



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:01 PM UTC

PDB ID : 4X3V / pdb_00004x3v
Title : Crystal structure of human ribonucleotide reductase 1 bound to inhibitor
Authors : Dealwis, C.G.; Ahmad, M.F.; Alam, I.
Deposited on : 2014-12-01
Resolution : 3.70 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

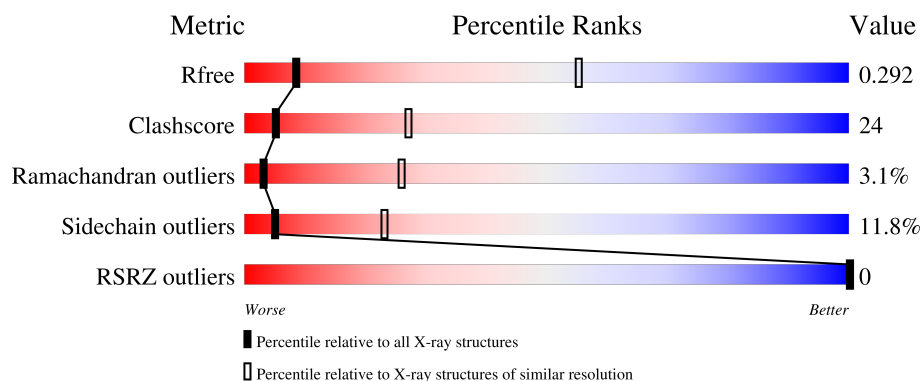
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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	792	
1	B	792	

2 Entry composition [i](#)

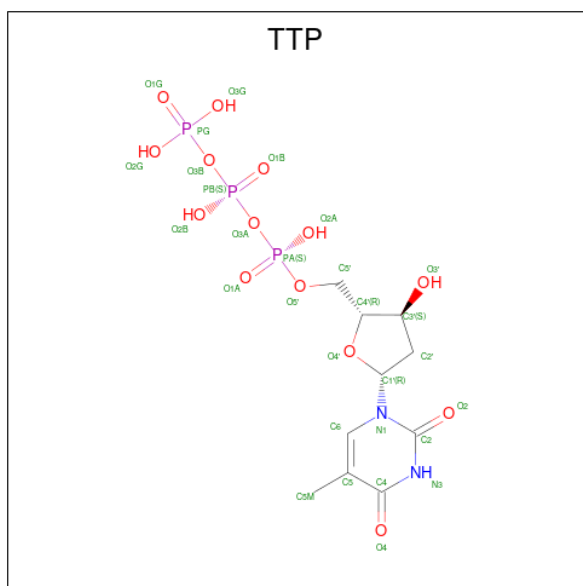
There are 3 unique types of molecules in this entry. The entry contains 11384 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ribonucleoside-diphosphate reductase large subunit.

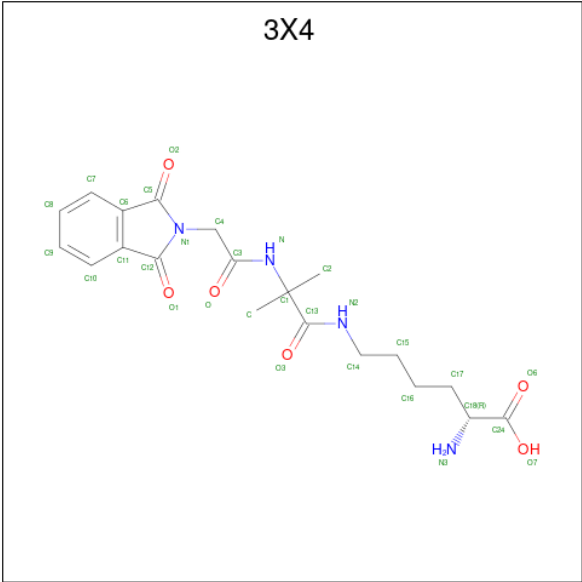
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	714	Total	C	N	O	S	7	0	0
			5545	3542	924	1047	32			
1	B	738	Total	C	N	O	S	0	0	0
			5751	3669	968	1080	34			

- Molecule 2 is THYMIDINE-5'-TRIPHOSPHATE (CCD ID: TTP) (formula: $C_{10}H_{17}N_2O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
2	B	1	Total	C	N	O	P	0	0
			29	10	2	14	3		

- Molecule 3 is N 6 -{N-[(1,3-dioxo-1,3-dihydro-2H-isoindol-2-yl)acetyl]-2-methyl-D-alanyl}-D-lysine (CCD ID: 3X4) (formula: $C_{20}H_{26}N_4O_6$).

