



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 08:33 AM UTC

PDB ID : 3DLH / pdb_00003dlh
Title : Crystal structure of the guide-strand-containing Argonaute protein silencing complex
Authors : Wang, Y.; Sheng, G.; Patel, D.J.
Deposited on : 2008-06-27
Resolution : 3.00 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
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

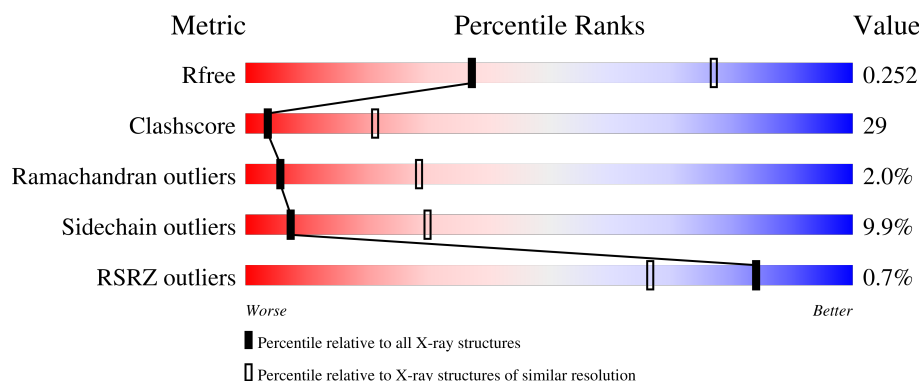
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	685	
1	B	685	
2	X	21	
2	Y	21	

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
6	ACY	B	687	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10986 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 Argonaute.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	673	Total	C	N	O	S	63	0	0
			5213	3337	973	896	7			
1	B	666	Total	C	N	O	S	38	0	0
			5079	3263	948	860	8			

- Molecule 2 is a DNA chain called DNA (5'-D(DTP*DGP*DAP*DGP*DGP*DTP*DAP*DG*DT)*DAP*DGP*DGP*DTP*DTP*DGP*DTP*DAP*DTP*DAP*DGP*DT)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	17	Total	C	N	O	P	0	0	1
			329	155	60	98	16			
2	Y	14	Total	C	N	O	P	0	0	1
			259	120	48	78	13			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		
3	Y	1	Total	Mg	0	0
			1	1		

- Molecule 4 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	X	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is ACETIC ACID (CCD ID: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

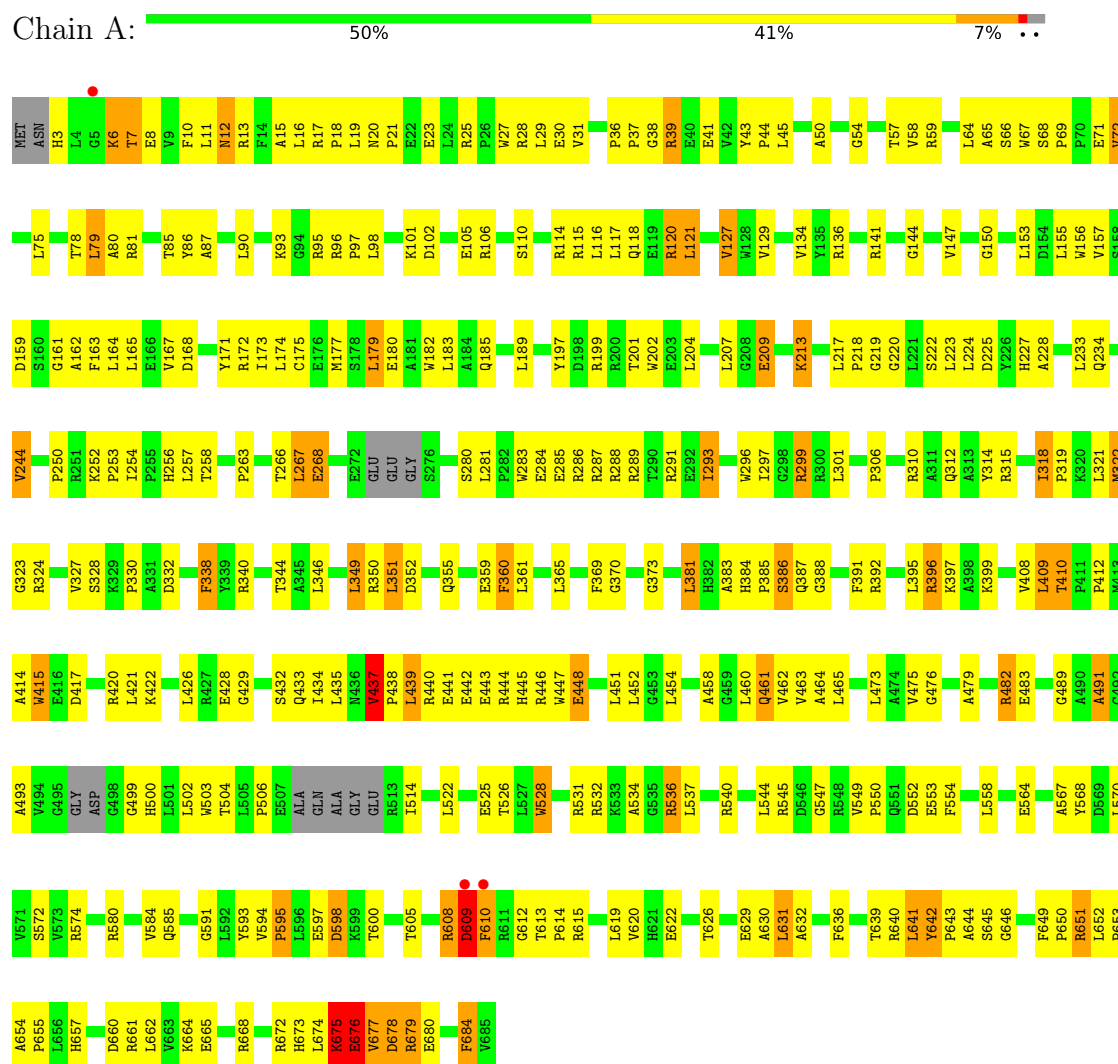
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	39	Total	O	0	0
			39	39		
7	B	35	Total	O	0	0
			35	35		
7	X	1	Total	O	0	0
			1	1		

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: Argonaute



• Molecule 1: Argonaute





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.74Å 114.63Å 175.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 30.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	93.0 (30.00-3.00) 92.9 (30.00-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.91Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.226 , 0.284 (Not available) , 0.252	Depositor DCC
R_{free} test set	2323 reflections (6.97%)	wwPDB-VP
Wilson B-factor (Å ²)	57.3	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 52.8	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	0.92	EDS
Total number of atoms	10986	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, ACY, MG, PGE

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	0.62	7/5336 (0.1%)	1.15	46/7250 (0.6%)
1	B	0.57	1/5199 (0.0%)	1.10	34/7071 (0.5%)
2	X	0.54	1/368 (0.3%)	1.01	1/565 (0.2%)
2	Y	0.54	1/289 (0.3%)	0.88	1/444 (0.2%)
All	All	0.59	10/11192 (0.1%)	1.11	82/15330 (0.5%)

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
2	X	0	1
2	Y	0	1
All	All	0	5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	608	ARG	C-O	-9.52	1.11	1.23
1	A	676	GLU	CA-C	-7.34	1.43	1.52
1	A	609	ASP	C-O	-7.05	1.14	1.23
1	A	676	GLU	N-CA	-7.01	1.37	1.46
1	A	609	ASP	CA-C	6.23	1.62	1.52
1	A	610	PHE	C-O	-6.13	1.16	1.24
2	X	17	DA	O3'-P	-5.99	1.52	1.61
1	B	2	ASN	CA-CB	-5.86	1.45	1.53
1	A	677	VAL	CA-C	-5.76	1.45	1.52
2	Y	118	DT	O3'-P	-5.35	1.53	1.61

