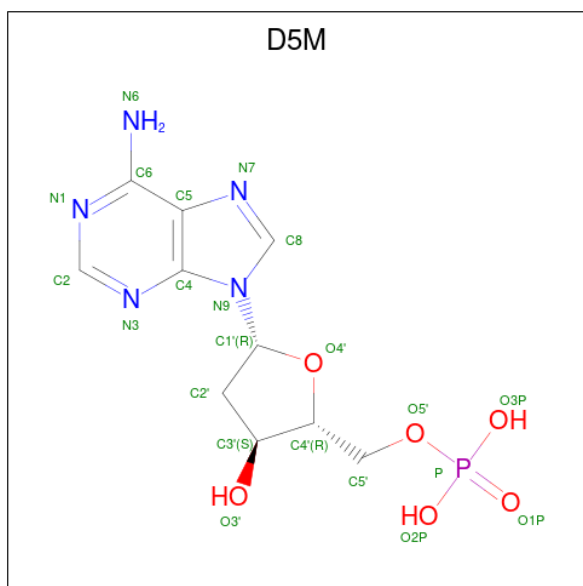
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mn 1 1	0	0
2	B	1	Total Mn 1 1	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is 2'-DEOXYADENOSINE-5'-MONOPHOSPHATE (CCD ID: D5M) (formula: $C_{10}H_{14}N_5O_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

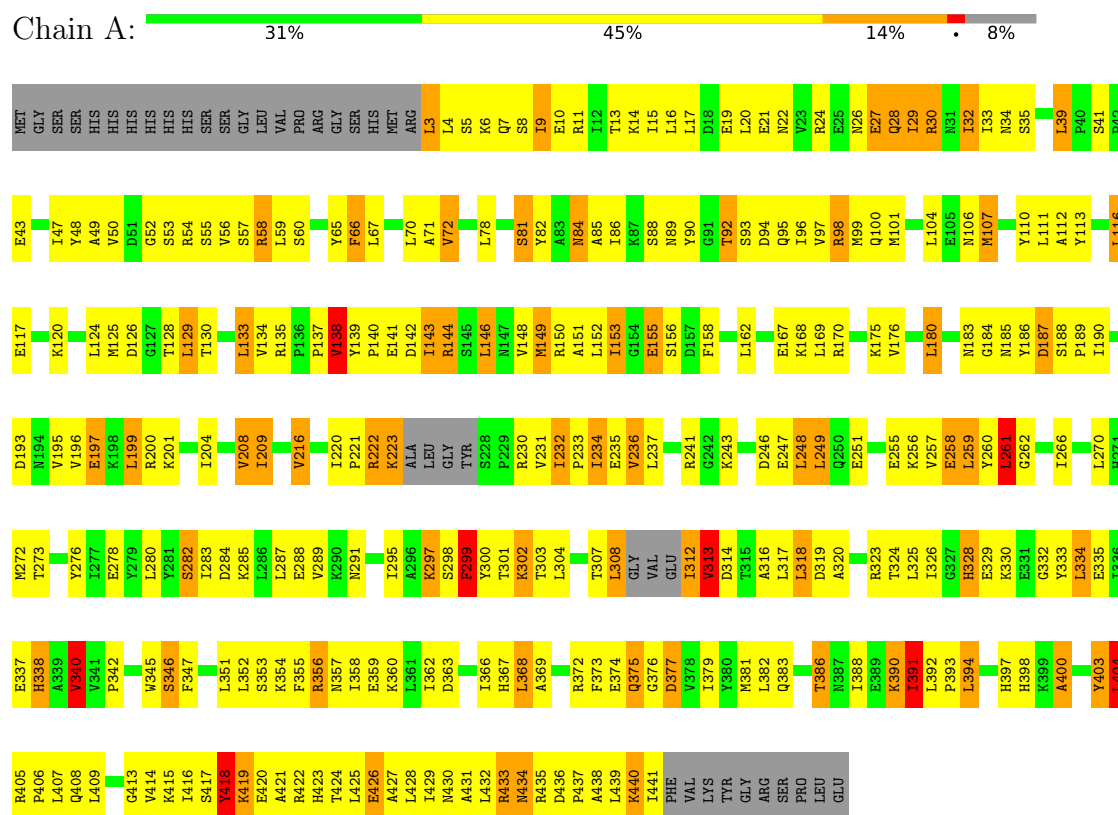
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	5	Total	O	0	0
			5	5		
5	B	4	Total	O	0	0
			4	4		

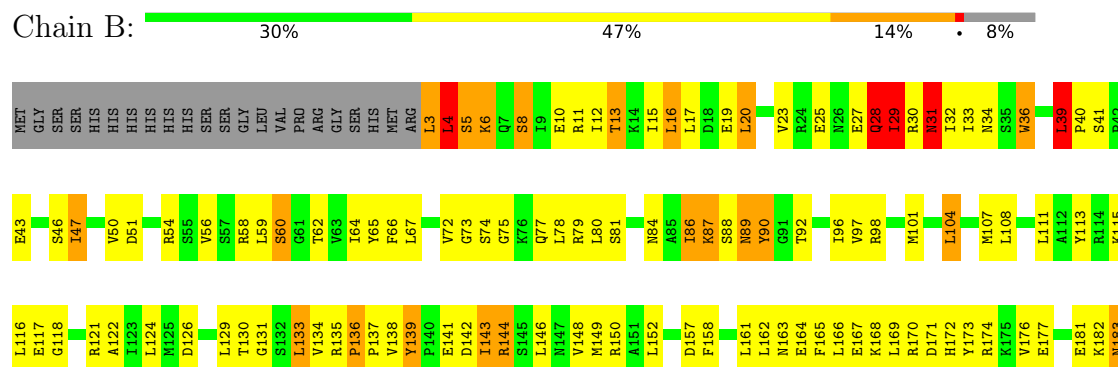
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: DNA double-strand break repair protein nurA



- Molecule 1: DNA double-strand break repair protein nurA





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.16Å 114.85Å 123.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.71 – 3.20 28.71 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.1 (28.71-3.20) 97.1 (28.71-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.191 , 0.279 (Not available) , 0.243	Depositor DCC
R_{free} test set	798 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	98.5	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 103.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7020	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MN, D5M

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	0.66	0/3546	1.07	14/4784 (0.3%)
1	B	0.60	0/3553	1.05	18/4796 (0.4%)
All	All	0.63	0/7099	1.06	32/9580 (0.3%)

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	B	0	3
All	All	0	6

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	88	SER	N-CA-C	7.12	120.53	109.07
1	B	39	LEU	N-CA-C	7.07	118.81	109.83
1	A	313	VAL	CB-CA-C	-6.65	105.49	111.74
1	B	60	SER	CB-CA-C	-6.51	109.05	116.54
1	A	404	LEU	N-CA-C	6.43	119.80	110.28
1	A	391	ILE	N-CA-C	6.36	116.52	110.42
1	B	136	PRO	CA-C-N	-6.25	113.11	120.11
1	B	136	PRO	C-N-CA	-6.25	113.11	120.11
1	A	375	GLN	CB-CA-C	-6.25	109.35	116.54
1	A	418	TYR	N-CA-C	-6.23	102.14	110.55
1	B	434	ASN	N-CA-C	6.12	118.73	108.02
1	B	139	TYR	CA-C-N	-5.86	112.51	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	139	TYR	C-N-CA	-5.86	112.51	119.84
1	B	437	PRO	N-CA-C	-5.86	105.38	113.53
1	A	155	GLU	N-CA-C	5.67	117.15	110.97
1	B	216	VAL	N-CA-C	5.64	114.58	107.70
1	B	339	ALA	N-CA-C	-5.63	101.97	110.24
1	A	261	LEU	N-CA-C	5.55	117.46	110.24
1	A	440	LYS	N-CA-C	-5.52	104.61	113.28
1	A	299	PHE	N-CA-C	-5.48	101.17	108.74
1	A	434	ASN	N-CA-C	5.47	117.21	108.41
1	A	84	ASN	N-CA-C	5.31	115.37	107.88
1	B	28	GLN	N-CA-C	-5.29	104.35	111.54
1	B	417	SER	N-CA-C	-5.28	106.83	113.28
1	A	340	VAL	N-CA-C	5.27	115.55	108.17
1	B	4	LEU	N-CA-C	5.27	122.02	110.80
1	B	266	ILE	CB-CA-C	-5.26	105.24	111.97
1	A	262	GLY	N-CA-C	5.22	118.64	111.54
1	B	89	ASN	N-CA-C	-5.21	100.75	109.24
1	B	412	HIS	N-CA-C	5.11	116.85	111.28
1	A	208	VAL	N-CA-C	5.11	117.08	108.81
1	B	352	LEU	N-CA-C	5.08	117.48	111.33

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3	LEU	Peptide
1	A	400	ALA	Peptide
1	A	417	SER	Peptide
1	B	374	GLU	Peptide
1	B	400	ALA	Peptide
1	B	8	SER	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3487	0	3609	344	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3494	0	3610	399	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	6	0	8	2	0
4	B	22	0	12	12	0
5	A	5	0	0	3	0
5	B	4	0	0	0	0
All	All	7020	0	7239	690	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 48.

