



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 08:45 PM UTC

PDB ID : 3T35 / pdb_00003t35
Title : Arabidopsis thaliana dynamin-related protein 1A in postfission state
Authors : Yan, L.M.; Ma, Y.Y.; Sun, Y.N.; Lou, Z.Y.
Deposited on : 2011-07-24
Resolution : 3.59 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

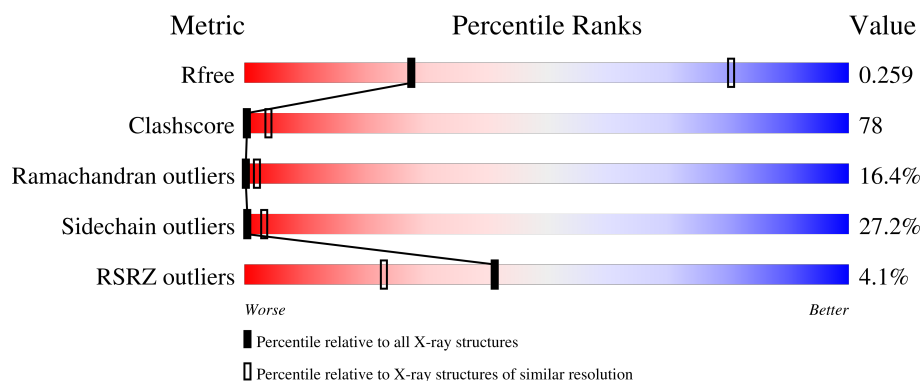
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.59 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	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	360	4% 16% 45% 29% 6%
1	B	360	4% 16% 46% 27% 5% 6%
1	C	360	4% 19% 41% 29% 6% 6%
1	D	360	4% 16% 47% 27% 6% 6%

2 Entry composition [i](#)

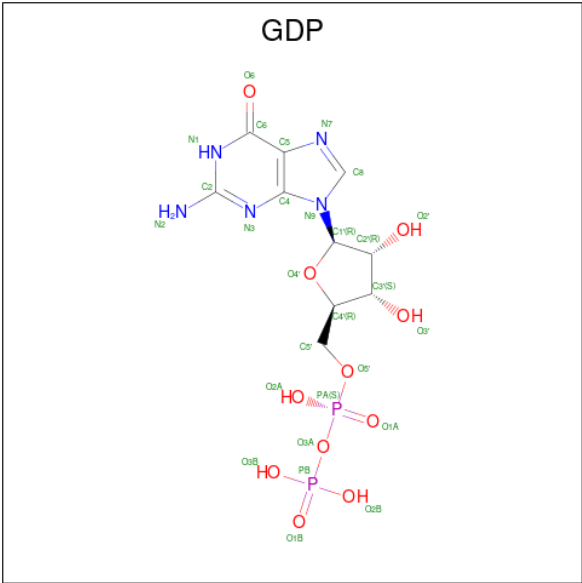
There are 3 unique types of molecules in this entry. The entry contains 11037 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dynamin-related protein 1A, LINKER, Dynamin-related protein 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	0	0
			2636	1649	472	508	7			
1	B	339	Total	C	N	O	S	0	0	0
			2636	1649	472	508	7			
1	C	339	Total	C	N	O	S	0	0	0
			2636	1649	472	508	7			
1	D	339	Total	C	N	O	S	0	0	0
			2636	1649	472	508	7			

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

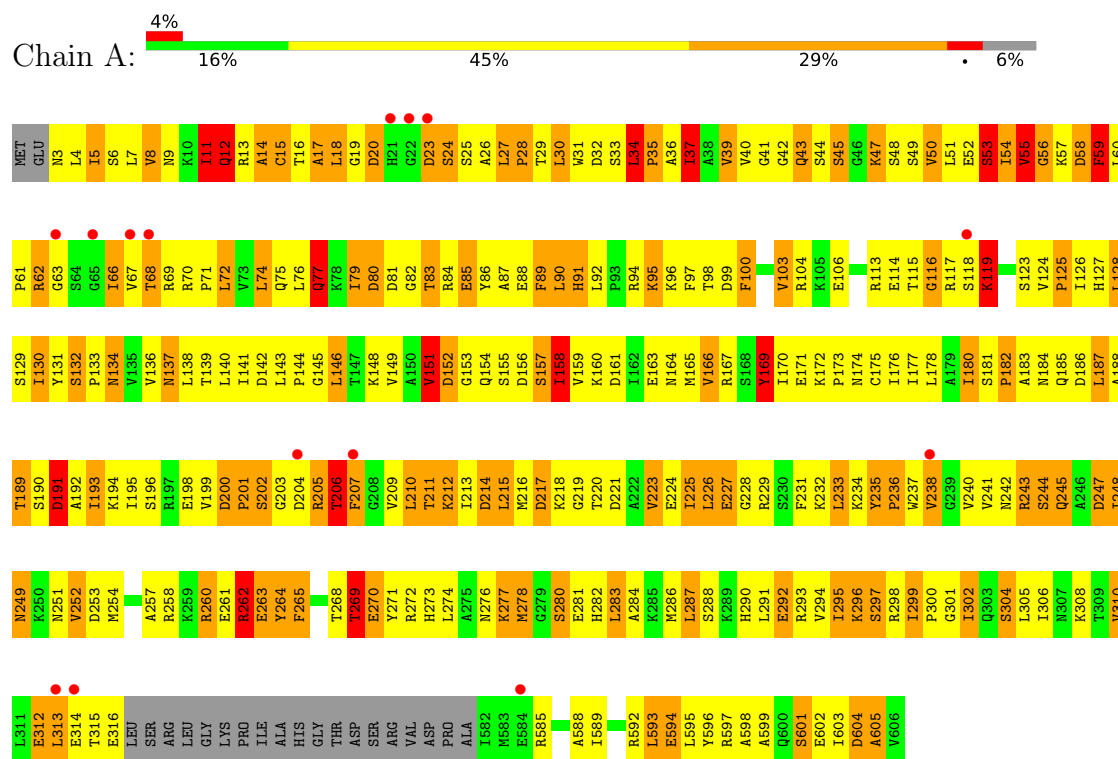
- Molecule 3 is water.

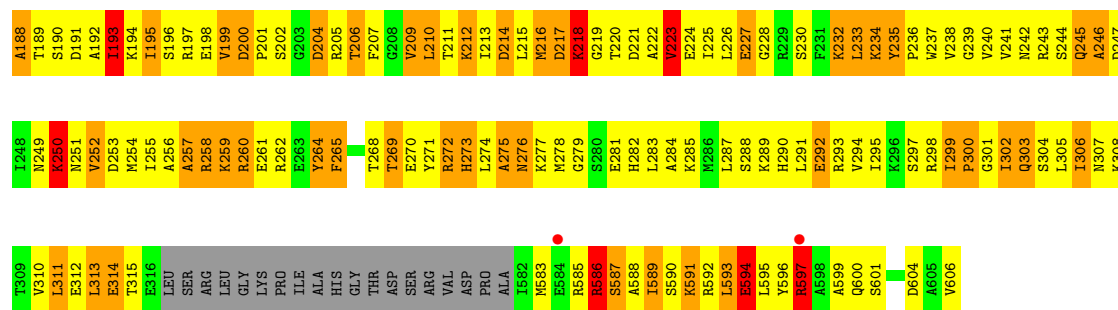
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	87	Total	O	0	0
			87	87		
3	B	121	Total	O	0	0
			121	121		
3	C	93	Total	O	0	0
			93	93		
3	D	80	Total	O	0	0
			80	80		

3 Residue-property plots

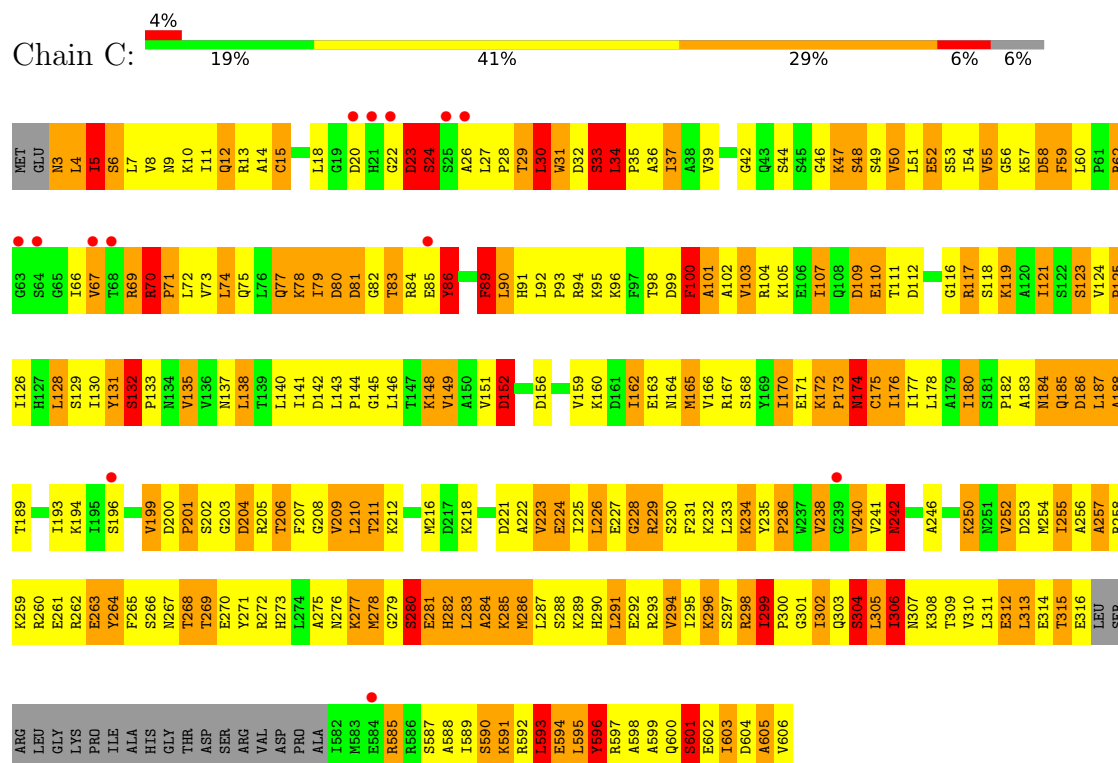
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Dynamin-related protein 1A, LINKER, Dynamin-related protein 1A

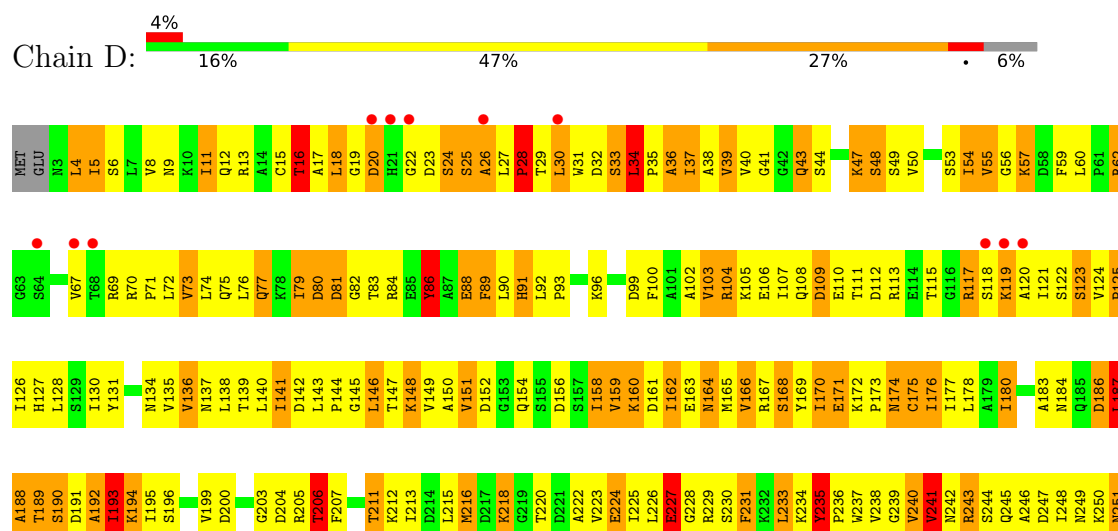




- Molecule 1: Dynamin-related protein 1A, LINKER, Dynamin-related protein 1A



- Molecule 1: Dynamin-related protein 1A, LINKER, Dynamin-related protein 1A



V252	D253	M254	I255	A256	A257	R258	K259	R260	E261	R262	E263	Y264	F265	S266	N267	T268	T269	E270	Y271	R272	H273	L274	A275	N276	K277	G279	S280	E281	H282	L283	A284	K285	M286	L287	S288	K289	H290	L291	E292	R293	V294	I295	K296	R297	R298	I299	P300	G301	I302	Q303	S304	L305	I306	N307	K308	T309	V310	L311
E312	L313	E314	T315	E316	LEU	SER	ARG	LEU	GLY	LYS	PRO	ILE	ALA	HIS	GLY	THR	ASP	SER	ARG	VAL	ASP	PRO	ALA	I582	H583	E584	R585	A588	I589	S590	R591	R592	I593	E594	I595	Y596	R597	A598	A599	D600	S601	E602	I603	D604	A605	Y606												

4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	146.16Å 146.16Å 204.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.32 – 3.59 43.32 – 3.59	Depositor EDS
% Data completeness (in resolution range)	87.2 (43.32-3.59) 98.5 (43.32-3.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 3.57Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.238 , 0.291 (Not available) , 0.259	Depositor DCC
R_{free} test set	1464 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	50.3	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 64.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.066 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	11037	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.60% 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: GDP

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	0.72	1/2671 (0.0%)	1.17	22/3605 (0.6%)
1	B	0.80	3/2671 (0.1%)	1.23	24/3605 (0.7%)
1	C	0.74	0/2671	1.20	31/3605 (0.9%)
1	D	0.67	0/2671	1.15	19/3605 (0.5%)
All	All	0.74	4/10684 (0.0%)	1.19	96/14420 (0.7%)

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	B	0	1
1	D	0	2
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	597	ARG	C-N	6.80	1.43	1.33
1	B	193	ILE	CA-CB	-5.42	1.48	1.54
1	B	302	ILE	CA-CB	5.20	1.60	1.54
1	A	37	ILE	CA-CB	-5.09	1.48	1.54

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	GLU	N-CA-C	-11.70	99.49	113.88
1	C	304	SER	N-CA-C	-9.40	101.33	113.17
1	D	235	TYR	CA-C-N	-9.28	108.24	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	235	TYR	C-N-CA	-9.28	108.24	119.84
1	D	34	LEU	CA-C-N	-9.25	108.28	119.84
1	D	34	LEU	C-N-CA	-9.25	108.28	119.84
1	B	234	LYS	N-CA-C	-9.24	104.08	114.62
1	C	34	LEU	CA-C-N	-8.90	108.72	119.84
1	C	34	LEU	C-N-CA	-8.90	108.72	119.84
1	C	601	SER	N-CA-C	-8.88	102.02	113.12
1	A	223	VAL	N-CA-C	8.79	118.86	110.42
1	D	187	LEU	N-CA-C	-8.76	103.11	113.88
1	B	30	LEU	N-CA-C	-8.72	100.96	111.69
1	D	303	GLN	N-CA-C	-8.68	101.73	111.71
1	B	302	ILE	N-CA-C	-8.37	103.62	113.42
1	A	54	ILE	N-CA-C	-8.30	103.09	111.88
1	B	17	ALA	N-CA-C	-7.80	101.56	113.89
1	C	588	ALA	N-CA-C	-7.79	103.61	113.43
1	A	299	ILE	CA-C-N	-7.51	110.45	119.84
1	A	299	ILE	C-N-CA	-7.51	110.45	119.84
1	C	52	GLU	N-CA-C	-7.43	105.39	114.75
1	C	250	LYS	N-CA-C	-7.30	102.64	112.94
1	A	138	LEU	N-CA-C	7.27	118.13	107.88
1	B	85	GLU	N-CA-C	7.25	118.97	111.14
1	D	301	GLY	N-CA-C	-7.22	103.88	115.66
1	C	70	ARG	CA-C-N	6.78	128.31	119.84
1	C	70	ARG	C-N-CA	6.78	128.31	119.84
1	A	103	VAL	N-CA-C	-6.74	103.84	113.07
1	A	304	SER	N-CA-C	-6.72	104.78	114.12
1	D	36	ALA	N-CA-C	-6.67	96.58	110.80
1	C	24	SER	N-CA-C	-6.62	104.79	114.39
1	D	170	ILE	N-CA-C	-6.60	106.80	113.47
1	B	213	ILE	N-CA-C	-6.58	107.46	113.71
1	B	181	SER	CA-C-N	6.51	127.02	119.99
1	B	181	SER	C-N-CA	6.51	127.02	119.99
1	C	132	SER	CA-C-N	6.49	127.95	119.84
1	C	132	SER	C-N-CA	6.49	127.95	119.84
1	C	89	PHE	N-CA-C	6.39	114.88	108.75
1	C	238	VAL	N-CA-C	-6.29	99.48	109.17
1	A	116	GLY	N-CA-C	6.28	119.34	110.74
1	C	15	CYS	N-CA-C	-6.12	106.14	113.97
1	D	160	LYS	N-CA-C	-6.11	106.80	114.56
1	D	171	GLU	N-CA-C	-6.07	106.54	112.97
1	B	276	ASN	N-CA-C	-6.00	106.56	114.31
1	B	172	LYS	CA-C-N	5.92	127.24	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	172	LYS	C-N-CA	5.92	127.24	119.84
1	C	289	LYS	N-CA-C	-5.78	105.06	111.71
1	B	121	ILE	N-CA-C	5.71	118.17	108.86
1	C	229	ARG	N-CA-C	-5.70	105.06	113.61
1	A	34	LEU	CA-C-N	-5.68	112.74	119.84
1	A	34	LEU	C-N-CA	-5.68	112.74	119.84
1	C	223	VAL	N-CA-C	5.67	115.80	110.30
1	C	121	ILE	N-CA-C	5.65	118.07	108.86
1	A	201	PRO	N-CA-C	-5.61	107.47	114.20
1	D	279	GLY	N-CA-C	-5.59	105.92	111.85
1	A	191	ASP	N-CA-C	-5.59	105.19	111.28
1	C	180	ILE	CB-CA-C	-5.56	103.36	110.98
1	D	602	GLU	N-CA-C	-5.55	106.28	113.16
1	B	214	ASP	N-CA-C	-5.53	106.03	112.89
1	A	219	GLY	N-CA-C	-5.49	108.16	115.40
1	B	199	VAL	CB-CA-C	-5.48	104.65	112.22
1	C	5	ILE	N-CA-C	-5.48	105.51	110.82
1	C	89	PHE	CA-C-O	5.47	121.78	118.33
1	A	169	TYR	N-CA-C	-5.46	106.66	113.38
1	B	180	ILE	CB-CA-C	-5.45	104.36	110.96
1	B	142	ASP	N-CA-C	-5.43	103.37	110.53
1	C	294	VAL	CB-CA-C	-5.41	104.95	111.88
1	B	170	ILE	N-CA-C	5.38	115.59	110.42
1	C	315	THR	CB-CA-C	-5.36	104.68	111.70
1	A	17	ALA	N-CA-C	-5.31	106.64	113.23
1	C	209	VAL	CB-CA-C	-5.30	102.42	110.95
1	B	55	VAL	N-CA-C	-5.30	108.11	113.20
1	B	27	LEU	CA-C-N	-5.26	113.26	119.84
1	B	27	LEU	C-N-CA	-5.26	113.26	119.84
1	A	53	SER	N-CA-C	-5.22	106.14	112.88
1	D	40	VAL	N-CA-C	5.21	114.80	106.88
1	A	20	ASP	N-CA-C	-5.17	106.66	113.17
1	C	110	GLU	N-CA-C	-5.17	105.27	112.45
1	B	66	ILE	N-CA-C	5.15	120.06	109.34
1	C	299	ILE	CA-C-N	-5.15	113.40	119.84
1	C	299	ILE	C-N-CA	-5.15	113.40	119.84
1	B	193	ILE	CB-CA-C	-5.14	105.31	112.04
1	C	595	LEU	N-CA-C	-5.14	108.76	114.62
1	C	596	TYR	N-CA-C	-5.13	105.33	111.03
1	D	239	GLY	N-CA-C	5.13	119.90	112.82
1	D	55	VAL	N-CA-C	-5.11	105.73	110.53
1	B	217	ASP	N-CA-C	5.10	117.04	108.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	VAL	N-CA-C	5.07	115.89	108.53
1	B	240	VAL	N-CA-C	5.07	116.00	108.65
1	D	39	VAL	N-CA-C	5.06	114.89	107.15
1	A	157	SER	N-CA-C	-5.06	107.66	113.88
1	A	245	GLN	N-CA-C	-5.04	105.79	111.28
1	D	24	SER	N-CA-C	-5.04	106.88	112.57
1	D	279	GLY	CA-C-O	-5.02	118.27	122.33
1	A	270	GLU	N-CA-C	5.01	117.47	111.71
1	C	201	PRO	N-CA-C	-5.01	108.09	114.35

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	34	LEU	Peptide
1	D	26	ALA	Peptide
1	D	28	PRO	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	2636	0	2705	439	0
1	B	2636	0	2705	401	1
1	C	2636	0	2705	440	0
1	D	2636	0	2705	441	1
2	A	28	0	12	7	0
2	B	28	0	12	7	0
2	C	28	0	12	6	0
2	D	28	0	12	8	0
3	A	87	0	0	12	0
3	B	121	0	0	18	0
3	C	93	0	0	34	0
3	D	80	0	0	32	0
All	All	11037	0	10868	1683	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 78.