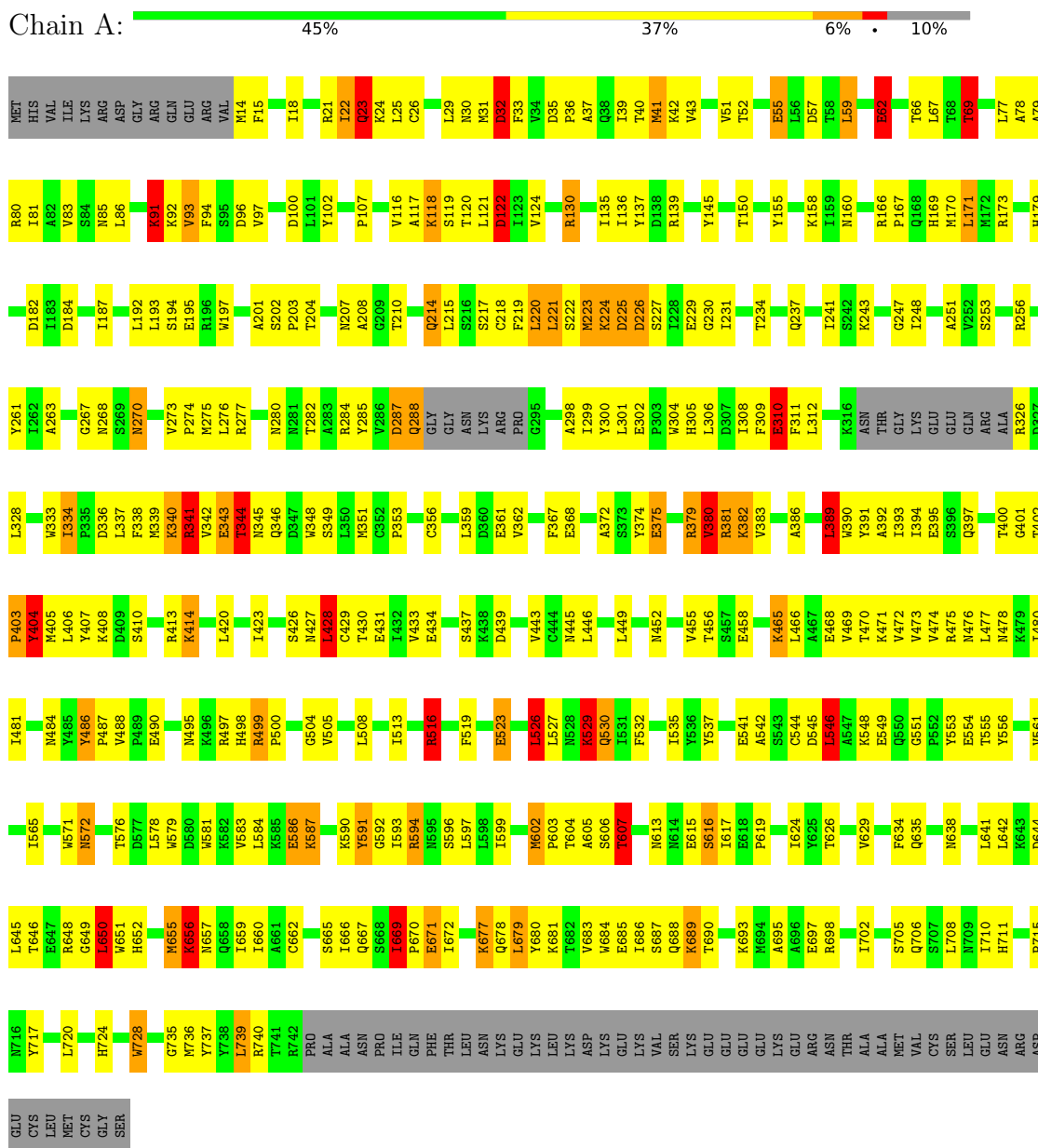


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			30	20	4	6		

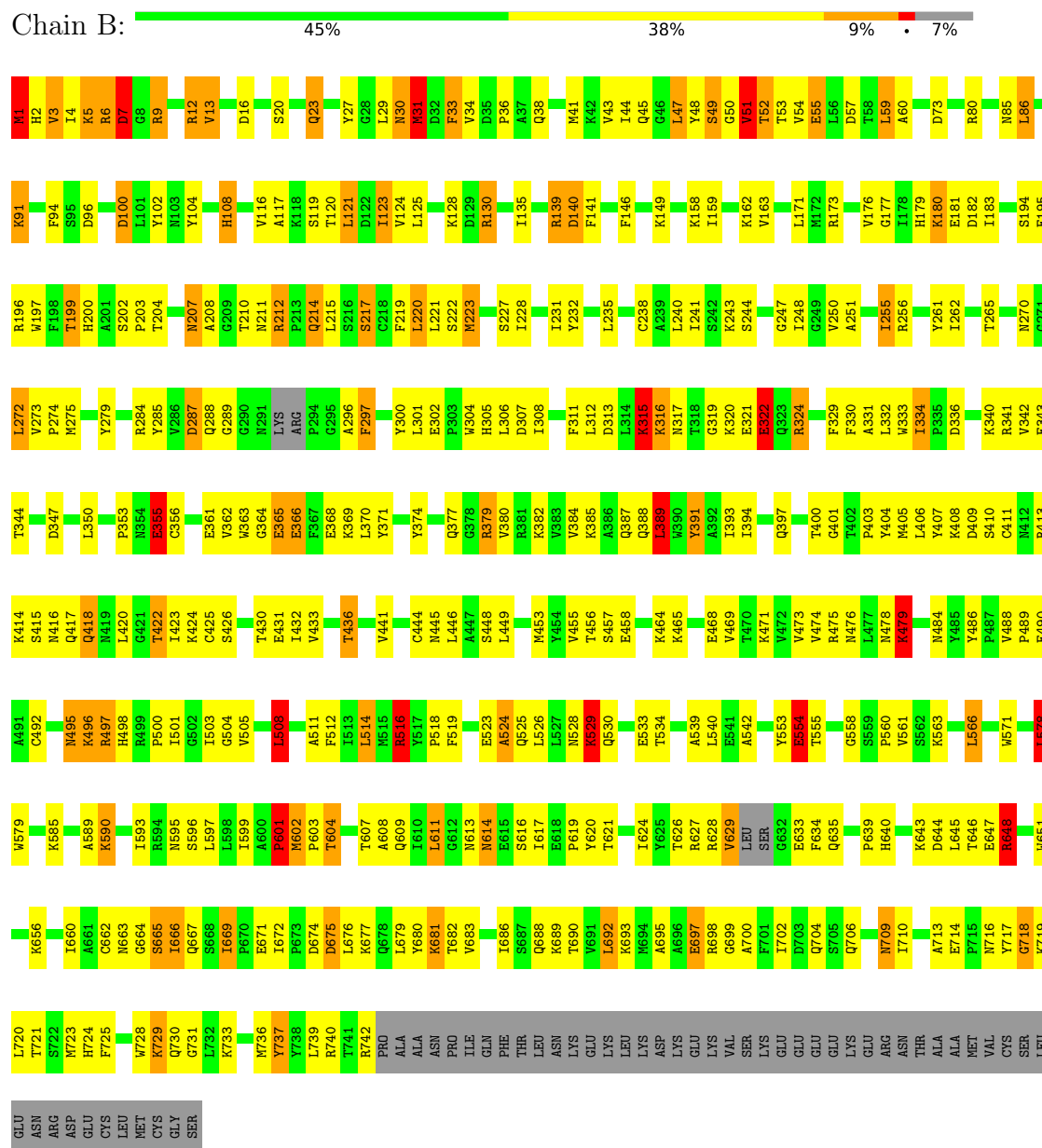
3 Residue-property plots

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: Ribonucleoside-diphosphate reductase large subunit



- Molecule 1: Ribonucleoside-diphosphate reductase large subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.88Å 110.50Å 216.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	108.36 – 3.70 108.36 – 3.70	Depositor EDS
% Data completeness (in resolution range)	95.8 (108.36-3.70) 90.0 (108.36-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 3.58Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.232 , 0.289 0.240 , 0.292	Depositor DCC
R_{free} test set	1987 reflections (9.61%)	wwPDB-VP
Wilson B-factor (Å ²)	110.3	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 74.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11384	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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: 3X4, TTP

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	0/5666	1.20	63/7709 (0.8%)
1	B	0.58	1/5877 (0.0%)	1.25	59/7989 (0.7%)
All	All	0.58	1/11543 (0.0%)	1.22	122/15698 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	8
All	All	0	14

