



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:26 PM UTC

PDB ID : 1MWH / pdb_00001mwh
Title : REOVIRUS POLYMERASE LAMBDA3 BOUND TO MRNA CAP ANALOG
Authors : Tao, Y.; Farsetta, D.L.; Nibert, M.L.; Harrison, S.C.
Deposited on : 2002-09-29
Resolution : 2.50 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

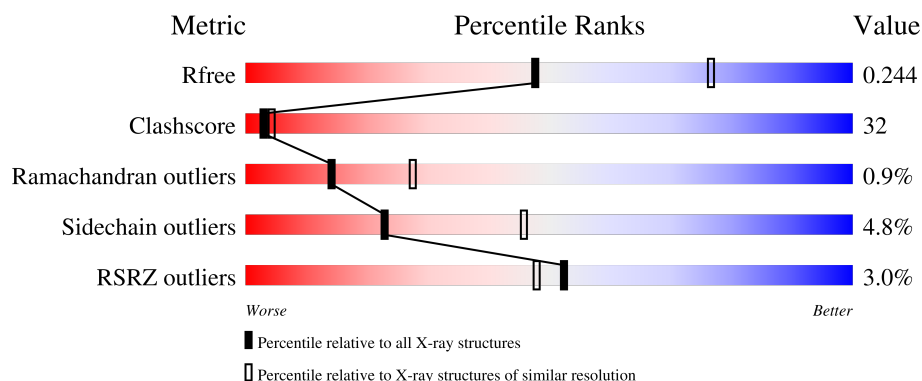
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	1267	 3% 58% 37% . .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10653 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.

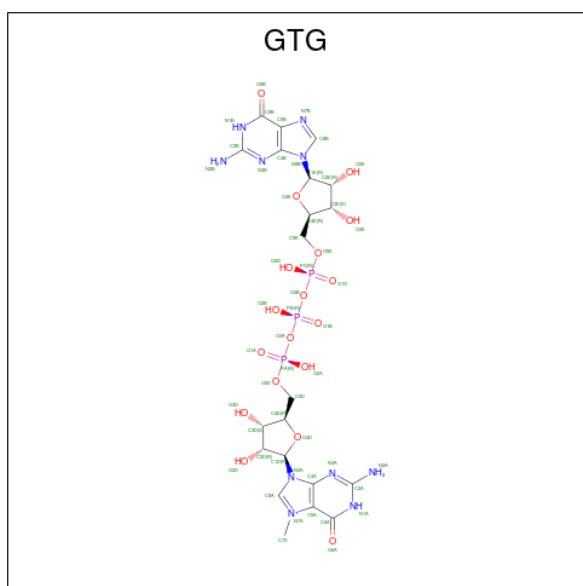
- Molecule 1 is a protein called MINOR CORE PROTEIN LAMBDA 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1256	Total	C	N	O	S	0	0	0
			9929	6337	1697	1831	64			

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

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

- Molecule 3 is 7-METHYL-GUANOSINE-5'-TRIPHOSPHATE-5'-GUANOSINE (CCD ID: GTG) (formula: C₂₁H₃₀N₁₀O₁₈P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			52	21	10	18	3		

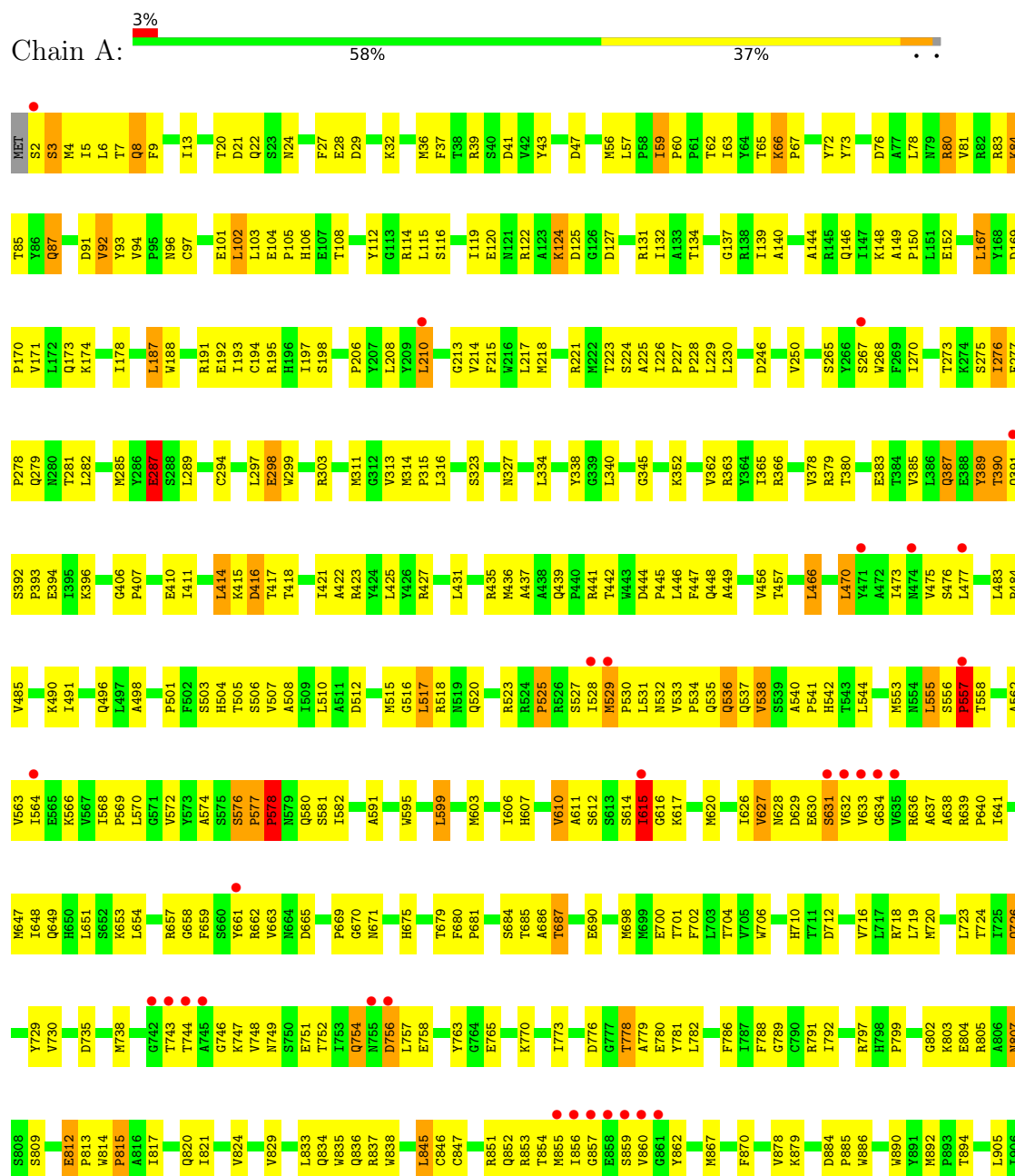
- Molecule 4 is water.

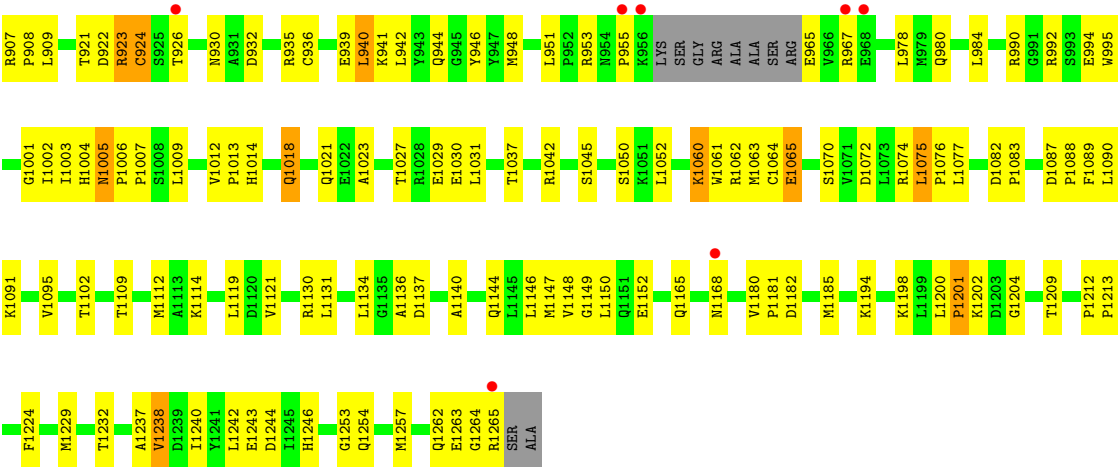
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	671	Total 671	O 671	0	0

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: MINOR CORE PROTEIN LAMBDA 3





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.89Å 84.94Å 249.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.88 – 2.50 49.88 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.1 (49.88-2.50) 93.1 (49.88-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.48Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.209 , 0.245 0.209 , 0.244	Depositor DCC
R_{free} test set	2636 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	32.3	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10653	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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

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	0.58	10/10181 (0.1%)	1.15	50/13828 (0.4%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	124	LYS	C-O	11.11	1.38	1.24
1	A	556	SER	CA-C	10.44	1.62	1.52
1	A	923	ARG	CA-C	7.44	1.62	1.52
1	A	36	MET	SD-CE	-6.83	1.62	1.79
1	A	924	CYS	N-CA	6.21	1.53	1.46
1	A	852	GLN	C-O	-5.99	1.16	1.23
1	A	555	LEU	C-N	5.53	1.41	1.33
1	A	407	PRO	C-N	-5.51	1.26	1.33
1	A	417	THR	CA-C	-5.40	1.45	1.52
1	A	556	SER	C-N	5.13	1.40	1.33