All (1683) 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:276:ASN:OD1	1:A:277:LYS:HD3	1.27	1.24
1:B:25:SER:O	1:B:308:LYS:CE	1.86	1.23
1:D:32:ASP:O	1:D:35:PRO:HD3	1.44	1.15
1:B:29:THR:HA	1:B:32:ASP:HB2	1.26	1.15
1:A:276:ASN:OD1	1:A:277:LYS:CD	1.95	1.14
1:D:170:ILE:HG22	1:D:199:VAL:HG11	1.29	1.13
1:A:11:ILE:HG22	1:A:12:GLN:H	1.05	1.12
1:B:313:LEU:HD23	1:B:597:ARG:NH2	1.65	1.11
1:D:16:THR:HA	1:D:20:ASP:H	1.03	1.11
1:C:183:ALA:HB1	1:C:216:MET:HE3	1.32	1.11
1:B:40:VAL:HG21	1:B:170:ILE:HD11	1.34	1.08
1:B:25:SER:O	1:B:308:LYS:HE3	1.53	1.07
1:D:140:LEU:HA	3:D:675:HOH:O	1.55	1.05
1:D:299:ILE:HG13	1:D:300:PRO:HD3	1.11	1.05
1:B:25:SER:O	1:B:308:LYS:NZ	1.90	1.02
1:B:60:LEU:HD23	1:B:61:PRO:HD2	1.42	1.01
1:C:27:LEU:HB3	1:C:31:TRP:HB2	1.37	1.01
1:D:16:THR:HA	1:D:20:ASP:N	1.76	1.01
1:C:83:THR:HG22	1:C:133:PRO:HG2	1.44	1.00
1:B:43:GLN:HE22	1:B:66:ILE:HB	1.26	1.00
1:A:11:ILE:HG22	1:A:12:GLN:N	1.75	1.00
1:A:92:LEU:HD13	1:A:95:LYS:HE3	1.41	0.99
1:A:23:ASP:HB2	1:A:26:ALA:HB3	1.45	0.99
1:B:92:LEU:HD11	1:B:95:LYS:HB3	1.43	0.99
1:C:66:ILE:HG22	1:C:119:LYS:HD2	1.45	0.99
1:B:313:LEU:HD23	1:B:597:ARG:HH22	1.21	0.99
1:C:42:GLY:HA2	1:C:146:LEU:HB2	1.39	0.98
1:A:183:ALA:HB2	1:A:210:LEU:HD22	1.42	0.98
1:C:189:THR:HA	1:D:148:LYS:HG2	1.45	0.98
1:A:293:ARG:HD3	1:C:306:ILE:HG21	1.46	0.97
1:D:299:ILE:CG1	1:D:300:PRO:HD3	1.94	0.97
1:C:298:ARG:HH11	1:C:298:ARG:HB2	1.26	0.97
1:D:299:ILE:HG13	1:D:300:PRO:CD	1.95	0.95
1:B:239:GLY:H	1:B:278:MET:HE1	1.28	0.95
1:C:305:LEU:O	1:C:307:ASN:N	1.98	0.95
1:D:140:LEU:HD23	3:D:675:HOH:O	1.66	0.94
1:A:12:GLN:O	1:A:15:CYS:HB3	1.68	0.94
1:D:176:ILE:H	1:D:176:ILE:HD12	1.30	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:585:ARG:HE	1:B:589:ILE:HD11	1.31	0.94
1:B:308:LYS:HD3	1:B:311:LEU:HD23	1.47	0.93
1:A:301:GLY:O	1:A:305:LEU:HB2	1.66	0.93
1:D:79:ILE:HD13	1:D:84:ARG:HD2	1.48	0.93
1:D:23:ASP:HB3	1:D:592:ARG:HD3	1.50	0.92
1:A:172:LYS:HE3	1:A:175:CYS:HB3	1.50	0.92
1:B:124:VAL:HG12	1:B:125:PRO:HD2	1.52	0.92
1:B:215:LEU:HD11	2:B:9001:GDP:C2	2.05	0.92
1:D:19:GLY:HA2	1:D:22:GLY:HA2	1.52	0.92
1:D:82:GLY:O	1:D:84:ARG:HG3	1.72	0.90
1:D:39:VAL:HG22	1:D:141:ILE:O	1.72	0.89
1:C:74:LEU:O	1:C:75:GLN:HG3	1.72	0.89
1:D:35:PRO:HA	1:D:174:ASN:O	1.73	0.89
1:A:32:ASP:O	1:A:35:PRO:HD3	1.71	0.89
1:B:39:VAL:HG13	1:B:142:ASP:HA	1.53	0.89
1:C:28:PRO:O	1:C:32:ASP:HB3	1.73	0.89
1:C:255:ILE:O	1:C:259:LYS:HB2	1.73	0.89
1:D:258:ARG:HE	1:D:281:GLU:HG2	1.38	0.89
1:A:234:LYS:HE2	1:C:597:ARG:CZ	2.01	0.89
1:B:212:LYS:HB3	1:B:215:LEU:HD12	1.52	0.89
1:A:238:VAL:HG11	1:A:283:LEU:HD13	1.55	0.88
1:D:75:GLN:HA	3:D:667:HOH:O	1.71	0.88
1:D:77:GLN:HG3	1:D:131:TYR:CE1	2.08	0.88
1:C:74:LEU:HD23	1:C:75:GLN:H	1.37	0.88
1:A:224:GLU:N	1:A:224:GLU:OE1	2.07	0.88
1:B:252:VAL:HG11	1:B:260:ARG:NH2	1.89	0.87
1:A:224:GLU:HG3	1:A:229:ARG:NH1	1.90	0.86
1:A:302:ILE:C	1:A:304:SER:H	1.80	0.86
1:A:29:THR:C	1:A:31:TRP:H	1.81	0.86
1:B:583:MET:HA	1:B:586:ARG:CZ	2.06	0.86
1:C:596:TYR:O	1:C:599:ALA:HB3	1.76	0.85
1:D:17:ALA:O	1:D:18:LEU:HB2	1.76	0.85
1:A:37:ILE:HG13	1:A:140:LEU:HD23	1.56	0.84
1:A:152:ASP:CG	1:A:153:GLY:H	1.82	0.84
1:D:11:ILE:HG22	3:D:625:HOH:O	1.76	0.84
1:D:193:ILE:HD12	1:D:193:ILE:H	1.40	0.84
1:D:193:ILE:HD12	1:D:193:ILE:N	1.93	0.84
1:D:256:ALA:HA	1:D:259:LYS:HB2	1.58	0.84
1:B:252:VAL:HG11	1:B:260:ARG:HH21	1.43	0.83
1:A:37:ILE:HG22	1:A:176:ILE:HB	1.60	0.83
1:A:226:LEU:HD22	1:A:278:MET:HE1	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:ASN:HD22	1:B:298:ARG:CD	1.91	0.83
1:A:183:ALA:HB2	1:A:210:LEU:CD2	2.08	0.83
1:B:23:ASP:OD2	1:B:26:ALA:HB3	1.80	0.82
1:C:290:HIS:HE1	3:C:673:HOH:O	1.62	0.82
1:B:29:THR:CA	1:B:32:ASP:HB2	2.08	0.82
1:D:69:ARG:HB3	1:D:121:ILE:HG22	1.61	0.82
1:B:174:ASN:HD22	1:B:298:ARG:HD3	1.41	0.82
1:A:39:VAL:HB	1:A:178:LEU:HD23	1.62	0.82
1:B:257:ALA:O	1:B:259:LYS:N	2.13	0.82
1:C:100:PHE:O	1:C:103:VAL:HG23	1.79	0.82
1:C:32:ASP:C	1:C:34:LEU:H	1.85	0.82
1:A:45:SER:O	1:A:182:PRO:HG3	1.77	0.81
1:A:42:GLY:HA2	1:A:146:LEU:H	1.43	0.81
1:B:5:ILE:HG23	1:B:6:SER:H	1.44	0.81
1:B:58:ASP:HB3	1:B:104:ARG:HH21	1.45	0.81
1:A:209:VAL:O	1:A:210:LEU:HB3	1.79	0.81
1:C:34:LEU:HD13	1:C:36:ALA:HB3	1.63	0.81
1:B:174:ASN:ND2	1:B:298:ARG:HE	1.77	0.81
1:C:276:ASN:OD1	1:C:277:LYS:HG3	1.81	0.81
1:D:224:GLU:OE2	1:D:229:ARG:HD3	1.80	0.80
1:C:234:LYS:O	1:C:235:TYR:CD2	2.34	0.80
1:C:238:VAL:HG11	1:C:283:LEU:HB2	1.63	0.80
1:A:24:SER:HB3	1:A:585:ARG:HH21	1.46	0.80
1:D:27:LEU:O	1:D:31:TRP:N	2.14	0.80
1:C:307:ASN:O	1:C:311:LEU:HG	1.80	0.80
1:C:55:VAL:HG21	1:C:59:PHE:CE2	2.16	0.80
1:C:234:LYS:O	1:C:235:TYR:HD2	1.64	0.80
1:A:588:ALA:O	1:A:592:ARG:HG3	1.82	0.80
1:D:131:TYR:HB2	3:D:640:HOH:O	1.82	0.80
1:D:138:LEU:HD11	1:D:288:SER:OG	1.80	0.80
1:B:34:LEU:HD11	1:B:36:ALA:HB3	1.63	0.80
1:B:159:VAL:HG12	1:B:160:LYS:N	1.94	0.79
1:B:176:ILE:HG22	1:B:177:ILE:H	1.47	0.79
1:B:290:HIS:O	1:B:294:VAL:HG23	1.82	0.79
1:C:69:ARG:HH21	1:C:119:LYS:HD3	1.47	0.79
1:C:305:LEU:C	1:C:307:ASN:H	1.90	0.79
1:A:15:CYS:HA	1:A:595:LEU:HD21	1.64	0.79
1:B:37:ILE:HD11	1:B:291:LEU:HD22	1.63	0.79
1:C:52:GLU:O	1:C:254:MET:HE2	1.82	0.79
1:B:583:MET:HA	1:B:586:ARG:NE	1.98	0.79
1:D:309:THR:HA	1:D:312:GLU:HB2	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:PRO:HG2	1:A:134:ASN:HD21	1.48	0.78
1:B:92:LEU:HD13	1:B:92:LEU:O	1.83	0.78
1:B:225:ILE:HG12	1:B:230:SER:OG	1.83	0.78
1:C:86:TYR:CE1	1:C:96:LYS:HD2	2.19	0.78
1:D:260:ARG:O	1:D:263:GLU:HB3	1.83	0.78
1:D:169:TYR:O	1:D:175:CYS:SG	2.41	0.78
1:D:79:ILE:O	1:D:81:ASP:N	2.16	0.78
1:A:29:THR:C	1:A:31:TRP:N	2.41	0.77
1:D:162:ILE:O	1:D:166:VAL:HG23	1.84	0.77
1:A:50:VAL:HG13	1:A:242:ASN:HD21	1.48	0.77
1:D:204:ASP:HA	1:D:234:LYS:CD	2.14	0.77
1:A:11:ILE:CG2	1:A:12:GLN:H	1.83	0.77
1:A:29:THR:O	1:A:31:TRP:N	2.18	0.77
1:C:291:LEU:O	1:C:291:LEU:HG	1.83	0.77
1:C:160:LYS:O	1:C:164:ASN:HB2	1.85	0.76
1:D:24:SER:HB2	1:D:592:ARG:NH1	1.99	0.76
1:C:74:LEU:HD23	1:C:75:GLN:N	2.00	0.76
1:C:240:VAL:HG12	1:C:261:GLU:OE2	1.84	0.76
1:C:600:GLN:O	1:C:600:GLN:HG2	1.85	0.76
1:C:302:ILE:HD11	1:C:603:ILE:HB	1.66	0.76
1:A:45:SER:HA	1:A:182:PRO:HG2	1.67	0.76
1:B:149:VAL:HA	3:B:682:HOH:O	1.86	0.75
1:A:282:HIS:O	1:A:283:LEU:C	2.28	0.75
1:C:66:ILE:CG2	1:C:119:LYS:HD2	2.16	0.75
1:D:282:HIS:O	1:D:282:HIS:ND1	2.19	0.75
1:B:15:CYS:O	1:B:17:ALA:N	2.13	0.75
1:B:606:VAL:HG13	3:B:676:HOH:O	1.85	0.75
1:A:82:GLY:O	1:A:84:ARG:N	2.16	0.75
1:B:183:ALA:HB1	1:B:216:MET:HE3	1.67	0.75
1:A:276:ASN:HB3	3:A:624:HOH:O	1.86	0.74
1:C:260:ARG:O	1:C:263:GLU:HB2	1.86	0.74
1:B:29:THR:HA	1:B:32:ASP:CB	2.14	0.74
1:B:305:LEU:O	1:B:307:ASN:N	2.21	0.74
1:B:178:LEU:O	1:B:180:ILE:HD12	1.87	0.74
1:C:11:ILE:O	1:C:12:GLN:C	2.31	0.74
1:A:300:PRO:C	1:A:302:ILE:H	1.95	0.74
1:C:301:GLY:C	1:C:302:ILE:O	2.29	0.74
1:C:39:VAL:HG22	1:C:142:ASP:HA	1.69	0.74
1:D:32:ASP:C	1:D:34:LEU:H	1.96	0.74
1:C:70:ARG:HH11	1:C:126:ILE:HD11	1.52	0.73
1:C:600:GLN:HA	1:C:603:ILE:HG13	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:ASN:O	1:C:138:LEU:HB3	1.88	0.73
1:D:193:ILE:H	1:D:193:ILE:CD1	2.00	0.73
1:C:27:LEU:O	1:C:31:TRP:N	2.21	0.73
1:C:69:ARG:NH2	1:C:119:LYS:HD3	2.03	0.73
1:C:598:ALA:O	1:C:602:GLU:HG3	1.89	0.73
1:D:86:TYR:CE1	1:D:96:LYS:HD3	2.24	0.73
1:B:212:LYS:CB	1:B:215:LEU:HD12	2.18	0.73
1:A:87:ALA:HB2	1:A:130:ILE:HG23	1.71	0.72
1:A:302:ILE:HA	1:A:305:LEU:HB3	1.72	0.72
1:C:27:LEU:HD22	1:C:31:TRP:CD1	2.23	0.72
1:C:39:VAL:CG2	1:C:142:ASP:HA	2.19	0.72
1:D:36:ALA:C	3:D:656:HOH:O	2.33	0.72
1:A:247:ASP:HB3	1:A:252:VAL:HG21	1.70	0.72
1:A:310:VAL:HG12	1:A:314:GLU:HB2	1.70	0.72
1:D:103:VAL:O	1:D:104:ARG:C	2.33	0.72
1:D:204:ASP:HA	1:D:234:LYS:HD2	1.71	0.72
1:A:13:ARG:O	1:A:15:CYS:N	2.23	0.72
1:D:307:ASN:HA	1:D:310:VAL:HG12	1.71	0.72
1:D:100:PHE:HA	1:D:103:VAL:HG23	1.71	0.72
1:A:119:LYS:HG3	1:A:154:GLN:HE21	1.53	0.72
1:D:24:SER:HB2	1:D:592:ARG:HH12	1.55	0.72
1:D:141:ILE:HD11	3:D:656:HOH:O	1.88	0.72
1:A:15:CYS:C	1:A:17:ALA:H	1.97	0.72
1:D:254:MET:HE3	1:D:254:MET:O	1.89	0.72
1:A:79:ILE:HD11	1:A:132:SER:HA	1.72	0.71
1:A:27:LEU:HD22	1:A:31:TRP:NE1	2.05	0.71
1:A:190:SER:HB2	1:A:193:ILE:HB	1.71	0.71
1:D:5:ILE:HD12	1:D:137:ASN:O	1.91	0.71
1:D:191:ASP:HB3	1:D:195:ILE:HD12	1.70	0.71
1:A:290:HIS:O	1:A:294:VAL:HG23	1.90	0.71
1:D:8:VAL:HG21	1:D:295:ILE:HD13	1.72	0.71
1:C:94:ARG:HD3	3:C:358:HOH:O	1.90	0.71
1:C:275:ALA:C	3:C:662:HOH:O	2.33	0.71
1:B:67:VAL:HG11	1:B:108:GLN:HE21	1.55	0.71
1:C:226:LEU:C	1:C:228:GLY:H	1.96	0.71
1:A:207:PHE:CZ	1:A:235:TYR:CE1	2.79	0.71
1:B:170:ILE:CG2	1:B:199:VAL:HG21	2.21	0.71
1:C:86:TYR:HE1	1:C:96:LYS:HD2	1.53	0.71
1:C:22:GLY:HA2	1:C:26:ALA:HB3	1.72	0.71
1:A:70:ARG:NH2	1:A:124:VAL:O	2.23	0.71
1:D:167:ARG:C	1:D:169:TYR:H	1.99	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:VAL:O	1:B:298:ARG:HG3	1.90	0.70
1:D:31:TRP:HA	1:D:172:LYS:HE2	1.73	0.70
1:A:27:LEU:N	1:A:28:PRO:CD	2.55	0.70
1:D:80:ASP:O	1:D:82:GLY:N	2.25	0.70
1:D:187:LEU:HB2	1:D:231:PHE:CD2	2.25	0.70
1:B:590:SER:O	1:B:594:GLU:HG3	1.91	0.70
1:A:137:ASN:ND2	3:A:659:HOH:O	2.22	0.70
1:D:241:VAL:HG12	1:D:241:VAL:O	1.90	0.70
1:A:6:SER:HB2	3:A:659:HOH:O	1.91	0.70
1:B:6:SER:HB2	1:B:77:GLN:OE1	1.91	0.70
1:A:89:PHE:HE1	1:A:106:GLU:HG2	1.56	0.70
1:C:8:VAL:HG21	1:C:295:ILE:HD13	1.74	0.70
1:D:49:SER:HA	1:D:62:ARG:HH12	1.56	0.70
1:A:234:LYS:HE2	1:C:597:ARG:NE	2.06	0.69
1:B:59:PHE:HD1	1:B:59:PHE:O	1.74	0.69
1:B:142:ASP:O	1:B:143:LEU:HD23	1.92	0.69
1:B:303:GLN:HA	1:B:306:ILE:HG22	1.72	0.69
1:A:36:ALA:HB1	1:A:139:THR:HG22	1.74	0.69
1:B:260:ARG:HG3	1:B:261:GLU:N	2.05	0.69
1:A:212:LYS:HG3	2:A:9001:GDP:C5	2.27	0.69
1:C:207:PHE:HD1	1:C:208:GLY:N	1.91	0.69
1:C:309:THR:N	3:C:675:HOH:O	2.24	0.69
1:D:192:ALA:HB3	1:D:193:ILE:HD12	1.74	0.69
1:A:182:PRO:HB3	1:A:212:LYS:HD3	1.74	0.69
1:B:67:VAL:HA	1:B:69:ARG:CZ	2.23	0.69
1:B:13:ARG:HB3	3:B:655:HOH:O	1.92	0.69
1:D:265:PHE:CE2	1:D:278:MET:HE1	2.27	0.69
1:D:299:ILE:O	1:D:302:ILE:HG22	1.93	0.69
1:B:70:ARG:NH2	1:B:124:VAL:H	1.90	0.69
1:B:305:LEU:C	1:B:307:ASN:N	2.50	0.69
2:C:9001:GDP:PA	3:C:667:HOH:O	2.49	0.69
1:C:225:ILE:HG12	1:C:230:SER:CB	2.23	0.69
1:D:105:LYS:O	1:D:109:ASP:HB2	1.93	0.69
1:A:272:ARG:HG3	1:A:272:ARG:HH11	1.56	0.69
1:D:227:GLU:HG2	1:D:229:ARG:CZ	2.23	0.69
1:D:300:PRO:HB3	1:D:303:GLN:OE1	1.92	0.69
1:A:71:PRO:HB2	1:A:125:PRO:HA	1.76	0.68
1:A:77:GLN:NE2	1:A:137:ASN:HD21	1.91	0.68
1:A:148:LYS:HB2	1:B:194:LYS:HG3	1.74	0.68
1:B:216:MET:HE1	1:B:222:ALA:HB2	1.74	0.68
1:C:34:LEU:HG	1:C:172:LYS:HE2	1.72	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:VAL:HG12	1:C:57:LYS:H	1.58	0.68
1:D:264:TYR:O	1:D:268:THR:HG23	1.93	0.68
1:B:31:TRP:CE3	1:B:172:LYS:HD3	2.28	0.68
1:C:200:ASP:OD2	1:C:206:THR:HB	1.92	0.68
1:A:243:ARG:HG2	1:A:247:ASP:HB2	1.75	0.68
1:C:12:GLN:HB3	1:C:75:GLN:HE22	1.58	0.68
1:C:29:THR:O	1:C:33:SER:HB3	1.94	0.68
1:D:30:LEU:O	1:D:30:LEU:HD23	1.93	0.68
1:C:33:SER:C	1:C:35:PRO:HD2	2.19	0.68
1:C:148:LYS:HG2	1:D:189:THR:HA	1.76	0.68
1:C:269:THR:HA	1:C:272:ARG:HB2	1.74	0.68
1:B:90:LEU:HB2	1:B:127:HIS:HB2	1.75	0.68
1:C:57:LYS:HG2	1:C:100:PHE:CE1	2.28	0.68
1:A:23:ASP:CB	1:A:26:ALA:HB3	2.23	0.68
1:A:42:GLY:HA2	1:A:146:LEU:HB2	1.74	0.68
1:A:63:GLY:HA3	1:A:67:VAL:HG22	1.76	0.68
1:B:56:GLY:O	1:B:57:LYS:HD3	1.92	0.68
1:C:173:PRO:O	1:C:175:CYS:N	2.25	0.68
1:B:34:LEU:CD1	1:B:36:ALA:HB3	2.22	0.68
1:B:253:ASP:HB3	3:B:632:HOH:O	1.91	0.68
1:B:295:ILE:O	1:B:299:ILE:HG22	1.93	0.68
1:C:27:LEU:HB3	1:C:31:TRP:CB	2.21	0.68
1:D:25:SER:O	1:D:28:PRO:HB2	1.93	0.68
1:B:143:LEU:HD11	1:B:169:TYR:HD2	1.59	0.68
1:A:126:ILE:HG22	1:A:126:ILE:O	1.94	0.67
1:B:37:ILE:HD12	1:B:37:ILE:H	1.58	0.67
1:C:90:LEU:HD23	1:C:90:LEU:O	1.92	0.67
1:C:302:ILE:C	1:C:304:SER:H	2.00	0.67
1:B:26:ALA:HB1	1:B:596:TYR:CE2	2.30	0.67
1:B:257:ALA:O	1:B:260:ARG:HG2	1.93	0.67
1:C:32:ASP:O	1:C:35:PRO:HD3	1.93	0.67
1:B:29:THR:O	1:B:33:SER:HB3	1.94	0.67
1:C:34:LEU:O	1:C:36:ALA:N	2.27	0.67
1:A:293:ARG:HD3	1:C:306:ILE:CG2	2.21	0.67
1:A:283:LEU:O	1:A:284:ALA:C	2.38	0.67
1:B:114:GLU:O	1:B:115:THR:HG23	1.95	0.67
1:D:23:ASP:N	1:D:26:ALA:HB3	2.10	0.67
1:D:244:SER:HB3	1:D:247:ASP:OD2	1.95	0.67
1:C:207:PHE:HD1	1:C:208:GLY:H	1.43	0.67
1:A:5:ILE:HG21	1:A:137:ASN:C	2.18	0.67
1:A:296:LYS:HG2	1:A:297:SER:N	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:ARG:HG3	1:A:14:ALA:N	2.10	0.67
1:A:48:SER:HB2	2:A:9001:GDP:PA	2.34	0.67
1:C:44:SER:HA	2:C:9001:GDP:O3B	1.95	0.67
1:D:593:LEU:O	1:D:594:GLU:C	2.36	0.67
1:A:27:LEU:N	1:A:28:PRO:HD2	2.09	0.67
1:B:143:LEU:HD21	1:B:169:TYR:CE2	2.29	0.67
1:D:180:ILE:HD13	1:D:180:ILE:H	1.59	0.67
1:D:36:ALA:HB1	1:D:139:THR:HG22	1.77	0.66
1:B:32:ASP:C	1:B:34:LEU:H	2.02	0.66
1:A:5:ILE:HG22	1:A:137:ASN:HD22	1.61	0.66
1:C:183:ALA:HB2	1:C:210:LEU:CD2	2.26	0.66
1:C:241:VAL:HG12	1:C:241:VAL:O	1.93	0.66
2:C:9001:GDP:O1A	3:C:667:HOH:O	2.12	0.66
1:D:176:ILE:HD12	1:D:176:ILE:N	2.08	0.66
1:D:227:GLU:HG2	1:D:229:ARG:NH1	2.09	0.66
1:D:267:ASN:HB3	3:D:662:HOH:O	1.96	0.66
1:C:30:LEU:HD23	1:C:34:LEU:HD23	1.76	0.66
1:C:55:VAL:HG11	1:C:59:PHE:CD2	2.30	0.66
1:A:200:ASP:C	1:A:202:SER:H	2.03	0.66
1:A:210:LEU:HB2	1:A:237:TRP:CZ3	2.31	0.66
1:C:33:SER:C	1:C:35:PRO:CD	2.68	0.66
1:C:290:HIS:C	1:C:292:GLU:H	2.04	0.66
1:D:23:ASP:OD2	1:D:26:ALA:HB2	1.95	0.66
1:D:230:SER:OG	1:D:231:PHE:N	2.29	0.66
1:A:190:SER:CB	1:A:193:ILE:HB	2.25	0.66
1:B:257:ALA:HA	1:B:260:ARG:HD2	1.76	0.66
1:D:37:ILE:HG23	1:D:176:ILE:HB	1.78	0.66
1:D:88:GLU:CD	1:D:96:LYS:HE2	2.21	0.66
1:B:243:ARG:HA	1:B:260:ARG:HH12	1.61	0.66
1:D:36:ALA:HB3	3:D:656:HOH:O	1.96	0.66
1:A:302:ILE:C	1:A:304:SER:N	2.53	0.66
1:B:70:ARG:O	1:B:72:LEU:N	2.28	0.66
1:B:265:PHE:HB3	1:B:275:ALA:HB2	1.78	0.66
1:C:130:ILE:HG22	1:C:131:TYR:N	2.10	0.66
1:C:257:ALA:O	1:C:261:GLU:N	2.22	0.66
2:C:9001:GDP:H3'	3:C:667:HOH:O	1.96	0.66
1:A:29:THR:O	1:A:33:SER:HB3	1.96	0.65
1:A:235:TYR:HB3	1:A:236:PRO:CD	2.26	0.65
1:C:252:VAL:HG12	1:C:253:ASP:N	2.11	0.65
1:D:260:ARG:HA	1:D:263:GLU:HB2	1.77	0.65
1:A:227:GLU:HG2	1:A:229:ARG:HE	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:ARG:CG	1:A:14:ALA:H	2.09	0.65
1:B:244:SER:OG	1:B:246:ALA:HB3	1.96	0.65
1:C:30:LEU:CD2	1:C:34:LEU:HD23	2.26	0.65
1:C:183:ALA:CB	1:C:216:MET:HE3	2.20	0.65
1:D:151:VAL:N	1:D:154:GLN:OE1	2.29	0.65
1:B:25:SER:HB2	1:B:308:LYS:HZ2	1.60	0.65
1:B:174:ASN:ND2	1:B:298:ARG:NE	2.43	0.65
1:C:149:VAL:HG22	1:D:188:ALA:HA	1.79	0.65
1:D:88:GLU:OE1	1:D:96:LYS:HE2	1.96	0.65
1:A:133:PRO:HG2	1:A:134:ASN:ND2	2.10	0.65
1:C:3:ASN:O	1:C:6:SER:OG	2.13	0.65
1:A:119:LYS:HG3	1:A:154:GLN:NE2	2.10	0.65
1:B:21:HIS:CD2	1:B:592:ARG:HH22	2.15	0.65
1:D:170:ILE:HG23	1:D:177:ILE:CD1	2.26	0.65
1:B:594:GLU:O	1:B:595:LEU:HD23	1.97	0.65
1:C:183:ALA:HB2	1:C:210:LEU:HD21	1.77	0.65
1:A:143:LEU:HD21	1:A:169:TYR:HD2	1.61	0.65
1:B:59:PHE:O	1:B:59:PHE:CD1	2.50	0.65
1:B:80:ASP:O	1:B:82:GLY:N	2.30	0.65
1:B:303:GLN:N	1:B:303:GLN:HE21	1.94	0.65
1:D:69:ARG:O	1:D:121:ILE:HG22	1.97	0.65
1:B:73:VAL:HG22	1:B:141:ILE:HG23	1.79	0.65
1:A:212:LYS:HB3	1:A:215:LEU:CD1	2.27	0.65
1:C:6:SER:HB2	1:C:77:GLN:NE2	2.11	0.65
1:A:13:ARG:HH12	1:A:129:SER:HB2	1.62	0.64
1:A:27:LEU:HD22	1:A:31:TRP:HE1	1.60	0.64
1:A:136:VAL:HG11	1:A:288:SER:HB3	1.80	0.64
1:B:174:ASN:HD22	1:B:298:ARG:NE	1.95	0.64
1:C:89:PHE:CD2	1:C:91:HIS:HB2	2.33	0.64
1:D:29:THR:C	1:D:31:TRP:H	2.05	0.64
1:B:26:ALA:HB1	1:B:596:TYR:HE2	1.62	0.64
1:C:186:ASP:HB2	1:D:44:SER:HB2	1.79	0.64
1:A:174:ASN:HB3	1:A:298:ARG:HH22	1.62	0.64
1:A:201:PRO:HB3	3:A:674:HOH:O	1.97	0.64
1:D:312:GLU:C	1:D:314:GLU:H	2.03	0.64
1:C:30:LEU:O	1:C:32:ASP:N	2.27	0.64
1:D:154:GLN:HE21	1:D:158:ILE:HG12	1.62	0.64
1:D:186:ASP:HB2	1:D:189:THR:HG23	1.77	0.64
1:C:252:VAL:HG12	1:C:253:ASP:H	1.63	0.64
1:D:27:LEU:C	1:D:29:THR:H	2.05	0.64
1:D:37:ILE:O	3:D:675:HOH:O	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:ASN:OD1	1:A:75:GLN:HG2	1.98	0.64
1:A:215:LEU:HD21	2:A:9001:GDP:N2	2.13	0.64
1:B:162:ILE:O	1:B:166:VAL:HG23	1.98	0.64
1:C:128:LEU:HD12	1:C:128:LEU:C	2.22	0.64
1:D:240:VAL:HG12	1:D:241:VAL:H	1.62	0.64
1:C:166:VAL:O	1:C:170:ILE:HG12	1.98	0.64
1:D:49:SER:HA	1:D:62:ARG:NH1	2.13	0.64
1:A:188:ALA:HB2	1:A:231:PHE:HZ	1.63	0.63
1:A:282:HIS:CE1	1:A:286:MET:HG3	2.33	0.63
1:B:46:GLY:O	1:B:47:LYS:C	2.40	0.63
1:B:70:ARG:NH1	3:B:679:HOH:O	2.31	0.63
1:C:301:GLY:HA2	1:C:304:SER:OG	1.97	0.63
1:C:589:ILE:HG22	1:C:589:ILE:O	1.98	0.63
1:A:58:ASP:O	1:A:59:PHE:CD2	2.52	0.63
1:B:275:ALA:HA	1:B:278:MET:HB2	1.79	0.63
1:C:32:ASP:C	1:C:34:LEU:N	2.53	0.63
1:C:302:ILE:HD13	3:C:658:HOH:O	1.98	0.63
1:D:151:VAL:HG22	1:D:152:ASP:CG	2.23	0.63
1:A:77:GLN:HG3	3:A:356:HOH:O	1.97	0.63
1:B:274:LEU:O	1:B:276:ASN:N	2.32	0.63
1:B:308:LYS:CD	1:B:311:LEU:HD23	2.27	0.63
1:C:302:ILE:O	1:C:304:SER:N	2.30	0.63
1:A:11:ILE:CG2	1:A:12:GLN:N	2.48	0.63
1:B:313:LEU:CD2	1:B:597:ARG:NH2	2.52	0.63
1:C:123:SER:HB3	1:C:165:MET:CE	2.27	0.63
1:C:189:THR:HA	1:D:148:LYS:CG	2.23	0.63
1:D:77:GLN:HG3	1:D:131:TYR:CD1	2.34	0.63
1:C:590:SER:C	1:C:592:ARG:H	2.06	0.63
1:A:18:LEU:HD11	1:A:595:LEU:HG	1.79	0.63
1:A:57:LYS:O	1:A:58:ASP:O	2.17	0.63
1:A:195:ILE:HD13	1:A:198:GLU:HG3	1.81	0.63
1:B:265:PHE:HB3	1:B:275:ALA:CB	2.28	0.63
1:C:183:ALA:HB1	1:C:216:MET:CE	2.19	0.63
1:D:187:LEU:C	1:D:189:THR:H	2.06	0.63
1:A:45:SER:O	1:A:182:PRO:CG	2.47	0.63
1:B:12:GLN:NE2	1:B:73:VAL:HG11	2.14	0.63
1:B:92:LEU:HD22	1:B:92:LEU:C	2.24	0.63
1:C:7:LEU:O	1:C:10:LYS:N	2.32	0.63
1:C:101:ALA:O	1:C:104:ARG:HB3	1.99	0.63
1:B:589:ILE:O	1:B:592:ARG:HB2	1.99	0.62
1:D:191:ASP:HA	1:D:194:LYS:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:LYS:HG2	1:A:96:LYS:N	2.13	0.62
1:A:254:MET:O	1:A:257:ALA:HB3	1.99	0.62
1:B:271:TYR:O	1:B:272:ARG:C	2.43	0.62
1:D:190:SER:HB3	1:D:192:ALA:HB3	1.81	0.62
1:A:34:LEU:O	1:A:36:ALA:N	2.32	0.62
1:A:245:GLN:O	1:A:249:ASN:ND2	2.33	0.62
1:B:25:SER:O	1:B:308:LYS:CD	2.46	0.62
1:B:146:LEU:HD11	1:B:195:ILE:HG21	1.82	0.62
1:B:260:ARG:HG3	1:B:261:GLU:H	1.63	0.62