All (690) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:ILE:CG2	1:B:378:VAL:HG21	1.69	1.21
1:A:441:ILE:HG21	1:B:378:VAL:CG2	1.71	1.19
1:B:310:VAL:HG22	1:B:311:GLU:H	1.09	1.11
1:B:229:PRO:HA	1:B:230:ARG:HB2	1.27	1.10
1:A:419:LYS:H	1:A:419:LYS:HD2	1.13	1.10
1:A:347:PHE:HB3	1:A:352:LEU:HD11	1.26	1.09
1:A:314:ASP:OD1	1:B:60:SER:HB3	1.54	1.08
1:A:230:ARG:HB3	1:B:234:ILE:HB	1.37	1.04
1:B:378:VAL:HG22	1:B:379:ILE:H	0.88	1.01
1:B:378:VAL:HG22	1:B:379:ILE:N	1.72	1.00
1:B:130:THR:HG23	1:B:383:GLN:HE22	1.29	0.98
1:B:378:VAL:CG2	1:B:379:ILE:H	1.75	0.97
1:B:162:LEU:HD21	1:B:354:LYS:HG3	1.47	0.96
1:A:435:ARG:HE	1:A:439:LEU:HD21	1.26	0.95
1:A:421:ALA:HA	1:A:424:THR:OG1	1.68	0.93
1:B:284:ASP:HB2	1:B:355:PHE:HB3	1.50	0.92
1:A:27:GLU:CD	1:A:27:GLU:H	1.78	0.92
1:A:54:ARG:HB3	1:A:101:MET:HE2	1.53	0.89
1:A:368:LEU:HB3	1:A:381:MET:HE1	1.54	0.89
1:A:236:VAL:HG23	1:A:259:LEU:HD11	1.56	0.87
1:A:441:ILE:HG21	1:B:378:VAL:HG21	0.89	0.87
1:B:138:VAL:HG22	1:B:141:GLU:HB3	1.54	0.87
1:A:302:LYS:HG2	1:B:89:ASN:ND2	1.90	0.87
1:B:259:LEU:HD23	1:B:260:TYR:N	1.89	0.87
1:B:310:VAL:HG22	1:B:311:GLU:N	1.89	0.86
1:B:419:LYS:HD2	1:B:422:ARG:HG3	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:ALA:HB1	1:B:434:ASN:ND2	1.91	0.86
1:A:302:LYS:HG2	1:B:89:ASN:HD21	1.39	0.85
1:B:131:GLY:HA3	4:B:453:D5M:H1	1.58	0.85
1:A:27:GLU:HG2	1:A:28:GLN:H	1.41	0.84
1:A:435:ARG:NE	1:A:439:LEU:HD21	1.91	0.83
1:B:144:ARG:O	1:B:148:VAL:HG23	1.79	0.83
1:B:422:ARG:NH1	1:B:423:HIS:HE1	1.76	0.83
1:A:295:ILE:HD11	1:A:382:LEU:HD13	1.61	0.82
1:B:135:ARG:NH2	1:B:306:ARG:HH12	1.76	0.82
1:B:229:PRO:HA	1:B:230:ARG:CB	2.10	0.82
1:A:419:LYS:HD2	1:A:419:LYS:N	1.95	0.81
1:B:130:THR:HG23	1:B:383:GLN:NE2	1.94	0.81
1:A:220:ILE:O	1:A:220:ILE:HD12	1.81	0.81
1:B:67:LEU:HD22	1:B:101:MET:HE2	1.63	0.81
1:A:53:SER:O	1:A:101:MET:HE1	1.80	0.80
1:A:325:LEU:HB3	1:A:326:ILE:HD12	1.64	0.79
1:B:29:ILE:HG12	1:B:33:ILE:HD13	1.65	0.79
1:A:162:LEU:HD21	1:A:354:LYS:HG3	1.65	0.79
1:B:27:GLU:OE2	1:B:30:ARG:HD2	1.83	0.78
1:A:129:LEU:HD13	1:A:366:ILE:HG12	1.65	0.78
1:A:144:ARG:HA	1:B:229:PRO:HG3	1.64	0.77
1:A:153:ILE:HD11	1:A:158:PHE:HA	1.67	0.77
1:B:421:ALA:HA	1:B:424:THR:OG1	1.85	0.77
1:B:222:ARG:HG3	1:B:223:LYS:HD3	1.67	0.77
1:B:419:LYS:H	1:B:419:LYS:HE2	1.50	0.76
1:B:241:ARG:HG2	1:B:242:GLY:H	1.49	0.76
1:B:29:ILE:HD11	1:B:326:ILE:HD11	1.68	0.75
1:B:342:PRO:HD2	1:B:362:ILE:HA	1.66	0.75
1:A:419:LYS:H	1:A:419:LYS:CD	1.95	0.75
1:B:12:ILE:O	1:B:15:ILE:HG22	1.85	0.75
1:A:427:ALA:O	1:A:430:ASN:HB2	1.86	0.75
1:B:86:ILE:CD1	1:B:87:LYS:HG2	2.16	0.75
1:B:150:ARG:NH2	1:B:350:PHE:CG	2.54	0.75
1:B:170:ARG:HH21	1:B:174:ARG:HH22	1.35	0.75
1:A:9:ILE:O	1:A:13:THR:HG23	1.86	0.74
1:A:170:ARG:HD2	1:A:170:ARG:O	1.87	0.74
1:B:229:PRO:CA	1:B:230:ARG:HB2	2.12	0.74
1:A:139:TYR:CD1	1:A:140:PRO:HA	2.23	0.74
1:A:302:LYS:CE	1:B:87:LYS:HG3	2.17	0.74
1:B:375:GLN:HG3	1:B:376:GLY:H	1.52	0.74
1:B:137:PRO:HG3	4:B:453:D5M:HN62	1.51	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:ARG:O	1:B:32:ILE:HG12	1.88	0.73
1:B:144:ARG:HD3	1:B:225:LEU:HD11	1.70	0.73
1:B:426:GLU:CD	1:B:426:GLU:H	1.96	0.73
1:A:230:ARG:HB3	1:B:234:ILE:CB	2.16	0.73
1:A:39:LEU:HD13	1:A:332:GLY:HA2	1.71	0.73
1:A:320:ALA:HA	1:B:436:ASP:OD2	1.89	0.73
1:A:441:ILE:O	1:A:441:ILE:HG22	1.87	0.73
1:B:144:ARG:HB2	1:B:225:LEU:CD1	2.19	0.72
1:B:130:THR:H	1:B:383:GLN:HE22	1.36	0.72
1:A:302:LYS:HE2	1:B:87:LYS:HG3	1.71	0.72
1:B:419:LYS:O	1:B:422:ARG:HB2	1.89	0.72
1:A:303:THR:HG22	1:A:307:THR:OG1	1.89	0.72
1:B:176:VAL:HG22	1:B:186:TYR:HE2	1.54	0.71
1:A:16:LEU:O	1:A:19:GLU:HB2	1.91	0.71
1:A:300:TYR:CG	1:A:301:THR:N	2.58	0.71
1:A:104:LEU:HD22	1:A:189:PRO:HB2	1.73	0.70
1:B:319:ASP:HA	1:B:379:ILE:CD1	2.21	0.70
1:A:6:LYS:HA	1:A:9:ILE:HB	1.74	0.70
1:B:342:PRO:CD	1:B:362:ILE:HA	2.21	0.70
1:A:232:ILE:HG13	1:B:232:ILE:HG23	1.73	0.70
1:B:217:LYS:HD3	1:B:260:TYR:CE2	2.27	0.70
1:B:176:VAL:HG13	1:B:186:TYR:HD2	1.55	0.69
1:B:137:PRO:HG3	4:B:453:D5M:N1	2.08	0.69
1:A:302:LYS:HE2	1:B:87:LYS:HZ3	1.56	0.69
1:A:320:ALA:HB1	1:B:434:ASN:HD21	1.55	0.69
1:A:300:TYR:C	1:A:304:LEU:HD12	2.17	0.69
1:B:336:ILE:HG12	1:B:368:LEU:HB2	1.75	0.69
1:A:358:ILE:O	1:A:362:ILE:HG12	1.92	0.69
1:B:4:LEU:C	1:B:6:LYS:H	1.99	0.69
1:B:162:LEU:CD2	1:B:166:LEU:HD11	2.23	0.68
1:B:392:LEU:HB3	1:B:393:PRO:HD3	1.75	0.68
1:B:220:ILE:HB	1:B:221:PRO:HD2	1.75	0.68
1:A:135:ARG:HH22	1:B:90:TYR:H	1.41	0.68
1:A:8:SER:CB	1:A:11:ARG:NH2	2.57	0.68
1:A:325:LEU:CB	1:A:326:ILE:HD12	2.23	0.68
1:B:333:TYR:HB2	1:B:371:VAL:HG22	1.77	0.67
1:B:118:GLY:H	1:B:121:ARG:NH2	1.91	0.67
1:B:86:ILE:HD12	1:B:87:LYS:HG2	1.77	0.67
1:A:314:ASP:OD1	1:B:60:SER:CB	2.39	0.67
1:A:375:GLN:HG3	1:A:376:GLY:H	1.58	0.67
1:B:342:PRO:HG2	1:B:362:ILE:HD13	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:ASP:OD1	1:B:378:VAL:N	2.26	0.67
1:B:335:GLU:HG3	1:B:388:ILE:HG13	1.77	0.67
1:B:176:VAL:HG13	1:B:186:TYR:CD2	2.30	0.66
1:A:241:ARG:O	1:B:246:ASP:OD2	2.13	0.66
1:B:196:VAL:HG23	1:B:274:LEU:HD12	1.76	0.66
1:B:310:VAL:CG2	1:B:311:GLU:H	1.93	0.66
1:A:149:MET:HE1	1:A:204:ILE:HD11	1.76	0.66
1:A:249:LEU:HD21	1:B:237:LEU:HB3	1.78	0.66
1:B:30:ARG:HG2	1:B:32:ILE:HG12	1.76	0.66
1:B:138:VAL:HG13	1:B:138:VAL:O	1.95	0.66
1:B:375:GLN:HG3	1:B:376:GLY:N	2.09	0.66
1:A:435:ARG:HH21	1:A:439:LEU:HD11	1.59	0.66
4:B:453:D5M:N3	4:B:453:D5M:H2'2	2.10	0.66
1:B:323:ARG:NH1	1:B:329:GLU:HG3	2.11	0.65
1:A:49:ALA:HA	1:A:124:LEU:HB3	1.78	0.65
1:B:67:LEU:CD2	1:B:101:MET:HE2	2.25	0.65
1:A:426:GLU:CD	1:A:426:GLU:H	2.03	0.65
1:A:302:LYS:CG	1:B:89:ASN:HD21	2.09	0.65
1:B:162:LEU:CD2	1:B:354:LYS:HG3	2.23	0.65
1:B:299:PHE:HD1	1:B:299:PHE:H	1.43	0.65
1:B:137:PRO:O	1:B:138:VAL:HG12	1.96	0.65
1:A:39:LEU:HD13	1:A:332:GLY:CA	2.27	0.65
1:B:325:LEU:HB3	1:B:326:ILE:HD12	1.78	0.65
1:B:56:VAL:HG12	1:B:65:TYR:HB3	1.78	0.64
1:B:436:ASP:O	1:B:439:LEU:HB2	1.97	0.64
1:A:312:ILE:C	1:A:313:VAL:HG12	2.22	0.64
1:B:135:ARG:HH21	1:B:306:ARG:HH12	1.45	0.64
1:B:420:GLU:O	1:B:424:THR:HG23	1.98	0.64
1:B:392:LEU:O	1:B:396:LEU:HD12	1.97	0.64
1:B:176:VAL:HG22	1:B:186:TYR:CE2	2.32	0.64
1:A:120:LYS:NZ	1:A:390:LYS:HE2	2.12	0.64
1:A:176:VAL:HG22	1:A:186:TYR:CE2	2.33	0.64
1:B:152:LEU:HG	1:B:207:LYS:HE2	1.79	0.63
1:B:440:LYS:HE3	1:B:440:LYS:HA	1.79	0.63
1:A:5:SER:C	1:A:7:GLN:H	2.05	0.63
1:B:173:TYR:CE1	1:B:281:TYR:HE2	2.17	0.63
1:A:104:LEU:CD2	1:A:189:PRO:HB2	2.28	0.63
1:B:322:ILE:CD1	1:B:323:ARG:HG3	2.28	0.63
1:B:144:ARG:HB2	1:B:225:LEU:HD11	1.80	0.63
1:B:4:LEU:C	1:B:6:LYS:N	2.57	0.62
1:B:245:VAL:HG12	1:B:249:LEU:HD12	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:TRP:CD1	1:B:345:TRP:C	2.77	0.62
1:A:372:ARG:HD3	1:A:375:GLN:O	1.99	0.62
1:A:295:ILE:CD1	1:A:382:LEU:HD13	2.29	0.62
1:A:124:LEU:HD21	1:A:404:LEU:HD12	1.81	0.62
1:B:86:ILE:HD12	1:B:87:LYS:H	1.64	0.62
1:B:228:SER:H	1:B:230:ARG:HG2	1.64	0.62
1:A:3:LEU:HD11	1:B:66:PHE:CZ	2.34	0.62
1:B:8:SER:HB2	1:B:11:ARG:NH2	2.15	0.62
1:B:355:PHE:CB	1:B:358:ILE:HD12	2.30	0.62
1:A:135:ARG:HH22	1:B:90:TYR:HB2	1.65	0.61
1:A:222:ARG:HA	1:A:230:ARG:NH1	2.15	0.61
1:A:142:ASP:OD2	1:A:143:ILE:HD13	1.99	0.61
1:B:115:LYS:HE2	1:B:181:GLU:OE2	2.00	0.61
1:B:98:ARG:HG2	4:B:453:D5M:HN61	1.63	0.61
1:B:342:PRO:HG2	1:B:362:ILE:HA	1.83	0.61
1:A:104:LEU:HD22	1:A:189:PRO:CB	2.30	0.61
1:B:399:LYS:HA	1:B:404:LEU:HA	1.81	0.61
1:B:422:ARG:HH11	1:B:423:HIS:HE1	1.48	0.61
1:B:436:ASP:HA	1:B:439:LEU:HD12	1.80	0.61
1:A:11:ARG:O	1:A:15:ILE:HG13	1.99	0.61
1:B:165:PHE:HD2	1:B:277:ILE:HG21	1.66	0.61
1:A:104:LEU:HA	1:A:107:MET:HE2	1.82	0.61