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	577	PRO	CA-C-N	47.85	179.66	119.84
1	A	577	PRO	C-N-CA	47.85	179.66	119.84
1	A	577	PRO	C-N-CD	-11.80	76.63	125.00
1	A	754	GLN	OE1-CD-NE2	-10.50	112.10	122.60
1	A	556	SER	CA-C-N	9.86	129.81	119.85
1	A	556	SER	C-N-CA	9.86	129.81	119.85
1	A	1018	GLN	OE1-CD-NE2	-9.85	112.75	122.60
1	A	1194	LYS	N-CA-C	8.44	120.56	111.36
1	A	287	GLU	N-CA-C	-8.39	102.08	111.82
1	A	557	PRO	CA-N-CD	-7.94	100.88	112.00
1	A	576	SER	CA-C-N	-7.73	112.42	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	576	SER	C-N-CA	-7.73	112.42	120.38
1	A	1264	GLY	CA-C-N	-7.61	108.00	121.70
1	A	1264	GLY	C-N-CA	-7.61	108.00	121.70
1	A	124	LYS	CA-C-O	-7.13	111.77	119.97
1	A	1075	LEU	N-CA-C	6.89	118.81	109.24
1	A	922	ASP	N-CA-C	-6.77	103.70	112.23
1	A	835	TRP	N-CA-C	6.76	119.22	111.11
1	A	1018	GLN	CG-CD-NE2	6.65	126.38	116.40
1	A	422	ALA	N-CA-C	-6.63	104.08	111.71
1	A	754	GLN	CG-CD-NE2	6.51	126.16	116.40
1	A	556	SER	N-CA-C	6.44	120.76	109.48
1	A	124	LYS	N-CA-C	-6.41	104.38	111.82
1	A	599	LEU	N-CA-C	6.41	118.27	111.28
1	A	578	PRO	CA-N-CD	-6.37	103.09	112.00
1	A	615	ILE	N-CA-C	6.15	122.12	109.34
1	A	124	LYS	O-C-N	6.06	129.73	122.27
1	A	449	ALA	N-CA-C	-5.97	104.86	111.36
1	A	553	MET	N-CA-C	5.89	120.63	113.38
1	A	812	GLU	CA-C-N	5.80	125.76	119.78
1	A	812	GLU	C-N-CA	5.80	125.76	119.78
1	A	1264	GLY	N-CA-C	-5.66	99.76	113.18
1	A	611	ALA	N-CA-C	5.63	120.60	111.37
1	A	1237	ALA	N-CA-C	-5.61	101.97	110.28
1	A	1070	SER	N-CA-C	-5.59	106.30	113.23
1	A	680	PHE	N-CA-C	5.50	116.63	109.64
1	A	59	ILE	CA-C-N	5.46	126.00	120.38
1	A	59	ILE	C-N-CA	5.46	126.00	120.38
1	A	103	LEU	N-CA-C	5.44	118.58	110.14
1	A	1165	GLN	N-CA-C	5.41	118.75	110.20
1	A	525	PRO	N-CA-C	5.33	123.45	112.47
1	A	389	TYR	CA-C-N	-5.27	111.68	122.58
1	A	389	TYR	C-N-CA	-5.27	111.68	122.58
1	A	1244	ASP	N-CA-C	5.24	116.81	108.79
1	A	529	MET	CA-C-N	5.23	126.38	119.84
1	A	529	MET	C-N-CA	5.23	126.38	119.84
1	A	8	GLN	N-CA-C	5.22	119.37	112.89
1	A	66	LYS	CA-C-N	5.09	125.09	120.21
1	A	66	LYS	C-N-CA	5.09	125.09	120.21
1	A	612	SER	N-CA-C	5.04	116.85	111.36

There are no chirality outliers.

There are no planarity outliers.

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	9929	0	9840	632	0
2	A	1	0	0	0	0
3	A	52	0	25	5	0
4	A	671	0	0	304	1
All	All	10653	0	9865	637	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 32.