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	384	HIS	N-CA-C	-15.02	92.86	110.13
1	A	677	VAL	N-CA-CB	12.72	127.92	111.90
1	A	675	LYS	CA-C-N	-12.46	101.41	122.33
1	A	675	LYS	C-N-CA	-12.46	101.41	122.33
1	B	2	ASN	N-CA-C	-11.79	98.20	112.59
1	A	610	PHE	N-CA-C	10.32	132.78	110.80
1	A	676	GLU	N-CA-C	9.64	125.76	108.69
1	A	429	GLY	N-CA-C	9.22	128.12	115.30
1	A	677	VAL	CB-CA-C	8.50	122.04	110.99
1	A	207	LEU	N-CA-C	-8.13	98.19	110.14
1	A	437	VAL	N-CA-C	8.12	126.41	108.88
1	A	537	LEU	N-CA-C	-7.62	100.15	110.36
1	B	292	GLU	N-CA-C	-7.43	103.32	112.38
1	B	333	ALA	N-CA-C	-7.15	104.82	113.97
1	B	642	TYR	CA-C-N	7.12	126.65	119.24
1	B	642	TYR	C-N-CA	7.12	126.65	119.24
1	A	438	PRO	N-CA-C	-7.11	97.71	112.36
1	A	7	THR	N-CA-C	7.07	118.83	108.86
1	A	324	ARG	N-CA-C	-6.93	103.78	111.82
1	A	385	PRO	N-CA-CB	6.87	110.81	103.39
1	A	677	VAL	CA-CB-CG2	6.87	122.08	110.40
1	B	385	PRO	N-CA-C	6.79	123.44	114.27
1	A	72	VAL	N-CA-C	-6.79	95.22	109.34
1	B	399	LYS	N-CA-C	-6.64	103.96	111.07
1	B	449	ASN	N-CA-C	-6.61	104.16	111.36
1	A	677	VAL	CA-C-O	6.57	127.71	120.48
1	B	684	PHE	N-CA-C	6.36	120.65	113.01
1	B	69	PRO	CA-C-N	6.20	126.39	119.32
1	B	69	PRO	C-N-CA	6.20	126.39	119.32
1	A	642	TYR	CA-C-N	6.18	127.56	119.84
1	A	642	TYR	C-N-CA	6.18	127.56	119.84
1	A	522	LEU	N-CA-C	-6.07	104.58	112.23
1	A	12	ASN	N-CA-C	-6.04	105.97	113.15
1	B	324	ARG	N-CA-C	-5.98	104.33	111.69
1	A	293	ILE	N-CA-C	-5.96	106.69	111.81
1	B	644	ALA	N-CA-C	5.94	121.27	113.20
1	B	228	ALA	N-CA-C	-5.85	104.98	111.36
1	A	323	GLY	N-CA-C	-5.79	99.46	113.18
1	A	595	PRO	N-CA-C	-5.76	102.04	111.21
1	A	209	GLU	N-CA-C	-5.74	106.27	113.28
1	B	168	ASP	CA-C-N	5.67	126.00	119.93
1	B	168	ASP	C-N-CA	5.67	126.00	119.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	TRP	N-CA-C	-5.65	106.93	113.88
1	A	679	ARG	N-CA-C	5.58	119.19	112.38
1	A	322	MET	N-CA-C	5.58	117.88	109.23
1	A	338	PHE	N-CA-C	5.58	118.34	110.14
1	A	199	ARG	N-CA-C	5.55	119.78	112.89
1	A	252	LYS	CA-C-N	5.55	125.47	119.76
1	A	252	LYS	C-N-CA	5.55	125.47	119.76
1	A	385	PRO	N-CA-C	-5.53	106.18	113.65
1	A	68	SER	CA-C-N	5.49	126.03	120.38
1	A	68	SER	C-N-CA	5.49	126.03	120.38
2	X	4	DG	N9-C1'-C2'	-5.42	105.37	113.50
1	B	462	VAL	N-CA-C	5.38	115.59	110.53
1	B	2	ASN	CA-C-N	5.37	131.80	121.54
1	B	2	ASN	C-N-CA	5.37	131.80	121.54
1	A	220	GLY	N-CA-C	-5.36	107.72	115.27
1	A	491	ALA	N-CA-C	5.35	117.32	109.24
2	Y	104	DG	N9-C1'-C2'	-5.34	105.48	113.50
1	A	678	ASP	N-CA-C	-5.32	102.42	110.24
1	B	304	GLY	N-CA-C	5.26	121.79	112.53
1	B	68	SER	CA-C-N	5.24	123.48	119.66
1	B	68	SER	C-N-CA	5.24	123.48	119.66
1	A	684	PHE	N-CA-C	5.22	119.65	113.28
1	B	200	ARG	N-CA-C	5.22	117.80	110.23
1	A	448	GLU	N-CA-C	-5.20	105.70	111.36
1	B	209	GLU	N-CA-C	-5.20	106.78	113.01
1	B	165	LEU	N-CA-C	5.17	117.83	109.40
1	A	197	TYR	N-CA-C	5.16	119.56	113.16
1	A	370	GLY	N-CA-C	-5.16	106.25	112.49
1	B	360	PHE	N-CA-C	5.15	116.71	111.14
1	B	437	VAL	CA-C-N	-5.15	113.40	119.84
1	B	437	VAL	C-N-CA	-5.15	113.40	119.84
1	B	338	PHE	N-CA-C	5.13	117.68	110.14
1	B	676	GLU	N-CA-C	-5.11	107.01	113.20
1	B	382	HIS	N-CA-C	5.10	119.51	113.28
1	A	651	ARG	N-CA-C	-5.09	105.81	112.23
1	A	514	ILE	N-CA-C	5.07	113.91	108.95
1	A	360	PHE	N-CA-C	5.06	116.87	111.36
1	A	120	ARG	N-CA-C	-5.03	105.88	111.36
1	B	514	ILE	CA-C-N	5.00	125.02	119.32
1	B	514	ILE	C-N-CA	5.00	125.02	119.32

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	608	ARG	Mainchain
1	A	609	ASP	Mainchain
1	A	676	GLU	Mainchain
2	X	7	DA	Sidechain
2	Y	104	DG	Sidechain

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	5213	0	5256	289	1
1	B	5079	0	5101	321	1
2	X	329	0	178	25	0
2	Y	259	0	137	14	0
3	A	2	0	0	0	0
3	Y	1	0	0	0	0
4	A	10	0	14	0	0
5	A	5	0	0	0	0
5	X	5	0	0	0	0
6	B	8	0	6	2	0
7	A	39	0	0	0	0
7	B	35	0	0	2	0
7	X	1	0	0	0	0
All	All	10986	0	10692	622	1

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 29.