1:B:374:GLU:HB3	1:B:375:GLN:HG2	1.82	0.61
1:A:32:ILE:HG22	1:A:33:ILE:HD13	1.83	0.61
1:A:241:ARG:HD3	1:B:246:ASP:OD1	2.00	0.61
1:B:86:ILE:HD11	1:B:87:LYS:HG2	1.82	0.61
1:B:284:ASP:CB	1:B:355:PHE:HB3	2.25	0.61
1:A:144:ARG:O	1:A:148:VAL:HG23	2.01	0.61
1:A:313:VAL:HG23	1:A:314:ASP:N	2.16	0.61
1:A:89:ASN:HB2	1:A:92:THR:HB	1.83	0.61
1:A:24:ARG:HH21	1:A:325:LEU:HD21	1.65	0.61
1:B:137:PRO:HG3	4:B:453:D5M:N6	2.14	0.60
1:A:419:LYS:HB2	1:A:422:ARG:HB2	1.83	0.60
1:A:60:SER:HB2	1:B:314:ASP:OD1	2.01	0.60
1:A:106:ASN:HB2	1:A:282:SER:OG	2.01	0.60
1:B:412:HIS:HA	1:B:415:LYS:HE2	1.83	0.60
1:B:310:VAL:O	1:B:312:ILE:HG23	2.02	0.60
1:B:440:LYS:HA	1:B:440:LYS:CE	2.31	0.60
1:A:308:LEU:HD23	1:A:308:LEU:H	1.67	0.60
1:A:392:LEU:HB3	1:A:393:PRO:HD3	1.82	0.60
1:B:6:LYS:HD3	1:B:6:LYS:C	2.26	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:VAL:HG12	1:B:199:LEU:HD23	1.82	0.60
1:B:58:ARG:O	1:B:59:LEU:HD23	2.01	0.60
1:B:258:GLU:O	1:B:259:LEU:HB2	2.02	0.59
1:B:80:LEU:HG	1:B:108:LEU:HD13	1.84	0.59
1:B:374:GLU:C	1:B:375:GLN:HG2	2.27	0.59
1:A:3:LEU:O	1:A:4:LEU:HG	2.01	0.59
1:A:439:LEU:O	1:A:440:LYS:HB3	2.01	0.59
1:B:16:LEU:O	1:B:19:GLU:HB2	2.02	0.59
1:B:336:ILE:HG13	1:B:368:LEU:O	2.03	0.59
1:A:85:ALA:O	1:B:15:ILE:HD13	2.03	0.59
1:A:308:LEU:HD23	1:A:308:LEU:N	2.18	0.59
1:B:29:ILE:O	1:B:33:ILE:HD12	2.02	0.59
1:A:291:ASN:HB3	1:A:391:ILE:HD11	1.85	0.59
1:A:369:ALA:HB2	1:A:388:ILE:HG13	1.85	0.59
1:B:319:ASP:HA	1:B:379:ILE:HD11	1.83	0.59
1:B:135:ARG:HH21	1:B:306:ARG:NH1	2.00	0.59
1:A:195:VAL:HG22	1:A:199:LEU:HD22	1.84	0.59
1:A:441:ILE:CG1	1:B:378:VAL:HG11	2.33	0.59
1:A:170:ARG:NH1	5:A:458:HOH:O	2.22	0.58
1:A:259:LEU:HD23	1:A:261:LEU:HD21	1.85	0.58
1:A:96:ILE:HD11	1:A:272:MET:CE	2.33	0.58
1:A:152:LEU:HD21	1:A:266:ILE:CD1	2.32	0.58
1:A:313:VAL:HG23	1:A:314:ASP:O	2.03	0.58
1:A:318:LEU:HD23	1:A:319:ASP:N	2.18	0.58
1:A:381:MET:HE3	1:A:383:GLN:HE21	1.68	0.58
1:A:439:LEU:C	1:A:441:ILE:H	2.11	0.58
1:B:17:LEU:HA	1:B:20:LEU:HG	1.85	0.58
1:B:259:LEU:HD23	1:B:260:TYR:H	1.69	0.58
1:A:120:LYS:NZ	1:A:394:LEU:HD11	2.19	0.58
1:B:54:ARG:HB3	1:B:101:MET:CE	2.34	0.58
1:B:319:ASP:HA	1:B:379:ILE:HD12	1.85	0.58
1:B:28:GLN:O	1:B:29:ILE:HG22	2.04	0.58
1:A:169:LEU:HD21	1:A:278:GLU:HG3	1.85	0.58
1:A:146:LEU:HD11	1:A:273:THR:HG23	1.86	0.57
1:B:17:LEU:O	1:B:20:LEU:HG	2.04	0.57
1:B:4:LEU:O	1:B:6:LYS:N	2.37	0.57
1:B:113:TYR:CG	1:B:289:VAL:HG22	2.40	0.57
1:B:131:GLY:HA3	4:B:453:D5M:C3'	2.32	0.57
1:B:201:LYS:HA	1:B:205:ASP:HB2	1.87	0.57
1:A:43:GLU:O	1:A:397:HIS:HB2	2.04	0.57
1:B:215:LYS:O	1:B:216:VAL:HG13	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:SER:HB2	1:A:8:SER:H	1.69	0.57
1:B:77:GLN:C	1:B:78:LEU:HD23	2.30	0.57
1:A:95:GLN:HB3	1:A:138:VAL:HG22	1.86	0.56
1:A:314:ASP:CG	1:B:60:SER:HB3	2.30	0.56
1:A:24:ARG:HH21	1:A:325:LEU:CD2	2.17	0.56
1:B:8:SER:HA	1:B:11:ARG:NH1	2.19	0.56
1:B:113:TYR:OH	1:B:290:LYS:HB2	2.04	0.56
1:A:66:PHE:CZ	1:A:421:ALA:HB3	2.40	0.56
1:A:342:PRO:HD2	1:A:362:ILE:HA	1.87	0.56
1:B:200:ARG:O	1:B:204:ILE:HB	2.06	0.56
1:B:323:ARG:HH11	1:B:329:GLU:HG3	1.70	0.56
1:A:413:GLY:O	1:A:416:ILE:HB	2.06	0.56
1:B:287:LEU:HB2	1:B:357:ASN:HB3	1.86	0.56
1:A:3:LEU:HD12	1:A:4:LEU:HA	1.88	0.56
1:B:279:TYR:CE2	1:B:283:ILE:HD11	2.41	0.56
1:B:130:THR:H	1:B:383:GLN:NE2	2.01	0.56
1:B:169:LEU:O	1:B:172:HIS:HB3	2.06	0.56
1:B:302:LYS:N	1:B:302:LYS:HD2	2.20	0.56
1:B:342:PRO:CG	1:B:362:ILE:HA	2.35	0.55
1:B:322:ILE:HD12	1:B:323:ARG:HG3	1.87	0.55
1:B:348:PRO:HB3	1:B:350:PHE:CE2	2.41	0.55
1:A:67:LEU:O	1:A:81:SER:HA	2.07	0.55
1:B:19:GLU:O	1:B:23:VAL:HG23	2.07	0.55
1:B:29:ILE:O	1:B:33:ILE:CD1	2.55	0.55
1:B:414:VAL:O	1:B:416:ILE:HD12	2.06	0.55
1:A:24:ARG:HE	1:A:325:LEU:HD21	1.72	0.55
1:A:151:ALA:HB1	1:A:233:PRO:HD3	1.87	0.55
1:A:323:ARG:HD3	1:A:329:GLU:OE1	2.06	0.55
1:B:107:MET:HG2	1:B:173:TYR:CE2	2.41	0.55
1:B:130:THR:O	1:B:133:LEU:HD23	2.06	0.55
1:B:224:ALA:O	1:B:225:LEU:HD12	2.06	0.55
1:A:27:GLU:CD	1:A:27:GLU:N	2.58	0.55
1:A:375:GLN:HG3	1:A:376:GLY:N	2.20	0.55
1:A:435:ARG:HG3	1:A:439:LEU:HD23	1.89	0.55
1:B:30:ARG:C	1:B:32:ILE:H	2.15	0.55
1:B:426:GLU:CD	1:B:426:GLU:N	2.63	0.55
1:B:149:MET:HE1	1:B:204:ILE:HD11	1.89	0.55
1:B:310:VAL:CG2	1:B:311:GLU:N	2.62	0.55
1:A:223:LYS:HD3	1:A:223:LYS:H	1.72	0.54
1:B:319:ASP:OD2	1:B:378:VAL:HG23	2.07	0.54
1:A:10:GLU:O	1:A:14:LYS:HD3	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:SER:C	1:A:101:MET:CE	2.81	0.54
1:A:146:LEU:CD1	1:A:273:THR:HG23	2.37	0.54
1:B:375:GLN:CG	1:B:376:GLY:N	2.66	0.54
1:A:312:ILE:C	1:A:313:VAL:CG1	2.81	0.54
1:A:373:PHE:CZ	1:A:404:LEU:HD21	2.42	0.54
1:A:434:ASN:ND2	1:A:437:PRO:HD3	2.23	0.54
1:A:435:ARG:HG3	1:A:439:LEU:CD2	2.38	0.54
1:B:183:ASN:N	1:B:183:ASN:ND2	2.55	0.54
1:B:137:PRO:CG	4:B:453:D5M:HN62	2.19	0.54
1:B:173:TYR:CE1	1:B:281:TYR:CE2	2.94	0.54
1:A:135:ARG:HH22	1:B:90:TYR:N	2.04	0.54
1:A:283:ILE:O	1:A:287:LEU:HG	2.07	0.54
1:A:326:ILE:HG21	1:A:328:HIS:CD2	2.42	0.54
1:A:301:THR:HG22	1:A:302:LYS:N	2.22	0.54
1:B:43:GLU:O	1:B:397:HIS:HB2	2.07	0.54
1:A:243:LYS:O	1:B:245:VAL:HG23	2.07	0.54
1:A:398:HIS:HE1	3:A:453:GOL:H2	1.73	0.54
1:B:158:PHE:O	1:B:161:LEU:HB3	2.08	0.54
1:B:209:ILE:HD13	1:B:209:ILE:N	2.23	0.54
1:B:326:ILE:HD12	1:B:326:ILE:N	2.23	0.54
1:A:436:ASP:O	1:A:439:LEU:HB2	2.08	0.54
1:A:3:LEU:HD11	1:B:66:PHE:HZ	1.73	0.53
1:B:54:ARG:HD2	1:B:97:VAL:HG12	1.90	0.53
1:B:170:ARG:NH2	1:B:174:ARG:HH22	2.05	0.53
1:B:336:ILE:CD1	1:B:338:HIS:O	2.56	0.53
1:A:188:SER:N	1:A:189:PRO:HD3	2.23	0.53
1:A:297:LYS:NZ	1:B:441:ILE:HA	2.23	0.53
1:B:17:LEU:HD22	1:B:20:LEU:HD11	1.89	0.53
1:B:117:GLU:HA	1:B:121:ARG:HH21	1.73	0.53
1:A:421:ALA:O	1:A:426:GLU:OE2	2.25	0.53
1:B:86:ILE:HD12	1:B:87:LYS:N	2.24	0.53
1:B:144:ARG:HB2	1:B:225:LEU:HD12	1.89	0.53
1:B:321:VAL:O	1:B:325:LEU:HB2	2.08	0.53
1:A:170:ARG:HD2	1:A:170:ARG:C	2.31	0.53
1:A:72:VAL:HG21	1:A:409:LEU:CB	2.38	0.53
1:A:316:ALA:HB2	1:B:440:LYS:HZ3	1.74	0.53
1:A:381:MET:HE3	1:A:383:GLN:HG2	1.90	0.53
1:B:165:PHE:CD2	1:B:277:ILE:HG21	2.42	0.53
1:A:230:ARG:HG2	1:B:234:ILE:HG13	1.90	0.53
1:B:89:ASN:HB2	1:B:92:THR:HB	1.89	0.53
1:B:430:ASN:HA	1:B:435:ARG:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:PHE:HB2	1:B:358:ILE:HD12	1.90	0.53
1:B:134:VAL:HG23	1:B:135:ARG:N	2.25	0.52
1:B:162:LEU:HD23	1:B:166:LEU:HD11	1.91	0.52
1:B:227:TYR:H	1:B:230:ARG:NH1	2.07	0.52
1:A:441:ILE:C	1:B:316:ALA:CB	2.81	0.52
1:A:441:ILE:HG13	1:B:378:VAL:HG11	1.90	0.52
1:B:150:ARG:NH2	1:B:350:PHE:CB	2.72	0.52
1:B:323:ARG:HG2	1:B:329:GLU:H	1.74	0.52
1:A:180:LEU:O	1:A:184:GLY:HA2	2.09	0.52
1:A:426:GLU:CD	1:A:426:GLU:N	2.67	0.52
1:A:170:ARG:NH2	5:A:458:HOH:O	2.36	0.52
1:B:411:HIS:C	1:B:411:HIS:CD2	2.87	0.52
1:A:88:SER:HA	1:A:93:SER:OG	2.10	0.52
1:A:113:TYR:O	1:A:116:LEU:HB2	2.10	0.52
1:A:314:ASP:HB3	1:A:317:LEU:HD12	1.90	0.52
1:A:324:THR:O	1:A:325:LEU:HD23	2.10	0.52
1:A:39:LEU:HD13	1:A:332:GLY:C	2.35	0.52
1:A:347:PHE:HD1	1:A:362:ILE:HD11	1.74	0.52
1:B:129:LEU:HG	1:B:294:TYR:CZ	2.45	0.52
1:B:47:ILE:HG13	1:B:122:ALA:O	2.10	0.52
1:B:28:GLN:C	1:B:30:ARG:H	2.18	0.52
1:B:280:LEU:HA	1:B:283:ILE:HG13	1.92	0.52
1:B:305:ALA:HA	1:B:310:VAL:O	2.09	0.52
1:B:422:ARG:HH11	1:B:423:HIS:CE1	2.28	0.52
1:A:120:LYS:HZ3	1:A:390:LYS:HE2	1.72	0.52
1:A:328:HIS:HB3	1:A:330:LYS:H	1.75	0.52
1:B:136:PRO:HG3	1:B:346:SER:HB2	1.92	0.52
1:B:245:VAL:HG12	1:B:249:LEU:CD1	2.39	0.52
1:A:176:VAL:HG22	1:A:186:TYR:HE2	1.74	0.51
1:A:299:PHE:O	1:A:300:TYR:HB2	2.10	0.51
1:B:65:TYR:CZ	1:B:84:ASN:HB3	2.45	0.51
1:B:86:ILE:HG13	1:B:87:LYS:O	2.10	0.51