All (637) 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:926:THR:HG21	1:A:1246:HIS:CG	1.61	1.36
1:A:277:PHE:HB2	4:A:2545:HOH:O	1.17	1.32
1:A:1146:LEU:HD22	4:A:2486:HOH:O	1.19	1.28
1:A:558:THR:HB	4:A:2600:HOH:O	1.14	1.27
1:A:197:ILE:HG12	4:A:2593:HOH:O	1.33	1.26
1:A:279:GLN:HB3	4:A:2648:HOH:O	1.28	1.23
1:A:1181:PRO:HD3	4:A:2611:HOH:O	1.30	1.23
1:A:1005:ASN:HB2	4:A:2454:HOH:O	1.39	1.22
1:A:529:MET:HG2	4:A:2531:HOH:O	1.39	1.20
1:A:718:ARG:HD2	4:A:2490:HOH:O	1.36	1.20
1:A:617:LYS:HE2	4:A:2414:HOH:O	1.43	1.19
1:A:1077:LEU:HD13	4:A:2652:HOH:O	1.37	1.19
1:A:637:ALA:HB3	4:A:2461:HOH:O	1.43	1.18
1:A:926:THR:CG2	1:A:1246:HIS:CD2	2.26	1.17
3:A:1425:GTG:O1G	4:A:2450:HOH:O	1.61	1.17
1:A:334:LEU:HD22	4:A:2597:HOH:O	1.46	1.14
1:A:1114:LYS:HE2	4:A:2580:HOH:O	1.49	1.11
1:A:93:TYR:HA	4:A:2501:HOH:O	1.49	1.11
1:A:447:PHE:CD2	4:A:2634:HOH:O	2.03	1.10
1:A:39:ARG:HB3	4:A:2613:HOH:O	1.52	1.07
1:A:860:VAL:HA	4:A:2578:HOH:O	1.53	1.06
1:A:879:LYS:HG3	4:A:2650:HOH:O	1.54	1.06
1:A:746:GLY:HA2	4:A:2474:HOH:O	1.54	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:719:LEU:HD12	4:A:2471:HOH:O	1.54	1.05
1:A:1262:GLN:HA	1:A:1265:ARG:HH11	1.16	1.05
1:A:93:TYR:HB2	4:A:2606:HOH:O	1.54	1.05
1:A:837:ARG:CD	4:A:2408:HOH:O	2.05	1.05
1:A:926:THR:HG21	1:A:1246:HIS:CD2	1.89	1.04
1:A:856:ILE:HB	4:A:2434:HOH:O	1.54	1.04
1:A:223:THR:HG22	1:A:225:ALA:H	1.24	1.02
1:A:859:SER:HB2	4:A:2463:HOH:O	1.57	1.02
1:A:1148:VAL:CG2	4:A:2667:HOH:O	2.07	1.02
1:A:1060:LYS:HE3	4:A:2555:HOH:O	1.60	1.02
1:A:926:THR:HG23	1:A:1246:HIS:CD2	1.91	1.02
1:A:1257:MET:SD	4:A:2547:HOH:O	2.19	1.01
1:A:505:THR:HA	4:A:2491:HOH:O	1.60	1.01
1:A:749:ASN:HD21	1:A:751:GLU:HB3	1.24	1.00
1:A:475:VAL:HA	4:A:2524:HOH:O	1.60	1.00
1:A:62:THR:HG23	4:A:2428:HOH:O	1.60	0.99
1:A:743:THR:HG22	1:A:744:THR:H	1.24	0.98
1:A:926:THR:CG2	1:A:1246:HIS:CG	2.45	0.98
1:A:323:SER:HB3	4:A:2645:HOH:O	1.64	0.98
1:A:669:PRO:HA	4:A:2493:HOH:O	1.64	0.97
1:A:278:PRO:HD3	4:A:2545:HOH:O	1.65	0.96
1:A:748:VAL:HG22	4:A:2443:HOH:O	1.65	0.96
1:A:1119:LEU:HD11	4:A:2563:HOH:O	1.65	0.96
1:A:557:PRO:HG2	1:A:781:TYR:OH	1.64	0.96
1:A:807:ASN:CG	4:A:2577:HOH:O	2.07	0.96
1:A:837:ARG:HD3	4:A:2408:HOH:O	1.63	0.95
1:A:362:VAL:HA	4:A:2488:HOH:O	1.66	0.95
1:A:747:LYS:HE3	4:A:2645:HOH:O	1.66	0.95
1:A:909:LEU:HD13	4:A:2643:HOH:O	1.65	0.94
1:A:1148:VAL:HG21	4:A:2667:HOH:O	1.66	0.94
1:A:735:ASP:CG	4:A:2423:HOH:O	2.11	0.94
1:A:743:THR:HG22	1:A:744:THR:N	1.81	0.92
1:A:905:LEU:HD23	1:A:1063:MET:HE1	1.53	0.91
1:A:724:THR:HG22	1:A:726:GLN:H	1.34	0.91
1:A:47:ASP:HA	4:A:2629:HOH:O	1.69	0.90
1:A:178:ILE:HD12	4:A:2408:HOH:O	1.70	0.90
1:A:770:LYS:HE2	4:A:2436:HOH:O	1.69	0.90
1:A:22:GLN:NE2	1:A:878:VAL:H	1.70	0.90
1:A:80:ARG:NE	4:A:2508:HOH:O	2.02	0.89
1:A:192:GLU:HG2	4:A:2644:HOH:O	1.72	0.89
1:A:1012:VAL:HG23	4:A:2563:HOH:O	1.72	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1140:ALA:HA	4:A:2655:HOH:O	1.73	0.87
1:A:475:VAL:CA	4:A:2524:HOH:O	2.18	0.87
1:A:1061:TRP:CE3	4:A:2543:HOH:O	2.26	0.87
1:A:303:ARG:NE	4:A:2588:HOH:O	2.01	0.87
1:A:747:LYS:CE	4:A:2645:HOH:O	2.20	0.86
1:A:791:ARG:NH1	4:A:2390:HOH:O	2.07	0.86
1:A:119:ILE:HG12	4:A:2550:HOH:O	1.76	0.86
1:A:749:ASN:HD22	1:A:752:THR:H	1.20	0.86
1:A:659:PHE:HA	4:A:2669:HOH:O	1.74	0.86
1:A:1074:ARG:CZ	4:A:2558:HOH:O	2.22	0.86
1:A:1004:HIS:C	1:A:1006:PRO:HD3	2.01	0.85
1:A:221:ARG:NE	4:A:2411:HOH:O	2.03	0.85
1:A:529:MET:HE2	1:A:661:TYR:CD1	2.11	0.85
1:A:1102:THR:HG21	4:A:2660:HOH:O	1.74	0.85
1:A:81:VAL:H	1:A:671:ASN:HD21	1.24	0.84
1:A:303:ARG:NH2	4:A:2588:HOH:O	2.10	0.84
1:A:965:GLU:N	4:A:2393:HOH:O	2.08	0.84
1:A:510:LEU:HD11	4:A:2646:HOH:O	1.78	0.84
1:A:1004:HIS:CD2	4:A:2487:HOH:O	2.30	0.84
1:A:859:SER:CB	4:A:2463:HOH:O	2.17	0.84
1:A:20:THR:HG21	4:A:2415:HOH:O	1.76	0.84
1:A:515:MET:HE2	1:A:527:SER:HB3	1.58	0.84
1:A:470:LEU:HD11	4:A:2491:HOH:O	1.77	0.83
1:A:749:ASN:ND2	1:A:751:GLU:HB3	1.94	0.83
1:A:758:GLU:HB3	4:A:2642:HOH:O	1.78	0.83
1:A:1119:LEU:HD21	4:A:2563:HOH:O	1.79	0.83
1:A:1074:ARG:NH2	4:A:2558:HOH:O	2.12	0.83
1:A:447:PHE:HD2	4:A:2634:HOH:O	1.45	0.82
1:A:1254:GLN:NE2	4:A:2547:HOH:O	2.12	0.81
1:A:505:THR:C	4:A:2521:HOH:O	2.23	0.81
1:A:924:CYS:HA	4:A:2395:HOH:O	1.81	0.81
1:A:1089:PHE:HB2	4:A:2476:HOH:O	1.78	0.81
1:A:1262:GLN:HA	1:A:1265:ARG:NH1	1.94	0.81
1:A:905:LEU:CD2	1:A:1063:MET:HE1	2.10	0.81
1:A:93:TYR:CB	4:A:2606:HOH:O	2.19	0.81
1:A:122:ARG:NH1	4:A:2550:HOH:O	2.07	0.81
1:A:529:MET:HE3	1:A:529:MET:HA	1.63	0.81
1:A:743:THR:CG2	1:A:744:THR:H	1.93	0.81
1:A:735:ASP:CB	4:A:2423:HOH:O	2.29	0.80
1:A:807:ASN:HB2	4:A:2577:HOH:O	1.80	0.80
1:A:847:CYS:SG	4:A:2537:HOH:O	2.38	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:992:ARG:HG3	1:A:1147:MET:HE3	1.64	0.80
1:A:641:ILE:HG12	4:A:2424:HOH:O	1.81	0.80
1:A:93:TYR:CA	4:A:2501:HOH:O	2.16	0.80
1:A:936:CYS:SG	1:A:940:LEU:HD11	2.22	0.79
1:A:173:GLN:OE1	4:A:2627:HOH:O	2.01	0.79
1:A:718:ARG:NH1	4:A:2490:HOH:O	2.07	0.79
1:A:653:LYS:HE2	4:A:2646:HOH:O	1.81	0.78
1:A:1001:GLY:O	4:A:2487:HOH:O	2.01	0.78
1:A:632:VAL:HA	4:A:2598:HOH:O	1.81	0.78
1:A:101:GLU:HG2	1:A:102:LEU:HD13	1.65	0.78
1:A:345:GLY:O	4:A:2417:HOH:O	2.02	0.77
1:A:747:LYS:CD	4:A:2442:HOH:O	2.31	0.77
1:A:1063:MET:HE2	1:A:1229:MET:HE2	1.66	0.76
1:A:628:ASN:OD1	4:A:2526:HOH:O	2.03	0.76
1:A:1137:ASP:HB3	4:A:2511:HOH:O	1.84	0.76
1:A:221:ARG:NH2	4:A:2411:HOH:O	2.18	0.76
1:A:1152:GLU:OE1	4:A:2664:HOH:O	2.02	0.76
1:A:770:LYS:CE	4:A:2436:HOH:O	2.32	0.76
1:A:314:MET:HE3	1:A:315:PRO:HD2	1.68	0.76
1:A:885:PRO:N	4:A:2650:HOH:O	2.19	0.76
1:A:92:VAL:C	4:A:2501:HOH:O	2.30	0.75
1:A:267:SER:HB3	4:A:2606:HOH:O	1.87	0.75
1:A:447:PHE:CE2	4:A:2634:HOH:O	2.34	0.75
1:A:704:THR:HB	4:A:2610:HOH:O	1.85	0.74
1:A:941:LYS:HE2	4:A:2438:HOH:O	1.85	0.74
1:A:303:ARG:CZ	4:A:2588:HOH:O	2.33	0.74
1:A:792:ILE:HD12	4:A:2488:HOH:O	1.87	0.74
1:A:562:ALA:HB1	4:A:2618:HOH:O	1.87	0.74
1:A:884:ASP:C	4:A:2650:HOH:O	2.29	0.74
1:A:626:ILE:HA	4:A:2424:HOH:O	1.87	0.74
1:A:29:ASP:OD1	4:A:2435:HOH:O	2.05	0.74
1:A:747:LYS:HD3	4:A:2442:HOH:O	1.86	0.74
1:A:1072:ASP:OD1	1:A:1074:ARG:HD3	1.88	0.74
1:A:476:SER:N	4:A:2524:HOH:O	2.20	0.74
1:A:637:ALA:CB	4:A:2461:HOH:O	2.15	0.74
1:A:654:LEU:CD1	4:A:2669:HOH:O	2.35	0.74
1:A:294:CYS:SG	1:A:577:PRO:HD2	2.28	0.73
1:A:56:MET:HG2	1:A:188:TRP:CE2	2.23	0.73
1:A:924:CYS:CA	4:A:2395:HOH:O	2.33	0.73
1:A:926:THR:HG21	1:A:1246:HIS:CB	2.18	0.73
1:A:144:ALA:O	4:A:2386:HOH:O	2.07	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:GLN:HA	1:A:536:GLN:HE21	1.53	0.73
1:A:807:ASN:CB	4:A:2577:HOH:O	2.28	0.73
1:A:114:ARG:HB2	1:A:215:PHE:HE1	1.52	0.73
1:A:114:ARG:HB2	1:A:215:PHE:CE1	2.23	0.73
1:A:855:MET:HE3	4:A:2633:HOH:O	1.86	0.73
1:A:152:GLU:HG2	4:A:2613:HOH:O	1.88	0.72
1:A:379:ARG:HH12	1:A:387:GLN:NE2	1.86	0.72
1:A:626:ILE:CA	4:A:2424:HOH:O	2.37	0.72
1:A:146:GLN:HE22	1:A:805:ARG:H	1.38	0.72
1:A:1062:ARG:NH1	4:A:2651:HOH:O	2.22	0.72
1:A:886:TRP:HA	4:A:2439:HOH:O	1.90	0.72
1:A:654:LEU:HD11	4:A:2669:HOH:O	1.88	0.72