All (622) 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:B:525:GLU:HG2	1:B:679:ARG:HH12	1.03	1.13
1:A:280:SER:HA	2:X:7:DA:H5'	1.30	1.10
1:B:286:ARG:HD2	1:B:613:THR:HG21	1.12	1.09
1:A:327:VAL:HG23	1:A:332:ASP:HB2	1.28	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:GLU:CB	1:B:141:ARG:HH21	1.66	1.08
1:A:286:ARG:HD2	1:A:613:THR:HG21	1.32	1.06
1:A:600:THR:HG22	1:A:620:VAL:HG22	1.32	1.05
1:B:531:ARG:HG2	1:B:531:ARG:HH21	1.19	1.03
1:B:54:GLY:HA3	1:B:73:LEU:HD23	1.39	1.03
1:B:528:TRP:HZ3	1:B:531:ARG:HH22	1.04	1.02
1:B:408:VAL:HB	1:B:434:ILE:HD13	1.41	1.02
1:B:330:PRO:HD2	1:B:646:GLY:HA2	1.41	0.98
1:B:100:PRO:O	1:B:106:ARG:HD2	1.64	0.97
2:X:1:DT:H5'	2:X:2:DG:H3'	1.47	0.97
1:B:51:ARG:HH21	1:B:51:ARG:HG3	1.28	0.96
1:B:645:SER:O	1:B:647:PHE:N	1.98	0.96
1:A:540:ARG:HH11	1:A:567:ALA:HB1	1.33	0.94
1:B:391:PHE:CE2	1:B:395:LEU:HD11	2.02	0.93
1:B:347:ALA:HB2	1:B:379:HIS:HB2	1.51	0.93
1:A:540:ARG:NH1	1:A:567:ALA:HB1	1.83	0.92
1:B:286:ARG:CD	1:B:613:THR:HG21	2.00	0.91
1:B:52:ARG:HE	1:B:79:LEU:HG	1.31	0.90
1:B:505:LEU:HD12	1:B:506:PRO:HD2	1.52	0.89
1:B:361:LEU:O	1:B:365:LEU:HD23	1.73	0.88
1:A:321:LEU:HD12	1:A:327:VAL:HG13	1.55	0.88
1:A:673:HIS:HD2	1:A:674:LEU:H	1.20	0.88
1:B:319:PRO:HG3	1:B:640:ARG:HD3	1.54	0.88
1:A:321:LEU:HD13	1:A:463:VAL:HG11	1.55	0.88
1:B:531:ARG:HH21	1:B:531:ARG:CG	1.87	0.87
1:B:222:SER:HB3	1:B:225:ASP:OD1	1.75	0.87
1:B:525:GLU:HG2	1:B:679:ARG:NH1	1.89	0.87
1:A:408:VAL:HB	1:A:434:ILE:HD13	1.57	0.86
1:A:360:PHE:HZ	1:A:439:LEU:HD13	1.39	0.86
1:B:351:LEU:HB2	1:B:410:THR:HG22	1.57	0.85
1:B:172:ARG:HH22	2:Y:109:DT:P	2.00	0.85
1:B:45:LEU:O	1:B:49:VAL:HG23	1.77	0.83
1:B:545:ARG:HD3	1:B:570:LEU:HD11	1.59	0.83
1:A:117:LEU:O	1:A:121:LEU:HB2	1.79	0.83
1:B:289:ARG:O	1:B:293:ILE:HG12	1.78	0.83
1:B:80:ALA:HB2	1:B:85:THR:HG22	1.62	0.82
1:B:286:ARG:HD2	1:B:613:THR:CG2	2.05	0.82
1:A:144:GLY:HA3	1:A:177:MET:HE2	1.59	0.82
1:B:69:PRO:HG2	1:B:72:VAL:HG23	1.60	0.82
1:A:322:MET:HA	1:A:327:VAL:HG12	1.61	0.81
1:A:409:LEU:HD23	1:A:437:VAL:HG22	1.60	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:TYR:HE2	1:A:595:PRO:HG2	1.43	0.80
1:A:213:LYS:HD2	1:A:224:LEU:HD22	1.61	0.80
1:A:350:ARG:HG3	1:A:350:ARG:HH11	1.46	0.79
1:B:138:GLU:CB	1:B:141:ARG:NH2	2.43	0.79
1:A:473:LEU:HD11	1:A:493:ALA:HB1	1.65	0.78
1:B:439:LEU:HD13	1:B:440:ARG:N	1.97	0.78
2:Y:106:DT:H2''	2:Y:107:DA:H5'	1.64	0.78
1:B:350:ARG:NH2	1:B:352:ASP:OD2	2.16	0.78
1:A:54:GLY:O	1:A:57:THR:HG22	1.83	0.78
1:B:446:ARG:O	1:B:449:ASN:N	2.17	0.78
1:B:346:LEU:O	1:B:346:LEU:HD23	1.85	0.77
1:A:97:PRO:C	1:A:98:LEU:HD12	2.10	0.76
1:A:351:LEU:CD1	1:A:410:THR:HB	2.15	0.76
1:A:202:TRP:HB2	1:A:244:VAL:CG2	2.17	0.75
1:A:673:HIS:CD2	1:A:674:LEU:H	2.03	0.75
1:A:153:LEU:HD22	1:A:167:VAL:HG22	1.67	0.75
1:B:50:ALA:HB2	1:B:64:LEU:HD22	1.68	0.75
1:A:410:THR:C	1:A:437:VAL:HG23	2.12	0.75
1:B:350:ARG:HG2	1:B:352:ASP:OD1	1.85	0.74
1:A:580:ARG:NH2	2:X:7:DA:OP2	2.19	0.74
1:A:254:ILE:HD12	2:X:20:DG:N2	2.02	0.74
1:A:437:VAL:HG12	1:A:437:VAL:O	1.86	0.73
1:A:660:ASP:OD1	1:A:664:LYS:HE3	1.88	0.73
1:B:319:PRO:HB3	1:B:637:HIS:CD2	2.23	0.73
1:B:11:LEU:C	1:B:13:ARG:H	1.94	0.73
1:A:640:ARG:HD2	1:A:640:ARG:N	2.04	0.72
1:B:447:TRP:O	1:B:451:LEU:HG	1.89	0.72
1:B:346:LEU:HA	1:B:403:VAL:HG13	1.72	0.72
1:A:440:ARG:O	1:A:443:GLU:HG2	1.90	0.72
1:A:253:PRO:O	1:A:254:ILE:HD13	1.89	0.71
1:B:172:ARG:CZ	1:B:172:ARG:HA	2.21	0.70
1:A:58:VAL:HG12	1:A:59:ARG:N	2.06	0.70
1:A:351:LEU:HD11	1:A:410:THR:HB	1.71	0.70
1:A:435:LEU:HD12	1:A:435:LEU:O	1.92	0.70
1:A:360:PHE:HB3	1:A:441:GLU:OE1	1.92	0.70
1:B:20:ASN:HB2	1:B:21:PRO:HD2	1.74	0.69
1:B:70:PRO:HA	1:B:73:LEU:HD12	1.73	0.69
1:A:491:ALA:HB3	1:A:504:THR:HG23	1.73	0.69
1:B:52:ARG:NE	1:B:79:LEU:HG	2.07	0.69
1:A:8:GLU:OE1	1:A:310:ARG:HD3	1.93	0.69
1:B:9:VAL:HG21	1:B:581:VAL:HG13	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:437:VAL:O	1:B:439:LEU:N	2.25	0.69
1:B:360:PHE:O	1:B:363:ARG:HG3	1.93	0.69
1:B:494:VAL:HG22	1:B:501:LEU:HD23	1.75	0.68
1:A:461:GLN:OE1	1:A:499:GLY:O	2.12	0.68
1:B:584:VAL:HG22	7:B:722:HOH:O	1.93	0.68
1:A:155:LEU:HD11	1:A:163:PHE:HB3	1.75	0.68
1:B:51:ARG:HG3	1:B:51:ARG:NH2	2.04	0.68
1:A:12:ASN:HD21	1:A:168:ASP:HB2	1.59	0.68
1:B:172:ARG:NH2	2:Y:109:DT:P	2.67	0.68
1:B:256:HIS:HD2	1:B:257:LEU:H	1.38	0.68
1:B:330:PRO:CD	1:B:646:GLY:HA2	2.19	0.68
1:B:472:GLU:CD	1:B:536:ARG:HH12	2.01	0.68
1:A:3:HIS:CB	1:A:6:LYS:HD3	2.24	0.68
1:A:327:VAL:CG2	1:A:332:ASP:HB2	2.15	0.67
1:A:289:ARG:O	1:A:293:ILE:HG13	1.95	0.67
1:B:540:ARG:NH1	1:B:567:ALA:HB1	2.08	0.67
1:A:202:TRP:HB2	1:A:244:VAL:HG22	1.77	0.67
1:B:446:ARG:HG2	2:Y:102:DG:C5	2.30	0.67
1:A:69:PRO:HG2	1:A:72:VAL:CG2	2.25	0.67
1:A:299:ARG:HG3	1:A:299:ARG:HH11	1.60	0.67
1:B:346:LEU:HD22	1:B:376:LEU:HD11	1.77	0.67
1:A:58:VAL:HG12	1:A:59:ARG:H	1.59	0.67
1:B:490:ALA:HB2	1:B:505:LEU:HD13	1.76	0.67
1:A:286:ARG:HD3	1:A:580:ARG:HD3	1.76	0.66
1:B:287:ARG:O	1:B:290:THR:HG22	1.96	0.66
1:B:266:THR:HG22	1:B:267:LEU:H	1.61	0.66
1:B:344:THR:O	1:B:376:LEU:HD12	1.96	0.66
1:B:504:THR:HG21	1:B:526:THR:OG1	1.96	0.66
1:B:256:HIS:CD2	1:B:257:LEU:H	2.13	0.65
1:B:365:LEU:HD21	1:B:451:LEU:HD22	1.77	0.65
1:A:280:SER:HA	2:X:7:DA:C5'	2.19	0.65
1:B:531:ARG:O	1:B:531:ARG:HG3	1.97	0.65
1:A:673:HIS:CD2	1:A:674:LEU:N	2.65	0.65
1:B:505:LEU:HD12	1:B:506:PRO:CD	2.26	0.65
1:A:69:PRO:HG2	1:A:72:VAL:HG23	1.79	0.65
1:B:232:ARG:HG3	1:B:232:ARG:HH11	1.62	0.65