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	692	LEU	C-O	7.28	1.32	1.24

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	578	LEU	N-CA-C	-13.05	97.11	111.07
1	B	315	LYS	N-CA-C	10.43	126.33	112.88
1	A	607	THR	N-CA-C	-10.35	100.06	112.89
1	B	590	LYS	CA-CB-CG	10.09	134.28	114.10
1	A	526	LEU	CA-CB-CG	10.00	151.29	116.30
1	B	366	GLU	N-CA-C	-9.64	99.05	112.45
1	B	590	LYS	N-CA-C	-9.62	100.36	111.03
1	B	495	ASN	N-CA-C	-9.60	101.26	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	669	ILE	CA-C-N	9.49	129.74	119.87
1	A	669	ILE	C-N-CA	9.49	129.74	119.87
1	A	122	ASP	N-CA-C	-9.41	100.12	111.69
1	B	689	LYS	N-CA-C	-9.00	101.55	111.36
1	B	6	ARG	N-CA-C	-8.97	99.98	112.45
1	B	643	LYS	N-CA-C	-8.61	101.98	111.36
1	A	586	GLU	N-CA-C	-8.42	103.44	114.31
1	B	590	LYS	N-CA-CB	8.24	121.93	109.98
1	A	541	GLU	N-CA-C	-7.90	102.27	112.23
1	B	410	SER	N-CA-C	-7.88	104.83	114.75
1	A	689	LYS	N-CA-C	-7.85	102.68	111.71
1	A	69	THR	N-CA-C	-7.77	102.72	112.90
1	B	334	ILE	N-CA-C	7.70	115.25	108.63
1	B	508	LEU	N-CA-C	-7.53	104.09	113.28
1	B	100	ASP	N-CA-C	-7.49	103.99	113.72
1	B	648	ARG	CB-CG-CD	7.41	128.34	111.30
1	B	648	ARG	CG-CD-NE	-7.39	95.74	112.00
1	A	334	ILE	N-CA-C	7.37	115.20	107.76
1	B	418	GLN	N-CA-C	-7.32	102.28	112.45
1	A	35	ASP	CA-C-N	7.29	127.30	119.28
1	A	35	ASP	C-N-CA	7.29	127.30	119.28
1	A	548	LYS	N-CA-C	-7.26	102.17	111.02
1	A	23	GLN	N-CA-CB	7.20	120.49	110.56
1	B	590	LYS	CB-CG-CD	7.18	127.81	111.30
1	B	1	MET	CB-CG-SD	-7.13	91.32	112.70
1	B	731	GLY	N-CA-C	6.90	123.89	114.92
1	B	558	GLY	N-CA-C	-6.85	106.25	113.58
1	B	355	GLU	N-CA-C	-6.82	103.92	111.36
1	B	255	ILE	N-CA-C	6.61	117.81	108.36
1	B	589	ALA	N-CA-C	6.51	118.38	111.28
1	B	108	HIS	N-CA-C	-6.45	104.10	112.68
1	A	656	LYS	CD-CE-NZ	6.36	132.24	111.90
1	A	689	LYS	CB-CG-CD	-6.31	96.78	111.30
1	B	139	ARG	CA-C-N	-6.31	112.58	122.73
1	B	139	ARG	C-N-CA	-6.31	112.58	122.73
1	A	591	TYR	N-CA-C	6.25	118.61	111.11
1	A	680	TYR	CA-C-N	-6.24	109.52	122.07
1	A	680	TYR	C-N-CA	-6.24	109.52	122.07
1	B	31	MET	CB-CG-SD	6.23	131.40	112.70
1	B	648	ARG	CA-CB-CG	6.13	126.36	114.10
1	A	42	LYS	N-CA-C	-6.12	105.85	113.38
1	A	428	LEU	N-CA-C	-6.11	105.83	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	202	SER	CA-C-N	-6.10	112.72	119.19
1	A	202	SER	C-N-CA	-6.10	112.72	119.19
1	A	616	SER	CB-CA-C	-6.09	109.56	116.63
1	A	379	ARG	CB-CG-CD	6.00	125.11	111.30
1	B	479	LYS	CB-CG-CD	-5.99	97.53	111.30
1	B	648	ARG	CB-CA-C	5.96	122.28	110.42
1	A	341	ARG	CB-CG-CD	5.95	124.98	111.30
1	A	551	GLY	CA-C-N	5.92	127.24	119.84
1	A	551	GLY	C-N-CA	5.92	127.24	119.84