1:A:855:MET:HB3	4:A:2633:HOH:O	1.88	0.71
1:A:1082:ASP:N	4:A:2476:HOH:O	2.22	0.71
1:A:1074:ARG:NH1	4:A:2558:HOH:O	2.22	0.71
1:A:924:CYS:N	4:A:2395:HOH:O	2.23	0.71
1:A:32:LYS:HD2	4:A:2435:HOH:O	1.91	0.71
1:A:797:ARG:HD2	4:A:2624:HOH:O	1.89	0.71
1:A:1082:ASP:O	4:A:2476:HOH:O	2.09	0.71
1:A:191:ARG:NH1	4:A:2629:HOH:O	2.24	0.71
1:A:365:ILE:HB	4:A:2488:HOH:O	1.90	0.71
1:A:506:SER:N	4:A:2521:HOH:O	2.24	0.71
1:A:1202:LYS:HB3	4:A:2651:HOH:O	1.90	0.71
1:A:1060:LYS:HG2	4:A:2459:HOH:O	1.91	0.70
1:A:197:ILE:O	1:A:221:ARG:NH1	2.20	0.70
1:A:93:TYR:N	4:A:2501:HOH:O	2.25	0.70
1:A:1061:TRP:CZ3	4:A:2543:HOH:O	2.42	0.70
1:A:470:LEU:CG	4:A:2491:HOH:O	2.38	0.70
1:A:1185:MET:HB3	4:A:2660:HOH:O	1.92	0.70
1:A:615:ILE:HG23	1:A:616:GLY:H	1.55	0.70
1:A:630:GLU:OE1	4:A:2526:HOH:O	2.08	0.70
1:A:41:ASP:OD2	4:A:2420:HOH:O	2.07	0.69
1:A:221:ARG:NH1	1:A:221:ARG:HB2	2.08	0.69
1:A:637:ALA:N	4:A:2461:HOH:O	2.25	0.69
1:A:718:ARG:NH2	4:A:2620:HOH:O	2.25	0.69
1:A:568:ILE:HG13	4:A:2614:HOH:O	1.90	0.69
1:A:80:ARG:NH2	4:A:2508:HOH:O	2.25	0.69
1:A:441:ARG:HD2	4:A:2427:HOH:O	1.92	0.69
1:A:754:GLN:O	1:A:758:GLU:HG3	1.93	0.69
1:A:821:ILE:HG23	1:A:845:LEU:HD13	1.75	0.69
1:A:941:LYS:CE	4:A:2438:HOH:O	2.39	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ARG:CB	4:A:2613:HOH:O	2.24	0.69
1:A:1005:ASN:HB2	1:A:1130:ARG:HH22	1.57	0.69
1:A:675:HIS:HD2	4:A:2412:HOH:O	1.77	0.68
1:A:475:VAL:C	4:A:2524:HOH:O	2.33	0.68
1:A:978:LEU:O	4:A:2626:HOH:O	2.10	0.68
1:A:80:ARG:CZ	4:A:2508:HOH:O	2.39	0.68
1:A:470:LEU:CD1	4:A:2491:HOH:O	2.34	0.68
1:A:807:ASN:HD22	1:A:807:ASN:H	1.41	0.68
1:A:847:CYS:HA	4:A:2537:HOH:O	1.92	0.68
1:A:457:THR:N	4:A:2592:HOH:O	2.26	0.68
1:A:83:ARG:HG2	1:A:92:VAL:HA	1.75	0.68
1:A:614:SER:O	4:A:2414:HOH:O	2.12	0.67
1:A:921:THR:HG23	1:A:932:ASP:HB2	1.74	0.67
1:A:470:LEU:HG	4:A:2491:HOH:O	1.94	0.67
1:A:633:VAL:HG13	4:A:2602:HOH:O	1.92	0.67
1:A:1263:GLU:OE1	4:A:2589:HOH:O	2.12	0.67
1:A:445:PRO:HD2	4:A:2467:HOH:O	1.93	0.67
1:A:444:ASP:CG	4:A:2467:HOH:O	2.37	0.67
1:A:536:GLN:HE22	1:A:685:THR:H	1.42	0.67
1:A:221:ARG:HB2	1:A:221:ARG:HH11	1.59	0.67
1:A:281:THR:O	1:A:285:MET:HG2	1.94	0.67
1:A:1198:LYS:NZ	4:A:2638:HOH:O	2.25	0.67
1:A:510:LEU:CD1	4:A:2646:HOH:O	2.35	0.67
1:A:1005:ASN:N	1:A:1006:PRO:HD3	2.10	0.66
1:A:747:LYS:NZ	4:A:2645:HOH:O	2.27	0.66
1:A:712:ASP:OD1	4:A:2513:HOH:O	2.12	0.66
1:A:528:ILE:O	1:A:530:PRO:HD3	1.95	0.66
1:A:1137:ASP:CA	4:A:2511:HOH:O	2.44	0.66
1:A:1077:LEU:CD1	4:A:2652:HOH:O	2.14	0.66
1:A:658:GLY:O	4:A:2669:HOH:O	2.13	0.65
1:A:1137:ASP:N	4:A:2511:HOH:O	2.29	0.65
1:A:718:ARG:CZ	4:A:2620:HOH:O	2.44	0.65
1:A:807:ASN:H	1:A:807:ASN:ND2	1.95	0.65
1:A:1005:ASN:HD21	1:A:1263:GLU:HB3	1.61	0.65
1:A:615:ILE:HG23	1:A:616:GLY:N	2.11	0.65
1:A:1140:ALA:HB2	4:A:2511:HOH:O	1.95	0.65
1:A:892:MET:HB2	1:A:1232:THR:HG23	1.78	0.65
1:A:1062:ARG:HD2	1:A:1243:GLU:OE2	1.97	0.65
1:A:923:ARG:C	4:A:2395:HOH:O	2.39	0.65
1:A:1005:ASN:ND2	1:A:1263:GLU:HB3	2.12	0.65
1:A:507:VAL:N	4:A:2521:HOH:O	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1140:ALA:CA	4:A:2655:HOH:O	2.34	0.64
1:A:637:ALA:CA	4:A:2461:HOH:O	2.44	0.64
1:A:1130:ARG:NH1	4:A:2454:HOH:O	2.03	0.64
1:A:856:ILE:HD13	4:A:2434:HOH:O	1.96	0.64
3:A:1425:GTG:H5B1	4:A:2615:HOH:O	1.96	0.64
1:A:313:VAL:HG21	4:A:2558:HOH:O	1.97	0.64
1:A:576:SER:O	1:A:577:PRO:C	2.40	0.64
1:A:995:TRP:CZ2	1:A:1006:PRO:HG3	2.33	0.64
1:A:20:THR:HG22	1:A:21:ASP:O	1.98	0.64
1:A:582:ILE:HG21	1:A:757:LEU:HD21	1.79	0.64
1:A:558:THR:HG22	1:A:558:THR:O	1.98	0.63
1:A:415:LYS:NZ	4:A:2499:HOH:O	2.11	0.63
1:A:1029:GLU:CD	1:A:1029:GLU:H	2.05	0.63
1:A:65:THR:HG23	4:A:2451:HOH:O	1.97	0.63
1:A:22:GLN:HE21	1:A:878:VAL:H	1.44	0.63
1:A:393:PRO:HD3	1:A:591:ALA:O	1.99	0.63
1:A:352:LYS:HG2	4:A:2661:HOH:O	1.98	0.63
1:A:425:LEU:HD13	1:A:698:MET:HE3	1.79	0.63
1:A:365:ILE:HD12	4:A:2488:HOH:O	1.99	0.63
1:A:955:PRO:HG3	1:A:1031:LEU:HA	1.81	0.62
1:A:298:GLU:HB2	1:A:311:MET:HE2	1.81	0.62
1:A:227:PRO:HB2	1:A:228:PRO:HD3	1.82	0.62
1:A:632:VAL:HG13	4:A:2552:HOH:O	1.98	0.62
1:A:1087:ASP:HB3	1:A:1088:PRO:HD3	1.81	0.62
1:A:617:LYS:CE	4:A:2414:HOH:O	2.17	0.62
1:A:1082:ASP:HB2	1:A:1083:PRO:CD	2.29	0.62
1:A:542:HIS:NE2	1:A:690:GLU:HG3	2.15	0.62
1:A:817:ILE:O	1:A:821:ILE:HG12	2.00	0.62
1:A:1201:PRO:HB2	1:A:1204:GLY:O	2.00	0.62
1:A:221:ARG:CZ	4:A:2411:HOH:O	2.38	0.62
1:A:515:MET:HE2	1:A:527:SER:CB	2.29	0.62
1:A:909:LEU:HB3	4:A:2643:HOH:O	1.99	0.62
1:A:1075:LEU:HG	4:A:2652:HOH:O	2.00	0.62
1:A:837:ARG:HG3	4:A:2408:HOH:O	2.00	0.62
1:A:416:ASP:CA	4:A:2557:HOH:O	2.47	0.61
1:A:776:ASP:OD1	1:A:778:THR:HB	2.00	0.61
1:A:572:VAL:HG13	1:A:789:GLY:O	2.00	0.61
1:A:653:LYS:NZ	4:A:2453:HOH:O	2.32	0.61
1:A:78:LEU:HD12	1:A:80:ARG:NH2	2.16	0.61
1:A:423:ARG:HE	1:A:427:ARG:NH2	1.98	0.61
1:A:362:VAL:CA	4:A:2488:HOH:O	2.38	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:994:GLU:OE1	4:A:2448:HOH:O	2.16	0.60
1:A:716:VAL:HG13	1:A:756:ASP:HB2	1.84	0.60
1:A:1061:TRP:HE3	4:A:2543:HOH:O	1.71	0.60
1:A:2:SER:N	1:A:6:LEU:HB2	2.17	0.60
1:A:2:SER:O	1:A:5:ILE:N	2.34	0.60
1:A:210:LEU:HB2	1:A:213:GLY:O	2.02	0.60
1:A:614:SER:HA	4:A:2414:HOH:O	2.01	0.60
1:A:1112:MET:CE	1:A:1150:LEU:HD11	2.32	0.60
1:A:1238:VAL:O	4:A:2401:HOH:O	2.16	0.59
1:A:807:ASN:HD22	1:A:807:ASN:N	1.98	0.59
1:A:926:THR:HG23	1:A:1246:HIS:HD2	1.58	0.59
1:A:437:ALA:HB2	1:A:610:VAL:HG22	1.84	0.59
1:A:221:ARG:HB3	4:A:2593:HOH:O	2.02	0.59
1:A:446:LEU:HD13	1:A:1149:GLY:HA3	1.83	0.59
3:A:1425:GTG:H4'	4:A:2591:HOH:O	2.03	0.59
1:A:146:GLN:NE2	1:A:805:ARG:H	2.01	0.59
1:A:1060:LYS:CE	4:A:2555:HOH:O	2.32	0.59
1:A:221:ARG:O	4:A:2593:HOH:O	2.16	0.58
1:A:1082:ASP:HB2	1:A:1083:PRO:HD2	1.84	0.58
1:A:137:GLY:HA2	4:A:2639:HOH:O	2.03	0.58
1:A:749:ASN:HD22	1:A:752:THR:N	1.98	0.58
1:A:879:LYS:HE2	4:A:2650:HOH:O	2.01	0.58
1:A:1014:HIS:O	1:A:1018:GLN:HG3	2.03	0.58
1:A:1112:MET:HE1	4:A:2667:HOH:O	2.03	0.58
1:A:491:ILE:N	4:A:2592:HOH:O	2.36	0.58
1:A:632:VAL:CA	4:A:2598:HOH:O	2.46	0.58
1:A:1224:PHE:HE2	4:A:2611:HOH:O	1.86	0.58
1:A:837:ARG:CG	4:A:2408:HOH:O	2.41	0.58
1:A:582:ILE:HG21	1:A:757:LEU:CD2	2.34	0.57
1:A:76:ASP:OD2	1:A:80:ARG:NH1	2.37	0.57
1:A:542:HIS:NE2	1:A:690:GLU:CG	2.66	0.57
1:A:557:PRO:HG2	1:A:781:TYR:HH	1.66	0.57
1:A:595:TRP:HA	1:A:599:LEU:HB2	1.86	0.57
1:A:627:VAL:N	4:A:2424:HOH:O	2.37	0.57
1:A:338:TYR:O	1:A:340:LEU:HG	2.04	0.57
1:A:557:PRO:HG2	1:A:781:TYR:CZ	2.39	0.57
1:A:2:SER:O	1:A:3:SER:C	2.48	0.57
1:A:137:GLY:O	4:A:2639:HOH:O	2.18	0.57
1:A:414:LEU:HD11	1:A:418:THR:HG21	1.86	0.57
1:A:1262:GLN:HG3	1:A:1265:ARG:NH1	2.19	0.57
1:A:1134:LEU:HD23	1:A:1257:MET:HE2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:907:ARG:HB3	1:A:908:PRO:HD3	1.86	0.56
1:A:416:ASP:N	4:A:2557:HOH:O	2.39	0.56
1:A:1007:PRO:HD2	1:A:1144:GLN:NE2	2.20	0.56
1:A:743:THR:CG2	1:A:744:THR:N	2.51	0.56
1:A:1137:ASP:O	4:A:2511:HOH:O	2.18	0.56
1:A:414:LEU:CD1	1:A:418:THR:HG21	2.35	0.56
1:A:854:THR:OG1	1:A:856:ILE:HD11	2.05	0.56
1:A:944:GLN:HB3	1:A:948:MET:CE	2.35	0.56
1:A:32:LYS:HG2	1:A:851:ARG:CZ	2.35	0.56