1:A:431:ALA:O	1:A:432:LEU:C	2.54	0.51
1:B:29:ILE:HG23	1:B:31:ASN:H	1.75	0.51
1:B:326:ILE:HG22	1:B:326:ILE:O	2.08	0.51
1:B:195:VAL:HG12	1:B:195:VAL:O	2.08	0.51
1:A:288:GLU:HG3	1:A:357:ASN:HD21	1.75	0.51
1:A:326:ILE:CG2	1:A:328:HIS:CD2	2.93	0.51
1:A:72:VAL:HG21	1:A:409:LEU:HB2	1.93	0.51
1:A:82:TYR:OH	1:A:193:ASP:HB2	2.10	0.51
1:B:54:ARG:HB3	1:B:101:MET:HE2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:TYR:CG	1:A:140:PRO:HA	2.45	0.51
1:A:209:ILE:O	1:A:216:VAL:HG12	2.11	0.51
1:B:8:SER:HA	1:B:11:ARG:HH12	1.74	0.51
1:B:54:ARG:N	1:B:101:MET:HE3	2.26	0.51
1:B:216:VAL:O	1:B:260:TYR:HA	2.11	0.51
1:B:228:SER:H	1:B:230:ARG:HH11	1.59	0.51
1:B:322:ILE:HD11	1:B:323:ARG:HG3	1.91	0.51
1:A:110:TYR:CD2	1:A:111:LEU:HD23	2.46	0.51
1:B:29:ILE:CG2	1:B:31:ASN:H	2.24	0.50
1:B:182:LYS:HB2	1:B:183:ASN:ND2	2.25	0.50
1:B:283:ILE:O	1:B:287:LEU:HG	2.12	0.50
1:B:104:LEU:CD2	1:B:189:PRO:HB2	2.40	0.50
1:B:204:ILE:HG22	1:B:205:ASP:N	2.26	0.50
1:A:223:LYS:H	1:A:223:LYS:CD	2.25	0.50
1:A:441:ILE:C	1:B:316:ALA:HB1	2.36	0.50
1:B:323:ARG:HG2	1:B:329:GLU:N	2.26	0.50
1:B:81:SER:O	1:B:189:PRO:HD3	2.11	0.50
1:A:403:TYR:C	1:A:403:TYR:CD2	2.89	0.50
1:A:433:ARG:HE	1:A:434:ASN:HB2	1.77	0.50
1:B:30:ARG:O	1:B:32:ILE:N	2.44	0.50
1:A:414:VAL:C	1:A:416:ILE:H	2.18	0.50
1:A:8:SER:HB3	1:A:11:ARG:NH2	2.27	0.50
1:A:120:LYS:HZ2	1:A:394:LEU:HD11	1.76	0.50
1:B:17:LEU:HA	1:B:20:LEU:CG	2.42	0.50
1:A:24:ARG:NH2	1:A:325:LEU:HD21	2.26	0.50
1:A:200:ARG:O	1:A:204:ILE:HB	2.12	0.50
1:A:287:LEU:HB3	1:A:357:ASN:HB3	1.93	0.50
1:A:312:ILE:HD12	1:A:313:VAL:N	2.27	0.50
1:A:5:SER:C	1:A:7:GLN:N	2.70	0.49
1:B:133:LEU:CD1	1:B:342:PRO:HB3	2.42	0.49
1:A:135:ARG:NH2	1:B:90:TYR:H	2.09	0.49
1:A:398:HIS:CE1	3:A:453:GOL:H2	2.47	0.49
1:A:196:VAL:HG13	1:A:197:GLU:N	2.27	0.49
1:B:98:ARG:CG	4:B:453:D5M:HN61	2.25	0.49
1:B:319:ASP:O	1:B:322:ILE:HG13	2.13	0.49
1:A:352:LEU:O	1:A:353:SER:C	2.56	0.49
1:A:302:LYS:HE2	1:B:87:LYS:NZ	2.26	0.49
1:A:316:ALA:HB2	1:B:440:LYS:NZ	2.27	0.49
1:A:334:LEU:C	1:A:334:LEU:HD12	2.38	0.49
1:A:67:LEU:HD21	1:A:97:VAL:HG13	1.95	0.49
1:B:333:TYR:HE2	1:B:335:GLU:HB2	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:TYR:CZ	1:A:84:ASN:HB3	2.48	0.49
1:A:113:TYR:CG	1:A:289:VAL:HG22	2.48	0.49
1:A:333:TYR:C	1:A:333:TYR:CD2	2.91	0.49
1:A:436:ASP:HB2	1:A:437:PRO:HD3	1.94	0.49
1:B:20:LEU:HD23	1:B:20:LEU:N	2.27	0.49
1:B:247:GLU:O	1:B:250:GLN:HB3	2.13	0.49
1:A:433:ARG:HE	1:A:434:ASN:CB	2.26	0.49
1:B:245:VAL:O	1:B:249:LEU:HD12	2.13	0.49
1:A:323:ARG:HD3	1:A:329:GLU:CG	2.43	0.49
1:A:220:ILE:CG1	1:A:257:VAL:HB	2.42	0.48
1:A:333:TYR:HE2	1:A:335:GLU:HB2	1.78	0.48
1:A:441:ILE:HG12	1:B:378:VAL:HG11	1.94	0.48
1:B:217:LYS:HD3	1:B:260:TYR:HE2	1.76	0.48
1:B:323:ARG:HH21	1:B:372:ARG:HH11	1.60	0.48
1:A:319:ASP:HA	1:A:379:ILE:HD12	1.95	0.48
1:A:340:VAL:HG13	1:A:366:ILE:O	2.14	0.48
1:A:400:ALA:HB2	1:A:405:ARG:HB2	1.95	0.48
1:A:258:GLU:HG3	1:A:260:TYR:OH	2.14	0.48
1:B:139:TYR:C	1:B:141:GLU:H	2.22	0.48
1:B:355:PHE:HB3	1:B:358:ILE:HD12	1.95	0.48
1:B:422:ARG:NH1	1:B:423:HIS:CE1	2.67	0.48
1:A:124:LEU:HD21	1:A:404:LEU:CD1	2.44	0.48
1:A:139:TYR:HA	1:A:140:PRO:C	2.37	0.48
1:A:234:ILE:HG12	1:B:227:TYR:CE2	2.48	0.48
1:B:13:THR:O	1:B:17:LEU:HG	2.14	0.48
1:B:116:LEU:HD23	1:B:121:ARG:HB3	1.96	0.48
1:A:8:SER:HB2	1:A:11:ARG:NH2	2.28	0.48
1:B:422:ARG:HD3	1:B:423:HIS:ND1	2.29	0.48
1:A:48:TYR:CD1	1:A:112:ALA:HB1	2.49	0.48
1:B:30:ARG:O	1:B:30:ARG:HG2	2.13	0.48
1:B:386:THR:CG2	1:B:391:ILE:HG12	2.44	0.48
1:A:139:TYR:HA	1:A:141:GLU:N	2.29	0.48
1:A:221:PRO:O	1:A:230:ARG:NH1	2.44	0.48
1:A:342:PRO:CD	1:A:362:ILE:HA	2.44	0.48
1:A:433:ARG:HH21	1:A:434:ASN:HA	1.79	0.48
1:B:250:GLN:O	1:B:254:GLU:HB2	2.14	0.48
1:A:144:ARG:HD2	1:B:228:SER:HB3	1.95	0.47
1:A:433:ARG:NH2	1:A:434:ASN:HA	2.29	0.47
1:B:3:LEU:HD22	1:B:4:LEU:HG	1.95	0.47
1:B:330:LYS:O	1:B:372:ARG:HD2	2.14	0.47
1:A:222:ARG:HD2	1:A:255:GLU:OE1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:MET:HE3	1:A:383:GLN:CG	2.43	0.47
1:A:169:LEU:HD11	1:A:278:GLU:HA	1.95	0.47
1:B:146:LEU:HG	1:B:273:THR:HG23	1.97	0.47
1:B:375:GLN:CG	1:B:376:GLY:H	2.16	0.47
1:A:223:LYS:HD2	1:A:230:ARG:CD	2.44	0.47
1:A:28:GLN:O	1:A:32:ILE:HG12	2.15	0.47
1:A:390:LYS:C	1:A:390:LYS:HD3	2.40	0.47
1:B:137:PRO:HG3	4:B:453:D5M:C6	2.44	0.47
1:A:129:LEU:O	1:A:133:LEU:HD22	2.15	0.47
1:A:320:ALA:HB2	1:B:436:ASP:HB2	1.95	0.47
1:B:51:ASP:OD2	1:B:126:ASP:CG	2.57	0.47
1:B:163:ASN:O	1:B:164:GLU:C	2.58	0.47
1:B:241:ARG:HG2	1:B:242:GLY:N	2.22	0.47
1:B:345:TRP:CD1	1:B:346:SER:N	2.83	0.47
1:B:433:ARG:HG3	1:B:434:ASN:N	2.29	0.47
1:B:201:LYS:HB3	1:B:205:ASP:OD2	2.15	0.47
1:B:382:LEU:HD12	1:B:383:GLN:N	2.30	0.47
1:A:95:GLN:HB3	1:A:138:VAL:HG13	1.97	0.47
1:A:129:LEU:HD13	1:A:366:ILE:CG1	2.42	0.47
1:A:137:PRO:C	1:A:138:VAL:HG23	2.39	0.47
1:B:51:ASP:OD2	1:B:126:ASP:OD2	2.33	0.47
1:B:73:GLY:C	1:B:75:GLY:H	2.21	0.47
1:B:124:LEU:HD12	1:B:293:ALA:HB3	1.96	0.47
1:B:437:PRO:O	1:B:440:LYS:HB2	2.15	0.47
1:A:175:LYS:HB2	1:A:175:LYS:HE3	1.71	0.46
1:A:176:VAL:HG22	1:A:186:TYR:CD2	2.50	0.46
1:A:297:LYS:HB3	1:A:297:LYS:HE3	1.46	0.46
1:B:201:LYS:HA	1:B:205:ASP:CG	2.40	0.46
1:A:209:ILE:H	1:A:209:ILE:HG12	1.65	0.46
1:A:345:TRP:CD1	1:A:345:TRP:C	2.93	0.46
1:B:124:LEU:HD12	1:B:293:ALA:CB	2.45	0.46
1:B:367:HIS:HB2	1:B:388:ILE:HD11	1.97	0.46
1:B:392:LEU:HG	1:B:396:LEU:CD1	2.45	0.46
1:B:118:GLY:H	1:B:121:ARG:CZ	2.28	0.46
1:B:201:LYS:HA	1:B:205:ASP:CB	2.46	0.46
1:A:326:ILE:HD12	1:A:326:ILE:N	2.31	0.46
1:B:142:ASP:OD2	1:B:143:ILE:N	2.45	0.46
1:B:302:LYS:O	1:B:303:THR:HG22	2.16	0.46
1:B:411:HIS:O	1:B:415:LYS:HG3	2.16	0.46
1:A:392:LEU:O	1:A:392:LEU:HD12	2.15	0.46
1:B:92:THR:HG22	1:B:96:ILE:HD11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:LYS:HE3	1:B:198:LYS:NZ	2.30	0.46
1:B:227:TYR:HB3	1:B:230:ARG:N	2.30	0.46
1:B:301:THR:O	1:B:304:LEU:HB2	2.16	0.46
1:A:337:GLU:HB2	1:A:338:HIS:CE1	2.51	0.46
1:A:316:ALA:HB3	1:B:60:SER:OG	2.16	0.46
1:B:27:GLU:O	1:B:30:ARG:N	2.49	0.46
1:A:8:SER:HB2	1:A:11:ARG:HH21	1.80	0.46
1:B:315:THR:O	1:B:316:ALA:C	2.57	0.46
1:A:304:LEU:HD23	1:A:304:LEU:HA	1.62	0.46
1:B:17:LEU:CD2	1:B:20:LEU:HD11	2.46	0.46
1:B:338:HIS:ND1	1:B:338:HIS:N	2.63	0.46
1:A:47:ILE:HG22	1:A:398:HIS:CE1	2.51	0.45
1:B:80:LEU:HB3	1:B:189:PRO:CG	2.46	0.45
1:B:219:LYS:HE2	1:B:256:LYS:HZ1	1.81	0.45
1:A:55:SER:HB3	1:A:66:PHE:HD2	1.79	0.45
1:A:152:LEU:HD21	1:A:266:ILE:HD11	1.98	0.45
1:A:235:GLU:H	1:A:235:GLU:CD	2.24	0.45
1:A:312:ILE:C	1:A:312:ILE:HD12	2.41	0.45
1:B:10:GLU:HA	1:B:13:THR:OG1	2.16	0.45
1:A:392:LEU:N	1:A:393:PRO:HD2	2.32	0.45
1:B:232:ILE:HG13	1:B:233:PRO:HD2	1.96	0.45
1:A:70:LEU:HD12	1:A:78:LEU:O	2.15	0.45
1:B:60:SER:OG	1:B:440:LYS:CD	2.64	0.45
1:B:233:PRO:HB2	1:B:236:VAL:HG22	1.98	0.45
1:A:284:ASP:OD2	1:A:355:PHE:HB3	2.16	0.45
1:B:287:LEU:HD13	1:B:357:ASN:O	2.17	0.45
1:A:180:LEU:HD22	1:A:180:LEU:HA	1.61	0.45
1:A:187:ASP:C	1:A:189:PRO:HD3	2.41	0.45
1:B:217:LYS:CD	1:B:260:TYR:CE2	2.99	0.45
1:A:54:ARG:HH22	1:A:98:ARG:NH2	2.14	0.45
1:A:230:ARG:CG	1:B:234:ILE:HG13	2.47	0.45
1:A:300:TYR:OH	1:A:302:LYS:HD3	2.17	0.45
1:A:374:GLU:O	1:A:377:ASP:HB2	2.18	0.45
1:A:421:ALA:HA	1:A:424:THR:HG1	1.72	0.45
1:B:39:LEU:HA	1:B:40:PRO:HD3	1.85	0.45
1:B:305:ALA:HB1	1:B:311:GLU:HA	1.99	0.45
1:A:26:ASN:HB3	1:A:30:ARG:HG2	1.99	0.44
1:A:100:GLN:HG2	1:A:190:ILE:HG13	1.99	0.44
1:A:135:ARG:NH2	1:B:90:TYR:HB2	2.31	0.44
1:B:39:LEU:HG	1:B:332:GLY:HA2	1.99	0.44
1:B:148:VAL:HG13	1:B:261:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:GLU:HG2	1:A:28:GLN:N	2.21	0.44
1:A:302:LYS:HD3	1:A:302:LYS:HA	1.53	0.44