1	B	578	LEU	CA-CB-CG	5.89	136.91	116.30
1	A	23	GLN	N-CA-C	-5.87	106.35	112.93
1	A	23	GLN	CA-CB-CG	5.84	125.77	114.10
1	A	22	ILE	CA-C-N	-5.79	113.03	122.65
1	A	22	ILE	C-N-CA	-5.79	113.03	122.65
1	B	31	MET	N-CA-C	-5.77	98.51	110.80
1	B	729	LYS	CA-C-N	-5.77	114.58	123.17
1	B	729	LYS	C-N-CA	-5.77	114.58	123.17
1	A	86	LEU	N-CA-C	-5.75	106.30	113.55
1	A	24	LYS	N-CA-C	-5.70	106.66	113.21
1	A	389	LEU	N-CA-C	-5.70	104.97	111.07
1	A	516	ARG	N-CA-C	-5.65	105.68	112.58
1	A	529	LYS	N-CA-C	-5.61	98.84	110.80
1	A	340	LYS	N-CA-C	5.61	118.93	111.75
1	B	389	LEU	N-CA-C	-5.61	105.26	111.71
1	A	678	GLN	N-CA-C	-5.55	105.63	112.90
1	A	526	LEU	CB-CA-C	-5.54	101.64	110.84
1	A	118	LYS	N-CA-C	-5.52	105.26	111.28
1	B	464	LYS	CB-CG-CD	5.51	123.98	111.30
1	B	718	GLY	CA-C-N	5.49	129.47	120.63
1	B	718	GLY	C-N-CA	5.49	129.47	120.63
1	B	514	LEU	N-CA-C	-5.47	106.45	113.23
1	B	3	VAL	CA-C-N	-5.46	115.33	122.37
1	B	3	VAL	C-N-CA	-5.46	115.33	122.37
1	B	30	ASN	CA-C-N	-5.46	111.12	121.54
1	B	30	ASN	C-N-CA	-5.46	111.12	121.54
1	A	344	THR	N-CA-C	-5.43	106.63	113.20
1	B	322	GLU	CA-C-N	5.42	128.46	119.35
1	B	322	GLU	C-N-CA	5.42	128.46	119.35
1	A	150	THR	N-CA-C	-5.36	105.88	112.90
1	A	32	ASP	CA-C-N	-5.36	114.11	122.73
1	A	32	ASP	C-N-CA	-5.36	114.11	122.73
1	A	341	ARG	CG-CD-NE	5.36	123.78	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	310	GLU	CA-CB-CG	5.35	124.81	114.10
1	A	267	GLY	CA-C-N	-5.33	114.94	122.94
1	A	267	GLY	C-N-CA	-5.33	114.94	122.94
1	A	310	GLU	N-CA-C	-5.33	106.75	113.20
1	B	496	LYS	CA-C-N	5.29	131.65	121.54
1	B	496	LYS	C-N-CA	5.29	131.65	121.54
1	B	496	LYS	N-CA-C	-5.29	105.97	112.90
1	A	587	LYS	CB-CA-C	-5.27	102.61	110.88
1	A	226	ASP	N-CA-C	-5.26	106.88	113.72
1	B	589	ALA	CA-C-O	-5.24	115.00	120.55
1	A	486	TYR	CA-C-N	5.23	124.55	118.85
1	A	486	TYR	C-N-CA	5.23	124.55	118.85
1	B	529	LYS	CB-CG-CD	5.23	123.32	111.30
1	B	55	GLU	N-CA-C	-5.22	106.75	113.02
1	A	380	VAL	CA-C-N	-5.21	113.97	122.26
1	A	380	VAL	C-N-CA	-5.21	113.97	122.26
1	A	437	SER	N-CA-C	5.19	114.88	108.19
1	A	223	MET	CB-CG-SD	5.16	128.18	112.70
1	A	529	LYS	CA-CB-CG	5.12	124.35	114.10
1	B	516	ARG	CA-CB-CG	5.12	124.34	114.10
1	A	666	ILE	N-CA-C	-5.11	107.32	112.17
1	B	585	LYS	N-CA-C	-5.10	105.61	111.07
1	B	212	ARG	CG-CD-NE	-5.10	100.78	112.00
1	A	657	ASN	N-CA-C	5.09	117.49	111.33
1	A	273	VAL	CA-C-N	-5.04	114.47	119.56
1	A	273	VAL	C-N-CA	-5.04	114.47	119.56
1	B	554	GLU	CB-CA-C	-5.04	100.40	110.42
1	B	714	GLU	CA-C-N	5.03	126.12	119.84
1	B	714	GLU	C-N-CA	5.03	126.12	119.84
1	B	578	LEU	CA-C-O	5.02	126.09	120.82