1:A:213:LYS:HD2	1:A:224:LEU:CD2	2.27	0.65
1:A:383:ALA:CB	1:A:391:PHE:HD1	2.10	0.65
1:A:256:HIS:HD2	1:A:257:LEU:H	1.45	0.64
1:A:408:VAL:HG12	1:A:410:THR:CG2	2.28	0.64
1:B:222:SER:HB3	1:B:225:ASP:CG	2.22	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:531:ARG:HG2	1:B:531:ARG:NH2	1.98	0.64
1:B:598:ASP:O	1:B:599:LYS:HB2	1.98	0.64
1:A:80:ALA:HB2	1:A:85:THR:HG22	1.77	0.64
1:B:231:GLY:O	1:B:234:GLN:HB2	1.98	0.64
1:B:9:VAL:CG2	1:B:581:VAL:HG13	2.27	0.64
1:B:525:GLU:CG	1:B:679:ARG:HH12	1.96	0.64
1:A:340:ARG:NH2	1:A:499:GLY:O	2.31	0.63
1:B:127:VAL:HG11	1:B:134:VAL:HG13	1.80	0.63
1:B:195:ASN:ND2	1:B:200:ARG:HB3	2.13	0.63
1:A:350:ARG:HG3	1:A:350:ARG:NH1	2.11	0.63
1:B:599:LYS:HG2	1:B:621:HIS:O	1.97	0.63
2:Y:106:DT:H2''	2:Y:107:DA:C5'	2.27	0.63
1:A:321:LEU:CD1	1:A:327:VAL:HG13	2.27	0.63
1:B:193:VAL:HG22	1:B:261:LEU:HB3	1.81	0.63
1:B:217:LEU:HD11	1:B:223:LEU:HA	1.80	0.63
1:A:97:PRO:O	1:A:98:LEU:HD12	1.98	0.63
1:B:349:LEU:HD22	1:B:351:LEU:HG	1.80	0.63
1:B:439:LEU:HD13	1:B:440:ARG:H	1.60	0.63
1:B:53:ALA:O	1:B:54:GLY:O	2.17	0.62
1:A:340:ARG:HH12	1:A:500:HIS:CD2	2.17	0.62
1:B:528:TRP:HZ3	1:B:531:ARG:NH2	1.87	0.62
1:A:8:GLU:HG2	1:A:310:ARG:HG2	1.80	0.62
1:A:78:THR:HG22	1:A:87:ALA:HA	1.79	0.62
1:A:283:TRP:HA	1:A:613:THR:HB	1.80	0.62
1:B:545:ARG:HG3	1:B:545:ARG:HH11	1.62	0.62
1:A:254:ILE:HD12	2:X:20:DG:H21	1.62	0.62
1:B:9:VAL:HG21	1:B:581:VAL:CG1	2.29	0.62
1:A:19:LEU:HD13	1:A:161:GLY:O	1.99	0.61
1:B:661:ARG:O	1:B:665:GLU:OE1	2.18	0.61
1:A:383:ALA:HB1	1:A:391:PHE:HD1	1.65	0.61
1:B:408:VAL:HB	1:B:434:ILE:CD1	2.23	0.61
1:B:363:ARG:O	1:B:366:LEU:N	2.34	0.61
1:A:250:PRO:HB3	1:A:482:ARG:HH21	1.65	0.61
1:B:142:GLY:HA3	1:B:145:TRP:CE2	2.34	0.61
1:A:528:TRP:CH2	1:B:1:MET:HE3	2.35	0.61
1:B:600:THR:HG22	1:B:620:VAL:HG22	1.82	0.61
1:B:38:GLY:O	1:B:41:GLU:HG2	2.01	0.60
1:B:531:ARG:HD3	1:B:536:ARG:O	2.01	0.60
1:B:455:LEU:HD22	1:B:460:LEU:HD22	1.83	0.60
1:B:350:ARG:HD2	1:B:356:GLY:O	2.02	0.60
1:A:297:ILE:HG23	1:A:301:LEU:HG	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:ARG:HG3	1:A:440:ARG:HH11	1.67	0.60
1:B:359:GLU:HG3	1:B:360:PHE:H	1.66	0.60
1:B:363:ARG:O	1:B:364:ALA:C	2.45	0.60
1:B:545:ARG:HG3	1:B:545:ARG:NH1	2.17	0.60
1:A:422:LYS:NZ	1:A:432:SER:O	2.34	0.60
1:B:193:VAL:CG2	1:B:261:LEU:HB3	2.31	0.60
1:A:626:THR:HG22	1:A:630:ALA:HB3	1.83	0.60
1:A:283:TRP:CE2	1:A:284:GLU:HG3	2.37	0.60
1:A:297:ILE:O	1:A:301:LEU:HB2	2.01	0.59
1:A:619:LEU:N	1:A:619:LEU:HD12	2.18	0.59
1:B:11:LEU:C	1:B:13:ARG:N	2.61	0.59
1:B:580:ARG:NH2	1:B:613:THR:HG23	2.17	0.59
1:A:121:LEU:HD22	1:A:129:VAL:HG11	1.84	0.59
1:A:408:VAL:HG12	1:A:410:THR:HG22	1.85	0.59
1:B:544:LEU:HD21	1:B:635:ILE:CD1	2.33	0.59
1:A:256:HIS:CD2	1:A:257:LEU:H	2.20	0.59
1:B:408:VAL:HG12	1:B:410:THR:HG23	1.85	0.59
1:A:79:LEU:HD22	1:A:79:LEU:O	2.02	0.59
1:A:360:PHE:HD1	1:A:360:PHE:H	1.50	0.59
1:A:636:PHE:O	1:A:639:THR:HB	2.02	0.59
1:A:349:LEU:HD22	1:A:351:LEU:HB3	1.83	0.58
1:B:444:ARG:HA	1:B:447:TRP:CE2	2.38	0.58
1:A:202:TRP:HB2	1:A:244:VAL:HG21	1.85	0.58
1:A:227:HIS:CE1	2:X:21:DT:H3'	2.38	0.58
1:A:491:ALA:HB3	1:A:504:THR:CG2	2.32	0.58
1:B:676:GLU:H	1:B:676:GLU:CD	2.10	0.58
1:A:665:GLU:HA	1:A:668:ARG:HB2	1.86	0.58
1:A:20:ASN:OD1	1:A:23:GLU:HG3	2.04	0.58
1:B:195:ASN:HD22	1:B:200:ARG:HB3	1.69	0.58
1:B:359:GLU:HG3	1:B:360:PHE:N	2.19	0.57
1:B:313:ALA:HB2	1:B:594:VAL:HG22	1.84	0.57
1:A:545:ARG:HD3	1:A:570:LEU:HD11	1.86	0.57
1:A:20:ASN:HB2	1:A:21:PRO:HD2	1.86	0.57
1:A:349:LEU:CD2	1:A:351:LEU:HB3	2.34	0.57
1:A:545:ARG:HG3	1:A:545:ARG:HH11	1.69	0.57
1:B:404:GLN:HG3	1:B:681:LYS:HE2	1.86	0.57
1:A:228:ALA:HB2	1:A:233:LEU:HD12	1.85	0.57
1:A:16:LEU:HD21	1:A:306:PRO:HB3	1.86	0.57
1:A:281:LEU:C	1:A:612:GLY:HA2	2.30	0.57
1:A:440:ARG:HD2	1:A:442:GLU:HB2	1.87	0.57
1:A:545:ARG:HD2	1:A:554:PHE:CE1	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:VAL:O	1:A:550:PRO:C	2.46	0.57
1:A:597:GLU:O	1:A:598:ASP:C	2.47	0.56
1:A:437:VAL:O	1:A:437:VAL:CG1	2.54	0.56
1:B:12:ASN:HD21	1:B:168:ASP:HB2	1.70	0.56
1:B:80:ALA:HA	1:B:85:THR:HA	1.87	0.56
1:B:580:ARG:NH2	2:Y:107:DA:OP2	2.27	0.56
1:A:71:GLU:OE2	1:A:75:LEU:HD11	2.06	0.56
1:A:172:ARG:HD3	2:X:9:DT:OP1	2.05	0.56
1:A:110:SER:OG	1:A:157:VAL:HG12	2.06	0.56
1:B:530:PHE:CD2	1:B:538:PRO:HD3	2.41	0.56
1:B:465:LEU:HG	1:B:641:LEU:HD23	1.87	0.56
2:Y:101:DT:H2''	2:Y:102:DG:OP1	2.06	0.56
1:A:675:LYS:O	1:A:676:GLU:CB	2.50	0.56
1:B:284:GLU:HG3	1:B:287:ARG:NH2	2.21	0.56
1:B:348:LEU:HD22	1:B:357:TRP:CE2	2.40	0.56
1:B:597:GLU:CB	6:B:687:ACY:H2	2.35	0.56
1:A:266:THR:HG22	1:A:267:LEU:N	2.21	0.55
1:A:399:LYS:HD2	1:A:428:GLU:O	2.06	0.55
1:B:43:TYR:HB2	1:B:44:PRO:HD3	1.87	0.55
1:B:352:ASP:HB3	1:B:437:VAL:HG21	1.88	0.55
1:A:127:VAL:HG21	1:A:134:VAL:CG2	2.37	0.55
1:A:654:ALA:HB3	1:A:655:PRO:HD3	1.88	0.55
1:B:46:LEU:HD12	1:B:59:ARG:HD2	1.87	0.55
1:A:286:ARG:CD	1:A:613:THR:HG21	2.21	0.55
1:A:657:HIS:O	1:A:661:ARG:HG2	2.06	0.55
1:B:378:LEU:HD12	1:B:378:LEU:N	2.21	0.55
1:B:202:TRP:HB3	1:B:245:ALA:O	2.06	0.55
1:A:286:ARG:HD2	1:A:613:THR:CG2	2.23	0.55
1:A:660:ASP:O	1:A:664:LYS:HG3	2.06	0.55
1:B:159:ASP:C	1:B:161:GLY:H	2.15	0.55
1:A:383:ALA:HB1	1:A:391:PHE:HA	1.88	0.55
1:A:280:SER:CA	2:X:7:DA:H5'	2.20	0.55
1:B:399:LYS:CD	1:B:430:LEU:HD11	2.36	0.55
1:B:545:ARG:NH2	1:B:622:GLU:OE1	2.38	0.55
1:B:13:ARG:HB3	1:B:164:LEU:HD21	1.89	0.54
1:A:121:LEU:HD22	1:A:129:VAL:CG1	2.37	0.54
1:B:121:LEU:HD22	1:B:134:VAL:HG22	1.89	0.54
1:B:506:PRO:HD3	1:B:522:LEU:CD2	2.38	0.54