1:B:98:ARG:CD	4:B:453:D5M:HN61	2.29	0.44
1:A:29:ILE:O	1:A:33:ILE:HG12	2.18	0.44
1:B:79:ARG:O	1:B:185:ASN:HA	2.16	0.44
1:A:32:ILE:HD13	1:A:32:ILE:HA	1.83	0.44
1:A:120:LYS:HZ1	1:A:390:LYS:HE2	1.81	0.44
1:A:423:HIS:C	1:A:426:GLU:OE1	2.61	0.44
1:A:24:ARG:NE	1:A:325:LEU:HD21	2.33	0.44
1:A:29:ILE:HA	1:A:29:ILE:HD12	1.75	0.44
1:A:141:GLU:HA	1:A:144:ARG:HD3	2.00	0.44
1:A:241:ARG:O	1:B:246:ASP:CG	2.61	0.44
1:B:215:LYS:HA	1:B:261:LEU:O	2.17	0.44
1:B:426:GLU:HA	1:B:429:ILE:HG13	1.99	0.44
1:A:8:SER:HA	1:A:11:ARG:CZ	2.48	0.44
1:B:32:ILE:HG22	1:B:334:LEU:HD21	2.00	0.44
1:B:162:LEU:O	1:B:166:LEU:HG	2.18	0.44
1:B:209:ILE:HD13	1:B:209:ILE:H	1.81	0.44
1:A:72:VAL:HG22	1:A:406:PRO:O	2.18	0.44
1:A:106:ASN:HD22	1:A:282:SER:HG	1.66	0.44
1:A:130:THR:O	1:A:134:VAL:HG13	2.18	0.44
1:A:170:ARG:CZ	5:A:458:HOH:O	2.63	0.44
1:A:220:ILE:HG12	1:A:257:VAL:HB	1.98	0.44
1:B:81:SER:O	1:B:189:PRO:CD	2.66	0.44
1:B:135:ARG:NH2	1:B:306:ARG:NH1	2.52	0.44
1:B:419:LYS:HB2	1:B:422:ARG:HB2	1.99	0.44
1:B:420:GLU:C	1:B:422:ARG:N	2.75	0.44
1:A:146:LEU:HD12	1:A:146:LEU:HA	1.76	0.43
1:B:232:ILE:HG12	1:B:233:PRO:O	2.17	0.43
1:B:367:HIS:ND1	1:B:387:ASN:HA	2.33	0.43
1:B:410:ALA:O	1:B:414:VAL:CG1	2.65	0.43
1:A:52:GLY:HA2	1:A:414:VAL:HG21	2.00	0.43
1:A:53:SER:C	1:A:101:MET:HE1	2.40	0.43
1:A:59:LEU:CD2	1:A:440:LYS:HA	2.48	0.43
1:A:249:LEU:HD21	1:B:237:LEU:CB	2.46	0.43
1:A:302:LYS:CG	1:B:89:ASN:ND2	2.69	0.43
1:B:133:LEU:HD11	1:B:342:PRO:HB3	1.99	0.43
1:A:106:ASN:CB	1:A:282:SER:OG	2.65	0.43
1:A:405:ARG:N	1:A:406:PRO:HD2	2.32	0.43
1:B:419:LYS:O	1:B:422:ARG:CB	2.64	0.43
1:A:404:LEU:H	1:A:404:LEU:HG	1.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:GLU:O	1:A:168:LYS:C	2.61	0.43
1:A:366:ILE:HG22	1:A:368:LEU:HD23	2.00	0.43
1:A:195:VAL:HG22	1:A:199:LEU:CD2	2.49	0.43
1:A:437:PRO:C	1:A:439:LEU:N	2.76	0.43
1:B:350:PHE:CD1	1:B:351:LEU:HD23	2.53	0.43
1:B:107:MET:O	1:B:111:LEU:HG	2.19	0.43
1:A:367:HIS:ND1	1:A:386:THR:C	2.77	0.43
1:B:124:LEU:HD13	1:B:395:ILE:HD12	2.00	0.43
1:B:252:LEU:HA	1:B:252:LEU:HD23	1.85	0.43
1:B:294:TYR:O	1:B:295:ILE:HD13	2.18	0.43
1:B:163:ASN:HA	1:B:166:LEU:HD12	2.01	0.43
1:A:70:LEU:HD12	1:A:71:ALA:H	1.84	0.43
1:A:302:LYS:HG2	1:A:302:LYS:HZ2	1.47	0.43
1:B:241:ARG:C	1:B:243:LYS:H	2.26	0.43
1:A:72:VAL:HG21	1:A:409:LEU:HB3	2.00	0.42
1:A:96:ILE:HD11	1:A:272:MET:HE2	2.01	0.42
1:A:299:PHE:O	1:A:300:TYR:CB	2.66	0.42
1:A:323:ARG:HD3	1:A:329:GLU:CD	2.44	0.42
1:A:420:GLU:OE1	1:A:420:GLU:N	2.52	0.42
1:B:342:PRO:CG	1:B:362:ILE:HD13	2.48	0.42
1:A:357:ASN:HA	1:A:360:LYS:HB3	2.01	0.42
1:B:116:LEU:O	1:B:121:ARG:NE	2.52	0.42
1:B:351:LEU:HD22	1:B:351:LEU:HA	1.76	0.42
1:B:372:ARG:HH12	1:B:379:ILE:HD11	1.84	0.42
1:A:302:LYS:NZ	1:B:87:LYS:HG3	2.35	0.42
1:B:33:ILE:O	1:B:36:TRP:HB3	2.19	0.42
1:B:134:VAL:CG2	1:B:135:ARG:N	2.82	0.42
1:A:247:GLU:O	1:A:251:GLU:HG3	2.20	0.42
1:A:433:ARG:HG3	1:A:434:ASN:H	1.84	0.42
1:B:115:LYS:HD2	1:B:115:LYS:HA	1.78	0.42
1:B:227:TYR:N	1:B:230:ARG:NH1	2.67	0.42
1:A:144:ARG:H	1:A:144:ARG:HG2	1.58	0.42
1:A:237:LEU:HD23	1:A:248:LEU:HD11	2.01	0.42
1:B:30:ARG:C	1:B:32:ILE:N	2.76	0.42
1:A:342:PRO:HG2	1:A:362:ILE:HD13	2.02	0.42
1:A:351:LEU:HD23	1:A:351:LEU:HA	1.75	0.42
1:B:36:TRP:CZ2	1:B:332:GLY:HA3	2.54	0.42
1:B:263:LYS:HD3	1:B:267:TYR:CZ	2.54	0.42
1:B:420:GLU:C	1:B:422:ARG:H	2.25	0.42
1:A:149:MET:SD	1:A:270:LEU:HA	2.60	0.42
1:B:342:PRO:HB2	1:B:362:ILE:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:VAL:O	1:A:152:LEU:HB2	2.19	0.42
1:A:280:LEU:HD23	1:A:280:LEU:HA	1.82	0.42
1:B:150:ARG:HH22	1:B:350:PHE:CB	2.32	0.42
1:B:233:PRO:O	1:B:236:VAL:HG23	2.20	0.42
1:B:310:VAL:HG12	1:B:338:HIS:CD2	2.55	0.42
1:B:323:ARG:NH2	1:B:372:ARG:HH11	2.18	0.42
1:B:414:VAL:O	1:B:414:VAL:CG2	2.68	0.42
1:A:223:LYS:HD2	1:A:230:ARG:HD2	2.02	0.41
1:A:345:TRP:CD1	1:A:346:SER:N	2.88	0.41
1:B:104:LEU:HD22	1:B:189:PRO:HB2	2.01	0.41
1:B:130:THR:OG1	1:B:131:GLY:N	2.51	0.41
1:B:301:THR:CG2	1:B:312:ILE:HG13	2.50	0.41
1:A:17:LEU:HD23	1:A:20:LEU:HD12	2.02	0.41
1:A:313:VAL:CG2	1:A:314:ASP:O	2.66	0.41
1:A:392:LEU:N	1:A:393:PRO:CD	2.84	0.41
1:A:58:ARG:HE	1:A:58:ARG:HB2	1.65	0.41
1:A:418:TYR:CD2	1:A:419:LYS:N	2.89	0.41
1:A:441:ILE:HD12	1:A:441:ILE:N	2.35	0.41
1:B:223:LYS:HD2	1:B:223:LYS:HA	1.81	0.41
1:B:340:VAL:HG11	1:B:368:LEU:HD11	2.03	0.41
1:B:420:GLU:H	1:B:420:GLU:HG2	1.60	0.41
1:A:299:PHE:N	1:A:299:PHE:CD1	2.89	0.41
1:A:400:ALA:HB3	1:A:403:TYR:O	2.21	0.41
1:B:104:LEU:HD11	1:B:189:PRO:HG2	2.01	0.41
1:B:162:LEU:HD23	1:B:166:LEU:CD1	2.49	0.41
1:B:227:TYR:CD1	1:B:229:PRO:O	2.74	0.41
1:B:299:PHE:CD1	1:B:299:PHE:N	2.84	0.41
1:B:303:THR:O	1:B:306:ARG:HB3	2.21	0.41
1:A:99:MET:CE	1:A:276:TYR:HD1	2.34	0.41
1:A:347:PHE:CD1	1:A:362:ILE:HD11	2.55	0.41
1:B:144:ARG:CB	1:B:225:LEU:HD11	2.49	0.41
1:A:300:TYR:O	1:A:301:THR:OG1	2.26	0.41
1:A:329:GLU:O	1:A:329:GLU:HG2	2.21	0.41
1:A:439:LEU:O	1:A:440:LYS:CB	2.67	0.41
1:B:36:TRP:CD1	1:B:36:TRP:C	2.98	0.41
1:B:65:TYR:HE2	1:B:86:ILE:HG22	1.86	0.41
1:B:412:HIS:O	1:B:415:LYS:HE2	2.20	0.41
1:A:403:TYR:OH	1:A:407:LEU:HG	2.21	0.41
1:B:46:SER:O	1:B:116:LEU:HD21	2.21	0.41
1:B:121:ARG:O	1:B:291:ASN:ND2	2.49	0.41
1:A:138:VAL:HG11	1:A:272:MET:HE1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:VAL:O	1:A:142:ASP:OD1	2.39	0.41
1:B:20:LEU:HD23	1:B:20:LEU:H	1.85	0.41
1:B:335:GLU:HA	1:B:369:ALA:HB2	2.02	0.41
1:B:360:LYS:HB2	1:B:360:LYS:HE3	1.73	0.41
1:A:39:LEU:CD1	1:A:332:GLY:C	2.94	0.41
1:A:52:GLY:CA	1:A:414:VAL:HG21	2.51	0.41
1:A:53:SER:O	1:A:101:MET:CE	2.57	0.41
1:A:144:ARG:HD2	1:B:228:SER:CB	2.51	0.41
1:A:195:VAL:HG22	1:A:195:VAL:O	2.21	0.41
1:A:285:LYS:HD2	1:A:285:LYS:HA	1.77	0.41
1:A:366:ILE:HG22	1:A:368:LEU:CD2	2.51	0.41
1:B:92:THR:HG22	1:B:96:ILE:CD1	2.51	0.41
1:B:124:LEU:HD12	1:B:124:LEU:HA	1.91	0.41
1:B:219:LYS:HD2	1:B:256:LYS:HE3	2.03	0.41
1:B:331:GLU:HB3	1:B:375:GLN:H	1.85	0.41
1:B:419:LYS:H	1:B:419:LYS:CE	2.26	0.41
1:A:222:ARG:HD2	1:A:255:GLU:CD	2.46	0.41
1:A:400:ALA:HB2	1:A:405:ARG:CB	2.51	0.41
1:B:405:ARG:HG2	1:B:406:PRO:HD3	2.02	0.41
1:A:420:GLU:C	1:A:422:ARG:H	2.28	0.40
1:B:195:VAL:O	1:B:195:VAL:CG1	2.68	0.40
1:A:26:ASN:CB	1:A:30:ARG:HG2	2.52	0.40
1:A:49:ALA:HA	1:A:124:LEU:O	2.22	0.40
1:A:98:ARG:HE	1:A:98:ARG:HB2	1.78	0.40
1:A:223:LYS:HD3	1:A:223:LYS:N	2.34	0.40
1:A:234:ILE:HG22	1:A:235:GLU:OE2	2.21	0.40
1:B:80:LEU:HB3	1:B:189:PRO:HG3	2.03	0.40
1:B:98:ARG:HG2	4:B:453:D5M:N6	2.34	0.40
1:A:16:LEU:HD21	1:B:62:THR:HG21	2.03	0.40
1:A:298:SER:HB2	1:B:60:SER:HA	2.04	0.40
1:A:356:ARG:HD3	1:A:356:ARG:HA	1.55	0.40
1:A:435:ARG:O	1:A:438:ALA:HB3	2.20	0.40
1:B:199:LEU:HD13	1:B:199:LEU:HA	1.76	0.40
1:B:304:LEU:C	1:B:306:ARG:N	2.76	0.40
1:B:315:THR:OG1	1:B:316:ALA:N	2.54	0.40
1:A:20:LEU:O	1:A:24:ARG:HG3	2.22	0.40
1:A:59:LEU:HD23	1:A:59:LEU:HA	1.77	0.40
1:A:116:LEU:HA	1:A:116:LEU:HD12	1.55	0.40
1:A:301:THR:CG2	1:A:302:LYS:N	2.85	0.40
1:A:425:LEU:C	1:A:425:LEU:HD13	2.46	0.40
1:B:144:ARG:CD	1:B:225:LEU:HD11	2.44	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:VAL:O	1:B:177:GLU:C	2.64	0.40
1:B:191:LEU:O	1:B:192:THR:C	2.65	0.40
1:B:287:LEU:CB	1:B:357:ASN:HB3	2.49	0.40
1:B:338:HIS:O	1:B:339:ALA:C	2.64	0.40
1:B:374:GLU:HB3	1:B:375:GLN:CG	2.51	0.40
1:B:436:ASP:O	1:B:437:PRO:C	2.64	0.40
1:A:356:ARG:O	1:A:359:GLU:N	2.54	0.40
1:B:65:TYR:CD2	1:B:65:TYR:N	2.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	426/471 (90%)	382 (90%)	41 (10%)	3 (1%)	18	52
1	B	427/471 (91%)	370 (87%)	52 (12%)	5 (1%)	10	42
All	All	853/942 (91%)	752 (88%)	93 (11%)	8 (1%)	14	47