1:A:829:VAL:HG13	1:A:890:TRP:CE2	2.40	0.56
1:A:837:ARG:CZ	4:A:2408:HOH:O	2.52	0.56
1:A:936:CYS:O	1:A:940:LEU:HG	2.06	0.56
1:A:670:GLY:N	4:A:2493:HOH:O	2.26	0.56
1:A:1027:THR:HG22	1:A:1030:GLU:CG	2.36	0.56
1:A:299:TRP:CD2	1:A:303:ARG:HG2	2.41	0.56
1:A:533:VAL:HB	1:A:534:PRO:HD3	1.87	0.56
1:A:716:VAL:O	1:A:720:MET:HG3	2.05	0.55
3:A:1425:GTG:C4E	4:A:2615:HOH:O	2.54	0.55
1:A:39:ARG:C	4:A:2613:HOH:O	2.48	0.55
1:A:1002:ILE:HD13	1:A:1136:ALA:HB2	1.88	0.55
1:A:1005:ASN:CB	1:A:1130:ARG:HH22	2.20	0.55
1:A:363:ARG:HH22	1:A:834:GLN:HE22	1.54	0.55
1:A:837:ARG:NE	4:A:2408:HOH:O	2.27	0.55
1:A:797:ARG:HG2	1:A:797:ARG:HH11	1.72	0.55
1:A:105:PRO:HG3	1:A:218:MET:HE2	1.88	0.55
1:A:582:ILE:HD12	1:A:757:LEU:HD11	1.89	0.55
1:A:626:ILE:C	4:A:2424:HOH:O	2.49	0.55
1:A:756:ASP:C	1:A:756:ASP:OD1	2.50	0.54
1:A:140:ALA:HB3	4:A:2639:HOH:O	2.07	0.54
1:A:246:ASP:O	1:A:250:VAL:HG23	2.08	0.54
1:A:125:ASP:HB2	4:A:2546:HOH:O	2.07	0.54
1:A:944:GLN:HB3	1:A:948:MET:HE2	1.89	0.54
1:A:87:GLN:HG2	1:A:268:TRP:CH2	2.43	0.54
1:A:1027:THR:HG22	1:A:1030:GLU:HG3	1.88	0.54
1:A:188:TRP:CZ2	1:A:192:GLU:HG3	2.42	0.54
1:A:541:PRO:HB2	1:A:648:ILE:HD11	1.89	0.54
1:A:120:GLU:O	1:A:124:LYS:HG3	2.08	0.53
1:A:1148:VAL:HG23	4:A:2667:HOH:O	1.90	0.53
1:A:385:VAL:HG22	1:A:515:MET:SD	2.48	0.53
1:A:744:THR:C	1:A:746:GLY:H	2.16	0.53
1:A:1063:MET:CE	1:A:1229:MET:HE2	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:879:LYS:CG	4:A:2650:HOH:O	2.33	0.53
1:A:303:ARG:HG3	1:A:303:ARG:HH11	1.72	0.53
1:A:490:LYS:C	4:A:2592:HOH:O	2.51	0.53
1:A:603:MET:HE1	1:A:651:LEU:HD23	1.88	0.53
1:A:856:ILE:CD1	4:A:2434:HOH:O	2.55	0.53
1:A:907:ARG:NH2	4:A:2459:HOH:O	2.42	0.53
1:A:1065:GLU:H	1:A:1065:GLU:CD	2.16	0.53
1:A:1119:LEU:CG	4:A:2563:HOH:O	2.55	0.53
1:A:859:SER:HB3	4:A:2434:HOH:O	2.09	0.53
1:A:1112:MET:HE1	1:A:1150:LEU:HD11	1.91	0.53
1:A:43:TYR:HE2	4:A:2613:HOH:O	1.91	0.53
1:A:195:ARG:HD3	4:A:2666:HOH:O	2.09	0.53
1:A:603:MET:HE1	1:A:651:LEU:HB3	1.89	0.53
1:A:441:ARG:CD	4:A:2427:HOH:O	2.51	0.53
1:A:421:ILE:HD11	1:A:701:THR:HG22	1.91	0.52
1:A:477:LEU:HB3	1:A:496:GLN:HB3	1.91	0.52
1:A:1063:MET:HE2	1:A:1229:MET:CE	2.38	0.52
1:A:614:SER:CA	4:A:2414:HOH:O	2.57	0.52
1:A:1137:ASP:C	4:A:2511:HOH:O	2.52	0.52
1:A:396:LYS:HD2	1:A:765:GLU:HB3	1.92	0.52
1:A:836:GLN:HE21	1:A:886:TRP:CG	2.27	0.52
1:A:1009:LEU:HA	4:A:2563:HOH:O	2.08	0.52
1:A:115:LEU:HD21	1:A:134:THR:HA	1.91	0.52
1:A:723:LEU:HG	4:A:2471:HOH:O	2.08	0.52
1:A:112:TYR:HB3	1:A:215:PHE:HB3	1.91	0.52
1:A:614:SER:C	4:A:2414:HOH:O	2.52	0.52
1:A:951:LEU:HD13	1:A:1037:THR:HG22	1.92	0.52
1:A:820:GLN:O	1:A:824:VAL:HG23	2.10	0.51
1:A:829:VAL:HG13	1:A:890:TRP:NE1	2.25	0.51
1:A:1119:LEU:CD2	4:A:2563:HOH:O	2.49	0.51
1:A:792:ILE:CD1	4:A:2488:HOH:O	2.52	0.51
1:A:770:LYS:HG2	4:A:2436:HOH:O	2.10	0.51
1:A:846:CYS:SG	1:A:870:PHE:CD1	3.04	0.51
1:A:3:SER:O	1:A:7:THR:N	2.41	0.51
1:A:22:GLN:HE22	1:A:878:VAL:H	1.53	0.51
1:A:617:LYS:HB2	4:A:2414:HOH:O	2.09	0.51
1:A:748:VAL:HA	4:A:2059:HOH:O	2.10	0.51
1:A:582:ILE:HB	1:A:738:MET:HB3	1.92	0.51
1:A:595:TRP:HB3	4:A:2608:HOH:O	2.09	0.51
1:A:797:ARG:HG2	1:A:797:ARG:NH1	2.25	0.51
1:A:1004:HIS:NE2	4:A:2487:HOH:O	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1119:LEU:CD1	4:A:2563:HOH:O	2.39	0.51
1:A:39:ARG:CA	4:A:2613:HOH:O	2.52	0.50
1:A:515:MET:HA	1:A:529:MET:HE1	1.92	0.50
1:A:289:LEU:HD21	1:A:316:LEU:HB3	1.92	0.50
1:A:171:VAL:HG11	1:A:1090:LEU:HD11	1.93	0.50
1:A:323:SER:CB	4:A:2645:HOH:O	2.41	0.50
1:A:298:GLU:HB2	1:A:311:MET:CE	2.42	0.50
1:A:617:LYS:NZ	4:A:2414:HOH:O	2.42	0.50
1:A:926:THR:HG1	1:A:1246:HIS:CD2	2.29	0.50
1:A:1012:VAL:CG2	4:A:2563:HOH:O	2.43	0.50
1:A:193:ILE:HD13	1:A:229:LEU:HD21	1.94	0.50
1:A:634:GLY:N	4:A:2522:HOH:O	2.44	0.50
1:A:686:ALA:O	1:A:687:THR:C	2.55	0.50
1:A:797:ARG:HD3	4:A:2497:HOH:O	2.10	0.49
1:A:1004:HIS:C	1:A:1006:PRO:CD	2.82	0.49
1:A:127:ASP:O	1:A:131:ARG:HG3	2.12	0.49
1:A:148:LYS:HG2	1:A:803:LYS:HB2	1.93	0.49
1:A:484:PRO:HB2	1:A:1021:GLN:HE21	1.77	0.49
1:A:704:THR:CB	4:A:2610:HOH:O	2.50	0.49
1:A:515:MET:CA	1:A:529:MET:HE1	2.43	0.49
1:A:516:GLY:O	1:A:517:LEU:HD12	2.13	0.49
1:A:1007:PRO:HD2	1:A:1144:GLN:HE22	1.76	0.49
3:A:1425:GTG:C4D	4:A:2591:HOH:O	2.58	0.49
1:A:93:TYR:CE1	1:A:379:ARG:HD3	2.48	0.49
1:A:223:THR:HG21	4:A:2200:HOH:O	2.10	0.49
1:A:837:ARG:HG2	4:A:2368:HOH:O	2.12	0.49
1:A:275:SER:O	1:A:278:PRO:HD2	2.12	0.49
1:A:847:CYS:CA	4:A:2537:HOH:O	2.53	0.49
1:A:1200:LEU:C	1:A:1200:LEU:HD23	2.38	0.49
1:A:570:LEU:HD21	1:A:730:VAL:HG21	1.94	0.48
1:A:297:LEU:HB2	4:A:2621:HOH:O	2.13	0.48
1:A:532:ASN:OD1	1:A:535:GLN:HG3	2.13	0.48
1:A:1064:CYS:HB3	1:A:1065:GLU:OE2	2.13	0.48
1:A:1121:VAL:HG13	4:A:2566:HOH:O	2.12	0.48
1:A:106:HIS:CE1	1:A:108:THR:H	2.31	0.48
1:A:563:VAL:HG12	1:A:568:ILE:HD11	1.95	0.48
1:A:1005:ASN:N	1:A:1006:PRO:CD	2.77	0.48
1:A:92:VAL:HG11	1:A:383:GLU:HB3	1.94	0.48
1:A:501:PRO:HB2	1:A:504:HIS:HD2	1.78	0.48
1:A:392:SER:HB3	1:A:393:PRO:HD2	1.95	0.48
1:A:1130:ARG:NH2	4:A:2454:HOH:O	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:LEU:O	1:A:730:VAL:HA	2.13	0.48
1:A:379:ARG:CB	4:A:2501:HOH:O	2.62	0.48
1:A:735:ASP:OD2	4:A:2423:HOH:O	2.19	0.48
1:A:757:LEU:HD22	1:A:773:ILE:HG21	1.96	0.48
1:A:856:ILE:O	4:A:2463:HOH:O	2.20	0.48
1:A:67:PRO:O	1:A:97:CYS:HB3	2.14	0.48
1:A:706:TRP:O	1:A:710:HIS:HD2	1.95	0.48
1:A:797:ARG:C	1:A:799:PRO:HD3	2.38	0.48
1:A:836:GLN:HE21	1:A:886:TRP:CD1	2.32	0.48
1:A:24:ASN:ND2	1:A:28:GLU:OE2	2.42	0.47
1:A:394:GLU:OE2	4:A:2641:HOH:O	2.20	0.47
1:A:564:ILE:HG22	1:A:1185:MET:HB2	1.96	0.47
1:A:566:LYS:HD3	1:A:782:LEU:O	2.14	0.47
1:A:631:SER:C	4:A:2598:HOH:O	2.56	0.47
1:A:410:GLU:N	1:A:649:GLN:OE1	2.38	0.47
1:A:606:ILE:O	1:A:610:VAL:HB	2.14	0.47
1:A:1075:LEU:HA	1:A:1076:PRO:HD3	1.80	0.47
1:A:20:THR:CG2	4:A:2415:HOH:O	2.47	0.47
1:A:285:MET:HG3	1:A:365:ILE:HD11	1.96	0.47
1:A:294:CYS:SG	1:A:314:MET:HB3	2.54	0.47
1:A:389:TYR:HD1	1:A:679:THR:HB	1.79	0.47
1:A:821:ILE:HD12	1:A:845:LEU:HD13	1.97	0.47
1:A:167:LEU:HD22	1:A:837:ARG:HD2	1.95	0.47
1:A:385:VAL:HG21	1:A:663:VAL:CG2	2.44	0.47
1:A:223:THR:HG22	1:A:224:SER:N	2.29	0.47
1:A:20:THR:CB	4:A:2415:HOH:O	2.63	0.47
1:A:92:VAL:CG1	1:A:383:GLU:HB3	2.44	0.47
1:A:149:ALA:HB1	1:A:150:PRO:CD	2.44	0.47
1:A:856:ILE:HD13	4:A:2176:HOH:O	2.14	0.47
1:A:746:GLY:CA	4:A:2474:HOH:O	2.35	0.47
1:A:829:VAL:HG13	1:A:890:TRP:CD1	2.49	0.47
1:A:390:THR:CG2	1:A:391:GLN:HG3	2.45	0.47
1:A:632:VAL:N	4:A:2598:HOH:O	2.47	0.47
1:A:855:MET:C	1:A:856:ILE:HD12	2.40	0.47
1:A:1029:GLU:CD	1:A:1029:GLU:N	2.72	0.47
1:A:518:ARG:HA	1:A:804:GLU:OE2	2.15	0.47
1:A:1240:ILE:C	4:A:2543:HOH:O	2.58	0.47
1:A:194:CYS:SG	1:A:206:PRO:HG2	2.55	0.46
1:A:671:ASN:N	1:A:671:ASN:HD22	2.12	0.46
1:A:797:ARG:CZ	4:A:2497:HOH:O	2.63	0.46
1:A:1027:THR:HG23	1:A:1030:GLU:H	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ARG:NH2	4:A:2629:HOH:O	2.48	0.46
1:A:990:ARG:HB3	4:A:2486:HOH:O	2.14	0.46
1:A:385:VAL:HG21	1:A:663:VAL:HG21	1.96	0.46
1:A:557:PRO:HG2	1:A:781:TYR:CE2	2.51	0.46