1:B:639:THR:HG23	1:B:650:PRO:O	2.06	0.54
1:A:314:TYR:CE2	1:A:595:PRO:HG2	2.34	0.54
1:B:360:PHE:HA	1:B:363:ARG:NE	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:484:SER:HA	1:B:549:VAL:HG13	1.90	0.54
1:A:10:PHE:CD2	1:A:287:ARG:NH2	2.75	0.54
1:B:554:PHE:O	1:B:558:LEU:HG	2.07	0.54
1:A:179:LEU:HD13	1:A:258:THR:HG22	1.90	0.54
1:B:29:LEU:HD23	1:B:90:LEU:HB3	1.90	0.54
1:B:52:ARG:HE	1:B:79:LEU:CG	2.13	0.54
1:B:232:ARG:HG3	1:B:232:ARG:NH1	2.23	0.54
1:B:449:ASN:ND2	2:Y:102:DG:H21	2.05	0.54
1:B:494:VAL:HG22	1:B:501:LEU:CD2	2.38	0.54
1:A:528:TRP:O	1:A:532:ARG:HG3	2.08	0.53
1:B:287:ARG:C	1:B:290:THR:HG22	2.33	0.53
1:A:360:PHE:CZ	1:A:439:LEU:HD13	2.31	0.53
1:A:504:THR:HG21	1:A:526:THR:OG1	2.08	0.53
1:A:584:VAL:HG23	1:A:585:GLN:N	2.22	0.53
1:B:81:ARG:O	1:B:82:MET:HB3	2.08	0.53
1:A:7:THR:OG1	1:A:8:GLU:N	2.40	0.53
1:A:156:TRP:CZ2	1:A:164:LEU:HD23	2.44	0.53
1:A:410:THR:O	1:A:437:VAL:HG23	2.08	0.53
1:B:147:VAL:HG22	1:B:173:ILE:HG12	1.90	0.53
1:A:165:LEU:HG	1:A:167:VAL:HG23	1.90	0.53
1:B:596:LEU:HG	6:B:687:ACY:O	2.09	0.53
1:B:654:ALA:HB3	1:B:655:PRO:HD3	1.91	0.53
1:A:202:TRP:CB	1:A:244:VAL:HG22	2.38	0.53
1:A:564:GLU:OE2	1:B:3:HIS:HA	2.09	0.53
1:B:50:ALA:HB2	1:B:64:LEU:CD2	2.37	0.53
2:X:5:DG:H2'	2:X:6:DT:H71	1.91	0.53
1:A:330:PRO:HB2	1:A:646:GLY:HA2	1.90	0.52
1:B:551:GLN:HE22	1:B:622:GLU:HB3	1.74	0.52
1:B:665:GLU:HG3	1:B:668:ARG:NH1	2.24	0.52
1:A:81:ARG:HG2	1:A:86:TYR:HE1	1.74	0.52
1:A:175:CYS:SG	1:A:263:PRO:HD2	2.50	0.52
1:A:525:GLU:OE1	1:A:679:ARG:NH2	2.42	0.52
1:A:360:PHE:HZ	1:A:439:LEU:CD1	2.15	0.52
1:A:545:ARG:HG3	1:A:545:ARG:NH1	2.25	0.52
1:B:596:LEU:HD22	1:B:602:LEU:HG	1.91	0.52
1:A:136:ARG:HD3	1:A:296:TRP:CH2	2.45	0.52
1:A:381:LEU:HD11	1:A:395:LEU:HD23	1.92	0.52
1:B:389:LEU:HD23	1:B:389:LEU:O	2.09	0.52
1:B:427:ARG:C	1:B:429:GLY:H	2.18	0.52
1:A:115:ARG:HA	1:A:118:GLN:HE21	1.75	0.52
1:B:600:THR:CG2	1:B:620:VAL:HG22	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:619:LEU:HD21	1:B:635:ILE:HG21	1.92	0.52
1:A:462:VAL:HG12	1:A:463:VAL:HG23	1.90	0.52
2:X:8:DG:H2''	2:X:9:DT:O5'	2.10	0.52
1:A:580:ARG:NH2	1:A:615:ARG:HG2	2.24	0.51
1:B:172:ARG:NH1	1:B:173:ILE:H	2.08	0.51
1:B:475:VAL:HB	1:B:493:ALA:HB2	1.92	0.51
1:B:34:ASP:HB3	1:B:87:ALA:HB3	1.93	0.51
1:A:38:GLY:O	1:A:39:ARG:C	2.53	0.51
1:A:153:LEU:CD2	1:A:167:VAL:HG22	2.39	0.51
1:A:351:LEU:HD12	1:A:410:THR:HB	1.90	0.51
1:A:463:VAL:HG12	1:A:464:ALA:N	2.26	0.51
1:B:89:ARG:HG3	1:B:91:TYR:CE1	2.46	0.51
1:A:81:ARG:O	1:A:81:ARG:HG3	2.11	0.51
1:B:338:PHE:CD2	1:B:462:VAL:HG12	2.45	0.51
1:B:523:LEU:HD21	1:B:561:LEU:HD21	1.92	0.51
1:B:180:GLU:OE2	1:B:240:ARG:HD3	2.10	0.51
1:A:597:GLU:HB3	1:A:600:THR:OG1	2.11	0.51
1:B:81:ARG:O	1:B:82:MET:CB	2.58	0.51
1:B:387:GLN:O	1:B:390:ALA:N	2.44	0.51
1:B:544:LEU:HD21	1:B:635:ILE:HD11	1.91	0.51
1:A:476:GLY:HA2	1:A:544:LEU:O	2.11	0.51
1:A:38:GLY:O	1:A:41:GLU:N	2.36	0.50
1:A:318:ILE:C	1:A:318:ILE:HD13	2.37	0.50
1:A:57:THR:HB	1:A:66:SER:HB2	1.94	0.50
1:A:554:PHE:O	1:A:558:LEU:HG	2.10	0.50
1:A:267:LEU:O	1:A:267:LEU:HD23	2.11	0.50
1:A:482:ARG:HG2	1:A:483:GLU:H	1.76	0.50
1:A:383:ALA:O	1:A:384:HIS:HB2	2.10	0.50
1:A:27:TRP:O	1:A:65:ALA:HA	2.12	0.50
1:A:528:TRP:HA	1:A:528:TRP:CE3	2.46	0.50
1:A:217:LEU:O	1:A:219:GLY:N	2.45	0.50
1:A:640:ARG:HG3	1:A:649:PHE:CD1	2.47	0.50
1:B:142:GLY:HA3	1:B:145:TRP:CZ2	2.47	0.50
1:B:289:ARG:HA	1:B:292:GLU:HG2	1.93	0.50
1:B:360:PHE:HA	1:B:363:ARG:HG3	1.93	0.50
1:B:1:MET:C	1:B:3:HIS:H	2.14	0.50
1:B:615:ARG:O	1:B:651:ARG:NH1	2.44	0.50
1:A:369:PHE:O	1:A:373:GLY:N	2.43	0.49
1:A:45:LEU:CD2	1:A:81:ARG:HD2	2.43	0.49
1:B:408:VAL:HG12	1:B:410:THR:CG2	2.42	0.49
1:A:444:ARG:O	1:A:448:GLU:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:ARG:NH2	1:B:78:THR:O	2.42	0.49
1:B:253:PRO:O	1:B:254:ILE:HD13	2.11	0.49
1:B:314:TYR:HE2	1:B:595:PRO:HG2	1.78	0.49
1:B:557:ALA:O	1:B:561:LEU:HG	2.13	0.49
1:A:433:GLN:HB3	1:A:454:LEU:HD23	1.93	0.49
1:A:147:VAL:HG22	1:A:173:ILE:HD13	1.95	0.49
2:X:11:DG:H2''	2:X:12:DG:OP2	2.12	0.49
1:B:365:LEU:O	1:B:369:PHE:HD1	1.96	0.49
1:A:597:GLU:HG2	1:A:598:ASP:H	1.78	0.49
1:A:43:TYR:HB2	1:A:44:PRO:HD3	1.95	0.49
1:B:506:PRO:HD3	1:B:522:LEU:HD21	1.94	0.49
1:B:121:LEU:HD22	1:B:134:VAL:CG2	2.43	0.48
1:B:387:GLN:CB	1:B:390:ALA:HB3	2.43	0.48
1:A:639:THR:HG23	1:A:650:PRO:O	2.13	0.48
1:B:127:VAL:CG1	1:B:134:VAL:HG13	2.42	0.48
1:B:202:TRP:HB2	1:B:244:VAL:HG22	1.94	0.48
1:B:376:LEU:HD23	1:B:378:LEU:HD11	1.94	0.48
1:B:445:HIS:CD2	1:B:647:PHE:CE2	3.01	0.48
1:A:609:ASP:CB	1:A:614:PRO:HA	2.43	0.48
1:B:58:VAL:HG11	1:B:111:ALA:HB1	1.96	0.48
1:B:446:ARG:O	1:B:447:TRP:C	2.56	0.48
1:B:202:TRP:HB2	1:B:244:VAL:CG2	2.42	0.48
1:A:19:LEU:HD11	1:A:157:VAL:HG23	1.96	0.48
1:A:69:PRO:HG2	1:A:72:VAL:HG21	1.94	0.48
1:B:434:ILE:HB	2:Y:101:DT:H4'	1.96	0.48
2:X:6:DT:H2''	2:X:7:DA:O5'	2.13	0.48
2:X:18:DT:H5''	2:X:18:DT:C6	2.48	0.48
1:A:286:ARG:HH11	1:A:613:THR:CG2	2.27	0.48
1:B:269:ASP:C	1:B:270:LEU:HD12	2.39	0.48
1:A:631:LEU:O	1:A:632:ALA:C	2.54	0.48
1:B:376:LEU:HG	1:B:377:ARG:N	2.28	0.48
1:A:528:TRP:CZ3	1:B:1:MET:HE3	2.49	0.48
1:B:56:VAL:HA	1:B:115:ARG:HG2	1.95	0.48
1:A:171:TYR:HB2	2:X:8:DG:H5''	1.95	0.47
1:B:340:ARG:NH2	1:B:461:GLN:HG3	2.29	0.47
1:B:222:SER:O	1:B:223:LEU:C	2.57	0.47
1:B:357:TRP:N	1:B:357:TRP:CD1	2.82	0.47
1:B:636:PHE:O	1:B:639:THR:HB	2.14	0.47
1:A:141:ARG:C	1:A:141:ARG:HD2	2.39	0.47
1:B:69:PRO:HG2	1:B:72:VAL:CG2	2.40	0.47