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	29	ILE
1	B	4	LEU
1	B	5	SER
1	B	31	ASN
1	A	328	HIS
1	A	231	VAL
1	B	439	LEU
1	A	138	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	387/419 (92%)	294 (76%)	93 (24%)	1	4
1	B	387/419 (92%)	299 (77%)	88 (23%)	1	5
All	All	774/838 (92%)	593 (77%)	181 (23%)	1	4

All (181) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ILE
1	A	21	GLU
1	A	22	ASN
1	A	27	GLU
1	A	28	GLN
1	A	29	ILE
1	A	30	ARG
1	A	32	ILE
1	A	34	ASN
1	A	35	SER
1	A	39	LEU
1	A	41	SER
1	A	50	VAL
1	A	56	VAL
1	A	57	SER
1	A	58	ARG
1	A	66	PHE
1	A	72	VAL
1	A	81	SER
1	A	86	ILE
1	A	90	TYR
1	A	92	THR
1	A	94	ASP
1	A	98	ARG
1	A	107	MET
1	A	116	LEU
1	A	117	GLU

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Mol	Chain	Res	Type
1	A	125	MET
1	A	126	ASP
1	A	128	THR
1	A	129	LEU
1	A	133	LEU
1	A	138	VAL
1	A	143	ILE
1	A	144	ARG
1	A	146	LEU
1	A	149	MET
1	A	150	ARG
1	A	153	ILE
1	A	155	GLU
1	A	156	SER
1	A	180	LEU
1	A	183	ASN
1	A	185	ASN
1	A	187	ASP
1	A	197	GLU
1	A	199	LEU
1	A	201	LYS
1	A	208	VAL
1	A	209	ILE
1	A	216	VAL
1	A	222	ARG
1	A	223	LYS
1	A	232	ILE
1	A	234	ILE
1	A	236	VAL
1	A	246	ASP
1	A	248	LEU
1	A	249	LEU
1	A	256	LYS
1	A	258	GLU
1	A	259	LEU
1	A	261	LEU
1	A	282	SER
1	A	297	LYS
1	A	299	PHE
1	A	302	LYS
1	A	308	LEU
1	A	312	ILE