1:D:189:THR:O	1:D:189:THR:OG1	2.17	0.62
1:D:238:VAL:HG13	1:D:278:MET:HG2	1.80	0.62
1:B:249:ASN:C	1:B:251:ASN:H	2.07	0.62
1:D:16:THR:HG21	1:D:125:PRO:CG	2.30	0.62
1:D:27:LEU:O	1:D:29:THR:N	2.33	0.62
1:B:13:ARG:O	1:B:17:ALA:HB2	1.99	0.62
1:B:167:ARG:HH21	1:B:195:ILE:HD11	1.65	0.62
1:D:257:ALA:O	1:D:261:GLU:N	2.29	0.62
1:D:69:ARG:HB3	1:D:121:ILE:CG2	2.30	0.62
1:A:79:ILE:O	1:A:81:ASP:N	2.30	0.62
1:A:45:SER:HA	1:A:182:PRO:CG	2.30	0.62
1:D:70:ARG:HG2	1:D:71:PRO:HD2	1.82	0.62
1:D:70:ARG:NH2	1:D:126:ILE:CD1	2.63	0.62
1:A:265:PHE:N	1:A:265:PHE:CD1	2.62	0.62
1:B:92:LEU:HD22	1:B:93:PRO:O	2.00	0.62
1:C:27:LEU:H	1:C:28:PRO:CD	2.11	0.62
1:D:15:CYS:C	1:D:17:ALA:H	2.08	0.62
1:D:16:THR:HG21	1:D:125:PRO:HG2	1.82	0.62
1:B:261:GLU:O	1:B:264:TYR:HB3	1.98	0.61
1:D:255:ILE:HD12	1:D:259:LYS:NZ	2.15	0.61
1:A:174:ASN:HA	1:A:298:ARG:HH12	1.65	0.61
1:B:257:ALA:HA	1:B:260:ARG:CD	2.30	0.61
1:D:213:ILE:HG13	3:D:654:HOH:O	2.01	0.61
1:A:16:THR:HA	1:A:20:ASP:HB2	1.81	0.61
1:A:55:VAL:HG11	1:A:59:PHE:CE2	2.35	0.61
1:A:185:GLN:NE2	1:B:185:GLN:NE2	2.49	0.61
1:A:223:VAL:HA	1:A:226:LEU:HD12	1.82	0.61
1:D:13:ARG:HG3	1:D:75:GLN:OE1	2.00	0.61
1:D:76:LEU:HD23	1:D:130:ILE:HB	1.81	0.61
1:B:204:ASP:HB2	3:B:681:HOH:O	2.00	0.61
1:C:51:LEU:N	3:C:634:HOH:O	2.32	0.61
1:C:238:VAL:HG21	1:C:283:LEU:HD13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:GLN:HE21	1:B:303:GLN:H	1.48	0.61
1:C:42:GLY:HA2	1:C:146:LEU:CB	2.25	0.61
1:C:148:LYS:HE2	1:D:148:LYS:HE2	1.82	0.61
1:D:282:HIS:C	3:D:660:HOH:O	2.44	0.61
1:B:243:ARG:HA	1:B:260:ARG:NH1	2.14	0.61
1:B:260:ARG:CG	1:B:261:GLU:H	2.13	0.61
1:C:600:GLN:HA	1:C:603:ILE:CG1	2.30	0.61
1:D:37:ILE:HD12	1:D:176:ILE:HD13	1.83	0.61
1:A:296:LYS:C	1:A:298:ARG:H	2.06	0.61
1:B:79:ILE:HD11	1:B:132:SER:HA	1.83	0.61
1:D:161:ASP:HA	1:D:164:ASN:OD1	2.00	0.61
1:D:241:VAL:O	1:D:241:VAL:CG1	2.48	0.61
1:D:312:GLU:C	1:D:314:GLU:N	2.55	0.61
1:A:13:ARG:HB2	1:A:90:LEU:HD21	1.82	0.61
1:A:59:PHE:CD1	1:A:59:PHE:C	2.78	0.61
1:B:585:ARG:NE	1:B:589:ILE:HD11	2.11	0.61
1:C:37:ILE:O	1:C:37:ILE:HG22	2.01	0.61
1:C:278:MET:N	3:C:662:HOH:O	2.34	0.61
1:D:56:GLY:HA2	1:D:254:MET:HE2	1.83	0.61
1:B:60:LEU:HD23	1:B:61:PRO:CD	2.25	0.61
1:C:66:ILE:HG23	1:C:69:ARG:HE	1.66	0.61
1:C:70:ARG:HG2	1:C:71:PRO:HD2	1.83	0.61
1:C:253:ASP:CG	1:C:254:MET:H	2.08	0.60
1:D:34:LEU:N	1:D:35:PRO:CD	2.64	0.60
1:A:23:ASP:HB3	1:A:592:ARG:HD3	1.81	0.60
1:C:27:LEU:N	1:C:28:PRO:CD	2.65	0.60
1:A:16:THR:CG2	1:A:30:LEU:HD13	2.31	0.60
1:A:79:ILE:HD11	1:A:132:SER:CA	2.31	0.60
1:C:266:SER:O	1:C:272:ARG:HG3	2.00	0.60
1:D:193:ILE:O	1:D:196:SER:N	2.31	0.60
1:A:13:ARG:CG	1:A:14:ALA:N	2.64	0.60
1:B:175:CYS:O	1:B:205:ARG:HD2	2.01	0.60
1:C:290:HIS:CE1	3:C:673:HOH:O	2.44	0.60
1:D:70:ARG:NH2	1:D:126:ILE:HD11	2.16	0.60
1:D:300:PRO:C	1:D:302:ILE:H	2.09	0.60
1:A:128:LEU:HD11	1:A:130:ILE:HG12	1.83	0.60
1:B:260:ARG:CG	1:B:261:GLU:N	2.63	0.60
1:A:13:ARG:HG3	1:A:14:ALA:H	1.66	0.60
1:C:234:LYS:C	1:C:235:TYR:CD2	2.79	0.60
1:C:30:LEU:C	1:C:32:ASP:H	2.09	0.60
1:D:186:ASP:HB2	3:D:659:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:187:LEU:O	1:D:189:THR:N	2.31	0.60
1:A:24:SER:CB	1:A:585:ARG:HH21	2.12	0.60
1:A:118:SER:C	1:A:119:LYS:HG2	2.26	0.60
1:A:224:GLU:HG3	1:A:229:ARG:CZ	2.32	0.60
1:B:596:TYR:O	1:B:599:ALA:HB3	2.00	0.60
1:C:194:LYS:HA	1:D:149:VAL:CG1	2.32	0.60
1:D:15:CYS:O	1:D:17:ALA:N	2.35	0.60
1:D:276:ASN:OD1	1:D:277:LYS:HG3	2.01	0.60
1:D:294:VAL:O	1:D:297:SER:HB3	2.01	0.60
1:B:215:LEU:HD11	2:B:9001:GDP:N2	2.16	0.60
1:C:23:ASP:OD1	1:C:26:ALA:HB2	2.02	0.60
1:C:226:LEU:C	1:C:228:GLY:N	2.60	0.60
1:D:263:GLU:O	1:D:267:ASN:HB2	2.02	0.60
1:A:30:LEU:HG	1:A:34:LEU:HD22	1.84	0.60
1:A:53:SER:O	1:A:280:SER:HB3	2.00	0.60
1:B:59:PHE:CD1	1:B:59:PHE:C	2.80	0.60
1:C:235:TYR:O	1:C:236:PRO:C	2.43	0.60
1:D:72:LEU:HD12	1:D:126:ILE:HB	1.84	0.59
1:A:16:THR:HG21	1:A:127:HIS:NE2	2.17	0.59
1:A:36:ALA:HB1	1:A:139:THR:CG2	2.32	0.59
1:A:207:PHE:N	1:A:207:PHE:CD2	2.70	0.59
1:B:285:LYS:O	1:B:289:LYS:HG2	2.03	0.59
1:C:186:ASP:O	1:C:188:ALA:N	2.34	0.59
1:B:92:LEU:HD21	1:B:95:LYS:HB2	1.83	0.59
1:B:207:PHE:CZ	1:B:235:TYR:CE1	2.90	0.59
1:B:183:ALA:HB1	1:B:216:MET:CE	2.32	0.59
1:C:302:ILE:HG13	1:C:603:ILE:HD12	1.83	0.59
1:D:234:LYS:HD3	1:D:235:TYR:CE2	2.37	0.59
1:B:235:TYR:N	1:B:235:TYR:CD2	2.69	0.59
1:D:15:CYS:HA	1:D:595:LEU:HD21	1.84	0.59
1:A:227:GLU:HG2	1:A:229:ARG:NE	2.17	0.59
1:A:300:PRO:C	1:A:302:ILE:N	2.58	0.59
1:B:119:LYS:HB2	1:B:154:GLN:HE21	1.68	0.59
1:B:247:ASP:O	1:B:252:VAL:HG23	2.02	0.59
1:B:593:LEU:C	1:B:595:LEU:H	2.10	0.59
1:C:44:SER:HB2	1:D:186:ASP:OD2	2.02	0.59
1:D:167:ARG:C	1:D:169:TYR:N	2.59	0.59
1:A:24:SER:HB3	1:A:585:ARG:NH2	2.16	0.59
1:C:592:ARG:O	1:C:593:LEU:C	2.46	0.59
1:C:593:LEU:HD23	1:C:593:LEU:H	1.68	0.59
1:A:33:SER:C	1:A:35:PRO:CD	2.76	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:LEU:CD2	1:C:11:ILE:HG12	2.33	0.59
1:C:80:ASP:O	1:C:82:GLY:N	2.36	0.59
1:C:225:ILE:HG12	1:C:230:SER:HB2	1.84	0.59
1:D:172:LYS:C	1:D:174:ASN:H	2.10	0.59
1:A:25:SER:C	1:A:28:PRO:HD2	2.28	0.59
1:D:88:GLU:O	1:D:89:PHE:HB2	2.02	0.59
1:A:42:GLY:HA2	1:A:146:LEU:N	2.16	0.58
1:A:204:ASP:OD1	1:A:234:LYS:NZ	2.36	0.58
1:D:189:THR:HG23	3:D:659:HOH:O	2.01	0.58
1:A:176:ILE:HD12	1:A:176:ILE:H	1.67	0.58
1:C:6:SER:CB	1:C:77:GLN:NE2	2.66	0.58
1:D:15:CYS:O	1:D:19:GLY:N	2.30	0.58
1:D:283:LEU:C	3:D:660:HOH:O	2.46	0.58
1:A:257:ALA:O	1:A:260:ARG:HB3	2.04	0.58
1:B:72:LEU:HD12	1:B:72:LEU:C	2.28	0.58
1:A:3:ASN:HA	1:A:137:ASN:ND2	2.19	0.58
1:A:59:PHE:HA	1:A:104:ARG:HB2	1.84	0.58
1:A:97:PHE:CD2	1:A:103:VAL:HG22	2.38	0.58
1:A:283:LEU:O	1:A:286:MET:N	2.36	0.58
1:B:591:LYS:O	1:B:595:LEU:HD12	2.04	0.58
1:C:7:LEU:HD23	1:C:11:ILE:HG12	1.86	0.58
1:D:259:LYS:HE3	3:D:643:HOH:O	2.02	0.58
1:A:31:TRP:HE3	1:A:172:LYS:HD3	1.68	0.58
1:A:34:LEU:HD23	1:A:172:LYS:HZ2	1.68	0.58
1:A:233:LEU:HD22	1:A:237:TRP:NE1	2.18	0.58
1:B:215:LEU:HD11	2:B:9001:GDP:N3	2.17	0.58
1:C:57:LYS:O	1:C:58:ASP:O	2.22	0.58
1:B:66:ILE:HG12	1:B:67:VAL:N	2.19	0.58
1:B:68:THR:O	1:B:68:THR:HG22	2.03	0.58
1:C:6:SER:HB3	1:C:137:ASN:ND2	2.19	0.58
1:C:51:LEU:C	3:C:636:HOH:O	2.47	0.58
1:A:123:SER:HB3	1:A:165:MET:HE2	1.84	0.58
1:C:148:LYS:HB3	1:D:194:LYS:HD2	1.84	0.58
1:D:313:LEU:HG	1:D:593:LEU:HD11	1.84	0.58
1:A:89:PHE:CE1	1:A:106:GLU:HG2	2.39	0.58
1:A:226:LEU:CD2	1:A:278:MET:HE1	2.32	0.58
1:B:77:GLN:HB2	1:B:131:TYR:CD1	2.38	0.58
1:B:232:LYS:HD3	3:B:649:HOH:O	2.02	0.58
1:B:257:ALA:HA	1:B:260:ARG:NE	2.19	0.58
1:C:132:SER:HB3	1:C:135:VAL:HG13	1.85	0.58
1:D:26:ALA:N	1:D:28:PRO:HD2	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:ARG:NH2	1:B:195:ILE:HD11	2.18	0.58
1:B:305:LEU:C	1:B:307:ASN:H	2.11	0.58
1:C:264:TYR:CD1	1:C:264:TYR:C	2.82	0.58
1:C:590:SER:C	1:C:592:ARG:N	2.59	0.58
1:D:25:SER:HA	1:D:28:PRO:HG2	1.86	0.58
1:B:5:ILE:O	1:B:7:LEU:N	2.37	0.58
1:D:235:TYR:HE1	3:D:628:HOH:O	1.87	0.58
1:A:37:ILE:HG23	1:A:176:ILE:HD13	1.85	0.57
1:A:234:LYS:HE2	1:C:597:ARG:NH2	2.18	0.57
1:A:258:ARG:HH21	1:A:281:GLU:HG2	1.68	0.57
1:B:5:ILE:HG23	1:B:6:SER:N	2.17	0.57
1:B:40:VAL:HG21	1:B:170:ILE:CD1	2.24	0.57
1:C:121:ILE:HD12	1:C:121:ILE:C	2.28	0.57
1:A:166:VAL:O	1:A:170:ILE:HG12	2.04	0.57
1:D:205:ARG:O	1:D:206:THR:HG23	2.04	0.57
1:D:274:LEU:HD23	1:D:277:LYS:HZ3	1.69	0.57
1:A:89:PHE:CE2	1:A:128:LEU:HB2	2.39	0.57
1:A:276:ASN:OD1	1:A:277:LYS:CE	2.52	0.57
1:B:176:ILE:HG22	1:B:177:ILE:N	2.19	0.57
1:C:82:GLY:O	1:C:84:ARG:N	2.33	0.57
1:A:33:SER:O	1:A:35:PRO:HD2	2.04	0.57
1:A:235:TYR:HB3	1:A:236:PRO:HD3	1.87	0.57
1:B:593:LEU:O	1:B:597:ARG:N	2.37	0.57
1:D:204:ASP:HA	1:D:234:LYS:CE	2.33	0.57
1:B:195:ILE:HG23	1:B:195:ILE:O	2.04	0.57
1:B:306:ILE:HG13	1:B:306:ILE:O	2.04	0.57
1:A:200:ASP:H	1:A:201:PRO:HD3	1.68	0.57
1:A:228:GLY:O	1:A:232:LYS:HG3	2.04	0.57
1:D:29:THR:O	1:D:31:TRP:N	2.38	0.57
1:A:86:TYR:CZ	1:A:131:TYR:CD2	2.93	0.57
1:C:27:LEU:CB	1:C:31:TRP:HB2	2.24	0.57
1:D:172:LYS:C	1:D:174:ASN:N	2.63	0.57
1:D:204:ASP:CA	1:D:234:LYS:HD2	2.33	0.57
1:A:37:ILE:CG1	1:A:140:LEU:HD23	2.30	0.57
1:A:42:GLY:O	1:A:43:GLN:C	2.48	0.57
1:B:97:PHE:CD2	1:B:103:VAL:HG23	2.40	0.57
1:B:252:VAL:O	1:B:253:ASP:C	2.48	0.57
1:B:590:SER:C	1:B:592:ARG:H	2.12	0.57
1:C:89:PHE:O	1:C:90:LEU:HB2	2.03	0.57
1:C:100:PHE:O	1:C:103:VAL:N	2.38	0.57
1:C:130:ILE:C	1:C:131:TYR:CD2	2.83	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:SER:HB3	2:D:9001:GDP:O1A	2.05	0.57
1:D:165:MET:C	1:D:167:ARG:H	2.11	0.57
1:D:599:ALA:C	1:D:601:SER:H	2.12	0.57
1:B:305:LEU:O	1:B:308:LYS:N	2.38	0.56
1:D:47:LYS:NZ	1:D:145:GLY:N	2.53	0.56
1:D:236:PRO:HD2	3:D:670:HOH:O	2.05	0.56
1:D:597:ARG:NH1	1:D:597:ARG:HG3	2.19	0.56
1:C:162:ILE:O	1:C:166:VAL:HG23	2.05	0.56
1:A:261:GLU:HG3	1:A:262:ARG:N	2.20	0.56
1:B:92:LEU:HD21	1:B:95:LYS:CB	2.36	0.56
1:B:157:SER:O	1:B:161:ASP:HB2	2.04	0.56
1:C:29:THR:O	1:C:33:SER:CB	2.53	0.56
1:C:46:GLY:HA2	1:C:49:SER:OG	2.05	0.56
1:C:295:ILE:C	1:C:297:SER:N	2.63	0.56
1:D:256:ALA:CA	1:D:259:LYS:HB2	2.31	0.56
1:A:136:VAL:CG1	1:A:288:SER:HB3	2.35	0.56
1:C:593:LEU:HD23	1:C:593:LEU:N	2.20	0.56
1:D:29:THR:O	1:D:33:SER:N	2.38	0.56
1:A:85:GLU:O	1:A:86:TYR:CD2	2.58	0.56
1:A:172:LYS:O	1:A:172:LYS:HG2	2.05	0.56
1:C:162:ILE:HG22	1:C:163:GLU:N	2.20	0.56
1:D:25:SER:C	1:D:28:PRO:HD2	2.31	0.56
1:D:86:TYR:CD1	1:D:86:TYR:C	2.83	0.56
1:D:302:ILE:CG1	1:D:600:GLN:HE21	2.18	0.56
1:A:293:ARG:NH1	1:C:604:ASP:OD2	2.39	0.56
1:D:215:LEU:HD11	2:D:9001:GDP:C2	2.40	0.56
1:A:8:VAL:HG21	1:A:295:ILE:HD13	1.88	0.56
1:A:24:SER:CB	1:A:585:ARG:NH2	2.68	0.56
1:B:223:VAL:O	1:B:227:GLU:HG3	2.06	0.56
1:D:23:ASP:CG	1:D:26:ALA:CB	2.79	0.56
1:D:27:LEU:C	1:D:29:THR:N	2.64	0.56
1:D:29:THR:C	1:D:31:TRP:N	2.61	0.56
1:D:305:LEU:O	1:D:306:ILE:C	2.48	0.56
1:A:293:ARG:HH22	1:C:604:ASP:CG	2.14	0.56
1:C:121:ILE:HD12	1:C:121:ILE:O	2.05	0.56
1:C:307:ASN:OD1	1:C:311:LEU:HD11	2.05	0.56
1:A:310:VAL:C	1:A:312:GLU:H	2.13	0.56
1:D:158:ILE:C	1:D:160:LYS:H	2.13	0.56
1:A:39:VAL:HG22	1:A:39:VAL:O	2.06	0.56
1:A:296:LYS:NZ	1:C:303:GLN:NE2	2.54	0.56
1:B:65:GLY:O	1:B:66:ILE:O	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:ASP:C	1:D:34:LEU:N	2.64	0.56
1:C:89:PHE:HD2	1:C:91:HIS:H	1.53	0.55
1:D:203:GLY:C	1:D:234:LYS:HD2	2.31	0.55
1:C:29:THR:O	1:C:33:SER:N	2.37	0.55
1:C:292:GLU:O	1:C:295:ILE:N	2.38	0.55
1:D:172:LYS:O	1:D:174:ASN:N	2.38	0.55
1:D:187:LEU:HD21	1:D:225:ILE:HD13	1.88	0.55
1:D:215:LEU:HD11	2:D:9001:GDP:N2	2.20	0.55
1:A:42:GLY:O	1:A:43:GLN:O	2.25	0.55
1:B:39:VAL:CG1	1:B:142:ASP:HA	2.32	0.55
1:C:49:SER:HB3	1:C:242:ASN:HD22	1.69	0.55
1:D:187:LEU:HD23	1:D:231:PHE:HD2	1.71	0.55
1:B:11:ILE:HG22	1:B:12:GLN:N	2.21	0.55
1:D:69:ARG:HD3	1:D:120:ALA:H	1.71	0.55
1:B:592:ARG:O	1:B:596:TYR:HB2	2.06	0.55
1:D:122:SER:O	1:D:123:SER:HB3	2.06	0.55
1:D:178:LEU:HD12	1:D:207:PHE:O	2.07	0.55
1:D:264:TYR:C	1:D:264:TYR:HD1	2.15	0.55
1:A:152:ASP:CG	1:A:153:GLY:N	2.56	0.55
1:C:295:ILE:O	1:C:297:SER:N	2.40	0.55
1:A:157:SER:O	1:A:161:ASP:N	2.39	0.55
1:A:306:ILE:HG22	1:A:306:ILE:O	2.07	0.55
1:B:14:ALA:O	1:B:15:CYS:O	2.25	0.55
1:A:15:CYS:C	1:A:17:ALA:N	2.63	0.55
1:A:299:ILE:C	1:A:301:GLY:H	2.14	0.55
1:B:15:CYS:C	1:B:17:ALA:H	2.09	0.55
1:B:253:ASP:O	1:B:256:ALA:HB3	2.07	0.55
1:B:257:ALA:O	1:B:258:ARG:C	2.50	0.55
1:C:27:LEU:H	1:C:28:PRO:HD2	1.71	0.55
1:C:137:ASN:O	1:C:138:LEU:CB	2.54	0.55
1:D:62:ARG:NH2	1:D:248:ILE:HD11	2.22	0.55
1:D:70:ARG:CZ	1:D:126:ILE:HD11	2.37	0.55
1:A:72:LEU:HG	1:A:74:LEU:HD13	1.88	0.55
1:B:59:PHE:HA	1:B:104:ARG:HB2	1.88	0.55
1:B:232:LYS:HD2	1:B:233:LEU:N	2.22	0.55
1:C:30:LEU:O	1:C:34:LEU:HB2	2.07	0.55
1:C:46:GLY:O	1:C:49:SER:HB2	2.07	0.55
1:C:162:ILE:C	1:C:164:ASN:H	2.13	0.55
1:D:289:LYS:N	3:D:636:HOH:O	2.17	0.55
1:D:604:ASP:O	1:D:606:VAL:HG12	2.06	0.55
1:A:51:LEU:HD22	1:A:140:LEU:HD13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:LEU:HD13	1:A:95:LYS:CE	2.28	0.55
1:A:296:LYS:CG	1:A:297:SER:N	2.69	0.55
1:B:159:VAL:O	1:B:161:ASP:N	2.40	0.55
1:C:221:ASP:OD1	1:C:223:VAL:HB	2.06	0.55
1:C:585:ARG:C	1:C:587:SER:N	2.63	0.55
1:D:142:ASP:O	1:D:143:LEU:HD23	2.06	0.55
1:D:296:LYS:O	1:D:298:ARG:N	2.41	0.55
1:D:306:ILE:O	1:D:307:ASN:C	2.49	0.55
1:A:8:VAL:O	1:A:12:GLN:HB2	2.07	0.54
1:A:286:MET:O	1:A:287:LEU:C	2.49	0.54
1:A:585:ARG:HA	1:A:588:ALA:HB3	1.87	0.54
1:B:70:ARG:HH21	1:B:124:VAL:H	1.55	0.54
1:D:308:LYS:O	1:D:312:GLU:HG2	2.07	0.54
1:A:18:LEU:HG	1:A:19:GLY:H	1.72	0.54
1:A:77:GLN:NE2	1:A:137:ASN:ND2	2.55	0.54
1:A:228:GLY:O	1:A:232:LYS:HE3	2.06	0.54
1:B:32:ASP:O	1:B:34:LEU:N	2.41	0.54
1:B:217:ASP:O	1:B:219:GLY:N	2.40	0.54
1:B:299:ILE:C	1:B:301:GLY:H	2.15	0.54
1:D:274:LEU:HD23	1:D:277:LYS:NZ	2.23	0.54
1:A:51:LEU:HA	1:A:54:ILE:HG22	1.88	0.54
1:C:279:GLY:O	1:C:281:GLU:N	2.41	0.54
1:D:90:LEU:HB3	1:D:127:HIS:HB2	1.89	0.54
1:D:170:ILE:CG2	1:D:199:VAL:HG11	2.21	0.54
1:D:223:VAL:O	1:D:227:GLU:HB2	2.07	0.54
1:A:596:TYR:O	1:A:599:ALA:HB3	2.08	0.54
1:B:88:GLU:HG3	1:B:95:LYS:O	2.07	0.54
1:A:30:LEU:O	1:A:34:LEU:HD22	2.07	0.54
1:A:174:ASN:CB	1:A:298:ARG:HH22	2.19	0.54
1:A:223:VAL:O	1:A:225:ILE:N	2.39	0.54
1:B:268:THR:O	1:B:270:GLU:N	2.41	0.54
1:D:70:ARG:HH21	1:D:126:ILE:HD13	1.71	0.54
1:D:298:ARG:HG3	1:D:298:ARG:HH11	1.73	0.54
1:A:23:ASP:O	1:A:25:SER:N	2.41	0.54
1:A:157:SER:O	1:A:158:ILE:C	2.51	0.54
1:B:216:MET:HE2	1:B:221:ASP:O	2.08	0.54
1:C:52:GLU:N	3:C:636:HOH:O	2.41	0.54
1:C:148:LYS:HB3	1:C:148:LYS:HZ2	1.73	0.54
1:D:227:GLU:HB3	1:D:229:ARG:HD2	1.90	0.54
1:B:124:VAL:HB	3:B:679:HOH:O	2.06	0.54
1:B:276:ASN:OD1	1:B:277:LYS:HG2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:LYS:HG2	1:C:100:PHE:CD1	2.43	0.54
1:A:176:ILE:HG21	1:A:207:PHE:HE2	1.73	0.54
1:A:221:ASP:OD1	1:A:221:ASP:C	2.50	0.54
1:B:299:ILE:O	1:B:302:ILE:HB	2.08	0.54
1:C:148:LYS:HE2	1:D:148:LYS:CE	2.38	0.54
1:C:148:LYS:CG	1:D:189:THR:HA	2.38	0.54
1:D:34:LEU:O	1:D:35:PRO:C	2.42	0.54
1:D:39:VAL:CG2	1:D:142:ASP:HA	2.37	0.54
1:B:261:GLU:O	1:B:262:ARG:C	2.51	0.54
1:C:260:ARG:HD2	1:C:260:ARG:C	2.32	0.54
1:C:302:ILE:HA	1:C:600:GLN:HE21	1.73	0.54
1:A:34:LEU:HG	1:A:172:LYS:HZ1	1.73	0.54
1:A:206:THR:HG22	1:A:206:THR:O	2.06	0.54
1:B:43:GLN:O	1:B:44:SER:HB2	2.07	0.54
1:B:190:SER:HB3	1:B:193:ILE:HB	1.89	0.54
1:B:22:GLY:HA3	1:B:27:LEU:HD12	1.90	0.53
1:C:109:ASP:HA	1:C:112:ASP:HB2	1.90	0.53
1:C:148:LYS:HE2	1:D:148:LYS:NZ	2.24	0.53
1:A:27:LEU:H	1:A:28:PRO:CD	2.21	0.53
1:A:97:PHE:HD2	1:A:103:VAL:HG22	1.73	0.53
1:A:160:LYS:HA	1:A:163:GLU:HG2	1.89	0.53
1:B:99:ASP:O	1:B:102:ALA:HB3	2.08	0.53
1:B:222:ALA:O	1:B:223:VAL:C	2.51	0.53
1:C:6:SER:HB2	1:C:77:GLN:HE21	1.70	0.53
1:C:223:VAL:HG13	1:C:224:GLU:N	2.22	0.53
1:C:256:ALA:O	1:C:257:ALA:C	2.52	0.53
1:C:305:LEU:C	1:C:307:ASN:N	2.56	0.53
1:D:70:ARG:HH21	1:D:126:ILE:CD1	2.21	0.53
1:D:289:LYS:O	1:D:293:ARG:HB3	2.09	0.53
1:A:265:PHE:O	1:A:272:ARG:HA	2.08	0.53
1:B:217:ASP:O	1:B:218:LYS:C	2.52	0.53
1:C:89:PHE:CE2	1:C:91:HIS:HB2	2.44	0.53
1:C:224:GLU:HB3	1:C:229:ARG:NH1	2.23	0.53
1:D:59:PHE:HD1	1:D:107:ILE:CD1	2.22	0.53
1:A:205:ARG:O	1:A:206:THR:CB	2.56	0.53
1:D:36:ALA:CB	3:D:656:HOH:O	2.55	0.53
1:D:264:TYR:C	1:D:264:TYR:CD1	2.86	0.53
1:B:209:VAL:HA	1:B:238:VAL:O	2.08	0.53
1:D:6:SER:HA	1:D:9:ASN:HB2	1.90	0.53
1:D:43:GLN:HG3	1:D:147:THR:HG22	1.90	0.53
1:D:47:LYS:HB3	2:D:9001:GDP:O1B	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:LEU:HB3	3:A:664:HOH:O	2.08	0.53
1:A:91:HIS:CE1	1:A:106:GLU:OE2	2.61	0.53
1:B:5:ILE:HG21	1:B:137:ASN:HB2	1.89	0.53
1:B:187:LEU:C	1:B:189:THR:H	2.16	0.53
1:B:294:VAL:O	1:B:297:SER:HB3	2.08	0.53
1:C:170:ILE:HG23	1:C:177:ILE:HD11	1.90	0.53
1:C:205:ARG:O	1:C:205:ARG:HG3	2.08	0.53
1:C:308:LYS:HE2	3:C:627:HOH:O	2.08	0.53
1:D:593:LEU:O	1:D:596:TYR:N	2.42	0.53
1:A:75:GLN:C	1:A:76:LEU:HD23	2.34	0.53
1:A:89:PHE:CD2	1:A:128:LEU:HB2	2.44	0.53
1:B:9:ASN:HD22	1:B:77:GLN:NE2	2.07	0.53
1:B:172:LYS:HG2	1:B:175:CYS:HB2	1.90	0.53
1:B:299:ILE:C	1:B:301:GLY:N	2.67	0.53
1:C:193:ILE:HA	1:C:196:SER:HB3	1.91	0.53
1:D:39:VAL:HG12	1:D:178:LEU:HD23	1.89	0.53
1:D:191:ASP:O	1:D:192:ALA:C	2.50	0.53
1:D:246:ALA:O	1:D:249:ASN:HB2	2.09	0.53
1:D:600:GLN:O	1:D:600:GLN:HG2	2.08	0.53
1:A:185:GLN:HE21	1:B:185:GLN:NE2	2.07	0.53
1:A:193:ILE:HA	1:A:196:SER:HB2	1.91	0.53
1:A:247:ASP:HB3	1:A:252:VAL:CG2	2.39	0.53
1:B:47:LYS:HG3	2:B:9001:GDP:O2B	2.09	0.53
1:B:207:PHE:CE1	1:B:235:TYR:CD1	2.97	0.53
1:B:313:LEU:HB3	1:B:597:ARG:HH21	1.73	0.53
1:C:9:ASN:O	3:C:351:HOH:O	2.18	0.53
1:C:11:ILE:O	1:C:14:ALA:N	2.41	0.53
1:D:193:ILE:O	1:D:194:LYS:C	2.51	0.53
1:A:187:LEU:C	1:A:189:THR:H	2.17	0.53
1:B:29:THR:HG21	1:B:596:TYR:CE1	2.44	0.53
1:B:583:MET:HA	1:B:586:ARG:CD	2.38	0.53
1:B:595:LEU:HD22	3:B:626:HOH:O	2.09	0.53
1:C:148:LYS:NZ	1:D:148:LYS:HZ1	2.07	0.53
1:C:253:ASP:OD2	1:C:255:ILE:HG12	2.09	0.53
1:D:82:GLY:O	1:D:84:ARG:CG	2.52	0.53
1:C:118:SER:C	1:C:119:LYS:HG2	2.33	0.52
1:D:34:LEU:O	1:D:36:ALA:N	2.42	0.52
1:D:296:LYS:O	1:D:297:SER:C	2.53	0.52
1:A:312:GLU:N	1:A:315:THR:OG1	2.42	0.52
1:C:83:THR:CG2	1:C:133:PRO:HG2	2.29	0.52
1:D:204:ASP:N	1:D:234:LYS:HD2	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:605:ALA:O	1:D:606:VAL:C	2.51	0.52
1:A:58:ASP:O	1:A:59:PHE:CB	2.57	0.52
1:A:59:PHE:C	1:A:104:ARG:HG3	2.34	0.52
1:B:118:SER:C	1:B:119:LYS:HG2	2.34	0.52
1:B:586:ARG:O	1:B:588:ALA:N	2.42	0.52
1:C:49:SER:CB	1:C:242:ASN:HD22	2.22	0.52
1:A:194:LYS:O	1:A:198:GLU:HG2	2.10	0.52
1:B:291:LEU:O	1:B:292:GLU:C	2.52	0.52
1:C:298:ARG:HB2	1:C:298:ARG:NH1	2.09	0.52
1:C:302:ILE:C	1:C:304:SER:N	2.68	0.52
1:D:71:PRO:O	1:D:125:PRO:HA	2.08	0.52
1:D:271:TYR:O	1:D:273:HIS:N	2.42	0.52
1:A:226:LEU:HB2	1:A:274:LEU:HD13	1.92	0.52
1:A:260:ARG:HG3	1:A:260:ARG:HH11	1.74	0.52
1:C:53:SER:HB3	1:C:280:SER:CB	2.40	0.52
1:C:599:ALA:O	1:C:603:ILE:HG12	2.09	0.52
1:D:23:ASP:CG	1:D:592:ARG:HB3	2.35	0.52
1:A:3:ASN:HA	1:A:137:ASN:HD21	1.75	0.52
1:B:8:VAL:O	1:B:9:ASN:C	2.53	0.52
1:B:302:ILE:HG22	1:B:303:GLN:NE2	2.24	0.52
1:C:52:GLU:C	1:C:254:MET:HE2	2.35	0.52
1:C:54:ILE:N	3:C:636:HOH:O	2.41	0.52