1:A:54:GLY:O	1:A:57:THR:CG2	2.60	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:TRP:O	1:A:451:LEU:HG	2.15	0.47
1:A:461:GLN:OE1	1:A:500:HIS:HA	2.15	0.47
1:B:528:TRP:O	1:B:532:ARG:HG3	2.14	0.47
1:A:120:ARG:HB2	1:A:301:LEU:CD1	2.45	0.47
1:B:7:THR:HG22	1:B:8:GLU:N	2.30	0.47
1:B:127:VAL:HG12	1:B:129:VAL:HG23	1.97	0.47
1:B:222:SER:CB	1:B:225:ASP:OD1	2.54	0.47
1:B:331:ALA:C	1:B:333:ALA:H	2.22	0.47
1:B:357:TRP:CD1	1:B:357:TRP:H	2.33	0.47
1:A:16:LEU:HD23	1:A:306:PRO:HA	1.96	0.47
1:A:652:LEU:N	1:A:652:LEU:HD12	2.29	0.47
1:B:78:THR:CG2	1:B:79:LEU:N	2.74	0.47
1:B:657:HIS:O	1:B:661:ARG:HG2	2.14	0.47
1:A:153:LEU:HD13	1:A:297:ILE:CD1	2.45	0.47
1:A:281:LEU:O	1:A:612:GLY:HA2	2.15	0.47
1:A:344:THR:HG21	1:A:458:ALA:HB1	1.97	0.47
1:A:609:ASP:O	2:X:6:DT:C5'	2.62	0.47
1:B:168:ASP:CG	1:B:580:ARG:HD3	2.40	0.47
1:B:399:LYS:HD2	1:B:430:LEU:HD11	1.96	0.47
1:B:422:LYS:NZ	1:B:432:SER:O	2.48	0.47
1:B:504:THR:CG2	1:B:526:THR:OG1	2.62	0.47
1:B:642:TYR:CE1	1:B:657:HIS:HD2	2.33	0.47
1:B:528:TRP:HA	1:B:528:TRP:CE3	2.50	0.47
1:A:11:LEU:C	1:A:13:ARG:H	2.22	0.47
1:A:81:ARG:HG2	1:A:86:TYR:CE1	2.50	0.47
1:B:472:GLU:OE1	1:B:536:ARG:NH1	2.47	0.47
1:A:531:ARG:HG2	1:B:627:PRO:HB3	1.97	0.47
1:B:593:TYR:CZ	1:B:595:PRO:HG3	2.50	0.46
1:A:102:ASP:O	1:A:106:ARG:HB2	2.15	0.46
1:A:396:ARG:HG3	1:A:397:LYS:N	2.29	0.46
1:A:408:VAL:HG11	1:A:421:LEU:HD21	1.98	0.46
1:A:662:LEU:HD13	1:A:684:PHE:CD2	2.50	0.46
1:B:368:ALA:C	1:B:370:GLY:H	2.23	0.46
1:A:410:THR:N	1:A:437:VAL:CG2	2.79	0.46
1:B:465:LEU:HG	1:B:641:LEU:CD2	2.46	0.46
1:B:640:ARG:HG3	1:B:649:PHE:CD2	2.50	0.46
1:A:127:VAL:HG21	1:A:134:VAL:HG23	1.97	0.46
1:A:189:LEU:HD12	1:A:189:LEU:H	1.81	0.46
1:A:489:GLY:O	1:A:506:PRO:CG	2.64	0.46
1:A:620:VAL:HG12	1:A:622:GLU:HG3	1.96	0.46
1:B:476:GLY:HA2	1:B:544:LEU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:531:ARG:CG	1:B:531:ARG:NH2	2.58	0.46
1:A:120:ARG:CB	1:A:301:LEU:HD13	2.46	0.46
1:A:168:ASP:OD1	1:A:580:ARG:HD2	2.16	0.46
1:A:525:GLU:HB3	1:A:679:ARG:HH22	1.79	0.46
1:B:346:LEU:HD12	1:B:454:LEU:HD11	1.97	0.46
1:B:363:ARG:O	1:B:365:LEU:N	2.49	0.46
1:B:547:GLY:HA2	1:B:572:SER:HB2	1.97	0.46
1:A:189:LEU:HD12	1:A:189:LEU:N	2.30	0.46
1:B:357:TRP:CZ2	1:B:378:LEU:HB3	2.50	0.46
1:B:36:PRO:HA	1:B:37:PRO:HD3	1.76	0.46
1:B:315:ARG:CZ	1:B:589:ALA:HB1	2.46	0.46
1:B:480:GLY:CA	1:B:663:VAL:HG11	2.46	0.46
1:A:222:SER:HB3	1:A:225:ASP:OD1	2.16	0.45
1:A:266:THR:HG22	1:A:267:LEU:H	1.80	0.45
2:Y:106:DT:H71	2:Y:107:DA:N6	2.31	0.45
1:B:434:ILE:HB	2:Y:101:DT:C4'	2.46	0.45
1:A:58:VAL:CG1	1:A:59:ARG:N	2.76	0.45
1:A:503:TRP:O	1:A:679:ARG:HD3	2.17	0.45
1:A:545:ARG:NH2	1:A:622:GLU:OE1	2.49	0.45
1:B:169:PRO:O	1:B:286:ARG:NH2	2.49	0.45
1:B:594:VAL:O	1:B:594:VAL:HG12	2.17	0.45
2:Y:106:DT:H71	2:Y:107:DA:H62	1.81	0.45
1:A:321:LEU:HD12	1:A:321:LEU:C	2.42	0.45
1:B:82:MET:C	1:B:84:GLN:H	2.23	0.45
1:B:148:LEU:CD1	1:B:174:LEU:HD11	2.47	0.45
1:A:383:ALA:HB3	1:A:391:PHE:HD1	1.82	0.45
1:A:597:GLU:HG2	1:A:598:ASP:N	2.31	0.45
1:A:299:ARG:HH11	1:A:299:ARG:CG	2.27	0.45
1:A:503:TRP:NE1	1:A:679:ARG:HA	2.31	0.45
1:A:79:LEU:HD13	1:A:79:LEU:N	2.32	0.45
1:B:287:ARG:O	1:B:291:ARG:HG3	2.16	0.45
1:B:346:LEU:CD2	1:B:376:LEU:HD11	2.46	0.45
1:B:531:ARG:HA	1:B:536:ARG:O	2.17	0.45
1:B:627:PRO:O	1:B:630:ALA:HB3	2.17	0.45
1:B:669:LEU:C	1:B:671:ILE:H	2.25	0.45
2:X:19:DA:H2'	2:X:20:DG:C8	2.51	0.45
1:A:321:LEU:HD12	1:A:321:LEU:O	2.16	0.45
1:A:386:SER:O	1:A:388:GLY:N	2.45	0.45
1:A:591:GLY:HA3	1:A:636:PHE:CZ	2.52	0.45
1:A:58:VAL:CG1	1:A:59:ARG:H	2.29	0.45
1:A:98:LEU:HB3	1:A:105:GLU:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:TRP:CZ2	1:A:284:GLU:HG3	2.52	0.45
1:A:319:PRO:HG2	1:A:640:ARG:HD3	1.98	0.45
1:A:410:THR:C	1:A:437:VAL:CG2	2.87	0.45
1:B:11:LEU:O	1:B:13:ARG:N	2.50	0.45
1:B:77:GLY:HA3	1:B:88:TYR:CE1	2.52	0.45
1:B:365:LEU:HD21	1:B:451:LEU:CD2	2.45	0.45
1:A:286:ARG:HH11	1:A:613:THR:HG22	1.82	0.45
1:A:640:ARG:HG3	1:A:649:PHE:CE1	2.52	0.45
1:B:598:ASP:O	1:B:599:LYS:CB	2.64	0.45
1:B:404:GLN:CG	1:B:681:LYS:HE2	2.46	0.44
2:X:9:DT:H6	2:X:9:DT:H2'	1.66	0.44
1:A:116:LEU:C	1:A:116:LEU:HD23	2.42	0.44
2:X:11:DG:H4'	2:X:11:DG:OP1	2.15	0.44
1:A:281:LEU:O	1:A:612:GLY:CA	2.66	0.44
1:B:628:LEU:O	1:B:629:GLU:C	2.61	0.44
1:A:153:LEU:HD13	1:A:297:ILE:HD11	2.00	0.44
1:A:475:VAL:O	1:A:475:VAL:HG13	2.16	0.44
1:A:677:VAL:O	1:A:678:ASP:C	2.55	0.44
1:B:51:ARG:NH2	1:B:51:ARG:CG	2.75	0.44
1:B:172:ARG:NH2	2:Y:109:DT:OP2	2.50	0.44
1:A:8:GLU:CD	1:A:310:ARG:HD3	2.42	0.44
1:B:601:PHE:CE2	1:B:619:LEU:HD13	2.53	0.44
1:B:197:TYR:CD1	1:B:232:ARG:HD2	2.52	0.44
1:B:266:THR:HG23	2:Y:109:DT:H5'	1.99	0.44
1:A:285:GLU:HG3	1:A:288:ARG:HH22	1.83	0.44
1:A:678:ASP:OD2	1:A:680:GLU:HB2	2.17	0.44
1:B:682:LEU:O	1:B:685:VAL:HG22	2.18	0.44
1:A:18:PRO:HA	1:A:162:ALA:HA	2.00	0.44
1:A:29:LEU:HB2	1:A:64:LEU:HB2	2.00	0.44
1:A:183:LEU:C	1:A:185:GLN:H	2.26	0.44
1:A:593:TYR:CZ	1:A:595:PRO:HG3	2.53	0.44
1:A:673:HIS:HD2	1:A:674:LEU:N	1.96	0.44
1:B:352:ASP:OD1	1:B:352:ASP:N	2.50	0.44
1:B:524:GLU:O	1:B:527:LEU:N	2.50	0.44
1:A:318:ILE:HD13	1:A:319:PRO:N	2.33	0.44
1:A:540:ARG:HH11	1:A:567:ALA:CB	2.17	0.44
1:B:69:PRO:HA	1:B:70:PRO:HD3	1.81	0.44
1:B:179:LEU:HD13	1:B:258:THR:HG22	2.00	0.44
1:B:233:LEU:HD22	1:B:238:GLY:H	1.83	0.44
1:B:369:PHE:HB3	1:B:374:ALA:O	2.17	0.44
1:A:318:ILE:HD13	1:A:319:PRO:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:GLY:O	1:B:39:ARG:C	2.60	0.43
1:B:51:ARG:O	1:B:51:ARG:HG2	2.18	0.43