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Mol	Chain	Res	Type
1	A	313	VAL
1	A	318	LEU
1	A	334	LEU
1	A	338	HIS
1	A	340	VAL
1	A	346	SER
1	A	356	ARG
1	A	363	ASP
1	A	368	LEU
1	A	377	ASP
1	A	386	THR
1	A	390	LYS
1	A	391	ILE
1	A	394	LEU
1	A	403	TYR
1	A	404	LEU
1	A	408	GLN
1	A	415	LYS
1	A	418	TYR
1	A	419	LYS
1	A	426	GLU
1	A	428	LEU
1	A	429	ILE
1	A	433	ARG
1	B	3	LEU
1	B	5	SER
1	B	6	LYS
1	B	13	THR
1	B	16	LEU
1	B	20	LEU
1	B	25	GLU
1	B	28	GLN
1	B	29	ILE
1	B	31	ASN
1	B	34	ASN
1	B	36	TRP
1	B	39	LEU
1	B	41	SER
1	B	47	ILE
1	B	50	VAL
1	B	64	ILE
1	B	72	VAL

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Mol	Chain	Res	Type
1	B	74	SER
1	B	86	ILE
1	B	87	LYS
1	B	90	TYR
1	B	104	LEU
1	B	133	LEU
1	B	143	ILE
1	B	144	ARG
1	B	157	ASP
1	B	167	GLU
1	B	171	ASP
1	B	183	ASN
1	B	185	ASN
1	B	187	ASP
1	B	190	ILE
1	B	201	LYS
1	B	206	THR
1	B	209	ILE
1	B	216	VAL
1	B	217	LYS
1	B	218	VAL
1	B	222	ARG
1	B	223	LYS
1	B	225	LEU
1	B	232	ILE
1	B	234	ILE
1	B	236	VAL
1	B	249	LEU
1	B	253	ASP
1	B	255	GLU
1	B	256	LYS
1	B	257	VAL
1	B	263	LYS
1	B	270	LEU
1	B	280	LEU
1	B	283	ILE
1	B	289	VAL
1	B	291	ASN
1	B	298	SER
1	B	299	PHE
1	B	303	THR
1	B	304	LEU