1:D:15:CYS:C	1:D:17:ALA:N	2.68	0.52
1:A:56:GLY:O	1:A:57:LYS:HD2	2.10	0.52
1:A:217:ASP:CG	1:A:218:LYS:H	2.17	0.52
1:B:301:GLY:HA3	3:B:708:HOH:O	2.09	0.52
1:C:77:GLN:O	1:C:131:TYR:HA	2.10	0.52
1:C:301:GLY:HA3	3:C:635:HOH:O	2.10	0.52
1:D:255:ILE:HD12	1:D:259:LYS:HZ3	1.74	0.52
1:A:47:LYS:HA	1:A:180:ILE:CD1	2.40	0.52
1:A:47:LYS:O	1:A:48:SER:C	2.53	0.52
1:A:50:VAL:O	1:A:54:ILE:HB	2.09	0.52
1:B:601:SER:HA	1:B:604:ASP:HB2	1.91	0.52
1:C:37:ILE:CG2	1:C:140:LEU:HG	2.39	0.52
1:C:111:THR:HG22	1:C:111:THR:O	2.10	0.52
1:D:170:ILE:HD12	1:D:177:ILE:HG12	1.92	0.52
1:D:309:THR:CA	1:D:312:GLU:HB2	2.35	0.52
1:A:42:GLY:HA2	1:A:146:LEU:CB	2.38	0.52
1:B:233:LEU:HD23	1:B:237:TRP:NE1	2.24	0.52
1:D:31:TRP:HZ3	1:D:171:GLU:O	1.92	0.52
1:B:226:LEU:C	1:B:228:GLY:H	2.19	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:GLY:C	1:C:281:GLU:N	2.68	0.52
1:D:166:VAL:HG12	1:D:166:VAL:O	2.08	0.52
1:D:298:ARG:HG3	1:D:298:ARG:NH1	2.25	0.52
1:A:124:VAL:O	1:A:125:PRO:O	2.28	0.51
1:A:299:ILE:C	1:A:301:GLY:N	2.66	0.51
1:A:301:GLY:O	1:A:305:LEU:CB	2.49	0.51
1:A:313:LEU:HD13	1:A:314:GLU:HG3	1.92	0.51
1:B:40:VAL:O	1:B:40:VAL:HG12	2.09	0.51
1:B:272:ARG:HB3	3:B:688:HOH:O	2.09	0.51
1:C:52:GLU:OE2	1:C:60:LEU:HB2	2.11	0.51
1:C:263:GLU:O	1:C:264:TYR:C	2.53	0.51
1:D:31:TRP:CE3	1:D:172:LYS:HG2	2.45	0.51
1:D:76:LEU:CD2	1:D:130:ILE:HB	2.40	0.51
1:D:170:ILE:HG22	1:D:199:VAL:CG1	2.19	0.51
1:A:52:GLU:O	1:A:254:MET:HE2	2.10	0.51
1:A:244:SER:HB3	1:A:247:ASP:OD2	2.11	0.51
1:A:296:LYS:O	1:A:298:ARG:N	2.43	0.51
1:C:50:VAL:HG11	1:C:240:VAL:HG21	1.93	0.51
1:D:288:SER:N	3:D:636:HOH:O	2.43	0.51
1:D:307:ASN:HA	1:D:310:VAL:CG1	2.39	0.51
1:C:203:GLY:O	1:C:204:ASP:C	2.53	0.51
1:D:37:ILE:CD1	1:D:176:ILE:HD13	2.40	0.51
1:D:187:LEU:HB2	1:D:231:PHE:CE2	2.45	0.51
1:D:192:ALA:CB	1:D:193:ILE:HD12	2.40	0.51
1:D:309:THR:HA	1:D:312:GLU:HG2	1.92	0.51
1:A:58:ASP:O	1:A:59:PHE:HB3	2.10	0.51
1:C:37:ILE:HG21	1:C:140:LEU:HG	1.92	0.51
1:C:200:ASP:N	1:C:201:PRO:HD3	2.24	0.51
1:C:308:LYS:CE	3:C:627:HOH:O	2.58	0.51
1:D:231:PHE:O	1:D:237:TRP:NE1	2.43	0.51
1:B:85:GLU:O	1:B:86:TYR:O	2.28	0.51
1:B:254:MET:O	1:B:257:ALA:N	2.25	0.51
1:C:51:LEU:HG	3:C:634:HOH:O	2.10	0.51
1:C:189:THR:C	1:D:148:LYS:HD3	2.35	0.51
1:C:309:THR:O	1:C:313:LEU:HG	2.10	0.51
1:D:37:ILE:CG2	1:D:176:ILE:HB	2.40	0.51
1:D:163:GLU:O	1:D:167:ARG:HG3	2.10	0.51
1:D:244:SER:C	1:D:246:ALA:H	2.18	0.51
2:D:9001:GDP:O2B	3:D:668:HOH:O	2.19	0.51
1:A:54:ILE:HG23	1:A:54:ILE:O	2.08	0.51
1:A:143:LEU:HD13	1:A:166:VAL:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:MET:HG2	1:C:166:VAL:N	2.26	0.51
1:C:183:ALA:O	1:C:216:MET:HG2	2.10	0.51
1:C:279:GLY:C	1:C:281:GLU:H	2.19	0.51
1:A:182:PRO:HA	1:A:211:THR:O	2.09	0.51
1:C:100:PHE:C	1:C:102:ALA:N	2.69	0.51
1:C:309:THR:HB	1:C:313:LEU:HD23	1.92	0.51
1:D:12:GLN:O	1:D:13:ARG:C	2.54	0.51
1:D:213:ILE:O	1:D:216:MET:HB3	2.11	0.51
1:A:27:LEU:H	1:A:28:PRO:HD2	1.75	0.51
1:B:79:ILE:HG12	1:B:132:SER:C	2.35	0.51
1:B:196:SER:C	1:B:198:GLU:N	2.67	0.51
1:B:277:LYS:O	1:B:282:HIS:CE1	2.64	0.51
1:D:90:LEU:O	1:D:93:PRO:HD3	2.10	0.51
1:D:256:ALA:HA	1:D:259:LYS:CB	2.34	0.51
1:D:302:ILE:HG13	1:D:600:GLN:HE21	1.75	0.51
1:A:238:VAL:CG1	1:A:283:LEU:HD13	2.35	0.51
1:C:34:LEU:O	1:C:35:PRO:C	2.50	0.51
1:C:54:ILE:HB	3:C:636:HOH:O	2.10	0.51
1:A:299:ILE:HD12	1:A:300:PRO:HD3	1.92	0.51
1:A:589:ILE:HA	1:A:592:ARG:HB2	1.93	0.51
1:B:215:LEU:CD1	2:B:9001:GDP:C2	2.87	0.51
1:C:235:TYR:O	1:C:236:PRO:O	2.29	0.51
1:D:23:ASP:H	1:D:26:ALA:HB3	1.75	0.51
1:A:134:ASN:ND2	1:A:134:ASN:N	2.59	0.50
1:A:189:THR:HA	1:B:148:LYS:CG	2.42	0.50
1:B:21:HIS:CD2	1:B:592:ARG:NH2	2.79	0.50
1:B:313:LEU:CD2	1:B:597:ARG:HH22	2.08	0.50
1:B:593:LEU:N	1:B:593:LEU:HD23	2.26	0.50
1:C:3:ASN:HA	1:C:6:SER:HB3	1.93	0.50
1:C:12:GLN:HB3	1:C:75:GLN:NE2	2.26	0.50
1:C:184:ASN:OD1	1:C:184:ASN:N	2.44	0.50
1:D:76:LEU:HB2	1:D:138:LEU:O	2.11	0.50
1:D:258:ARG:O	1:D:260:ARG:N	2.44	0.50
1:D:302:ILE:HD11	1:D:600:GLN:HE21	1.76	0.50
1:B:92:LEU:CD1	1:B:95:LYS:HB3	2.28	0.50
1:C:600:GLN:HA	1:C:603:ILE:CD1	2.42	0.50
1:D:253:ASP:OD2	1:D:255:ILE:HG13	2.10	0.50
1:A:170:ILE:HG23	1:A:177:ILE:HD11	1.92	0.50
1:A:207:PHE:N	1:A:207:PHE:HD2	2.09	0.50
1:C:77:GLN:HE22	1:C:137:ASN:HD21	1.57	0.50
1:C:226:LEU:CD2	1:C:278:MET:SD	2.99	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ILE:HA	1:A:209:VAL:HB	1.92	0.50
1:B:34:LEU:HD12	1:B:172:LYS:HE3	1.93	0.50
1:B:108:GLN:O	1:B:108:GLN:HG2	2.11	0.50
1:B:593:LEU:O	1:B:595:LEU:N	2.44	0.50
1:D:34:LEU:HG	1:D:172:LYS:NZ	2.26	0.50
1:D:195:ILE:HG22	1:D:195:ILE:O	2.11	0.50
1:A:47:LYS:HB3	1:A:180:ILE:HD12	1.93	0.50
1:A:251:ASN:O	1:A:252:VAL:C	2.55	0.50
1:B:77:GLN:HG3	1:B:131:TYR:CE1	2.46	0.50
1:C:86:TYR:HD1	1:C:96:LYS:HB3	1.75	0.50
1:D:594:GLU:O	1:D:595:LEU:C	2.55	0.50
1:A:23:ASP:HB2	1:A:26:ALA:CB	2.29	0.50
1:B:66:ILE:CG1	1:B:67:VAL:N	2.75	0.50
1:D:69:ARG:CB	1:D:121:ILE:HG22	2.39	0.50
1:D:204:ASP:HA	1:D:234:LYS:HE2	1.92	0.50
1:A:30:LEU:O	1:A:34:LEU:CD2	2.59	0.50
1:A:214:ASP:OD2	1:A:214:ASP:N	2.41	0.50
1:B:243:ARG:HG2	1:B:260:ARG:NH1	2.26	0.50
1:B:586:ARG:C	1:B:588:ALA:N	2.70	0.50
1:C:257:ALA:O	1:C:260:ARG:N	2.44	0.50
1:A:245:GLN:OE1	1:A:248:ILE:HD11	2.11	0.50
1:B:93:PRO:O	1:B:94:ARG:C	2.55	0.50
1:B:211:THR:O	1:B:212:LYS:O	2.29	0.50
1:C:100:PHE:HA	1:C:103:VAL:HG23	1.94	0.50
1:C:276:ASN:N	3:C:662:HOH:O	2.43	0.50
1:C:295:ILE:C	1:C:297:SER:H	2.20	0.50
1:A:49:SER:O	1:A:52:GLU:N	2.44	0.50
1:A:186:ASP:OD1	1:A:187:LEU:N	2.45	0.50
1:B:32:ASP:C	1:B:34:LEU:N	2.67	0.50
1:B:75:GLN:NE2	3:B:655:HOH:O	2.32	0.50
1:B:86:TYR:HA	1:B:97:PHE:O	2.12	0.50
1:B:90:LEU:C	1:B:92:LEU:N	2.69	0.50
1:B:190:SER:OG	1:B:192:ALA:HB3	2.12	0.50
1:C:132:SER:CB	1:C:135:VAL:HG13	2.41	0.50
1:D:9:ASN:OD1	1:D:75:GLN:HG2	2.11	0.50
1:A:69:ARG:HD3	1:A:119:LYS:HB3	1.92	0.49
1:B:196:SER:O	1:B:198:GLU:N	2.45	0.49
1:B:238:VAL:HG11	1:B:283:LEU:HD13	1.94	0.49
1:C:46:GLY:HA3	1:C:211:THR:HG21	1.94	0.49
1:C:142:ASP:OD2	1:C:143:LEU:N	2.45	0.49
1:D:37:ILE:N	1:D:37:ILE:HD13	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:ILE:CG2	1:D:177:ILE:CD1	2.89	0.49
1:D:236:PRO:HG2	1:D:238:VAL:CG2	2.42	0.49
1:D:286:MET:O	1:D:290:HIS:HD2	1.94	0.49
1:B:11:ILE:O	1:B:14:ALA:N	2.42	0.49
1:C:3:ASN:C	1:C:6:SER:OG	2.55	0.49
1:C:124:VAL:O	1:C:125:PRO:O	2.30	0.49
1:C:162:ILE:C	1:C:164:ASN:N	2.69	0.49
1:D:23:ASP:OD2	1:D:592:ARG:HB3	2.12	0.49
1:D:250:LYS:O	1:D:251:ASN:C	2.55	0.49
1:A:200:ASP:C	1:A:202:SER:N	2.70	0.49
1:A:308:LYS:HG3	3:A:650:HOH:O	2.12	0.49
1:C:48:SER:HB3	1:C:60:LEU:HD13	1.93	0.49
1:C:66:ILE:HG23	1:C:66:ILE:O	2.12	0.49
1:C:309:THR:OG1	3:C:675:HOH:O	2.18	0.49
1:D:226:LEU:C	1:D:228:GLY:N	2.70	0.49
1:D:309:THR:HA	1:D:312:GLU:CB	2.37	0.49
1:D:603:ILE:O	1:D:606:VAL:HB	2.12	0.49
1:B:257:ALA:C	1:B:260:ARG:HG2	2.38	0.49
1:C:27:LEU:N	1:C:28:PRO:HD2	2.26	0.49
1:C:273:HIS:ND1	3:C:668:HOH:O	2.35	0.49
1:C:316:GLU:HA	3:C:684:HOH:O	2.13	0.49
1:D:311:LEU:O	1:D:315:THR:HG23	2.12	0.49
1:A:5:ILE:HD13	1:A:137:ASN:O	2.12	0.49
1:A:187:LEU:HB2	1:A:231:PHE:CD2	2.47	0.49
1:A:207:PHE:CE1	1:A:235:TYR:CD1	3.00	0.49
1:C:258:ARG:O	1:C:259:LYS:C	2.55	0.49
1:D:277:LYS:O	1:D:282:HIS:CE1	2.66	0.49
1:D:604:ASP:O	1:D:605:ALA:C	2.55	0.49
1:A:28:PRO:HB3	1:A:308:LYS:NZ	2.27	0.49
1:A:593:LEU:O	1:A:594:GLU:C	2.56	0.49
1:B:118:SER:O	1:B:119:LYS:HG2	2.13	0.49
1:B:143:LEU:HD21	1:B:169:TYR:HE2	1.75	0.49
1:B:154:GLN:O	1:B:155:SER:C	2.56	0.49
1:B:282:HIS:CG	1:B:282:HIS:O	2.66	0.49
1:C:128:LEU:HD12	1:C:128:LEU:O	2.12	0.49
1:D:47:LYS:HZ2	1:D:145:GLY:N	2.10	0.49
1:D:56:GLY:O	1:D:57:LYS:HB2	2.12	0.49
1:A:224:GLU:CG	1:A:229:ARG:NH1	2.71	0.49
1:A:235:TYR:CB	1:A:236:PRO:CD	2.91	0.49
1:B:12:GLN:HA	1:B:15:CYS:SG	2.53	0.49
1:B:305:LEU:O	1:B:306:ILE:C	2.56	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:ILE:O	1:C:79:ILE:HD12	2.12	0.49
1:C:82:GLY:O	1:C:84:ARG:HG3	2.12	0.49
1:C:148:LYS:NZ	1:D:148:LYS:NZ	2.60	0.49
1:C:312:GLU:O	1:C:314:GLU:N	2.46	0.49
1:D:28:PRO:HA	1:D:31:TRP:HB2	1.95	0.49
1:D:70:ARG:NH2	1:D:126:ILE:HD13	2.28	0.49
1:D:250:LYS:O	1:D:252:VAL:N	2.46	0.49
1:D:256:ALA:O	1:D:257:ALA:C	2.54	0.49
1:D:305:LEU:O	1:D:307:ASN:N	2.45	0.49
1:D:589:ILE:HA	1:D:592:ARG:HG3	1.93	0.49
1:B:90:LEU:C	1:B:92:LEU:H	2.20	0.49
1:B:124:VAL:CG1	1:B:125:PRO:HD2	2.34	0.49
1:C:302:ILE:HG12	1:C:600:GLN:HG3	1.95	0.49
1:D:27:LEU:N	1:D:28:PRO:CD	2.75	0.49
1:D:41:GLY:HA3	1:D:180:ILE:HG12	1.94	0.49
1:D:247:ASP:O	1:D:248:ILE:C	2.56	0.49
1:A:23:ASP:HB3	1:A:592:ARG:CD	2.43	0.49
1:A:167:ARG:O	1:A:171:GLU:HG3	2.13	0.49
1:A:272:ARG:HG3	1:A:272:ARG:NH1	2.27	0.49
1:B:158:ILE:HG23	1:B:159:VAL:H	1.78	0.49
1:D:136:VAL:HB	1:D:138:LEU:CD1	2.43	0.49
1:A:55:VAL:HG11	1:A:59:PHE:HE2	1.75	0.49
1:A:158:ILE:HG22	1:A:159:VAL:N	2.27	0.49
1:B:300:PRO:C	1:B:302:ILE:H	2.21	0.49
1:C:296:LYS:HA	1:C:299:ILE:HD13	1.95	0.49
1:A:31:TRP:CE3	1:A:172:LYS:HD3	2.46	0.48
1:A:51:LEU:HA	1:A:54:ILE:CG2	2.43	0.48
1:D:255:ILE:O	1:D:259:LYS:HB2	2.12	0.48
1:A:189:THR:HA	1:B:148:LYS:HG3	1.96	0.48
1:B:62:ARG:HD2	1:B:62:ARG:HA	1.47	0.48
1:C:39:VAL:HG12	1:C:178:LEU:HD23	1.95	0.48
1:C:228:GLY:O	1:C:232:LYS:HE2	2.13	0.48
1:D:23:ASP:CG	1:D:26:ALA:HB2	2.38	0.48
1:D:35:PRO:HG3	1:D:174:ASN:HB3	1.95	0.48
1:A:296:LYS:HZ1	1:C:303:GLN:NE2	2.11	0.48
1:B:27:LEU:N	1:B:28:PRO:CD	2.77	0.48
1:B:42:GLY:O	1:B:43:GLN:C	2.54	0.48
1:B:89:PHE:HB3	1:B:91:HIS:HB3	1.95	0.48
1:B:233:LEU:HB3	1:B:234:LYS:H	1.44	0.48
1:B:257:ALA:CA	1:B:260:ARG:HD2	2.42	0.48
1:C:186:ASP:O	1:C:187:LEU:C	2.55	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:THR:O	1:C:313:LEU:N	2.46	0.48
1:D:80:ASP:C	1:D:82:GLY:N	2.72	0.48
1:D:597:ARG:O	1:D:598:ALA:O	2.31	0.48
1:A:224:GLU:C	1:A:225:ILE:HG12	2.34	0.48
1:B:42:GLY:HA2	1:B:146:LEU:HB2	1.94	0.48
1:C:301:GLY:O	1:C:305:LEU:HD12	2.13	0.48
1:D:15:CYS:SG	3:D:625:HOH:O	2.60	0.48
1:A:149:VAL:HB	1:B:188:ALA:HA	1.96	0.48
1:B:586:ARG:N	1:B:586:ARG:HD2	2.29	0.48
1:C:263:GLU:O	1:C:265:PHE:N	2.47	0.48
1:C:310:VAL:HA	1:C:313:LEU:HG	1.96	0.48
1:A:34:LEU:HG	1:A:172:LYS:NZ	2.28	0.48
1:A:224:GLU:HG3	1:A:229:ARG:HH12	1.72	0.48
1:A:299:ILE:C	1:A:299:ILE:HD12	2.37	0.48
1:C:5:ILE:HG21	1:C:138:LEU:HA	1.95	0.48
1:D:262:ARG:O	1:D:263:GLU:C	2.56	0.48
1:A:100:PHE:HZ	1:A:130:ILE:HG21	1.77	0.48
1:A:151:VAL:O	1:A:152:ASP:HB3	2.14	0.48
1:B:119:LYS:CB	1:B:154:GLN:HE21	2.27	0.48
1:B:138:LEU:HD21	1:B:288:SER:HB2	1.95	0.48
1:C:276:ASN:OD1	1:C:277:LYS:N	2.47	0.48
1:D:91:HIS:HE2	1:D:110:GLU:CD	2.21	0.48
1:A:83:THR:HA	1:A:133:PRO:HG3	1.95	0.48
1:A:238:VAL:HG12	1:A:238:VAL:O	2.13	0.48
1:B:90:LEU:O	1:B:92:LEU:N	2.47	0.48
1:B:105:LYS:HG3	1:B:109:ASP:OD2	2.13	0.48
1:B:606:VAL:HA	3:B:676:HOH:O	2.13	0.48
1:D:302:ILE:C	1:D:305:LEU:H	2.22	0.48
1:A:89:PHE:HB3	1:A:91:HIS:HB3	1.95	0.48
1:A:252:VAL:HG12	1:A:253:ASP:O	2.14	0.48
1:B:59:PHE:C	1:B:104:ARG:HB2	2.39	0.48
1:B:168:SER:O	1:B:169:TYR:C	2.54	0.48
1:B:199:VAL:HG23	1:B:200:ASP:N	2.28	0.48
1:C:47:LYS:C	1:C:49:SER:H	2.22	0.48
1:C:130:ILE:HG22	1:C:131:TYR:H	1.77	0.48
1:C:593:LEU:O	1:C:595:LEU:N	2.47	0.48
1:A:302:ILE:HA	1:A:305:LEU:CB	2.40	0.48
1:B:311:LEU:C	3:B:656:HOH:O	2.56	0.48
1:C:91:HIS:NE2	1:C:110:GLU:CD	2.72	0.48
1:A:296:LYS:C	1:A:298:ARG:N	2.70	0.47
1:C:47:LYS:C	1:C:49:SER:N	2.69	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:277:LYS:C	1:C:282:HIS:CE1	2.92	0.47
1:A:18:LEU:CD1	1:A:595:LEU:HG	2.44	0.47
1:A:66:ILE:HG23	1:A:119:LYS:HD2	1.95	0.47
1:A:82:GLY:O	1:A:84:ARG:HG3	2.14	0.47
1:A:172:LYS:CE	1:A:175:CYS:HB3	2.35	0.47
1:C:187:LEU:C	1:C:189:THR:H	2.21	0.47
1:D:8:VAL:O	1:D:11:ILE:HB	2.13	0.47
1:D:57:LYS:HE2	1:D:100:PHE:CD1	2.49	0.47
1:D:170:ILE:HG23	1:D:177:ILE:HD11	1.95	0.47
1:A:128:LEU:CD1	1:A:130:ILE:HG12	2.45	0.47
1:B:15:CYS:C	1:B:17:ALA:N	2.71	0.47
1:B:54:ILE:HG22	1:B:54:ILE:O	2.14	0.47
1:B:180:ILE:HD12	1:B:180:ILE:H	1.79	0.47
1:C:56:GLY:O	1:C:254:MET:HG3	2.14	0.47
1:C:591:LYS:O	1:C:595:LEU:HD12	2.14	0.47
1:D:124:VAL:O	1:D:125:PRO:O	2.32	0.47
1:D:222:ALA:C	1:D:224:GLU:H	2.21	0.47
1:A:176:ILE:HG21	1:A:207:PHE:CE2	2.49	0.47
1:A:200:ASP:OD2	1:A:205:ARG:O	2.32	0.47
1:B:244:SER:HB3	2:B:9001:GDP:HN22	1.78	0.47
1:B:313:LEU:HD23	1:B:597:ARG:HH21	1.65	0.47
1:D:137:ASN:HA	3:D:655:HOH:O	2.15	0.47
1:D:222:ALA:C	1:D:224:GLU:N	2.68	0.47
1:D:302:ILE:CD1	1:D:600:GLN:HE21	2.27	0.47
1:D:597:ARG:HG3	1:D:597:ARG:HH11	1.78	0.47
1:D:599:ALA:C	1:D:601:SER:N	2.73	0.47
1:A:72:LEU:HB3	1:A:142:ASP:HB3	1.95	0.47
1:A:143:LEU:CD2	1:A:169:TYR:HD2	2.24	0.47
1:B:243:ARG:HB3	1:B:247:ASP:HB2	1.96	0.47
1:B:256:ALA:O	1:B:257:ALA:O	2.33	0.47
1:B:295:ILE:C	1:B:297:SER:N	2.72	0.47
1:D:99:ASP:OD2	1:D:102:ALA:HB2	2.14	0.47
1:D:299:ILE:CB	1:D:300:PRO:HD3	2.44	0.47
1:A:8:VAL:O	1:A:11:ILE:HB	2.15	0.47
1:A:92:LEU:CD1	1:A:95:LYS:HE3	2.30	0.47
1:A:113:ARG:C	1:A:114:GLU:HG3	2.40	0.47
1:B:200:ASP:OD2	1:B:205:ARG:HG2	2.14	0.47
1:B:315:THR:HG21	1:B:589:ILE:HD13	1.96	0.47
1:C:246:ALA:O	1:C:250:LYS:HG3	2.15	0.47
1:A:43:GLN:H	1:A:146:LEU:N	2.12	0.47
1:A:233:LEU:HD12	1:A:233:LEU:HA	1.69	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:ILE:O	1:B:140:LEU:HA	2.15	0.47
1:B:52:GLU:HG3	1:B:60:LEU:HD12	1.96	0.47
1:B:59:PHE:CE1	1:B:60:LEU:HG	2.49	0.47
1:B:222:ALA:C	1:B:224:GLU:N	2.71	0.47
1:C:11:ILE:O	1:C:13:ARG:N	2.48	0.47
1:C:13:ARG:NE	3:C:351:HOH:O	2.47	0.47
1:C:100:PHE:O	1:C:101:ALA:C	2.58	0.47
1:D:8:VAL:CG2	1:D:295:ILE:HG21	2.45	0.47
1:D:57:LYS:O	1:D:59:PHE:HD2	1.97	0.47
1:D:143:LEU:HD23	1:D:143:LEU:HA	1.46	0.47
1:D:205:ARG:O	1:D:205:ARG:HG3	2.15	0.47
1:D:211:THR:O	1:D:212:LYS:HB2	2.15	0.47
1:D:265:PHE:CE2	1:D:278:MET:CE	2.97	0.47
1:A:39:VAL:HG23	1:A:180:ILE:HD11	1.96	0.47
1:B:283:LEU:O	1:B:284:ALA:C	2.56	0.47
1:C:6:SER:HB3	1:C:137:ASN:HD21	1.79	0.47
1:C:182:PRO:HB2	1:C:212:LYS:HD2	1.97	0.47
1:D:5:ILE:HD12	1:D:137:ASN:C	2.40	0.47
1:D:156:ASP:C	1:D:158:ILE:H	2.23	0.47
1:A:215:LEU:HD21	2:A:9001:GDP:C2	2.49	0.47
1:A:601:SER:HA	1:A:604:ASP:HB2	1.97	0.47
1:B:172:LYS:CG	1:B:175:CYS:HB2	2.44	0.47
1:D:146:LEU:HD12	1:D:191:ASP:HB3	1.96	0.47
1:D:271:TYR:O	1:D:272:ARG:C	2.57	0.47
1:A:23:ASP:O	1:A:24:SER:OG	2.30	0.47
1:A:44:SER:OG	1:B:186:ASP:HB2	2.14	0.47
1:A:47:LYS:HE3	1:A:143:LEU:O	2.14	0.47
1:A:90:LEU:HB3	3:A:646:HOH:O	2.14	0.47
1:B:33:SER:O	1:B:33:SER:OG	2.31	0.47
1:B:244:SER:O	1:B:245:GLN:C	2.58	0.47
1:C:140:LEU:HD23	1:C:141:ILE:N	2.30	0.47
1:D:285:LYS:N	3:D:660:HOH:O	2.48	0.47
1:D:307:ASN:O	1:D:311:LEU:HD23	2.15	0.47
1:C:187:LEU:C	1:C:189:THR:N	2.73	0.46
1:C:253:ASP:CG	1:C:254:MET:N	2.73	0.46
1:C:302:ILE:CG1	1:C:603:ILE:HD12	2.46	0.46
1:D:167:ARG:O	1:D:169:TYR:N	2.48	0.46
1:B:30:LEU:O	1:B:34:LEU:HB2	2.15	0.46
1:B:67:VAL:C	1:B:69:ARG:HD2	2.40	0.46
1:C:264:TYR:O	1:C:267:ASN:N	2.45	0.46
1:C:277:LYS:O	1:C:278:MET:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:80:ASP:O	1:D:81:ASP:C	2.57	0.46
1:D:118:SER:C	1:D:119:LYS:HG2	2.41	0.46
1:D:141:ILE:CD1	3:D:656:HOH:O	2.57	0.46
1:A:34:LEU:HD23	1:A:172:LYS:NZ	2.30	0.46
1:A:59:PHE:HD1	1:A:59:PHE:O	1.98	0.46
1:A:286:MET:HE1	1:C:604:ASP:HB2	1.96	0.46
1:A:301:GLY:O	1:A:305:LEU:N	2.48	0.46
1:B:13:ARG:CB	3:B:655:HOH:O	2.57	0.46
1:C:95:LYS:HG3	1:C:96:LYS:N	2.31	0.46
1:C:199:VAL:O	1:C:200:ASP:HB3	2.15	0.46
1:C:241:VAL:HG21	1:C:264:TYR:CE2	2.50	0.46
1:D:165:MET:O	1:D:167:ARG:N	2.48	0.46
1:D:258:ARG:O	1:D:259:LYS:C	2.58	0.46
1:D:278:MET:HE2	1:D:278:MET:HB2	1.59	0.46
1:A:6:SER:HB2	1:A:77:GLN:HE21	1.80	0.46
1:A:157:SER:C	1:A:159:VAL:N	2.70	0.46
1:B:249:ASN:C	1:B:251:ASN:N	2.74	0.46
1:C:57:LYS:HG2	1:C:100:PHE:HE1	1.79	0.46
1:C:103:VAL:O	1:C:107:ILE:HG12	2.15	0.46
1:C:130:ILE:CG2	1:C:131:TYR:N	2.77	0.46
1:C:593:LEU:C	1:C:595:LEU:H	2.23	0.46
1:A:33:SER:C	1:A:35:PRO:HD2	2.41	0.46
1:A:69:ARG:HD3	1:A:119:LYS:HA	1.97	0.46
1:B:154:GLN:HB3	1:B:158:ILE:HG21	1.96	0.46
1:C:28:PRO:O	1:C:32:ASP:CB	2.53	0.46
1:C:148:LYS:HZ1	1:D:148:LYS:NZ	2.13	0.46
1:A:59:PHE:CZ	1:A:74:LEU:HD21	2.51	0.46
1:A:69:ARG:CD	1:A:119:LYS:HA	2.46	0.46
1:A:80:ASP:C	1:A:82:GLY:H	2.24	0.46
1:A:213:ILE:O	1:A:216:MET:HB3	2.15	0.46
1:B:155:SER:OG	1:B:156:ASP:N	2.47	0.46
1:B:606:VAL:CG1	3:B:676:HOH:O	2.54	0.46
1:C:7:LEU:O	1:C:8:VAL:C	2.58	0.46
1:C:128:LEU:C	1:C:128:LEU:CD1	2.89	0.46
1:C:132:SER:HB3	1:C:135:VAL:CG1	2.44	0.46
1:C:178:LEU:HD12	1:C:178:LEU:HA	1.80	0.46
1:C:605:ALA:O	1:C:606:VAL:C	2.58	0.46
1:D:165:MET:C	1:D:167:ARG:N	2.74	0.46
1:A:55:VAL:HG11	1:A:59:PHE:CD2	2.51	0.46
1:A:62:ARG:HB2	1:A:62:ARG:HH11	1.80	0.46
1:A:191:ASP:HB2	3:A:649:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:VAL:O	1:B:107:ILE:HG13	2.15	0.46
1:B:159:VAL:HG12	1:B:160:LYS:HG3	1.97	0.46
1:B:261:GLU:O	1:B:265:PHE:N	2.48	0.46
1:C:233:LEU:HG	1:C:234:LYS:H	1.80	0.46
1:D:50:VAL:O	1:D:50:VAL:HG12	2.16	0.46
1:D:54:ILE:HG22	1:D:55:VAL:N	2.29	0.46
1:B:18:LEU:HD12	1:B:18:LEU:O	2.14	0.46
1:B:69:ARG:HD2	1:B:69:ARG:N	2.31	0.46
1:B:585:ARG:O	1:B:588:ALA:N	2.43	0.46
1:D:123:SER:HA	1:D:165:MET:HE1	1.97	0.46
1:A:118:SER:C	1:A:119:LYS:CG	2.89	0.46
1:A:183:ALA:HB1	1:A:216:MET:CE	2.45	0.46
1:B:52:GLU:CG	1:B:60:LEU:HD12	2.45	0.46
1:C:290:HIS:C	1:C:290:HIS:ND1	2.73	0.46
1:D:38:ALA:HA	1:D:141:ILE:HG13	1.98	0.46
1:D:151:VAL:HG22	1:D:152:ASP:OD2	2.16	0.46
1:B:5:ILE:CG2	1:B:6:SER:H	2.22	0.46
1:B:94:ARG:NH1	1:B:94:ARG:HB2	2.30	0.46
1:B:124:VAL:HG12	1:B:125:PRO:CD	2.33	0.46
1:C:301:GLY:C	1:C:305:LEU:HD12	2.40	0.46
1:C:312:GLU:O	1:C:313:LEU:C	2.59	0.46
1:D:34:LEU:N	1:D:35:PRO:HD3	2.30	0.46
1:D:136:VAL:HG23	1:D:284:ALA:HB1	1.96	0.46
1:A:79:ILE:HD11	1:A:132:SER:N	2.31	0.45
1:B:37:ILE:HD12	1:B:37:ILE:N	2.27	0.45
1:B:40:VAL:HG13	1:B:166:VAL:CG1	2.46	0.45
1:B:57:LYS:C	1:B:254:MET:HG3	2.41	0.45
1:C:34:LEU:N	1:C:35:PRO:CD	2.79	0.45
1:C:290:HIS:C	1:C:292:GLU:N	2.65	0.45
1:D:597:ARG:HH11	1:D:597:ARG:CG	2.29	0.45
1:A:234:LYS:CE	1:C:597:ARG:NH2	2.80	0.45
1:C:79:ILE:O	1:C:80:ASP:C	2.59	0.45
1:C:142:ASP:C	1:C:143:LEU:HG	2.42	0.45
1:C:606:VAL:HG12	1:C:606:VAL:O	2.16	0.45