1:A:702:PHE:HB2	1:A:763:TYR:CE2	2.50	0.46
1:A:616:GLY:C	1:A:617:LYS:HG3	2.40	0.46
1:A:1134:LEU:HA	1:A:1257:MET:CE	2.46	0.46
1:A:1027:THR:CG2	1:A:1030:GLU:H	2.29	0.46
1:A:299:TRP:CE2	1:A:303:ARG:HG2	2.51	0.46
1:A:456:VAL:HA	4:A:2592:HOH:O	2.15	0.46
1:A:542:HIS:CE1	1:A:690:GLU:HG3	2.50	0.46
1:A:698:MET:HE2	1:A:698:MET:HA	1.97	0.46
1:A:879:LYS:CE	4:A:2650:HOH:O	2.60	0.46
1:A:9:PHE:O	1:A:13:ILE:HG13	2.16	0.46
1:A:389:TYR:OH	1:A:527:SER:HB2	2.16	0.46
1:A:448:GLN:NE2	1:A:620:MET:H	2.14	0.46
1:A:633:VAL:HA	4:A:2244:HOH:O	2.16	0.46
1:A:930:ASN:ND2	4:A:2395:HOH:O	2.47	0.46
1:A:379:ARG:HB3	4:A:2501:HOH:O	2.16	0.46
1:A:512:ASP:HB3	1:A:662:ARG:HG3	1.98	0.46
1:A:833:LEU:HD12	1:A:838:TRP:CD2	2.51	0.46
1:A:223:THR:CG2	1:A:224:SER:N	2.79	0.45
1:A:747:LYS:NZ	4:A:2442:HOH:O	2.15	0.45
1:A:779:ALA:HB3	1:A:786:PHE:HB2	1.96	0.45
1:A:1254:GLN:CD	4:A:2547:HOH:O	2.54	0.45
1:A:935:ARG:O	1:A:939:GLU:HG3	2.16	0.45
1:A:909:LEU:HD22	4:A:2643:HOH:O	2.17	0.45
1:A:557:PRO:HD2	1:A:730:VAL:HG12	1.97	0.45
1:A:577:PRO:HD3	1:A:788:PHE:HA	1.99	0.45
1:A:724:THR:HG22	1:A:726:GLN:N	2.15	0.45
1:A:809:SER:CB	4:A:2577:HOH:O	2.63	0.45
1:A:20:THR:HG22	1:A:21:ASP:N	2.31	0.45
1:A:665:ASP:HB3	1:A:671:ASN:HB2	1.98	0.45
1:A:833:LEU:HD12	1:A:838:TRP:CE3	2.52	0.45
1:A:1140:ALA:CB	4:A:2655:HOH:O	2.62	0.45
1:A:389:TYR:HE2	1:A:515:MET:CE	2.30	0.45
1:A:83:ARG:NH1	1:A:84:LYS:O	2.49	0.45
1:A:94:VAL:HG22	1:A:139:ILE:HG23	1.99	0.45
1:A:314:MET:HE3	1:A:315:PRO:CD	2.43	0.45
1:A:421:ILE:HD11	1:A:701:THR:CG2	2.47	0.44
1:A:456:VAL:C	4:A:2592:HOH:O	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:VAL:HG13	1:A:651:LEU:HB2	1.98	0.44
1:A:748:VAL:HA	4:A:2443:HOH:O	2.16	0.44
1:A:940:LEU:HG	1:A:940:LEU:H	1.70	0.44
1:A:3:SER:O	1:A:7:THR:HB	2.17	0.44
1:A:221:ARG:HH11	1:A:221:ARG:CB	2.30	0.44
1:A:1140:ALA:CB	4:A:2511:HOH:O	2.59	0.44
1:A:198:SER:HA	1:A:217:LEU:HD21	1.98	0.44
1:A:287:GLU:HB2	4:A:2310:HOH:O	2.16	0.44
1:A:926:THR:O	1:A:926:THR:HG22	2.17	0.44
1:A:1002:ILE:HG21	1:A:1136:ALA:HB2	2.00	0.44
1:A:56:MET:HG2	1:A:188:TRP:CD2	2.53	0.44
1:A:273:THR:O	1:A:276:ILE:HG12	2.17	0.44
1:A:436:MET:HE3	1:A:544:LEU:HD13	1.99	0.44
1:A:965:GLU:C	1:A:967:ARG:N	2.74	0.44
1:A:580:GLN:OE1	1:A:747:LYS:HB2	2.18	0.44
1:A:279:GLN:HG3	1:A:327:ASN:HD22	1.83	0.44
1:A:501:PRO:HD2	1:A:504:HIS:CD2	2.53	0.44
1:A:837:ARG:NH1	4:A:2408:HOH:O	2.51	0.44
1:A:946:TYR:OH	1:A:1050:SER:HB3	2.17	0.44
1:A:1112:MET:HE3	1:A:1150:LEU:HD11	2.00	0.44
1:A:421:ILE:HD13	1:A:763:TYR:HE1	1.82	0.43
1:A:537:GLN:O	1:A:647:MET:HE2	2.18	0.43
1:A:555:LEU:HB3	1:A:729:TYR:O	2.18	0.43
1:A:149:ALA:HB1	1:A:150:PRO:HD2	2.00	0.43
1:A:485:VAL:HG12	1:A:1021:GLN:CG	2.48	0.43
1:A:568:ILE:N	1:A:569:PRO:CD	2.80	0.43
1:A:659:PHE:CE2	1:A:681:PRO:HD3	2.52	0.43
1:A:39:ARG:HH11	1:A:39:ARG:HG2	1.84	0.43
1:A:87:GLN:HB3	1:A:268:TRP:CZ2	2.54	0.43
1:A:1130:ARG:CZ	4:A:2454:HOH:O	2.58	0.43
1:A:441:ARG:NH1	4:A:2580:HOH:O	2.39	0.43
1:A:470:LEU:HD23	1:A:477:LEU:HD21	2.00	0.43
1:A:1180:VAL:HA	4:A:2611:HOH:O	2.18	0.43
1:A:20:THR:CG2	1:A:21:ASP:N	2.81	0.43
1:A:814:TRP:CD2	1:A:815:PRO:HB3	2.53	0.43
1:A:948:MET:HE2	1:A:1042:ARG:HA	2.01	0.43
1:A:1002:ILE:HD13	1:A:1136:ALA:CB	2.49	0.43
1:A:525:PRO:HD3	4:A:2001:HOH:O	2.19	0.43
1:A:473:ILE:HG13	1:A:475:VAL:HG23	2.01	0.43
1:A:845:LEU:HD23	1:A:845:LEU:HA	1.90	0.43
1:A:169:ASP:HA	1:A:170:PRO:HD3	1.90	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:ALA:HB3	1:A:541:PRO:HD3	2.01	0.43
1:A:2:SER:O	1:A:4:MET:N	2.52	0.42
1:A:39:ARG:HE	1:A:208:LEU:HD22	1.84	0.42
1:A:47:ASP:CA	4:A:2629:HOH:O	2.47	0.42
1:A:379:ARG:HH12	1:A:387:GLN:HE22	1.61	0.42
1:A:406:GLY:HA3	1:A:630:GLU:O	2.19	0.42
1:A:639:ARG:HA	1:A:640:PRO:HD3	1.92	0.42
1:A:1109:THR:HG22	1:A:1168:ASN:HD21	1.83	0.42
1:A:32:LYS:CD	4:A:2435:HOH:O	2.59	0.42
1:A:379:ARG:NH2	4:A:2011:HOH:O	2.50	0.42
1:A:859:SER:HB3	4:A:2463:HOH:O	2.02	0.42
1:A:515:MET:HA	1:A:529:MET:CE	2.49	0.42
1:A:187:LEU:HD23	1:A:187:LEU:HA	1.87	0.42
1:A:287:GLU:N	4:A:2505:HOH:O	2.49	0.42
1:A:3:SER:O	1:A:7:THR:CB	2.67	0.42
1:A:270:ILE:HA	4:A:2235:HOH:O	2.20	0.42
1:A:435:ARG:O	1:A:439:GLN:HG3	2.19	0.42
1:A:281:THR:OG1	1:A:282:LEU:N	2.48	0.42
1:A:942:LEU:HD23	1:A:942:LEU:C	2.45	0.42
1:A:59:ILE:HA	1:A:60:PRO:HD3	1.93	0.42
1:A:603:MET:HE3	1:A:648:ILE:HG23	2.02	0.42
1:A:1201:PRO:HA	1:A:1242:LEU:O	2.19	0.42
1:A:1253:GLY:O	1:A:1257:MET:HG3	2.20	0.42
1:A:27:PHE:CG	1:A:867:MET:HB3	2.54	0.42
1:A:72:TYR:O	1:A:83:ARG:HD2	2.20	0.42
1:A:125:ASP:CB	4:A:2546:HOH:O	2.66	0.42
1:A:380:THR:OG1	1:A:383:GLU:HG2	2.20	0.42
1:A:603:MET:CE	1:A:651:LEU:HB3	2.50	0.42
1:A:834:GLN:NE2	4:A:2003:HOH:O	2.50	0.42
1:A:1007:PRO:HD2	1:A:1144:GLN:CD	2.45	0.42
1:A:1212:PRO:HA	1:A:1213:PRO:HD3	1.89	0.42
1:A:385:VAL:CG2	1:A:515:MET:SD	3.08	0.42
1:A:654:LEU:HD12	4:A:2669:HOH:O	2.09	0.42
1:A:268:TRP:N	4:A:2606:HOH:O	2.50	0.41
1:A:390:THR:HG23	1:A:391:GLN:HG3	2.02	0.41
1:A:529:MET:HG3	1:A:661:TYR:CZ	2.55	0.41
1:A:558:THR:CB	4:A:2600:HOH:O	2.03	0.41
1:A:39:ARG:HH11	1:A:39:ARG:CG	2.33	0.41
1:A:389:TYR:HE2	1:A:515:MET:HE1	1.84	0.41
1:A:416:ASP:CB	4:A:2557:HOH:O	2.68	0.41
1:A:626:ILE:CG2	1:A:638:ALA:HB1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:941:LYS:HE3	4:A:2438:HOH:O	2.15	0.41
1:A:1003:ILE:HG12	1:A:1131:LEU:HD21	2.02	0.41
1:A:780:GLU:CD	1:A:780:GLU:C	2.87	0.41
1:A:1012:VAL:HB	1:A:1013:PRO:HD3	2.01	0.41
1:A:96:ASN:OD1	1:A:265:SER:HA	2.20	0.41
1:A:193:ILE:O	1:A:197:ILE:HG13	2.20	0.41
1:A:744:THR:C	1:A:746:GLY:N	2.79	0.41
1:A:66:LYS:HA	1:A:67:PRO:HD3	1.89	0.41
1:A:436:MET:HE2	1:A:442:THR:OG1	2.20	0.41
1:A:879:LYS:CD	4:A:2650:HOH:O	2.65	0.41
1:A:629:ASP:O	1:A:636:ARG:HA	2.20	0.41
1:A:980:GLN:HE21	1:A:980:GLN:HB3	1.69	0.41
1:A:1201:PRO:HG3	1:A:1209:THR:HG21	2.01	0.41
1:A:73:TYR:HB2	1:A:132:ILE:HG23	2.03	0.41
1:A:523:ARG:HD2	4:A:2548:HOH:O	2.21	0.41
1:A:531:LEU:HD11	1:A:684:SER:HB2	2.03	0.41
1:A:411:ILE:C	1:A:411:ILE:HD12	2.45	0.41
1:A:466:LEU:HD12	1:A:508:ALA:HB1	2.02	0.41
1:A:520:GLN:OE1	1:A:523:ARG:NH1	2.54	0.41
1:A:542:HIS:NE2	1:A:690:GLU:HG2	2.35	0.41
1:A:574:ALA:HB1	1:A:581:SER:HB3	2.03	0.41
1:A:188:TRP:CE2	1:A:192:GLU:HG3	2.55	0.41
1:A:1021:GLN:C	1:A:1023:ALA:H	2.29	0.41
1:A:1091:LYS:O	1:A:1095:VAL:HB	2.22	0.41
1:A:298:GLU:CB	1:A:311:MET:HE2	2.50	0.40
1:A:483:LEU:HA	1:A:483:LEU:HD23	1.81	0.40
1:A:812:GLU:HA	1:A:813:PRO:HD3	1.87	0.40
1:A:226:ILE:O	1:A:230:LEU:HG	2.21	0.40
1:A:444:ASP:HA	4:A:2467:HOH:O	2.20	0.40
1:A:532:ASN:OD1	1:A:534:PRO:HD2	2.21	0.40
1:A:853:ARG:HA	1:A:862:TYR:CD1	2.56	0.40
1:A:948:MET:HE1	1:A:1042:ARG:HG3	2.03	0.40
1:A:104:GLU:HG3	1:A:116:SER:HB2	2.03	0.40
1:A:425:LEU:HB2	1:A:698:MET:HE1	2.04	0.40
1:A:631:SER:OG	4:A:2574:HOH:O	2.04	0.40
1:A:289:LEU:HD12	1:A:289:LEU:HA	1.92	0.40
1:A:456:VAL:CA	4:A:2592:HOH:O	2.70	0.40
1:A:501:PRO:HB2	1:A:504:HIS:CD2	2.57	0.40
1:A:607:HIS:HB2	1:A:648:ILE:HG21	2.04	0.40
1:A:799:PRO:HB2	1:A:802:GLY:HA3	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2299:HOH:O	4:A:2582:HOH:O[4_475]	2.11	0.09