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	287	ASP	Peptide
1	A	403	PRO	Peptide
1	A	546	LEU	Peptide
1	A	571	TRP	Peptide
1	A	655	MET	Peptide
1	A	91	LYS	Peptide
1	B	1	MET	Peptide

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Mol	Chain	Res	Type	Group
1	B	30	ASN	Peptide
1	B	315	LYS	Peptide
1	B	322	GLU	Peptide
1	B	524	ALA	Peptide
1	B	601	PRO	Peptide
1	B	614	ASN	Peptide
1	B	648	ARG	Peptide

5.2 Too-close contacts [i](#)

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	5545	0	5342	259	0
1	B	5751	0	5586	292	0
2	A	29	0	13	4	0
2	B	29	0	13	4	0
3	A	30	0	25	3	0
All	All	11384	0	10979	547	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (547) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:497:ARG:HG3	1:B:554:GLU:HG2	1.30	1.14
1:A:446:LEU:HB3	1:A:602:MET:HE1	1.40	1.00
1:A:667:GLN:HE21	1:A:677:LYS:HB2	1.26	0.97
1:B:624:ILE:HD11	1:B:635:GLN:HE21	1.32	0.95
1:B:1:MET:H2	1:B:12:ARG:HE	1.09	0.93
1:B:363:TRP:HD1	1:B:422:THR:HG23	1.31	0.93
1:A:52:THR:H	1:A:55:GLU:HG3	1.37	0.89
1:A:523:GLU:HA	1:A:526:LEU:HD23	1.53	0.89
1:A:404:TYR:HD1	1:A:404:TYR:H	1.18	0.86
1:B:365:GLU:HA	1:B:368:GLU:HG2	1.56	0.85
1:B:1:MET:N	1:B:12:ARG:HE	1.75	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:ASN:HB3	1:B:274:PRO:HG2	1.59	0.83
1:A:337:LEU:HG	1:A:368:GLU:HG2	1.58	0.83
1:B:455:VAL:HG11	1:B:514:LEU:HD22	1.58	0.83
1:B:361:GLU:HG2	1:B:424:LYS:HE2	1.60	0.83
1:A:302:GLU:HG2	1:A:333:TRP:HB3	1.59	0.82
1:B:611:LEU:HD12	1:B:613:ASN:ND2	1.94	0.81
1:B:227:SER:HA	2:B:801:TTP:H5'1	1.65	0.79
1:B:315:LYS:HD2	1:B:330:PHE:CD2	2.17	0.79
1:A:57:ASP:OD2	1:A:85:ASN:ND2	2.15	0.79
1:A:52:THR:N	1:A:55:GLU:HG3	1.99	0.77
1:A:336:ASP:HA	1:A:728:TRP:HE1	1.50	0.77
1:A:667:GLN:HE21	1:A:677:LYS:CB	1.97	0.76
1:B:418:GLN:HE21	1:B:560:PRO:HG3	1.50	0.76
1:A:256:ARG:NH2	1:A:261:TYR:O	2.19	0.76
1:B:1:MET:HG2	1:B:2:HIS:HB2	1.68	0.75
1:A:340:LYS:O	1:A:344:THR:OG1	2.05	0.75
1:B:256:ARG:NH2	2:B:801:TTP:O3B	2.20	0.75
1:A:397:GLN:HB3	1:A:739:LEU:HD12	1.69	0.75
1:A:395:GLU:HG3	1:A:717:TYR:HE1	1.52	0.75
1:B:215:LEU:N	1:B:484:ASN:OD1	2.20	0.75
1:B:363:TRP:CD1	1:B:422:THR:HG23	2.20	0.74
1:B:501:ILE:HG12	1:B:595:ASN:HD22	1.52	0.74
1:A:118:LYS:O	1:A:122:ASP:HB2	1.86	0.74
1:B:315:LYS:HD2	1:B:330:PHE:HD2	1.51	0.74
1:B:667:GLN:HA	1:B:677:LYS:HD3	1.70	0.74
1:B:44:ILE:HA	1:B:47:LEU:HD12	1.69	0.73
1:B:1:MET:HA	1:B:12:ARG:HH11	1.53	0.73
1:B:730:GLN:O	1:B:730:GLN:HG2	1.87	0.73
1:B:406:LEU:HD11	1:B:430:THR:HB	1.71	0.73
1:A:171:LEU:HD23	1:A:193:LEU:HB3	1.70	0.72
1:B:214:GLN:HG3	1:B:244:SER:HB3	1.71	0.72
1:B:709:ASN:OD1	1:B:740:ARG:NH2	2.16	0.72
1:A:662:CYS:HB3	1:A:665:SER:HB3	1.72	0.71
1:A:310:GLU:N	1:A:310:GLU:OE1	2.24	0.71
1:A:312:LEU:HD22	1:A:393:ILE:HA	1.72	0.71
1:B:1:MET:HB3	1:B:13:VAL:HG23	1.72	0.71