1:D:43:GLN:HE21	1:D:43:GLN:HB3	1.49	0.45
1:D:89:PHE:HE2	1:D:128:LEU:HB2	1.79	0.45
1:A:76:LEU:HD23	1:A:76:LEU:N	2.31	0.45
1:A:195:ILE:HA	1:A:198:GLU:HG2	1.97	0.45
1:B:239:GLY:H	1:B:278:MET:CE	2.15	0.45
1:B:252:VAL:CG1	1:B:260:ARG:HH21	2.23	0.45
1:D:585:ARG:O	1:D:588:ALA:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:VAL:HA	1:A:178:LEU:HB3	1.97	0.45
1:A:79:ILE:HG13	1:A:133:PRO:N	2.32	0.45
1:A:164:ASN:O	1:A:165:MET:C	2.60	0.45
1:A:589:ILE:HG22	1:A:589:ILE:O	2.15	0.45
1:B:143:LEU:HD21	1:B:169:TYR:CD2	2.51	0.45
1:B:170:ILE:HG22	1:B:199:VAL:HG21	1.99	0.45
1:C:186:ASP:O	1:C:189:THR:N	2.47	0.45
1:C:216:MET:SD	1:C:222:ALA:HB2	2.55	0.45
1:D:99:ASP:O	1:D:102:ALA:HB3	2.16	0.45
1:B:39:VAL:HG23	1:B:180:ILE:HD11	1.98	0.45
1:B:67:VAL:O	1:B:69:ARG:HD2	2.15	0.45
1:B:284:ALA:O	1:B:285:LYS:C	2.60	0.45
1:C:30:LEU:C	1:C:32:ASP:N	2.75	0.45
1:D:187:LEU:C	1:D:189:THR:N	2.73	0.45
1:A:8:VAL:CG1	1:A:33:SER:O	2.64	0.45
1:A:174:ASN:CG	1:A:298:ARG:HH22	2.24	0.45
1:B:34:LEU:HA	1:B:34:LEU:HD22	1.44	0.45
1:B:245:GLN:O	1:B:246:ALA:C	2.59	0.45
1:C:78:LYS:HB2	1:C:135:VAL:O	2.16	0.45
1:D:47:LYS:NZ	1:D:145:GLY:H	2.15	0.45
1:D:598:ALA:O	1:D:601:SER:N	2.49	0.45
1:A:47:LYS:CA	1:A:180:ILE:HD12	2.47	0.45
1:A:68:THR:O	1:A:144:PRO:HB3	2.17	0.45
1:A:86:TYR:CZ	1:A:131:TYR:HD2	2.35	0.45
1:A:213:ILE:HG23	1:A:216:MET:CE	2.46	0.45
1:B:15:CYS:HB2	1:B:16:THR:H	1.46	0.45
1:B:170:ILE:HG21	1:B:199:VAL:HG21	1.96	0.45
1:B:283:LEU:HD12	1:B:283:LEU:HA	1.85	0.45
1:B:586:ARG:C	1:B:588:ALA:H	2.25	0.45
1:C:77:GLN:NE2	1:C:137:ASN:HD21	2.15	0.45
1:C:148:LYS:CE	1:D:148:LYS:NZ	2.80	0.45
1:C:283:LEU:HG	1:C:284:ALA:N	2.31	0.45
1:D:313:LEU:HD21	1:D:597:ARG:HH21	1.81	0.45
1:A:166:VAL:HG12	1:A:167:ARG:N	2.31	0.45
1:A:204:ASP:HA	1:A:234:LYS:NZ	2.32	0.45
1:B:16:THR:HG21	1:B:30:LEU:HD13	1.98	0.45
1:B:241:VAL:HG12	1:B:241:VAL:O	2.17	0.45
1:C:187:LEU:HA	1:C:187:LEU:HD12	1.71	0.45
1:C:225:ILE:HG22	1:C:225:ILE:O	2.17	0.45
1:D:74:LEU:N	1:D:140:LEU:O	2.47	0.45
1:A:95:LYS:HG2	1:A:96:LYS:H	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:SER:O	1:B:308:LYS:HD2	2.17	0.45
1:B:76:LEU:HD13	1:B:135:VAL:HB	1.98	0.45
1:B:593:LEU:O	1:B:596:TYR:N	2.41	0.45
1:C:86:TYR:HE1	1:C:96:LYS:CD	2.25	0.45
1:C:176:ILE:HD11	1:C:290:HIS:CE1	2.52	0.45
1:D:8:VAL:HG21	1:D:295:ILE:HG21	1.99	0.45
1:D:23:ASP:OD2	1:D:26:ALA:CB	2.63	0.45
1:D:73:VAL:HG12	3:D:653:HOH:O	2.17	0.45
1:A:218:LYS:C	1:A:220:THR:H	2.25	0.45
1:B:7:LEU:O	1:B:11:ILE:N	2.48	0.45
1:B:291:LEU:HD12	1:B:291:LEU:HA	1.52	0.45
1:C:89:PHE:CD2	1:C:91:HIS:CB	3.00	0.45
1:D:34:LEU:HG	1:D:172:LYS:HZ2	1.81	0.45
1:D:112:ASP:HA	1:D:115:THR:OG1	2.17	0.45
1:D:183:ALA:O	1:D:216:MET:HE3	2.17	0.45
1:D:290:HIS:O	1:D:294:VAL:HB	2.17	0.45
1:A:43:GLN:H	1:A:146:LEU:H	1.65	0.44
1:A:273:HIS:CD2	1:A:274:LEU:HD23	2.52	0.44
1:A:604:ASP:O	1:A:605:ALA:C	2.60	0.44
1:B:27:LEU:H	1:B:28:PRO:CD	2.30	0.44
1:B:264:TYR:CD1	1:B:264:TYR:C	2.94	0.44
1:C:9:ASN:C	1:C:11:ILE:N	2.75	0.44
1:D:186:ASP:O	1:D:187:LEU:HD13	2.17	0.44
1:A:195:ILE:HA	1:A:198:GLU:CG	2.47	0.44
1:A:261:GLU:O	1:A:265:PHE:CE1	2.71	0.44
1:B:586:ARG:O	1:B:587:SER:C	2.61	0.44
1:C:23:ASP:CG	1:C:26:ALA:HB2	2.42	0.44
1:C:140:LEU:HD23	1:C:140:LEU:C	2.43	0.44
1:C:260:ARG:C	1:C:260:ARG:CD	2.90	0.44
1:D:108:GLN:C	1:D:110:GLU:N	2.75	0.44
1:D:170:ILE:CG2	1:D:177:ILE:HD11	2.47	0.44
1:A:249:ASN:C	1:A:251:ASN:H	2.25	0.44
1:A:291:LEU:O	1:A:295:ILE:HG13	2.17	0.44
1:B:590:SER:C	1:B:592:ARG:N	2.75	0.44
1:C:23:ASP:HB2	1:C:24:SER:H	1.66	0.44
1:C:173:PRO:HB2	1:C:174:ASN:H	1.47	0.44
1:C:310:VAL:HG23	3:C:675:HOH:O	2.17	0.44
1:B:47:LYS:O	1:B:48:SER:C	2.61	0.44
1:C:23:ASP:H	1:C:26:ALA:HB2	1.83	0.44
1:C:187:LEU:HB2	3:C:666:HOH:O	2.17	0.44
1:C:264:TYR:HE1	1:C:268:THR:HG1	1.62	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:THR:CG2	1:D:125:PRO:HG2	2.47	0.44
1:D:274:LEU:CD2	1:D:277:LYS:NZ	2.80	0.44
1:D:596:TYR:O	1:D:597:ARG:C	2.59	0.44
1:C:79:ILE:O	1:C:81:ASP:N	2.51	0.44
1:C:98:THR:C	1:C:100:PHE:H	2.26	0.44
1:C:283:LEU:HD11	1:C:287:LEU:HD11	2.00	0.44
1:C:302:ILE:CD1	3:C:658:HOH:O	2.60	0.44
1:A:224:GLU:CG	1:A:229:ARG:HH12	2.31	0.44
1:B:172:LYS:O	1:B:174:ASN:N	2.50	0.44
1:B:212:LYS:HB3	1:B:215:LEU:CD1	2.37	0.44
1:B:315:THR:HG21	1:B:589:ILE:CD1	2.48	0.44
1:C:7:LEU:HD23	1:C:7:LEU:C	2.42	0.44
1:C:188:ALA:HA	1:D:149:VAL:HG23	1.98	0.44
1:D:59:PHE:O	1:D:104:ARG:HA	2.16	0.44
1:D:158:ILE:HD11	1:D:162:ILE:HD11	1.99	0.44
1:D:598:ALA:O	1:D:599:ALA:C	2.60	0.44
1:A:245:GLN:HA	1:A:248:ILE:HG12	1.98	0.44
1:B:7:LEU:HD23	1:B:7:LEU:C	2.42	0.44
1:B:41:GLY:O	1:B:47:LYS:HD3	2.18	0.44
1:B:165:MET:HE3	1:B:165:MET:HB2	1.92	0.44
1:D:168:SER:O	1:D:172:LYS:HE3	2.18	0.44
1:D:193:ILE:O	1:D:195:ILE:N	2.50	0.44
1:D:305:LEU:O	1:D:308:LYS:N	2.39	0.44
1:A:37:ILE:CD1	1:A:140:LEU:HD23	2.48	0.44
1:B:100:PHE:O	1:B:103:VAL:N	2.46	0.44
1:C:47:LYS:O	1:C:49:SER:N	2.51	0.44
1:C:171:GLU:HA	1:C:199:VAL:HG11	2.00	0.44
1:C:252:VAL:CG1	1:C:253:ASP:N	2.80	0.44
1:D:4:LEU:HD13	1:D:295:ILE:HB	1.99	0.44
1:D:86:TYR:HE1	1:D:96:LYS:HD3	1.78	0.44
1:D:245:GLN:HG3	1:D:245:GLN:O	2.18	0.44
1:A:62:ARG:HA	1:A:62:ARG:HD3	1.71	0.44
1:A:169:TYR:HD1	1:A:169:TYR:HA	1.75	0.44
1:B:250:LYS:H	1:B:250:LYS:HG2	1.45	0.44
1:B:312:GLU:C	1:B:314:GLU:N	2.74	0.44
1:C:167:ARG:O	1:C:170:ILE:N	2.43	0.44
1:C:585:ARG:C	1:C:587:SER:H	2.26	0.44
1:A:47:LYS:CB	1:A:180:ILE:HD12	2.48	0.43
1:A:187:LEU:C	1:A:189:THR:N	2.76	0.43
1:A:200:ASP:N	1:A:201:PRO:HD3	2.29	0.43
1:B:118:SER:C	1:B:119:LYS:CG	2.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:ASP:O	1:C:101:ALA:N	2.51	0.43
1:C:222:ALA:N	1:C:271:TYR:OH	2.48	0.43
1:D:199:VAL:HG12	1:D:200:ASP:N	2.30	0.43
1:D:227:GLU:OE2	1:D:274:LEU:HD11	2.18	0.43
1:D:310:VAL:O	1:D:310:VAL:HG13	2.18	0.43
1:A:212:LYS:CG	2:A:9001:GDP:C5	3.00	0.43
1:B:61:PRO:HB2	1:B:67:VAL:HB	2.00	0.43
1:B:222:ALA:O	1:B:224:GLU:N	2.51	0.43
1:C:51:LEU:HD23	1:C:51:LEU:HA	1.79	0.43
1:C:62:ARG:NE	3:C:667:HOH:O	2.50	0.43
1:C:313:LEU:HD12	1:C:314:GLU:HG3	2.00	0.43
1:C:600:GLN:HA	1:C:603:ILE:HD11	2.00	0.43
1:D:77:GLN:O	1:D:131:TYR:HA	2.18	0.43
1:D:245:GLN:O	1:D:249:ASN:OD1	2.36	0.43
1:A:71:PRO:O	1:A:72:LEU:HB2	2.16	0.43
1:A:203:GLY:O	1:A:234:LYS:HD3	2.18	0.43
1:A:603:ILE:O	1:A:604:ASP:C	2.61	0.43
1:C:235:TYR:HA	1:C:236:PRO:HD2	1.69	0.43
1:D:287:LEU:C	3:D:636:HOH:O	2.61	0.43
1:D:309:THR:C	1:D:312:GLU:H	2.26	0.43
1:A:181:SER:O	1:A:210:LEU:HA	2.18	0.43
1:B:50:VAL:O	1:B:53:SER:HB2	2.19	0.43
1:B:239:GLY:N	1:B:278:MET:HE1	2.12	0.43
1:C:151:VAL:O	1:C:152:ASP:HB2	2.17	0.43
1:D:62:ARG:HH21	1:D:248:ILE:HD11	1.82	0.43
1:D:309:THR:HA	1:D:312:GLU:CG	2.48	0.43
1:A:4:LEU:HB2	3:A:609:HOH:O	2.18	0.43
1:A:41:GLY:O	1:A:145:GLY:HA2	2.18	0.43
1:A:258:ARG:HE	1:A:281:GLU:HG3	1.84	0.43
1:B:199:VAL:O	1:B:201:PRO:HD3	2.19	0.43
1:D:92:LEU:CD1	1:D:106:GLU:OE2	2.67	0.43
1:D:227:GLU:OE2	1:D:274:LEU:HD21	2.18	0.43
1:A:258:ARG:C	1:A:260:ARG:H	2.25	0.43
1:A:291:LEU:O	1:A:294:VAL:HB	2.19	0.43
1:B:177:ILE:HB	1:B:206:THR:HG23	2.00	0.43
1:C:148:LYS:HG3	1:D:189:THR:C	2.43	0.43
1:C:160:LYS:O	1:C:164:ASN:CB	2.62	0.43
1:C:200:ASP:C	1:C:202:SER:H	2.26	0.43
1:C:203:GLY:O	1:C:206:THR:N	2.52	0.43
1:D:235:TYR:N	1:D:235:TYR:CD2	2.86	0.43
1:D:300:PRO:C	1:D:302:ILE:N	2.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:SER:O	1:A:60:LEU:HD13	2.18	0.43
1:A:149:VAL:O	1:A:151:VAL:HG12	2.18	0.43
1:A:598:ALA:O	1:A:602:GLU:HB2	2.18	0.43
1:B:5:ILE:O	1:B:8:VAL:N	2.51	0.43
1:B:298:ARG:O	1:B:301:GLY:N	2.48	0.43
1:C:149:VAL:HG11	1:D:193:ILE:HB	1.99	0.43
1:C:173:PRO:C	1:C:175:CYS:H	2.25	0.43
1:D:15:CYS:SG	1:D:595:LEU:HD11	2.58	0.43
1:D:117:ARG:HG3	1:D:117:ARG:HH11	1.82	0.43
1:A:99:ASP:O	1:A:99:ASP:OD2	2.36	0.43
1:A:143:LEU:HD12	1:A:166:VAL:HG22	2.00	0.43
1:A:588:ALA:HB1	1:A:592:ARG:HE	1.84	0.43
1:C:89:PHE:HB3	1:C:90:LEU:H	1.55	0.43
1:C:142:ASP:OD2	1:C:142:ASP:C	2.61	0.43
1:C:211:THR:O	1:C:212:LYS:C	2.61	0.43
1:C:278:MET:HB2	3:C:662:HOH:O	2.18	0.43
1:D:131:TYR:CB	3:D:640:HOH:O	2.56	0.43
1:A:4:LEU:N	3:A:609:HOH:O	2.39	0.43
1:B:226:LEU:C	1:B:228:GLY:N	2.75	0.43
1:B:287:LEU:O	1:B:290:HIS:N	2.50	0.43
1:C:66:ILE:O	1:C:69:ARG:NE	2.51	0.43
1:C:260:ARG:O	1:C:263:GLU:N	2.52	0.43
1:D:113:ARG:HG2	1:D:113:ARG:HH11	1.83	0.43
1:D:164:ASN:ND2	1:D:164:ASN:C	2.77	0.43
1:A:74:LEU:HA	1:A:74:LEU:HD12	1.77	0.43
1:A:74:LEU:HD11	1:A:128:LEU:CD2	2.49	0.43
1:A:588:ALA:C	1:A:592:ARG:HG3	2.43	0.43
1:B:39:VAL:HG23	1:B:180:ILE:CD1	2.49	0.43
1:B:103:VAL:HG12	1:B:104:ARG:N	2.34	0.43
1:B:244:SER:HB3	2:B:9001:GDP:N2	2.33	0.43
1:B:264:TYR:O	1:B:268:THR:OG1	2.36	0.43
1:C:105:LYS:O	1:C:109:ASP:HB2	2.19	0.43
1:C:597:ARG:O	1:C:600:GLN:N	2.52	0.43
1:D:235:TYR:HB3	1:D:236:PRO:CD	2.48	0.43
1:D:302:ILE:C	1:D:304:SER:N	2.74	0.43
1:D:593:LEU:HD23	1:D:593:LEU:HA	1.67	0.43
1:A:268:THR:O	1:A:269:THR:C	2.62	0.42
1:B:25:SER:HB2	1:B:308:LYS:NZ	2.31	0.42
1:C:205:ARG:O	1:C:205:ARG:CG	2.66	0.42
1:C:263:GLU:O	1:C:266:SER:N	2.39	0.42
1:D:59:PHE:CE1	1:D:60:LEU:HG	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:ASN:C	1:D:138:LEU:HD12	2.44	0.42
1:A:90:LEU:HB2	1:A:127:HIS:HB2	2.00	0.42
1:B:119:LYS:HD3	1:B:119:LYS:N	2.35	0.42
1:B:586:ARG:CD	1:B:586:ARG:H	2.29	0.42
1:C:86:TYR:CD2	1:C:86:TYR:O	2.73	0.42
1:C:283:LEU:O	1:C:285:LYS:N	2.51	0.42
1:C:295:ILE:O	1:C:296:LYS:C	2.62	0.42
1:D:50:VAL:HG22	1:D:242:ASN:HD21	1.83	0.42
1:D:106:GLU:HA	1:D:109:ASP:HB3	2.01	0.42
1:D:243:ARG:O	2:D:9001:GDP:O2'	2.37	0.42
1:D:286:MET:N	3:D:660:HOH:O	2.17	0.42
1:A:283:LEU:O	1:A:286:MET:HB2	2.19	0.42
1:A:302:ILE:O	1:A:304:SER:N	2.52	0.42
1:B:72:LEU:HA	1:B:126:ILE:HB	2.01	0.42
1:B:293:ARG:O	1:B:294:VAL:C	2.62	0.42
1:C:116:GLY:O	1:C:117:ARG:HB2	2.18	0.42
1:C:143:LEU:HA	1:C:144:PRO:HD3	1.89	0.42
1:C:177:ILE:HB	1:C:206:THR:OG1	2.19	0.42
1:C:265:PHE:O	1:C:272:ARG:HA	2.19	0.42
1:C:292:GLU:O	1:C:293:ARG:C	2.63	0.42
1:A:293:ARG:HH21	1:C:600:GLN:HG2	1.85	0.42
1:C:58:ASP:HB3	1:C:59:PHE:H	1.57	0.42
1:C:315:THR:O	1:C:316:GLU:CD	2.62	0.42
1:D:4:LEU:HD23	1:D:4:LEU:HA	1.78	0.42
1:D:291:LEU:C	1:D:291:LEU:HD12	2.44	0.42
1:A:33:SER:C	1:A:35:PRO:HD3	2.44	0.42
1:A:207:PHE:CZ	1:A:235:TYR:HE1	2.35	0.42
1:A:299:ILE:HD12	1:A:300:PRO:CD	2.50	0.42
1:B:211:THR:O	1:B:212:LYS:C	2.62	0.42
1:B:295:ILE:C	1:B:297:SER:H	2.26	0.42
1:B:305:LEU:HB2	1:B:600:GLN:OE1	2.19	0.42
1:C:262:ARG:O	1:C:263:GLU:O	2.37	0.42
1:C:295:ILE:O	1:C:298:ARG:N	2.52	0.42
1:D:303:GLN:HA	1:D:306:ILE:HD11	2.01	0.42
1:A:136:VAL:O	1:A:137:ASN:C	2.61	0.42
1:A:593:LEU:HA	1:A:593:LEU:HD23	1.79	0.42
1:B:79:ILE:CD1	1:B:132:SER:HA	2.49	0.42
1:B:143:LEU:HD23	1:B:143:LEU:HA	1.70	0.42
1:D:71:PRO:HA	1:D:142:ASP:O	2.19	0.42
1:D:108:GLN:C	1:D:110:GLU:H	2.27	0.42
1:D:236:PRO:O	1:D:238:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:597:ARG:NH1	1:D:597:ARG:CG	2.82	0.42
1:A:183:ALA:HB3	1:A:212:LYS:O	2.20	0.42
1:C:230:SER:OG	1:C:231:PHE:HD2	2.02	0.42
1:C:283:LEU:O	1:C:286:MET:N	2.52	0.42
1:D:57:LYS:N	1:D:254:MET:HG3	2.34	0.42
1:D:75:GLN:HG3	3:D:653:HOH:O	2.20	0.42
1:A:27:LEU:HD22	1:A:31:TRP:CD1	2.55	0.42
1:A:155:SER:HB2	3:A:638:HOH:O	2.20	0.42
1:A:225:ILE:C	1:A:228:GLY:H	2.27	0.42
1:B:4:LEU:O	1:B:4:LEU:HD23	2.19	0.42
1:B:314:GLU:C	3:B:656:HOH:O	2.63	0.42
1:C:241:VAL:HG21	1:C:264:TYR:CD2	2.55	0.42
1:C:302:ILE:N	1:C:305:LEU:HD12	2.35	0.42
1:D:16:THR:HG21	1:D:125:PRO:HG3	2.02	0.42
1:D:91:HIS:NE2	1:D:110:GLU:CD	2.78	0.42
1:D:233:LEU:HD13	1:D:233:LEU:HA	1.73	0.42
1:A:60:LEU:HA	1:A:61:PRO:HD3	1.93	0.42
1:A:216:MET:HG2	1:A:217:ASP:N	2.34	0.42
1:C:72:LEU:C	1:C:72:LEU:HD12	2.44	0.42
1:C:91:HIS:CE1	1:C:110:GLU:CD	2.97	0.42
1:C:185:GLN:HB2	3:C:623:HOH:O	2.18	0.42
1:C:286:MET:O	1:C:290:HIS:HB2	2.20	0.42
1:C:296:LYS:HD2	1:C:296:LYS:O	2.20	0.42
1:D:19:GLY:O	1:D:20:ASP:C	2.63	0.42
1:D:218:LYS:NZ	1:D:218:LYS:HB3	2.35	0.42
1:D:284:ALA:O	1:D:285:LYS:C	2.63	0.42
1:D:299:ILE:N	1:D:300:PRO:CD	2.83	0.42
1:A:3:ASN:O	1:A:6:SER:HB3	2.20	0.42
1:A:263:GLU:O	1:A:264:TYR:O	2.38	0.42
1:B:190:SER:C	1:B:192:ALA:N	2.76	0.42
1:C:92:LEU:HA	1:C:93:PRO:HD2	1.88	0.42
1:C:110:GLU:OE2	1:C:110:GLU:HA	2.20	0.42
1:C:187:LEU:HD11	1:C:193:ILE:HD11	2.01	0.42
1:D:176:ILE:H	1:D:176:ILE:CD1	2.08	0.42
1:D:274:LEU:CD2	1:D:277:LYS:HZ1	2.32	0.42
2:D:9001:GDP:PB	3:D:631:HOH:O	2.77	0.42
1:A:300:PRO:O	1:A:302:ILE:O	2.38	0.41
1:D:147:THR:O	1:D:159:VAL:HG12	2.20	0.41
1:D:158:ILE:C	1:D:160:LYS:N	2.78	0.41
1:D:244:SER:C	1:D:246:ALA:N	2.76	0.41
1:A:244:SER:HB2	2:A:9001:GDP:N2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:LYS:HB2	1:B:48:SER:H	1.75	0.41
1:B:235:TYR:N	1:B:235:TYR:HD2	2.16	0.41
1:C:4:LEU:O	1:C:4:LEU:HD22	2.20	0.41
1:C:5:ILE:O	1:C:6:SER:C	2.63	0.41
1:C:207:PHE:CD1	1:C:208:GLY:N	2.81	0.41
1:C:225:ILE:HG12	1:C:230:SER:HB3	1.98	0.41
1:C:273:HIS:N	3:C:668:HOH:O	2.53	0.41
1:C:302:ILE:CA	1:C:305:LEU:HD12	2.50	0.41
1:C:307:ASN:C	3:C:675:HOH:O	2.62	0.41
1:D:48:SER:N	2:D:9001:GDP:O1B	2.47	0.41
1:A:34:LEU:HD12	1:A:36:ALA:HB3	2.01	0.41
1:A:57:LYS:C	1:A:254:MET:HG3	2.46	0.41
1:A:70:ARG:HH22	1:A:124:VAL:HG23	1.84	0.41
1:C:223:VAL:CG1	1:C:224:GLU:N	2.83	0.41
1:C:598:ALA:O	1:C:602:GLU:CG	2.63	0.41
1:C:600:GLN:O	1:C:600:GLN:CG	2.60	0.41
1:D:268:THR:O	1:D:269:THR:C	2.62	0.41
1:A:16:THR:OG1	1:A:127:HIS:NE2	2.53	0.41
1:A:56:GLY:C	1:A:254:MET:HB3	2.45	0.41
1:A:69:ARG:NH1	1:A:116:GLY:O	2.52	0.41
1:A:104:ARG:HG2	1:A:104:ARG:O	2.20	0.41
1:A:293:ARG:HE	1:C:600:GLN:CD	2.28	0.41
1:A:299:ILE:O	1:A:302:ILE:HB	2.20	0.41
1:C:305:LEU:HB2	1:C:600:GLN:NE2	2.35	0.41
1:A:56:GLY:O	1:A:254:MET:HB3	2.20	0.41
1:A:209:VAL:O	1:A:238:VAL:O	2.39	0.41
1:B:4:LEU:O	1:B:4:LEU:CD2	2.69	0.41
1:B:70:ARG:NH2	1:B:124:VAL:N	2.63	0.41
1:B:180:ILE:HA	1:B:209:VAL:HB	2.02	0.41
1:C:256:ALA:O	1:C:257:ALA:O	2.38	0.41
1:C:264:TYR:C	1:C:264:TYR:HD1	2.26	0.41
1:C:283:LEU:O	1:C:284:ALA:C	2.63	0.41
1:C:290:HIS:O	1:C:292:GLU:N	2.53	0.41
1:C:299:ILE:N	1:C:300:PRO:CD	2.84	0.41
1:D:47:LYS:HZ2	1:D:144:PRO:C	2.29	0.41
1:D:310:VAL:O	1:D:314:GLU:OE1	2.38	0.41
1:A:148:LYS:HE3	1:B:191:ASP:N	2.35	0.41
1:A:593:LEU:O	1:A:595:LEU:N	2.53	0.41
1:C:185:GLN:HG3	3:C:623:HOH:O	2.21	0.41
1:C:599:ALA:O	1:C:603:ILE:CG1	2.68	0.41
1:D:23:ASP:CG	1:D:26:ALA:HB3	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:103:VAL:O	1:D:106:GLU:N	2.35	0.41
1:D:108:GLN:O	1:D:110:GLU:N	2.53	0.41
1:A:7:LEU:O	1:A:8:VAL:C	2.63	0.41
1:A:27:LEU:O	1:A:29:THR:N	2.47	0.41
1:A:57:LYS:CA	1:A:254:MET:HG3	2.51	0.41
1:A:233:LEU:HD22	1:A:237:TRP:HE1	1.84	0.41
1:B:110:GLU:O	1:B:111:THR:C	2.64	0.41
1:B:264:TYR:HE1	1:B:268:THR:HG21	1.85	0.41
1:C:5:ILE:C	1:C:7:LEU:N	2.79	0.41
1:C:7:LEU:CD2	1:C:7:LEU:C	2.94	0.41
1:C:12:GLN:O	1:C:15:CYS:HB2	2.21	0.41
1:C:32:ASP:O	1:C:34:LEU:N	2.54	0.41
1:C:69:ARG:HH21	1:C:119:LYS:CD	2.27	0.41
1:C:75:GLN:O	1:C:130:ILE:N	2.53	0.41
1:A:272:ARG:NH1	1:A:272:ARG:CG	2.83	0.41
1:B:16:THR:HA	1:B:19:GLY:H	1.85	0.41
1:B:312:GLU:O	1:B:313:LEU:C	2.62	0.41
1:C:46:GLY:C	1:C:49:SER:HB2	2.46	0.41
1:C:91:HIS:CE1	1:C:110:GLU:OE2	2.74	0.41
1:B:12:GLN:O	1:B:13:ARG:C	2.60	0.41
1:B:69:ARG:HH21	1:B:119:LYS:HD2	1.86	0.41
1:B:196:SER:C	1:B:198:GLU:H	2.28	0.41
1:B:268:THR:O	1:B:268:THR:HG22	2.21	0.41
1:C:7:LEU:C	1:C:9:ASN:N	2.78	0.41
1:A:45:SER:HA	1:A:182:PRO:CD	2.51	0.41
1:A:287:LEU:HD23	1:A:287:LEU:HA	1.83	0.41
1:B:8:VAL:HG12	1:B:9:ASN:N	2.35	0.41
1:B:43:GLN:NE2	1:B:66:ILE:HB	2.11	0.41
1:B:58:ASP:CB	1:B:104:ARG:HH21	2.22	0.41
1:C:49:SER:OG	2:C:9001:GDP:O1A	2.38	0.41
1:C:257:ALA:O	1:C:258:ARG:C	2.63	0.41
1:D:23:ASP:HB3	1:D:592:ARG:CD	2.36	0.41
1:A:55:VAL:O	1:A:55:VAL:CG1	2.69	0.40
1:A:57:LYS:HG2	1:A:100:PHE:HD1	1.85	0.40
1:A:225:ILE:HG22	1:A:237:TRP:CD1	2.56	0.40
1:A:293:ARG:HH21	1:C:600:GLN:CG	2.34	0.40
1:B:41:GLY:C	1:B:47:LYS:HD3	2.47	0.40
1:B:57:LYS:HD3	1:B:57:LYS:HA	1.93	0.40
1:B:128:LEU:O	1:B:128:LEU:HG	2.20	0.40
1:B:225:ILE:HG12	1:B:230:SER:HG	1.83	0.40
1:B:254:MET:O	1:B:257:ALA:CB	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:601:SER:C	1:C:603:ILE:N	2.79	0.40
1:D:27:LEU:O	1:D:30:LEU:N	2.54	0.40
1:D:57:LYS:HG2	1:D:100:PHE:CE1	2.56	0.40
1:D:143:LEU:O	1:D:144:PRO:C	2.63	0.40
1:D:227:GLU:CG	1:D:229:ARG:NH1	2.83	0.40
1:A:30:LEU:HG	1:A:30:LEU:O	2.22	0.40
1:A:49:SER:O	1:A:52:GLU:HB2	2.21	0.40
1:A:245:GLN:HB2	2:A:9001:GDP:O3'	2.22	0.40
1:A:310:VAL:C	1:A:312:GLU:N	2.79	0.40
1:B:50:VAL:HG12	1:B:51:LEU:N	2.34	0.40
1:C:124:VAL:HA	1:C:125:PRO:HD3	1.88	0.40
1:D:226:LEU:O	1:D:227:GLU:C	2.62	0.40
1:A:4:LEU:C	1:A:6:SER:N	2.77	0.40
1:A:88:GLU:O	1:A:89:PHE:CG	2.74	0.40
1:A:167:ARG:NH2	1:A:195:ILE:CD1	2.84	0.40
1:B:161:ASP:HA	1:B:164:ASN:HD21	1.86	0.40
1:B:273:HIS:CG	3:B:688:HOH:O	2.74	0.40
1:C:49:SER:OG	2:C:9001:GDP:PA	2.80	0.40
1:C:299:ILE:HG12	1:C:300:PRO:HD3	2.02	0.40
1:D:9:ASN:HA	1:D:75:GLN:HE21	1.86	0.40
1:A:34:LEU:CG	1:A:172:LYS:NZ	2.85	0.40
1:A:59:PHE:CD1	1:A:59:PHE:O	2.74	0.40
1:B:44:SER:O	1:B:45:SER:C	2.64	0.40
1:B:79:ILE:HG12	1:B:132:SER:CA	2.51	0.40
1:B:94:ARG:HB2	1:B:94:ARG:HH11	1.86	0.40
1:B:143:LEU:HA	1:B:144:PRO:HD2	1.65	0.40
1:B:144:PRO:HG2	1:B:165:MET:SD	2.61	0.40
1:B:154:GLN:O	1:B:155:SER:O	2.39	0.40
1:B:252:VAL:CG1	1:B:260:ARG:NH2	2.72	0.40
1:D:69:ARG:C	1:D:121:ILE:HG22	2.46	0.40
1:D:170:ILE:C	1:D:172:LYS:H	2.30	0.40
1:A:23:ASP:OD2	1:A:26:ALA:HB3	2.22	0.40
1:A:90:LEU:HA	1:A:90:LEU:HD12	1.67	0.40
1:A:244:SER:N	1:A:247:ASP:OD2	2.55	0.40
1:A:291:LEU:O	1:A:292:GLU:C	2.64	0.40
1:B:146:LEU:CD1	1:B:195:ILE:HG21	2.50	0.40
1:B:172:LYS:HA	1:B:173:PRO:HD2	1.84	0.40
1:B:183:ALA:HB2	1:B:210:LEU:HD13	2.02	0.40
1:C:12:GLN:CB	1:C:75:GLN:NE2	2.84	0.40
1:C:22:GLY:HA2	1:C:26:ALA:CB	2.46	0.40
1:C:74:LEU:O	1:C:75:GLN:CG	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:VAL:O	1:C:104:ARG:C	2.65	0.40
1:C:149:VAL:HG12	1:D:194:LYS:HB2	2.03	0.40
1:D:47:LYS:O	1:D:49:SER:N	2.55	0.40
1:D:84:ARG:O	1:D:86:TYR:HB3	2.22	0.40
1:D:296:LYS:C	1:D:298:ARG:N	2.79	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:B:234:LYS:NZ	1:D:313:LEU:CD1[1_655]	1.86	0.34