1:B:205:LEU:C	1:B:206:ARG:HG3	2.42	0.43
1:B:447:TRP:HA	1:B:450:ALA:HB3	2.00	0.43
1:B:626:THR:O	1:B:627:PRO:C	2.61	0.43
1:A:286:ARG:HD3	1:A:580:ARG:CD	2.47	0.43
1:B:338:PHE:HB3	1:B:462:VAL:HA	2.00	0.43
2:X:1:DT:H5'	2:X:2:DG:C3'	2.34	0.43
1:A:202:TRP:CB	1:A:244:VAL:CG2	2.92	0.43
1:A:217:LEU:C	1:A:219:GLY:H	2.27	0.43
1:A:360:PHE:CD1	1:A:360:PHE:N	2.84	0.43
1:A:446:ARG:HG2	2:X:2:DG:C5	2.53	0.43
1:A:465:LEU:HG	1:A:641:LEU:HD23	2.00	0.43
1:A:327:VAL:HG23	1:A:332:ASP:CB	2.21	0.43
1:A:36:PRO:HA	1:A:37:PRO:HD3	1.76	0.43
1:A:321:LEU:HD12	1:A:327:VAL:CG1	2.39	0.43
1:B:349:LEU:HD22	1:B:351:LEU:CG	2.46	0.43
1:B:410:THR:CA	1:B:437:VAL:HG23	2.49	0.43
1:B:411:PRO:O	1:B:412:PRO:C	2.60	0.43
1:A:45:LEU:HD21	1:A:81:ARG:HD2	2.00	0.43
1:A:605:THR:HG21	1:A:651:ARG:O	2.18	0.43
1:B:503:TRP:HB2	1:B:662:LEU:HD22	2.01	0.43
1:A:177:MET:HE3	1:A:182:TRP:HE3	1.84	0.43
1:B:177:MET:HB3	1:B:181:ALA:HB3	1.99	0.43
1:B:396:ARG:HA	1:B:399:LYS:HE3	2.01	0.43
1:B:540:ARG:HA	1:B:567:ALA:O	2.19	0.43
1:B:594:VAL:O	1:B:595:PRO:C	2.61	0.43
1:A:101:LYS:HA	1:A:159:ASP:OD2	2.19	0.43
1:A:283:TRP:CA	1:A:613:THR:HB	2.48	0.43
1:A:361:LEU:O	1:A:365:LEU:HD23	2.19	0.43
1:B:53:ALA:O	1:B:54:GLY:C	2.62	0.43
1:B:351:LEU:HD21	1:B:385:PRO:HD3	2.01	0.43
1:B:540:ARG:HH11	1:B:567:ALA:HB1	1.80	0.43
1:B:661:ARG:HB2	1:B:684:PHE:HD1	1.84	0.43
1:A:31:VAL:HG22	1:A:90:LEU:CD2	2.49	0.42
1:A:183:LEU:C	1:A:185:GLN:N	2.77	0.42
1:B:165:LEU:HD21	1:B:297:ILE:HG21	1.99	0.42
1:B:415:TRP:HH2	1:B:668:ARG:HE	1.66	0.42
1:A:568:TYR:C	1:A:568:TYR:CD2	2.97	0.42
1:A:653:PRO:O	1:A:654:ALA:C	2.62	0.42
1:B:503:TRP:O	1:B:503:TRP:CD2	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:536:ARG:HB3	1:B:537:LEU:H	1.51	0.42
1:B:640:ARG:HA	1:B:649:PHE:CD2	2.54	0.42
1:B:653:PRO:O	1:B:654:ALA:C	2.61	0.42
1:A:434:ILE:O	2:X:1:DT:H4'	2.19	0.42
1:B:351:LEU:HB2	1:B:410:THR:CG2	2.41	0.42
1:B:359:GLU:OE1	1:B:363:ARG:NH2	2.52	0.42
1:B:570:LEU:HB3	1:B:623:ALA:HB3	2.01	0.42
1:A:153:LEU:CD1	1:A:297:ILE:HD11	2.50	0.42
1:B:230:LYS:HB2	1:B:232:ARG:HG2	2.00	0.42
1:B:283:TRP:CG	1:B:284:GLU:N	2.87	0.42
1:B:572:SER:OG	1:B:620:VAL:HB	2.19	0.42
1:A:134:VAL:O	1:A:150:GLY:HA3	2.19	0.42
1:A:344:THR:OG1	1:A:460:LEU:HD11	2.19	0.42
1:A:644:ALA:O	1:A:645:SER:HB3	2.19	0.42
1:B:154:ASP:O	1:B:165:LEU:HD12	2.19	0.42
1:B:584:VAL:HG23	1:B:585:GLN:N	2.35	0.42
1:B:291:ARG:C	1:B:293:ILE:N	2.75	0.42
1:B:524:GLU:C	1:B:526:THR:N	2.77	0.42
1:A:350:ARG:NH1	1:A:350:ARG:CG	2.80	0.42
1:B:8:GLU:OE1	1:B:310:ARG:HD3	2.19	0.42
1:B:91:TYR:O	1:B:92:PRO:C	2.62	0.42
1:B:287:ARG:O	1:B:290:THR:CG2	2.65	0.42
1:B:360:PHE:CG	1:B:361:LEU:N	2.88	0.42
1:A:609:ASP:O	2:X:6:DT:H5'	2.19	0.42
1:B:160:SER:O	1:B:161:GLY:C	2.61	0.42
1:B:266:THR:HG22	1:B:267:LEU:N	2.31	0.42
1:B:357:TRP:HE3	1:B:361:LEU:HD22	1.85	0.42
1:A:534:ALA:C	1:A:536:ARG:H	2.28	0.42
1:B:82:MET:O	1:B:82:MET:SD	2.78	0.42
1:B:391:PHE:CD2	1:B:395:LEU:HD11	2.50	0.42
1:B:437:VAL:C	1:B:439:LEU:N	2.77	0.42
1:A:268:GLU:H	1:A:268:GLU:HG3	1.58	0.41
2:X:19:DA:H2''	2:X:20:DG:C5'	2.49	0.41
1:B:104:GLY:HA3	7:B:700:HOH:O	2.20	0.41
1:B:411:PRO:O	1:B:413:MET:N	2.52	0.41
1:B:426:LEU:O	1:B:429:GLY:N	2.45	0.41
1:B:446:ARG:O	1:B:448:GLU:N	2.53	0.41
1:B:641:LEU:HD22	1:B:641:LEU:HA	1.88	0.41
1:A:50:ALA:O	1:A:57:THR:HG23	2.20	0.41
1:A:346:LEU:HG	1:A:454:LEU:HD11	2.02	0.41
1:A:414:ALA:O	1:A:415:TRP:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:ARG:C	1:B:448:GLU:N	2.79	0.41
1:A:25:ARG:O	1:A:95:ARG:NH1	2.53	0.41
1:A:217:LEU:C	1:A:219:GLY:N	2.78	0.41
1:B:473:LEU:HB3	1:B:541:VAL:HG12	2.03	0.41
1:A:631:LEU:HD12	1:A:631:LEU:HA	1.90	0.41
1:A:642:TYR:HA	1:A:643:PRO:HD2	1.73	0.41
1:B:329:LYS:HE3	1:B:332:ASP:OD1	2.20	0.41
1:B:389:LEU:O	1:B:392:ARG:HG2	2.20	0.41
1:B:555:ALA:O	1:B:559:GLU:HG2	2.20	0.41
1:A:16:LEU:O	1:A:17:ARG:C	2.64	0.41
1:A:318:ILE:HA	1:A:319:PRO:HD3	1.93	0.41
1:A:594:VAL:O	1:A:595:PRO:C	2.63	0.41
1:A:645:SER:HB2	2:X:3:DA:H4'	2.02	0.41
1:B:506:PRO:HD3	1:B:522:LEU:HD23	2.02	0.41
1:A:266:THR:HB	1:A:268:GLU:HG3	2.03	0.41
1:A:672:ARG:O	1:A:673:HIS:HB2	2.20	0.41
1:B:198:ASP:OD1	1:B:199:ARG:N	2.53	0.41
1:B:442:GLU:HG3	1:B:443:GLU:N	2.36	0.41
1:B:642:TYR:HA	1:B:643:PRO:HD2	1.82	0.41
1:A:30:GLU:OE1	1:A:93:LYS:HD2	2.21	0.41
1:A:180:GLU:OE2	1:A:258:THR:OG1	2.33	0.41
1:A:327:VAL:HG22	1:A:328:SER:N	2.36	0.41
1:A:417:ASP:HA	1:A:420:ARG:HB3	2.02	0.41
1:A:444:ARG:HA	1:A:447:TRP:NE1	2.36	0.41
1:B:18:PRO:HA	1:B:162:ALA:HA	2.03	0.41
1:A:15:ALA:HA	1:A:164:LEU:HD12	2.03	0.41
1:B:16:LEU:HB3	1:B:303:LEU:O	2.21	0.41
1:B:524:GLU:HG3	1:B:528:TRP:CD1	2.56	0.41
1:A:120:ARG:HG3	1:A:120:ARG:HH11	1.85	0.40
1:A:547:GLY:HA2	1:A:572:SER:HB2	2.03	0.40
1:B:35:PRO:HA	1:B:36:PRO:HD3	1.98	0.40
1:B:406:VAL:O	1:B:432:SER:HA	2.21	0.40
1:B:410:THR:O	1:B:436:ASN:HA	2.20	0.40
1:B:541:VAL:O	1:B:568:TYR:HA	2.22	0.40
1:A:479:ALA:HA	1:A:489:GLY:HA2	2.02	0.40
1:B:159:ASP:C	1:B:161:GLY:N	2.80	0.40
1:B:427:ARG:C	1:B:429:GLY:N	2.78	0.40
1:B:57:THR:HG21	1:B:73:LEU:CD2	2.52	0.40
1:B:205:LEU:HD21	1:B:245:ALA:HB2	2.03	0.40
1:B:215:LEU:HD13	1:B:223:LEU:HD12	2.03	0.40
1:B:444:ARG:HA	1:B:447:TRP:NE1	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:VAL:CG1	1:A:464:ALA:N	2.84	0.40
1:B:313:ALA:CB	1:B:594:VAL:HG22	2.49	0.40
1:B:415:TRP:CZ2	1:B:668:ARG:HD3	2.56	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	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:GLU:OE2	1:B:139:HIS:O[3_545]	2.18	0.02