1:A:337:LEU:HB3	1:A:341:ARG:HD3	1.73	0.71
1:A:546:LEU:HD12	1:A:594:ARG:HB2	1.71	0.71
1:A:624:ILE:HD13	1:A:660:ILE:HG12	1.73	0.70
1:B:604:THR:HB	1:B:607:THR:HG23	1.71	0.70
1:B:256:ARG:NH1	1:B:261:TYR:O	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:TRP:HB2	1:A:386:ALA:HB2	1.74	0.69
1:B:140:ASP:OD1	1:B:140:ASP:N	2.22	0.69
1:A:516:ARG:NH2	1:A:644:ASP:OD2	2.26	0.69
1:B:616:SER:OG	1:B:617:ILE:N	2.19	0.69
1:B:80:ARG:HD3	1:B:141:PHE:HB3	1.75	0.68
1:A:537:TYR:CE2	1:A:579:TRP:HB3	2.29	0.68
1:A:23:GLN:HB3	1:A:26:CYS:HB2	1.75	0.68
1:A:504:GLY:HA3	1:A:602:MET:SD	2.34	0.68
1:B:725:PHE:O	1:B:729:LYS:HB2	1.93	0.67
1:A:499:ARG:HE	1:A:594:ARG:HD2	1.58	0.67
1:B:341:ARG:HD3	1:B:347:ASP:O	1.95	0.67
1:B:418:GLN:NE2	1:B:560:PRO:HG3	2.10	0.67
1:A:270:ASN:H	2:A:801:TTP:HM52	1.59	0.67
1:B:603:PRO:HA	1:B:616:SER:HB2	1.76	0.67
1:A:516:ARG:NH1	1:A:679:LEU:HD13	2.09	0.66
1:A:261:TYR:HA	1:A:268:ASN:HD22	1.60	0.66
1:B:530:GLN:HB3	1:B:578:LEU:HD21	1.77	0.66
1:B:602:MET:HE2	1:B:604:THR:HG22	1.78	0.66
1:A:284:ARG:NH1	1:B:322:GLU:O	2.28	0.66
1:A:465:LYS:HA	1:A:468:GLU:HB2	1.78	0.66
1:A:481:ILE:HG23	1:A:495:ASN:ND2	2.11	0.66
1:B:498:HIS:HB2	1:B:500:PRO:HD3	1.76	0.66
1:B:43:VAL:HG22	1:B:59:LEU:HD22	1.76	0.66
1:A:667:GLN:NE2	1:A:677:LYS:HB2	2.06	0.66
1:B:300:TYR:HE2	1:B:406:LEU:HD13	1.61	0.66
1:A:179:HIS:HB3	1:A:182:ASP:HB3	1.77	0.65
1:B:401:GLY:HA2	1:B:739:LEU:HB2	1.78	0.65
1:B:423:ILE:HD13	1:B:433:VAL:HG12	1.78	0.65
1:A:471:LYS:HA	1:A:542:ALA:HB2	1.78	0.65
1:B:397:GLN:HB3	1:B:739:LEU:HD12	1.79	0.65
1:B:52:THR:HG23	1:B:55:GLU:HB3	1.79	0.65
1:B:504:GLY:HA3	1:B:602:MET:HG2	1.78	0.64
1:B:647:GLU:O	1:B:648:ARG:HB3	1.97	0.64
1:B:365:GLU:CD	1:B:413:ARG:HH22	2.05	0.64
1:A:537:TYR:CD1	1:A:584:LEU:HD22	2.33	0.64
1:A:446:LEU:HB3	1:A:602:MET:CE	2.22	0.64
1:A:69:THR:HG21	1:A:656:LYS:NZ	2.12	0.64
1:B:256:ARG:HH12	1:B:262:ILE:HA	1.61	0.64
1:A:650:LEU:HG	1:A:650:LEU:O	1.98	0.64
1:A:337:LEU:CG	1:A:368:GLU:HG2	2.28	0.64
1:B:614:ASN:HD21	1:B:620:TYR:HA	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:TYR:HE2	1:A:561:VAL:HG23	1.64	0.63
1:B:7:ASP:HB3	1:B:9:ARG:H	1.64	0.63
1:B:52:THR:HG23	1:B:55:GLU:CB	2.29	0.63
1:A:270:ASN:N	2:A:801:TTP:HM52	2.13	0.63
1:B:355:GLU:O	1:B:379:ARG:HD2	1.99	0.63
1:A:423:ILE:HD13	1:A:433:VAL:HG12	1.81	0.63
1:B:48:TYR:O	1:B:50:GLY:N	2.31	0.63
1:B:297:PHE:HD1	1:B:297:PHE:N	1.97	0.63
1:A:449:LEU:H	1:A:505:VAL:HA	1.62	0.62
1:A:256:ARG:NH1	2:A:801:TTP:O1B	2.32	0.62
1:B:1:MET:H2	1:B:12:ARG:NE	1.89	0.62
1:B:31:MET:HA	1:B:34:VAL:HB	1.80	0.62
1:B:272:LEU:HD11	1:B:305:HIS:CE1	2.33	0.62
1:A:170:MET:HG2	1:A:173:ARG:HH21	1.63	0.62
1:A:23:GLN:C	1:A:25:LEU:H	2.07	0.62
1:B:676:LEU:HD22	1:B:680:TYR:HE1	1.64	0.62
1:B:179:HIS:HB3	1:B:182:ASP:HB3	1.81	0.61