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/360 (93%)	201 (60%)	80 (24%)	54 (16%)	0	2
1	B	335/360 (93%)	194 (58%)	81 (24%)	60 (18%)	0	1
1	C	335/360 (93%)	205 (61%)	73 (22%)	57 (17%)	0	2
1	D	335/360 (93%)	192 (57%)	94 (28%)	49 (15%)	0	3
All	All	1340/1440 (93%)	792 (59%)	328 (24%)	220 (16%)	0	2

All (220) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	ILE
1	A	14	ALA
1	A	43	GLN
1	A	58	ASP
1	A	72	LEU

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Mol	Chain	Res	Type
1	A	80	ASP
1	A	83	THR
1	A	91	HIS
1	A	125	PRO
1	A	200	ASP
1	A	206	THR
1	A	235	TYR
1	A	236	PRO
1	A	264	TYR
1	A	605	ALA
1	B	6	SER
1	B	15	CYS
1	B	16	THR
1	B	25	SER
1	B	47	LYS
1	B	66	ILE
1	B	81	ASP
1	B	86	TYR
1	B	91	HIS
1	B	155	SER
1	B	159	VAL
1	B	246	ALA
1	B	257	ALA
1	B	258	ARG
1	B	260	ARG
1	B	272	ARG
1	B	275	ALA
1	B	306	ILE
1	C	12	GLN
1	C	31	TRP
1	C	58	ASP
1	C	62	ARG
1	C	80	ASP
1	C	81	ASP
1	C	83	THR
1	C	85	GLU
1	C	90	LEU
1	C	100	PHE
1	C	117	ARG
1	C	125	PRO
1	C	173	PRO
1	C	174	ASN