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1252/1267 (99%)	1175 (94%)	66 (5%)	11 (1%)	14 27

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	578	PRO
1	A	615	ILE
1	A	498	ALA
1	A	687	THR
1	A	1201	PRO
1	A	91	ASP
1	A	631	SER
1	A	1005	ASN
1	A	276	ILE
1	A	857	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1076/1083 (99%)	1024 (95%)	52 (5%)	23	46

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	37	PHE
1	A	57	LEU
1	A	63	ILE
1	A	80	ARG
1	A	84	LYS
1	A	85	THR
1	A	87	GLN
1	A	92	VAL
1	A	102	LEU
1	A	167	LEU
1	A	174	LYS
1	A	187	LEU
1	A	210	LEU
1	A	214	VAL
1	A	287	GLU
1	A	298	GLU
1	A	366	ARG
1	A	378	VAL
1	A	387	GLN
1	A	390	THR
1	A	414	LEU
1	A	416	ASP
1	A	431	LEU
1	A	466	LEU
1	A	470	LEU
1	A	503	SER
1	A	517	LEU
1	A	536	GLN
1	A	538	VAL
1	A	557	PRO
1	A	578	PRO
1	A	610	VAL
1	A	627	VAL
1	A	657	ARG
1	A	700	GLU
1	A	726	GLN
1	A	756	ASP