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Mol	Chain	Res	Type
1	B	307	THR
1	B	318	LEU
1	B	333	TYR
1	B	338	HIS
1	B	340	VAL
1	B	345	TRP
1	B	349	ASP
1	B	351	LEU
1	B	355	PHE
1	B	361	LEU
1	B	379	ILE
1	B	387	ASN
1	B	389	GLU
1	B	390	LYS
1	B	391	ILE
1	B	396	LEU
1	B	403	TYR
1	B	404	LEU
1	B	414	VAL
1	B	416	ILE
1	B	419	LYS
1	B	420	GLU
1	B	422	ARG
1	B	426	GLU
1	B	429	ILE
1	B	432	LEU
1	B	433	ARG
1	B	440	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	31	ASN
1	A	250	GLN
1	A	328	HIS
1	A	338	HIS
1	A	397	HIS
1	A	398	HIS
1	B	89	ASN
1	B	147	ASN
1	B	183	ASN

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Mol	Chain	Res	Type
1	B	383	GLN
1	B	387	ASN
1	B	411	HIS
1	B	423	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	D5M	B	453	-	24,24,24	0.58	0	35,36,36	0.56	1 (2%)
3	GOL	A	453	-	5,5,5	0.58	0	5,5,5	0.74	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	D5M	B	453	-	-	4/10/22/22	0/3/3/3
3	GOL	A	453	-	-	4/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	453	D5M	O2P-P-O1P	2.07	118.88	110.83

There are no chirality outliers.

All (8) torsion outliers are listed below:

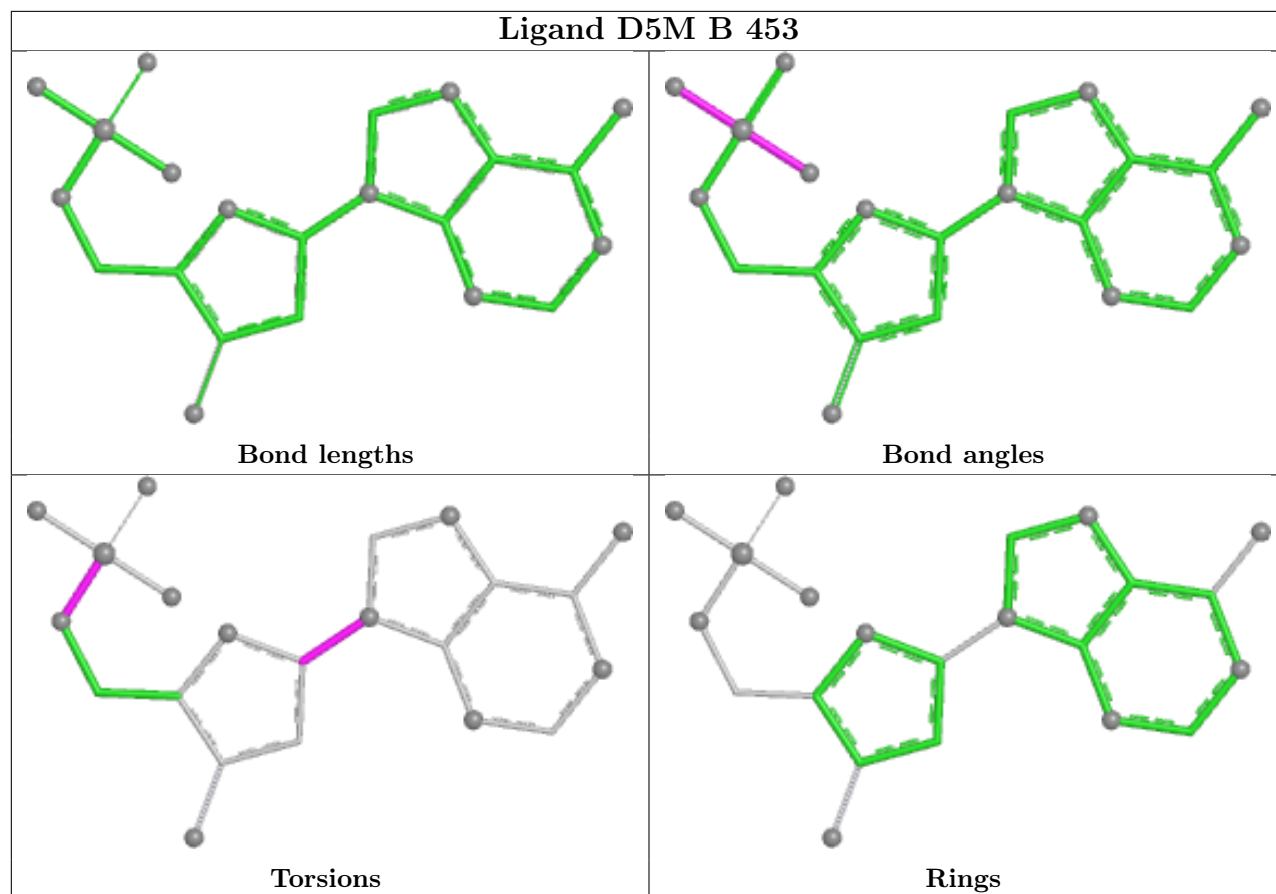
Mol	Chain	Res	Type	Atoms
3	A	453	GOL	O1-C1-C2-C3
4	B	453	D5M	C5'-O5'-P-O1P
3	A	453	GOL	O1-C1-C2-O2
4	B	453	D5M	C2'-C1'-N9-C4
4	B	453	D5M	C2'-C1'-N9-C8
3	A	453	GOL	C1-C2-C3-O3
3	A	453	GOL	O2-C2-C3-O3
4	B	453	D5M	C5'-O5'-P-O3P

There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	453	D5M	12	0
3	A	453	GOL	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	432/471 (91%)	-0.78	0 100 100	51, 94, 153, 179	0
1	B	433/471 (91%)	-0.67	0 100 100	62, 114, 169, 227	0
All	All	865/942 (91%)	-0.73	0 100 100	51, 106, 163, 227	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

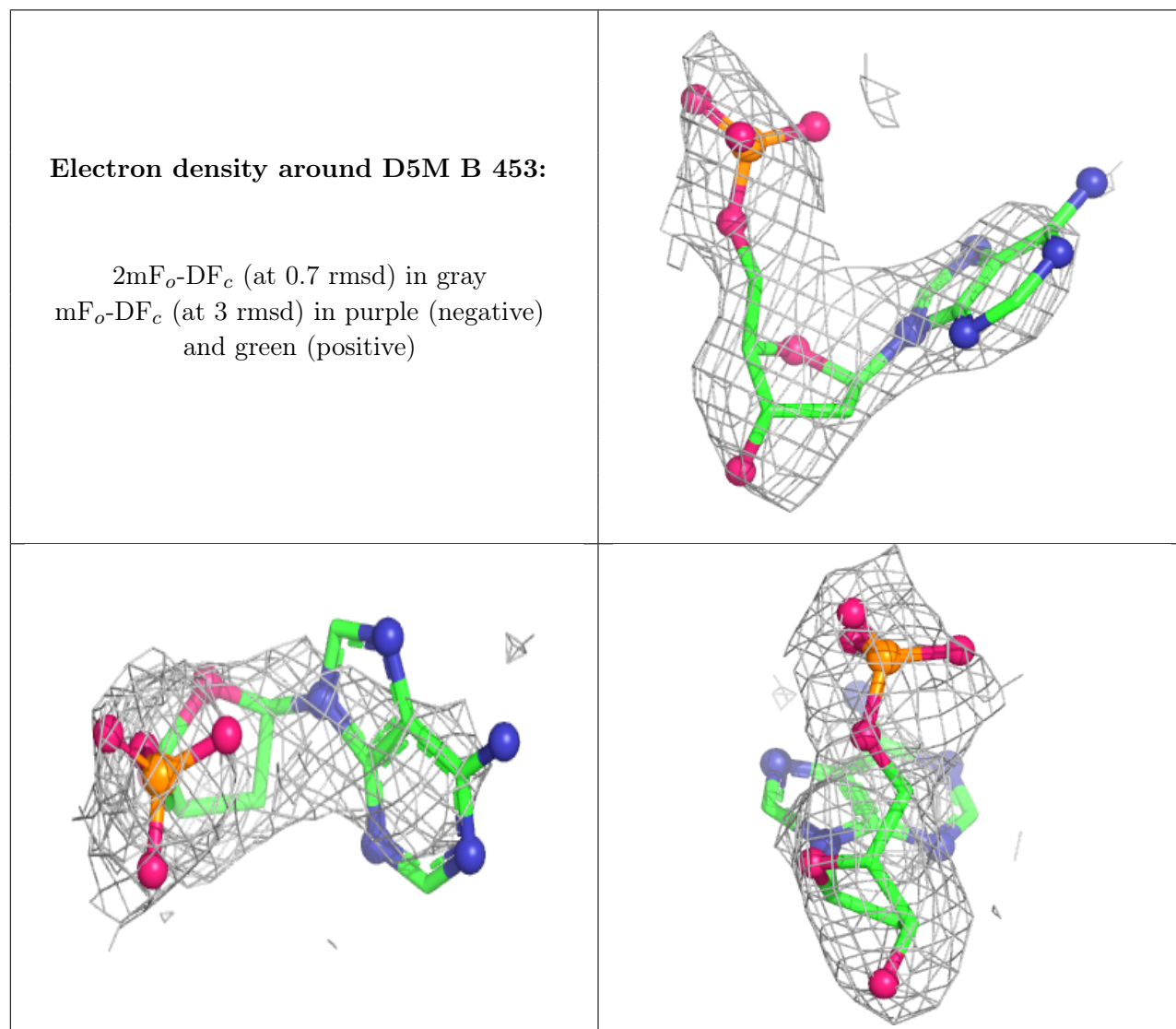
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	A	453	6/6	0.86	0.10	69,90,110,113	0
4	D5M	B	453	22/22	0.88	0.07	137,179,188,189	0
2	MN	B	452	1/1	0.98	0.05	91,91,91,91	0
2	MN	A	452	1/1	0.99	0.04	73,73,73,73	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers ⓘ

There are no such residues in this entry.