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Mol	Chain	Res	Type
1	C	187	LEU
1	C	204	ASP
1	C	236	PRO
1	C	263	GLU
1	C	264	TYR
1	C	284	ALA
1	C	296	LYS
1	C	306	ILE
1	C	605	ALA
1	D	16	THR
1	D	18	LEU
1	D	20	ASP
1	D	25	SER
1	D	80	ASP
1	D	81	ASP
1	D	91	HIS
1	D	123	SER
1	D	125	PRO
1	D	194	LYS
1	D	235	TYR
1	D	251	ASN
1	D	257	ALA
1	D	272	ARG
1	D	306	ILE
1	D	598	ALA
1	D	599	ALA
1	A	12	GLN
1	A	15	CYS
1	A	30	LEU
1	A	34	LEU
1	A	59	PHE
1	A	85	GLU
1	A	152	ASP
1	A	158	ILE
1	A	192	ALA
1	A	252	VAL
1	A	283	LEU
1	A	296	LYS
1	B	18	LEU
1	B	22	GLY
1	B	33	SER
1	B	58	ASP

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Mol	Chain	Res	Type
1	B	94	ARG
1	B	144	PRO
1	B	156	ASP
1	B	197	ARG
1	B	212	LYS
1	B	259	LYS
1	B	264	TYR
1	B	279	GLY
1	B	587	SER
1	B	594	GLU
1	B	597	ARG
1	C	6	SER
1	C	34	LEU
1	C	119	LYS
1	C	228	GLY
1	C	242	ASN
1	C	257	ALA
1	C	280	SER
1	C	291	LEU
1	C	302	ILE
1	C	313	LEU
1	C	590	SER
1	C	591	LYS
1	C	593	LEU
1	C	594	GLU
1	D	30	LEU
1	D	47	LYS
1	D	48	SER
1	D	89	PHE
1	D	103	VAL
1	D	104	ARG
1	D	159	VAL
1	D	168	SER
1	D	188	ALA
1	D	206	THR
1	D	259	LYS
1	D	297	SER
1	A	23	ASP
1	A	24	SER
1	A	77	GLN
1	A	119	LYS
1	A	217	ASP

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Mol	Chain	Res	Type
1	A	287	LEU
1	A	297	SER
1	A	313	LEU
1	A	604	ASP
1	B	29	THR
1	B	117	ARG
1	B	160	LYS
1	B	173	PRO
1	B	187	LEU
1	B	218	LYS
1	B	223	VAL
1	B	269	THR
1	B	586	ARG
1	C	33	SER
1	C	47	LYS
1	C	145	GLY
1	C	152	ASP
1	C	188	ALA
1	C	252	VAL
1	D	119	LYS
1	D	173	PRO
1	D	186	ASP
1	D	594	GLU
1	A	28	PRO
1	A	56	GLY
1	A	89	PHE
1	A	94	ARG
1	A	115	THR
1	A	212	LYS
1	A	244	SER
1	A	262	ARG
1	A	269	THR
1	A	312	GLU
1	A	594	GLU
1	B	71	PRO
1	B	115	THR
1	B	125	PRO
1	B	188	ALA
1	B	252	VAL
1	B	265	PHE
1	B	300	PRO
1	B	591	LYS

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Mol	Chain	Res	Type
1	C	30	LEU
1	C	48	SER
1	C	86	TYR
1	C	138	LEU
1	C	186	ASP
1	C	283	LEU
1	D	28	PRO
1	D	33	SER
1	D	57	LYS
1	D	86	TYR
1	D	109	ASP
1	D	150	ALA
1	D	166	VAL
1	D	192	ALA
1	D	258	ARG
1	D	305	LEU
1	D	600	GLN
1	A	45	SER
1	A	55	VAL
1	A	263	GLU
1	B	99	ASP
1	B	161	ASP
1	B	250	LYS
1	B	593	LEU
1	C	269	THR
1	C	299	ILE
1	C	585	ARG
1	D	117	ARG
1	B	9	ASN
1	B	292	GLU
1	C	23	ASP
1	C	101	ALA
1	D	193	ILE
1	D	227	GLU
1	A	35	PRO
1	A	182	PRO
1	C	67	VAL
1	D	241	VAL
1	A	295	ILE
1	B	34	LEU
1	D	34	LEU
1	B	236	PRO

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Mol	Chain	Res	Type
1	C	55	VAL
1	B	5	ILE
1	B	46	GLY
1	C	71	PRO
1	A	173	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	294/313 (94%)	214 (73%)	80 (27%)	0	3
1	B	294/313 (94%)	218 (74%)	76 (26%)	0	4
1	C	294/313 (94%)	209 (71%)	85 (29%)	0	2
1	D	294/313 (94%)	215 (73%)	79 (27%)	0	3
All	All	1176/1252 (94%)	856 (73%)	320 (27%)	0	3

All (320) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	8	VAL
1	A	11	ILE
1	A	12	GLN
1	A	18	LEU
1	A	27	LEU
1	A	34	LEU
1	A	37	ILE
1	A	39	VAL
1	A	40	VAL
1	A	47	LYS
1	A	50	VAL
1	A	53	SER
1	A	55	VAL
1	A	59	PHE
1	A	62	ARG

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Mol	Chain	Res	Type
1	A	66	ILE
1	A	68	THR
1	A	74	LEU
1	A	77	GLN
1	A	79	ILE
1	A	90	LEU
1	A	95	LYS
1	A	98	THR
1	A	100	PHE
1	A	117	ARG
1	A	119	LYS
1	A	128	LEU
1	A	130	ILE
1	A	132	SER
1	A	134	ASN
1	A	137	ASN
1	A	141	ILE
1	A	146	LEU
1	A	151	VAL
1	A	156	ASP
1	A	158	ILE
1	A	166	VAL
1	A	169	TYR
1	A	180	ILE
1	A	184	ASN
1	A	187	LEU
1	A	189	THR
1	A	191	ASP
1	A	193	ILE
1	A	199	VAL
1	A	202	SER
1	A	205	ARG
1	A	206	THR
1	A	207	PHE
1	A	210	LEU
1	A	211	THR
1	A	214	ASP
1	A	215	LEU
1	A	225	ILE
1	A	226	LEU
1	A	233	LEU
1	A	238	VAL

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Mol	Chain	Res	Type
1	A	240	VAL
1	A	241	VAL
1	A	243	ARG
1	A	247	ASP
1	A	248	ILE
1	A	249	ASN
1	A	260	ARG
1	A	262	ARG
1	A	265	PHE
1	A	269	THR
1	A	270	GLU
1	A	271	TYR
1	A	277	LYS
1	A	278	MET
1	A	280	SER
1	A	292	GLU
1	A	302	ILE
1	A	310	VAL
1	A	316	GLU
1	A	593	LEU
1	A	597	ARG
1	A	601	SER
1	B	4	LEU
1	B	7	LEU
1	B	8	VAL
1	B	11	ILE
1	B	15	CYS
1	B	23	ASP
1	B	27	LEU
1	B	29	THR
1	B	34	LEU
1	B	39	VAL
1	B	50	VAL
1	B	59	PHE
1	B	62	ARG
1	B	67	VAL
1	B	69	ARG
1	B	72	LEU
1	B	74	LEU
1	B	84	ARG
1	B	86	TYR
1	B	90	LEU

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Mol	Chain	Res	Type
1	B	92	LEU
1	B	103	VAL
1	B	105	LYS
1	B	115	THR
1	B	117	ARG
1	B	126	ILE
1	B	128	LEU
1	B	136	VAL
1	B	140	LEU
1	B	141	ILE
1	B	142	ASP
1	B	143	LEU
1	B	148	LYS
1	B	160	LYS
1	B	161	ASP
1	B	164	ASN
1	B	165	MET
1	B	170	ILE
1	B	176	ILE
1	B	178	LEU
1	B	181	SER
1	B	184	ASN
1	B	193	ILE
1	B	195	ILE
1	B	200	ASP
1	B	202	SER
1	B	204	ASP
1	B	206	THR
1	B	209	VAL
1	B	210	LEU
1	B	214	ASP
1	B	216	MET
1	B	218	LYS
1	B	220	THR
1	B	223	VAL
1	B	227	GLU
1	B	232	LYS
1	B	233	LEU
1	B	235	TYR
1	B	242	ASN
1	B	245	GLN
1	B	250	LYS

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Mol	Chain	Res	Type
1	B	255	ILE
1	B	269	THR
1	B	273	HIS
1	B	281	GLU
1	B	299	ILE
1	B	303	GLN
1	B	304	SER
1	B	310	VAL
1	B	311	LEU
1	B	313	LEU
1	B	314	GLU
1	B	586	ARG
1	B	589	ILE
1	B	594	GLU
1	C	3	ASN
1	C	4	LEU
1	C	5	ILE
1	C	18	LEU
1	C	20	ASP
1	C	23	ASP
1	C	24	SER
1	C	29	THR
1	C	30	LEU
1	C	33	SER
1	C	34	LEU
1	C	37	ILE
1	C	50	VAL
1	C	59	PHE
1	C	67	VAL
1	C	69	ARG
1	C	70	ARG
1	C	73	VAL
1	C	74	LEU
1	C	77	GLN
1	C	78	LYS
1	C	79	ILE
1	C	86	TYR
1	C	89	PHE
1	C	100	PHE
1	C	103	VAL
1	C	107	ILE
1	C	109	ASP

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Mol	Chain	Res	Type
1	C	123	SER
1	C	128	LEU
1	C	129	SER
1	C	131	TYR
1	C	132	SER
1	C	135	VAL
1	C	148	LYS
1	C	149	VAL
1	C	152	ASP
1	C	156	ASP
1	C	159	VAL
1	C	162	ILE
1	C	165	MET
1	C	168	SER
1	C	170	ILE
1	C	172	LYS
1	C	174	ASN
1	C	175	CYS
1	C	176	ILE
1	C	180	ILE
1	C	184	ASN
1	C	185	GLN
1	C	199	VAL
1	C	206	THR
1	C	209	VAL
1	C	210	LEU
1	C	211	THR
1	C	218	LYS
1	C	224	GLU
1	C	226	LEU
1	C	227	GLU
1	C	234	LYS
1	C	240	VAL
1	C	242	ASN
1	C	255	ILE
1	C	268	THR
1	C	270	GLU
1	C	277	LYS
1	C	278	MET
1	C	280	SER
1	C	281	GLU
1	C	282	HIS

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Mol	Chain	Res	Type
1	C	285	LYS
1	C	286	MET
1	C	288	SER
1	C	294	VAL
1	C	298	ARG
1	C	299	ILE
1	C	304	SER
1	C	305	LEU
1	C	306	ILE
1	C	312	GLU
1	C	593	LEU
1	C	594	GLU
1	C	596	TYR
1	C	601	SER
1	C	603	ILE
1	D	4	LEU
1	D	5	ILE
1	D	11	ILE
1	D	16	THR
1	D	34	LEU
1	D	37	ILE
1	D	43	GLN
1	D	53	SER
1	D	54	ILE
1	D	62	ARG
1	D	67	VAL
1	D	73	VAL
1	D	77	GLN
1	D	79	ILE
1	D	83	THR
1	D	86	TYR
1	D	88	GLU
1	D	111	THR
1	D	134	ASN
1	D	135	VAL
1	D	136	VAL
1	D	141	ILE
1	D	146	LEU
1	D	148	LYS
1	D	151	VAL
1	D	158	ILE
1	D	162	ILE

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Mol	Chain	Res	Type
1	D	164	ASN
1	D	174	ASN
1	D	175	CYS
1	D	176	ILE
1	D	180	ILE
1	D	184	ASN
1	D	187	LEU
1	D	189	THR
1	D	190	SER
1	D	193	ILE
1	D	206	THR
1	D	211	THR
1	D	216	MET
1	D	218	LYS
1	D	220	THR
1	D	224	GLU
1	D	227	GLU
1	D	231	PHE
1	D	233	LEU
1	D	240	VAL
1	D	241	VAL
1	D	243	ARG
1	D	252	VAL
1	D	253	ASP
1	D	255	ILE
1	D	259	LYS
1	D	260	ARG
1	D	264	TYR
1	D	268	THR
1	D	269	THR
1	D	270	GLU
1	D	273	HIS
1	D	278	MET
1	D	280	SER
1	D	283	LEU
1	D	288	SER
1	D	293	ARG
1	D	295	ILE
1	D	299	ILE
1	D	305	LEU
1	D	306	ILE
1	D	310	VAL

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Mol	Chain	Res	Type
1	D	311	LEU
1	D	312	GLU
1	D	313	LEU
1	D	314	GLU
1	D	316	GLU
1	D	590	SER
1	D	593	LEU
1	D	594	GLU
1	D	595	LEU
1	D	597	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	GLN
1	A	91	HIS
1	A	134	ASN
1	A	154	GLN
1	A	174	ASN
1	A	185	GLN
1	A	242	ASN
1	A	273	HIS
1	A	282	HIS
1	A	290	HIS
1	B	12	GLN
1	B	21	HIS
1	B	43	GLN
1	B	108	GLN
1	B	154	GLN
1	B	164	ASN
1	B	174	ASN
1	B	185	GLN
1	B	245	GLN
1	B	303	GLN
1	C	12	GLN
1	C	43	GLN
1	C	75	GLN
1	C	127	HIS
1	C	137	ASN
1	C	174	ASN
1	C	185	GLN
1	C	242	ASN

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Mol	Chain	Res	Type
1	C	290	HIS
1	C	303	GLN
1	D	43	GLN
1	D	75	GLN
1	D	185	GLN
1	D	242	ASN
1	D	290	HIS
1	D	600	GLN

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](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GDP	B	9001	-	29,30,30	1.12	2 (6%)	45,47,47	1.86	8 (17%)
2	GDP	A	9001	-	29,30,30	1.23	4 (13%)	45,47,47	2.06	13 (28%)
2	GDP	D	9001	-	29,30,30	1.19	4 (13%)	45,47,47	1.93	10 (22%)
2	GDP	C	9001	-	29,30,30	1.23	4 (13%)	45,47,47	1.84	6 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GDP	B	9001	-	-	2/16/32/32	0/3/3/3
2	GDP	A	9001	-	-	6/16/32/32	0/3/3/3
2	GDP	D	9001	-	-	5/16/32/32	0/3/3/3
2	GDP	C	9001	-	-	0/16/32/32	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	9001	GDP	C5-C4	3.06	1.47	1.38
2	B	9001	GDP	C5-C4	2.97	1.46	1.38
2	A	9001	GDP	C5-C4	2.90	1.46	1.38
2	C	9001	GDP	C6-N1	-2.83	1.33	1.38
2	A	9001	GDP	C6-N1	-2.77	1.33	1.38
2	D	9001	GDP	C5-C4	2.69	1.46	1.38
2	D	9001	GDP	PA-O3A	2.66	1.62	1.59
2	A	9001	GDP	PA-O3A	2.47	1.62	1.59
2	D	9001	GDP	C5-N7	-2.38	1.34	1.39
2	D	9001	GDP	C6-N1	-2.36	1.34	1.38
2	B	9001	GDP	C6-N1	-2.35	1.34	1.38
2	A	9001	GDP	C5-N7	-2.09	1.34	1.39
2	C	9001	GDP	C5-N7	-2.09	1.34	1.39
2	C	9001	GDP	PA-O3A	2.05	1.61	1.59

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	9001	GDP	C5-C4-N3	-6.56	117.95	128.39
2	A	9001	GDP	C5-C4-N3	-6.52	118.01	128.39
2	B	9001	GDP	C5-C4-N3	-6.19	118.54	128.39
2	D	9001	GDP	C5-C4-N3	-5.48	119.67	128.39
2	A	9001	GDP	C2-N3-C4	5.30	121.43	112.30
2	C	9001	GDP	C2-N3-C4	5.18	121.22	112.30
2	A	9001	GDP	N9-C4-N3	5.16	136.26	125.95
2	B	9001	GDP	C2-N3-C4	5.03	120.96	112.30
2	B	9001	GDP	N9-C4-N3	4.93	135.81	125.95
2	C	9001	GDP	N9-C4-N3	4.90	135.75	125.95
2	D	9001	GDP	C2-N3-C4	4.59	120.20	112.30
2	D	9001	GDP	N9-C4-N3	4.12	134.19	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	9001	GDP	C6-C5-N7	3.29	136.28	130.29
2	B	9001	GDP	C6-C5-N7	3.26	136.23	130.29
2	D	9001	GDP	O4'-C1'-N9	3.23	115.69	108.36
2	A	9001	GDP	C6-C5-N7	3.21	136.14	130.29
2	D	9001	GDP	O6-C6-C5	-3.04	118.52	126.53
2	C	9001	GDP	C6-C5-N7	2.86	135.49	130.29
2	B	9001	GDP	O3B-PB-O3A	2.66	113.56	104.64
2	A	9001	GDP	C4-C5-N7	-2.64	106.49	110.67
2	D	9001	GDP	C4-C5-N7	-2.59	106.56	110.67
2	B	9001	GDP	C4-C5-N7	-2.50	106.71	110.67
2	A	9001	GDP	O4'-C1'-C2'	-2.49	101.29	106.62
2	A	9001	GDP	O4'-C1'-N9	2.42	113.85	108.36
2	A	9001	GDP	O6-C6-C5	-2.42	120.16	126.53
2	C	9001	GDP	O6-C6-C5	-2.40	120.19	126.53
2	C	9001	GDP	C4-C5-N7	-2.38	106.90	110.67
2	A	9001	GDP	C5'-C4'-C3'	-2.32	106.87	115.21
2	B	9001	GDP	O6-C6-C5	-2.29	120.49	126.53
2	D	9001	GDP	O3B-PB-O3A	2.28	112.29	104.64
2	A	9001	GDP	O2B-PB-O3A	2.28	112.27	104.64
2	D	9001	GDP	C8-N7-C5	2.13	108.06	104.26
2	A	9001	GDP	C8-N7-C5	2.11	108.02	104.26
2	B	9001	GDP	C8-N7-C5	2.11	108.01	104.26
2	A	9001	GDP	C2'-C1'-N9	-2.09	107.44	113.25
2	A	9001	GDP	O2A-PA-O3A	2.03	112.75	107.27
2	D	9001	GDP	C3'-C2'-C1'	-2.01	97.67	101.46