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Mol	Chain	Res	Type
1	A	778	THR
1	A	807	ASN
1	A	815	PRO
1	A	845	LEU
1	A	894	THR
1	A	940	LEU
1	A	953	ARG
1	A	984	LEU
1	A	1045	SER
1	A	1052	LEU
1	A	1060	LYS
1	A	1065	GLU
1	A	1182	ASP
1	A	1238	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	22	GLN
1	A	87	GLN
1	A	121	ASN
1	A	146	GLN
1	A	387	GLN
1	A	448	GLN
1	A	504	HIS
1	A	536	GLN
1	A	628	ASN
1	A	646	ASN
1	A	664	ASN
1	A	671	ASN
1	A	675	HIS
1	A	710	HIS
1	A	749	ASN
1	A	754	GLN
1	A	755	ASN
1	A	807	ASN
1	A	820	GLN
1	A	834	GLN
1	A	852	GLN
1	A	917	ASN
1	A	980	GLN

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Mol	Chain	Res	Type
1	A	1014	HIS
1	A	1021	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GTG	A	1425	-	57,57,57	2.85	18 (31%)	85,90,90	3.17	26 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GTG	A	1425	-	-	13/32/64/64	0/6/6/6

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1425	GTG	PA-O3A	-12.41	1.46	1.59
3	A	1425	GTG	PG-O3B	7.99	1.68	1.59
3	A	1425	GTG	PB-O3B	6.04	1.66	1.59
3	A	1425	GTG	C2D-C3D	-5.51	1.38	1.53
3	A	1425	GTG	PA-O5D	-5.15	1.39	1.59
3	A	1425	GTG	PB-O1B	3.86	1.64	1.50
3	A	1425	GTG	C3D-C4D	-3.81	1.43	1.53
3	A	1425	GTG	C2E-C3E	-3.47	1.44	1.53
3	A	1425	GTG	O3D-C3D	-3.37	1.34	1.43
3	A	1425	GTG	C1D-N9A	2.89	1.55	1.47
3	A	1425	GTG	O4E-C4E	-2.67	1.39	1.45
3	A	1425	GTG	C5D-C4D	-2.66	1.43	1.51
3	A	1425	GTG	C6B-N1B	2.61	1.43	1.38
3	A	1425	GTG	PG-O5E	2.44	1.68	1.59
3	A	1425	GTG	C2B-N1B	2.44	1.43	1.37
3	A	1425	GTG	C2D-C1D	2.10	1.60	1.53
3	A	1425	GTG	C8A-N7A	-2.03	1.29	1.33
3	A	1425	GTG	PG-O1G	2.00	1.57	1.50

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1425	GTG	O2B-PB-O3B	10.44	135.49	107.27
3	A	1425	GTG	O2G-PG-O3B	-9.70	81.06	107.27
3	A	1425	GTG	O4D-C4D-C5D	7.91	134.67	109.33
3	A	1425	GTG	O3A-PB-O1B	-6.97	89.75	110.70
3	A	1425	GTG	O3A-PA-O1A	6.94	131.59	110.70
3	A	1425	GTG	PA-O5D-C5D	6.88	160.77	121.35
3	A	1425	GTG	O5E-C5E-C4E	6.47	131.03	108.99
3	A	1425	GTG	O3D-C3D-C4D	6.40	129.47	111.08
3	A	1425	GTG	O2B-PB-O1B	-6.11	84.04	112.44
3	A	1425	GTG	O2A-PA-O3A	-5.76	91.70	107.27
3	A	1425	GTG	O3B-PB-O1B	-5.51	94.12	110.70
3	A	1425	GTG	C5D-C4D-C3D	-5.48	95.48	115.21
3	A	1425	GTG	O4D-C4D-C3D	5.16	115.39	105.15
3	A	1425	GTG	O5E-PG-O1G	5.10	129.13	108.94
3	A	1425	GTG	O3B-PG-O1G	-4.04	98.54	110.70
3	A	1425	GTG	C7X-N7A-C5A	3.88	131.63	126.80
3	A	1425	GTG	O5D-PA-O1A	3.78	123.94	108.94
3	A	1425	GTG	C3D-C2D-C1D	3.66	108.39	101.46
3	A	1425	GTG	O2G-PG-O1G	3.33	127.93	112.44
3	A	1425	GTG	O2G-PG-O5E	-3.23	92.92	107.57
3	A	1425	GTG	C3E-C2E-C1E	3.16	107.44	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1425	GTG	PG-O5E-C5E	-3.15	103.32	121.35
3	A	1425	GTG	C8A-N7A-C5A	-3.08	103.94	107.78
3	A	1425	GTG	C2D-C1D-N9A	2.92	121.39	113.25
3	A	1425	GTG	O5D-C5D-C4D	-2.09	101.88	108.99
3	A	1425	GTG	N9B-C8B-N7B	2.02	117.15	113.40

There are no chirality outliers.

All (13) torsion outliers are listed below:

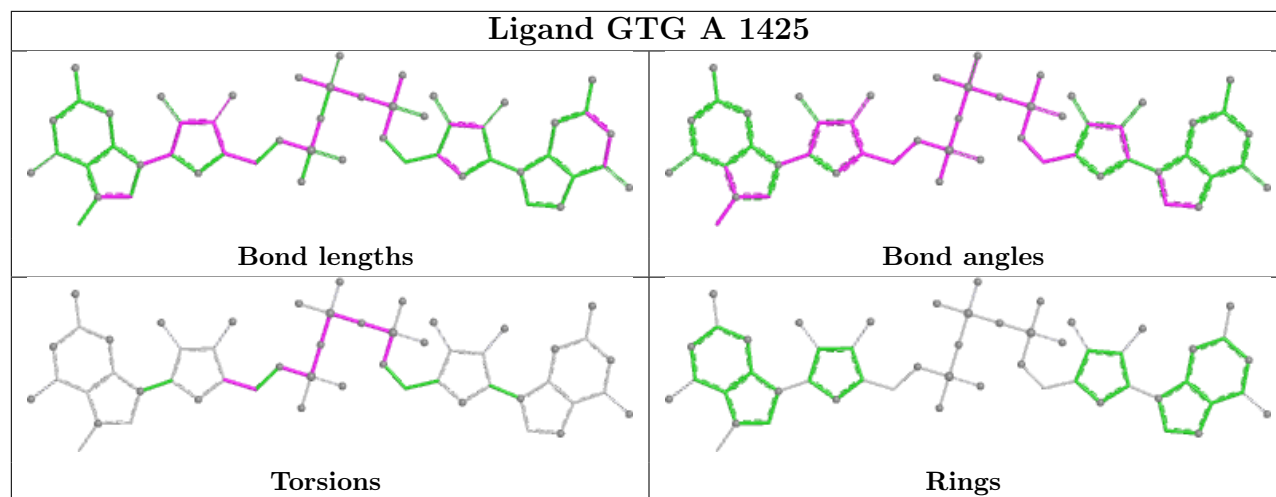
Mol	Chain	Res	Type	Atoms
3	A	1425	GTG	C5D-O5D-PA-O1A
3	A	1425	GTG	C5D-O5D-PA-O2A
3	A	1425	GTG	C5D-O5D-PA-O3A
3	A	1425	GTG	O4D-C4D-C5D-O5D
3	A	1425	GTG	C5E-O5E-PG-O3B
3	A	1425	GTG	C5E-O5E-PG-O1G
3	A	1425	GTG	C3D-C4D-C5D-O5D
3	A	1425	GTG	PB-O3B-PG-O5E
3	A	1425	GTG	PG-O3B-PB-O2B
3	A	1425	GTG	C5E-O5E-PG-O2G
3	A	1425	GTG	PB-O3B-PG-O1G
3	A	1425	GTG	PB-O3A-PA-O2A
3	A	1425	GTG	PA-O3A-PB-O1B

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1425	GTG	5	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	1256/1267 (99%)	0.06	38 (3%)	52 48	17, 31, 53, 83	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	756	ASP	5.1
1	A	2	SER	4.4
1	A	857	GLY	4.2
1	A	856	ILE	4.1
1	A	855	MET	4.0
1	A	744	THR	3.8
1	A	926	THR	3.8
1	A	745	ALA	3.7
1	A	557	PRO	3.5
1	A	471	TYR	3.4
1	A	860	VAL	3.3
1	A	267	SER	3.1
1	A	859	SER	3.1
1	A	755	ASN	2.9
1	A	632	VAL	2.9
1	A	743	THR	2.9
1	A	391	GLN	2.7
1	A	661	TYR	2.7
1	A	858	GLU	2.7
1	A	634	GLY	2.6
1	A	633	VAL	2.6
1	A	477	LEU	2.6
1	A	631	SER	2.4
1	A	1265	ARG	2.4
1	A	861	GLY	2.3
1	A	742	GLY	2.3
1	A	210	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	529	MET	2.2
1	A	956	LYS	2.2
1	A	564	ILE	2.2
1	A	967	ARG	2.2
1	A	955	PRO	2.1
1	A	615	ILE	2.1
1	A	1168	ASN	2.1
1	A	474	ASN	2.0
1	A	968	GLU	2.0
1	A	528	ILE	2.0
1	A	635	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

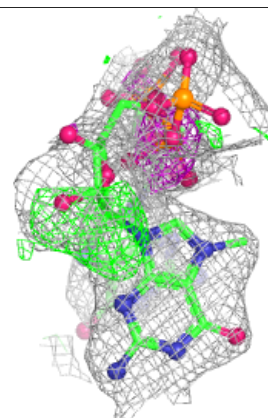
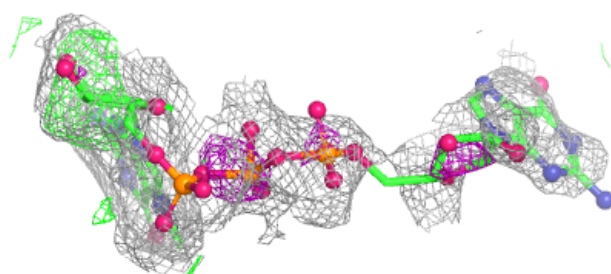
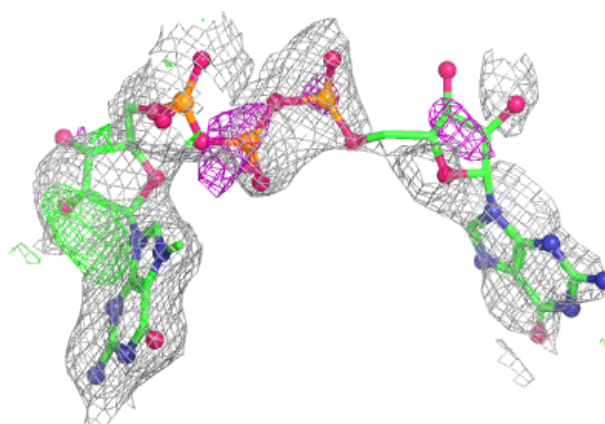
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GTG	A	1425	52/52	0.76	0.17	43,81,90,91	0
2	MN	A	1500	1/1	0.99	0.06	54,54,54,54	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 GTG A 1425:

$2mF_o-DF_c$ (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.