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	665/685 (97%)	601 (90%)	52 (8%)	12 (2%)	6	31
1	B	654/685 (96%)	569 (87%)	70 (11%)	15 (2%)	5	25
All	All	1319/1370 (96%)	1170 (89%)	122 (9%)	27 (2%)	6	28

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	ARG
1	A	355	GLN
1	B	39	ARG
1	B	374	ALA
1	B	597	GLU
1	B	646	GLY
1	A	352	ASP
1	A	387	GLN
1	A	598	ASP
1	A	610	PHE

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Mol	Chain	Res	Type
1	A	675	LYS
1	B	12	ASN
1	B	54	GLY
1	B	388	GLY
1	B	412	PRO
1	A	386	SER
1	B	82	MET
1	A	218	PRO
1	A	412	PRO
1	A	415	TRP
1	B	332	ASP
1	B	339	TYR
1	B	364	ALA
1	B	369	PHE
1	B	5	GLY
1	A	437	VAL
1	B	218	PRO

5.3.2 Protein sidechains [i](#)

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	512/549 (93%)	465 (91%)	47 (9%)	8	33
1	B	488/549 (89%)	436 (89%)	52 (11%)	6	26
All	All	1000/1098 (91%)	901 (90%)	99 (10%)	7	30

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	28	ARG
1	A	79	LEU
1	A	96	ARG
1	A	114	ARG
1	A	121	LEU

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Mol	Chain	Res	Type
1	A	127	VAL
1	A	174	LEU
1	A	179	LEU
1	A	201	THR
1	A	204	LEU
1	A	209	GLU
1	A	213	LYS
1	A	223	LEU
1	A	234	GLN
1	A	244	VAL
1	A	267	LEU
1	A	268	GLU
1	A	291	ARG
1	A	299	ARG
1	A	312	GLN
1	A	315	ARG
1	A	318	ILE
1	A	338	PHE
1	A	349	LEU
1	A	351	LEU
1	A	359	GLU
1	A	381	LEU
1	A	392	ARG
1	A	396	ARG
1	A	409	LEU
1	A	410	THR
1	A	426	LEU
1	A	439	LEU
1	A	445	HIS
1	A	452	LEU
1	A	461	GLN
1	A	482	ARG
1	A	502	LEU
1	A	528	TRP
1	A	536	ARG
1	A	552	ASP
1	A	553	GLU
1	A	574	ARG
1	A	629	GLU
1	A	631	LEU
1	A	641	LEU
1	B	3	HIS

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Mol	Chain	Res	Type
1	B	30	GLU
1	B	51	ARG
1	B	52	ARG
1	B	57	THR
1	B	58	VAL
1	B	67	TRP
1	B	78	THR
1	B	79	LEU
1	B	93	LYS
1	B	117	LEU
1	B	118	GLN
1	B	127	VAL
1	B	137	ARG
1	B	141	ARG
1	B	166	GLU
1	B	172	ARG
1	B	179	LEU
1	B	191	LYS
1	B	202	TRP
1	B	204	LEU
1	B	206	ARG
1	B	223	LEU
1	B	234	GLN
1	B	244	VAL
1	B	269	ASP
1	B	283	TRP
1	B	291	ARG
1	B	292	GLU
1	B	315	ARG
1	B	343	GLU
1	B	346	LEU
1	B	389	LEU
1	B	392	ARG
1	B	399	LYS
1	B	404	GLN
1	B	409	LEU
1	B	410	THR
1	B	426	LEU
1	B	452	LEU
1	B	475	VAL
1	B	504	THR
1	B	505	LEU

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Mol	Chain	Res	Type
1	B	531	ARG
1	B	548	ARG
1	B	552	ASP
1	B	587	ARG
1	B	592	LEU
1	B	599	LYS
1	B	631	LEU
1	B	640	ARG
1	B	641	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	48	GLN
1	A	84	GLN
1	A	118	GLN
1	A	227	HIS
1	A	256	HIS
1	A	342	GLN
1	A	382	HIS
1	A	404	GLN
1	A	500	HIS
1	A	621	HIS
1	A	673	HIS
1	B	12	ASN
1	B	48	GLN
1	B	84	GLN
1	B	256	HIS
1	B	379	HIS
1	B	445	HIS
1	B	551	GLN
1	B	657	HIS

5.3.3 RNA ⓘ

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 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 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	PGE	A	688	-	9,9,9	0.52	0	8,8,8	0.79	0
5	PO4	A	689	-	4,4,4	1.71	0	6,6,6	0.47	0
6	ACY	B	687	-	3,3,3	2.72	1 (33%)	3,3,3	0.73	0
5	PO4	X	22	-	4,4,4	1.76	1 (25%)	6,6,6	0.45	0
6	ACY	B	686	-	3,3,3	2.71	1 (33%)	3,3,3	0.90	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	PGE	A	688	-	-	2/7/7/7	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	687	ACY	O-C	4.66	1.42	1.22
6	B	686	ACY	O-C	4.63	1.42	1.22
5	X	22	PO4	P-O2	-2.07	1.48	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	688	PGE	O3-C5-C6-O4
4	A	688	PGE	O2-C3-C4-O3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	687	ACY	2	0

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	672/685 (98%)	-0.19	3 (0%) 88 76	24, 52, 82, 95	18 (2%)
1	B	666/685 (97%)	-0.08	3 (0%) 87 72	18, 59, 89, 104	12 (1%)
2	X	17/21 (80%)	0.21	1 (5%) 28 14	32, 51, 150, 150	0
2	Y	14/21 (66%)	0.76	2 (14%) 6 3	55, 70, 129, 135	1 (7%)
All	All	1369/1412 (96%)	-0.12	9 (0%) 84 66	18, 56, 88, 150	31 (2%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	609	ASP	7.1
2	Y	119	DA	5.1
1	A	5	GLY	3.0
2	X	12	DG	3.0
1	B	407	LEU	2.6
1	B	438	PRO	2.1
2	Y	109	DT	2.1
1	B	246	ASP	2.0
1	A	610	PHE	2.0

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
5	PO4	A	689	5/5	0.47	0.12	149,150,150,150	0
5	PO4	X	22	5/5	0.55	0.16	147,147,147,148	0
4	PGE	A	688	10/10	0.68	0.15	102,107,108,108	0
6	ACY	B	687	4/4	0.84	0.16	60,61,61,62	0
6	ACY	B	686	4/4	0.89	0.12	44,45,45,46	0
3	MG	A	687	1/1	0.89	0.07	57,57,57,57	0
3	MG	Y	2	1/1	0.95	0.07	26,26,26,26	0
3	MG	A	686	1/1	0.95	0.08	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.