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	9001	GDP	C5'-O5'-PA-O3A
2	A	9001	GDP	O4'-C4'-C5'-O5'
2	D	9001	GDP	C5'-O5'-PA-O3A
2	D	9001	GDP	C5'-O5'-PA-O2A
2	A	9001	GDP	C3'-C4'-C5'-O5'
2	D	9001	GDP	C3'-C4'-C5'-O5'
2	D	9001	GDP	O4'-C4'-C5'-O5'
2	A	9001	GDP	C5'-O5'-PA-O1A
2	D	9001	GDP	C5'-O5'-PA-O1A
2	A	9001	GDP	PB-O3A-PA-O1A
2	A	9001	GDP	PB-O3A-PA-O2A
2	B	9001	GDP	PA-O3A-PB-O1B

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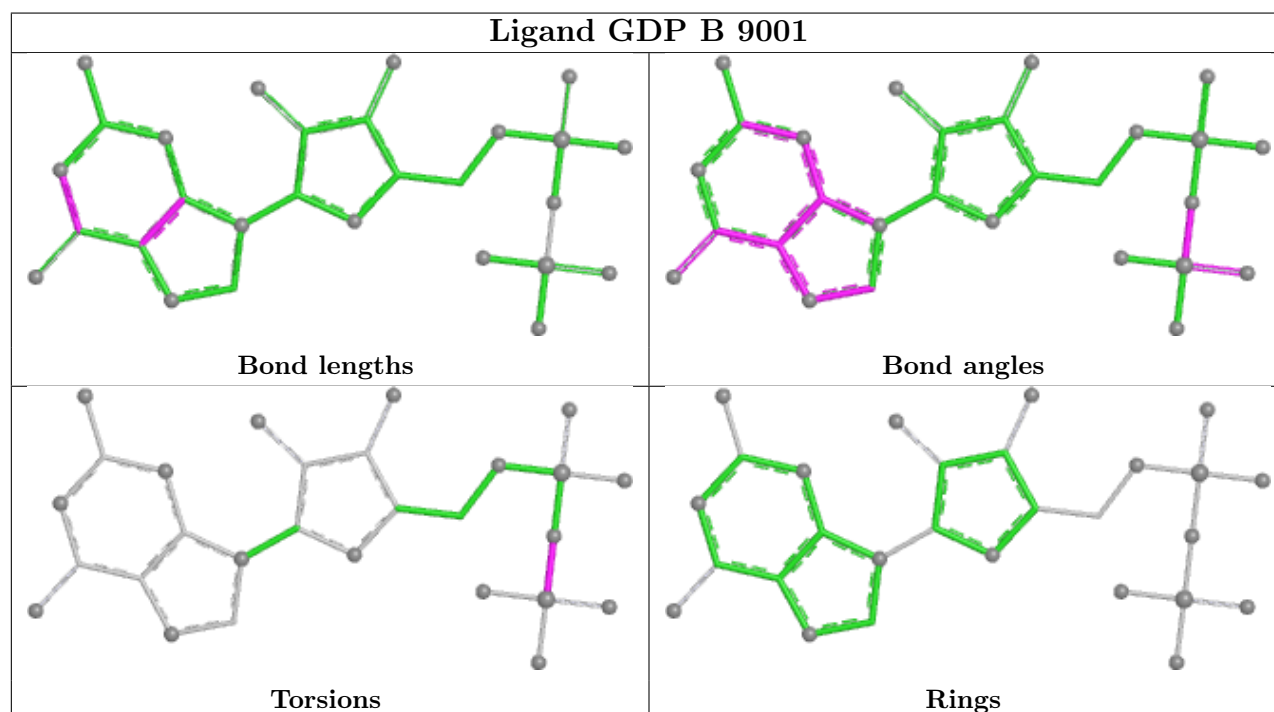
Mol	Chain	Res	Type	Atoms
2	B	9001	GDP	PA-O3A-PB-O3B

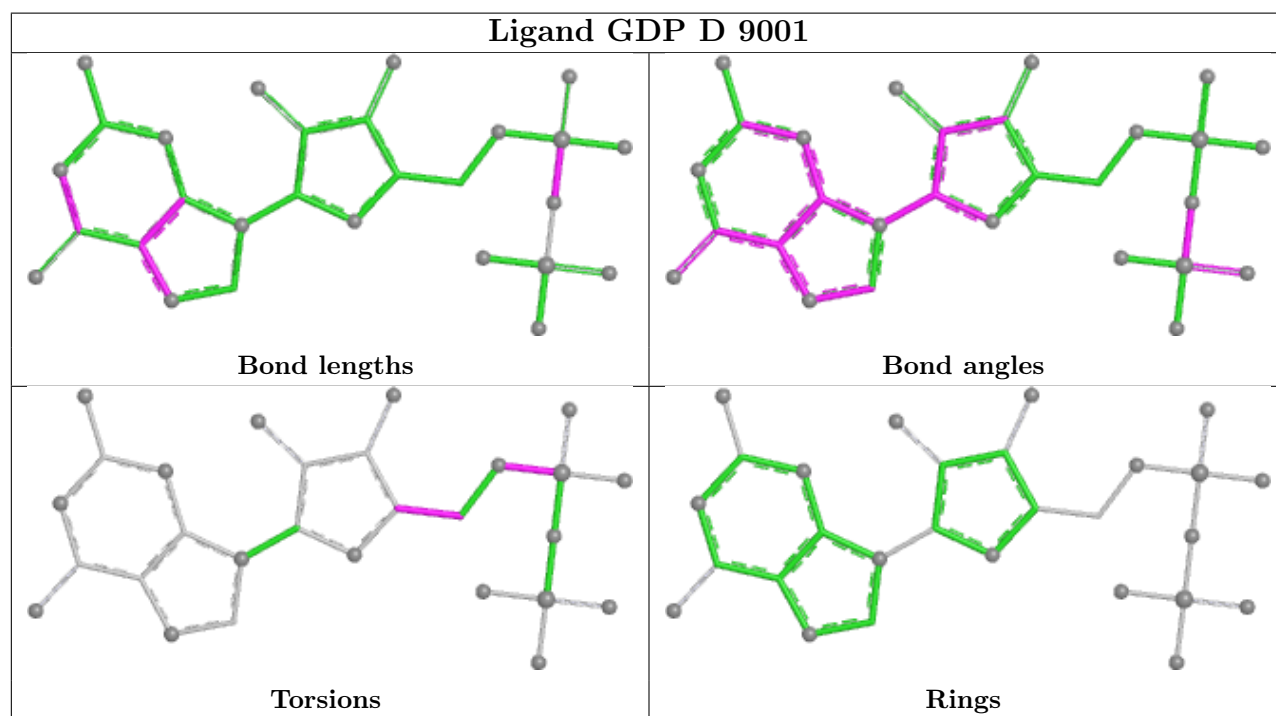
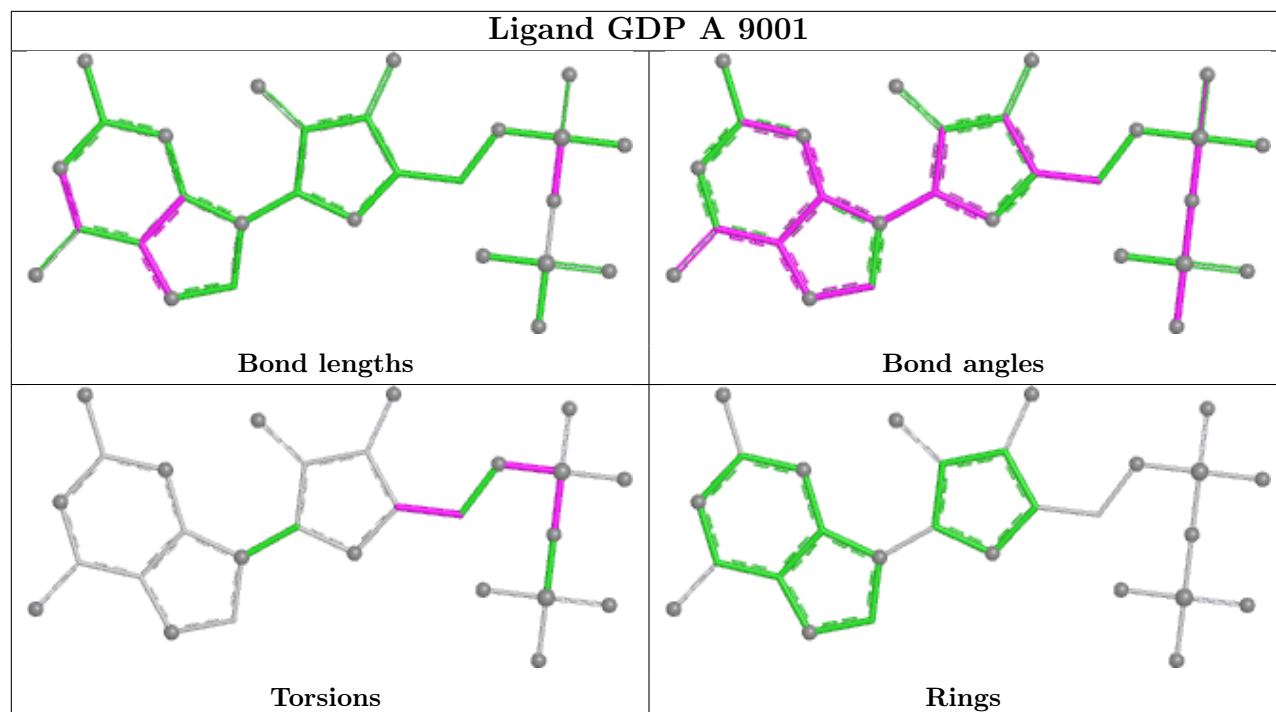
There are no ring outliers.

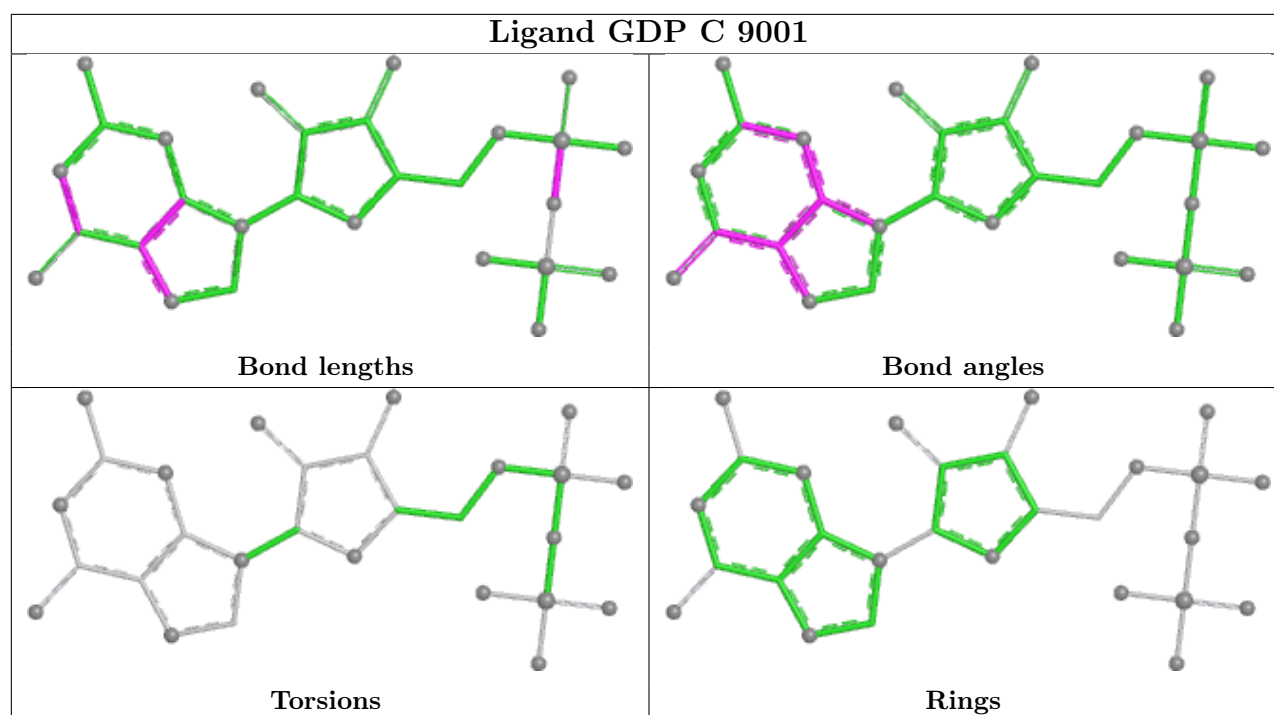
4 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	9001	GDP	7	0
2	A	9001	GDP	7	0
2	D	9001	GDP	8	0
2	C	9001	GDP	6	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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	339/360 (94%)	0.35	14 (4%)	41 23	20, 44, 118, 146	0
1	B	339/360 (94%)	0.17	15 (4%)	39 22	18, 38, 104, 162	0
1	C	339/360 (94%)	0.35	13 (3%)	44 25	22, 51, 130, 174	0
1	D	339/360 (94%)	0.52	13 (3%)	44 25	31, 62, 118, 173	0
All	All	1356/1440 (94%)	0.35	55 (4%)	41 23	18, 48, 118, 174	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	65	GLY	3.9
1	C	21	HIS	3.7
1	C	584	GLU	3.7
1	B	20	ASP	3.5
1	D	584	GLU	3.4
1	D	118	SER	3.4
1	D	64	SER	3.4
1	A	22	GLY	3.3
1	D	22	GLY	3.2
1	D	20	ASP	3.1
1	D	120	ALA	3.1
1	A	118	SER	3.1
1	D	68	THR	3.1
1	B	25	SER	3.0
1	D	21	HIS	2.9
1	A	67	VAL	2.9
1	B	584	GLU	2.7
1	C	64	SER	2.7
1	B	23	ASP	2.6
1	C	20	ASP	2.6
1	B	27	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	64	SER	2.6
1	D	30	LEU	2.6
1	D	26	ALA	2.4
1	B	26	ALA	2.4
1	B	65	GLY	2.4
1	C	196	SER	2.3
1	A	68	THR	2.3
1	B	597	ARG	2.3
1	A	23	ASP	2.3
1	A	314	GLU	2.3
1	B	121	ILE	2.3
1	A	63	GLY	2.3
1	A	238	VAL	2.3
1	C	22	GLY	2.3
1	D	119	LYS	2.3
1	A	204	ASP	2.3
1	C	25	SER	2.2
1	C	63	GLY	2.2
1	B	32	ASP	2.2
1	A	313	LEU	2.2
1	B	67	VAL	2.1
1	B	120	ALA	2.1
1	A	207	PHE	2.1
1	B	30	LEU	2.1
1	A	21	HIS	2.1
1	C	68	THR	2.1
1	C	26	ALA	2.1
1	D	67	VAL	2.0
1	A	584	GLU	2.0
1	C	85	GLU	2.0
1	B	24	SER	2.0
1	D	276	ASN	2.0
1	C	239	GLY	2.0
1	C	67	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates [i](#)

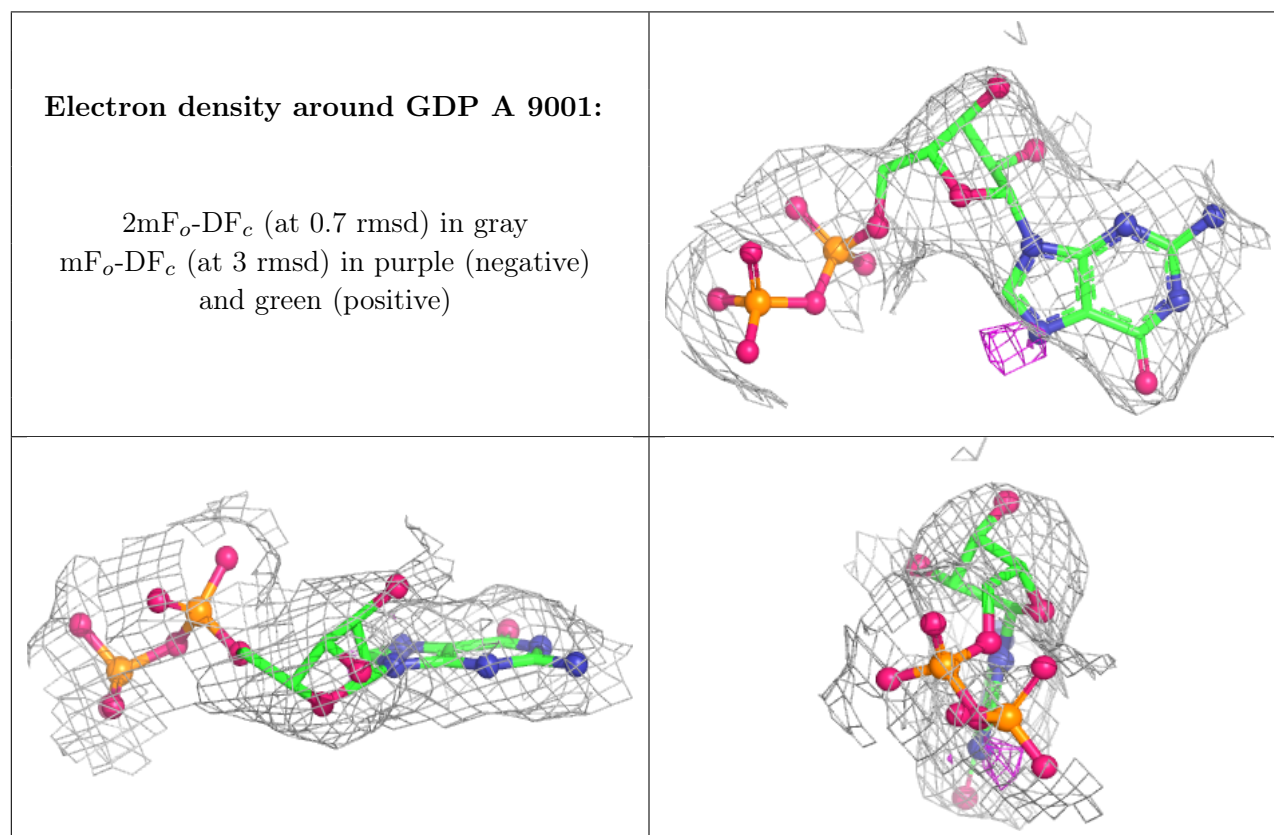
There are no oligosaccharides in this entry.

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.

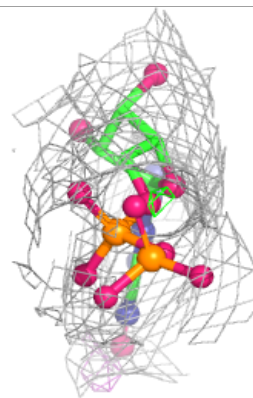
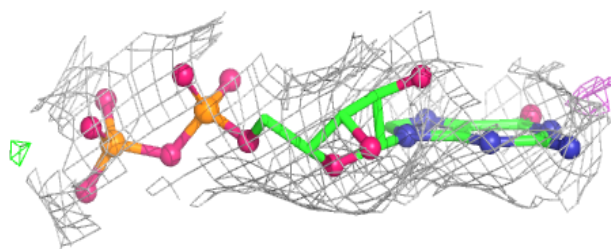
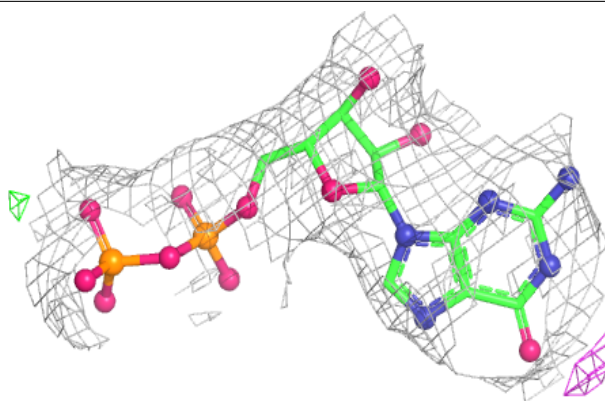
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GDP	A	9001	28/28	0.93	0.11	24,41,56,61	0
2	GDP	D	9001	28/28	0.93	0.09	34,42,47,48	0
2	GDP	C	9001	28/28	0.94	0.10	33,47,52,54	0
2	GDP	B	9001	28/28	0.97	0.07	22,27,33,37	0

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.

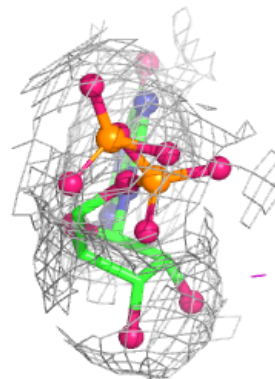
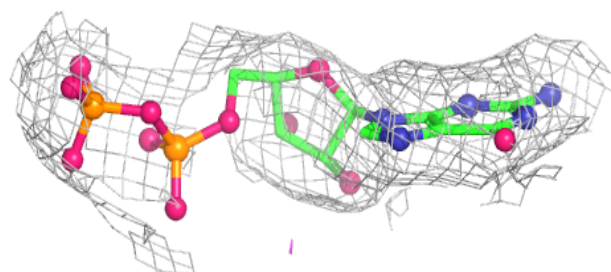


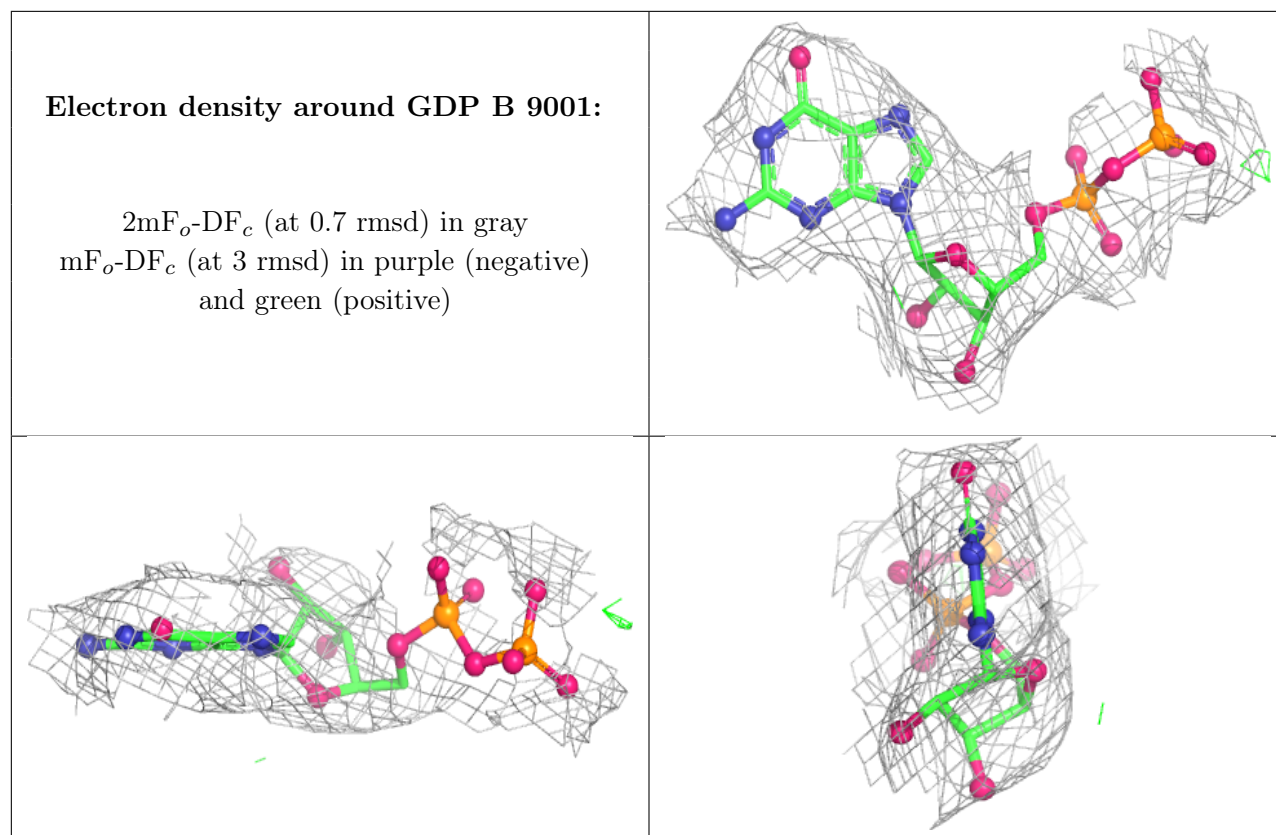
Electron density around GDP D 9001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around GDP C 9001:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.