1:B:207:ASN:OD1	1:B:207:ASN:N	2.33	0.61
1:B:341:ARG:HH12	1:B:371:TYR:HE2	1.49	0.61
1:A:486:TYR:OH	1:A:495:ASN:ND2	2.27	0.61
1:B:604:THR:OG1	1:B:608:ALA:HB2	2.00	0.61
1:A:445:ASN:HD21	1:A:481:ILE:HG12	1.66	0.61
1:B:475:ARG:O	1:B:479:LYS:HG3	2.01	0.61
1:A:375:GLU:HA	1:A:375:GLU:OE1	2.00	0.60
1:A:452:ASN:ND2	1:A:613:ASN:OD1	2.28	0.60
1:B:1:MET:HB3	1:B:13:VAL:CG2	2.31	0.60
1:B:690:THR:O	1:B:693:LYS:HB3	2.02	0.60
1:B:341:ARG:NH1	1:B:371:TYR:HE2	2.00	0.60
3:A:802:3X4:C3	3:A:802:3X4:H23	2.15	0.60
1:A:192:LEU:HA	1:A:197:TRP:HD1	1.67	0.59
1:A:402:THR:HG22	1:A:404:TYR:CE1	2.37	0.59
1:B:57:ASP:HA	1:B:60:ALA:HB3	1.84	0.59
1:B:468:GLU:HA	1:B:471:LYS:HB2	1.84	0.59
1:A:340:LYS:HA	1:A:343:GLU:OE2	2.01	0.59
1:A:237:GLN:HG2	1:A:488:VAL:HG11	1.84	0.59
1:B:251:ALA:HB2	1:B:425:CYS:HB3	1.84	0.59
1:A:32:ASP:OD1	1:A:32:ASP:N	2.35	0.59
1:A:739:LEU:C	1:A:740:ARG:HG2	2.27	0.59
1:B:331:ALA:HB2	1:B:404:TYR:HD2	1.67	0.59
1:B:611:LEU:HD12	1:B:613:ASN:HD22	1.67	0.59
1:B:297:PHE:N	1:B:297:PHE:CD1	2.69	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:TYR:HD2	1:A:379:ARG:HD2	1.67	0.58
1:B:621:THR:HA	1:B:683:VAL:HG12	1.85	0.58
1:A:285:TYR:O	1:B:270:ASN:ND2	2.35	0.58
1:A:275:MET:HE2	1:A:276:LEU:HD12	1.85	0.58
1:A:275:MET:HG3	1:B:285:TYR:CZ	2.38	0.58
1:A:341:ARG:HH12	1:A:346:GLN:HE21	1.52	0.58
1:B:302:GLU:HG2	1:B:333:TRP:HB3	1.86	0.58
1:B:405:MET:HG3	1:B:724:HIS:CE1	2.37	0.58
1:B:528:ASN:HD21	1:B:698:ARG:HH21	1.52	0.58
1:B:709:ASN:HD21	1:B:737:TYR:HD2	1.50	0.58
1:A:300:TYR:HE2	1:A:406:LEU:HD13	1.69	0.58
1:B:149:LYS:HD2	1:B:629:VAL:HG21	1.85	0.58
1:A:404:TYR:CD1	1:A:404:TYR:N	2.70	0.57
1:B:287:ASP:HB2	1:B:289:GLY:H	1.69	0.57
1:B:377:GLN:OE1	1:B:379:ARG:NH2	2.25	0.57
1:B:501:ILE:HG12	1:B:595:ASN:ND2	2.19	0.57
1:B:57:ASP:OD2	1:B:85:ASN:ND2	2.37	0.57
1:A:690:THR:HA	1:A:693:LYS:HB2	1.86	0.57
1:B:29:LEU:HD22	1:B:73:ASP:HB3	1.86	0.57
1:B:139:ARG:NH1	1:B:194:SER:OG	2.38	0.57
1:B:350:LEU:HB2	1:B:382:LYS:HB2	1.86	0.57
1:A:410:SER:O	1:A:414:LYS:HG3	2.04	0.57
1:B:397:GLN:HG3	1:B:403:PRO:HD2	1.86	0.57
1:B:524:ALA:O	1:B:528:ASN:N	2.35	0.57
1:B:203:PRO:HG2	1:B:217:SER:HA	1.87	0.57
1:B:614:ASN:ND2	1:B:620:TYR:HA	2.20	0.57
1:A:497:ARG:HA	1:A:554:GLU:HG2	1.87	0.57
1:A:626:THR:HG22	1:A:635:GLN:HA	1.86	0.57
1:B:688:GLN:O	1:B:692:LEU:HD12	2.04	0.57
1:A:603:PRO:HA	1:A:616:SER:HB2	1.86	0.57
1:A:655:MET:SD	1:A:669:ILE:HD12	2.45	0.57
1:B:33:PHE:CE2	1:B:646:THR:HB	2.40	0.56
1:A:69:THR:HG21	1:A:656:LYS:HZ2	1.70	0.56
1:A:222:SER:HA	1:A:251:ALA:HB3	1.86	0.56
1:B:611:LEU:HD12	1:B:613:ASN:HD21	1.70	0.56
1:A:67:LEU:C	1:A:69:THR:H	2.12	0.56
1:A:139:ARG:NH1	1:A:194:SER:OG	2.39	0.56
1:A:404:TYR:HD1	1:A:404:TYR:N	1.98	0.56
1:B:227:SER:O	1:B:231:ILE:N	2.37	0.56
1:B:256:ARG:HH22	2:B:801:TTP:PG	2.29	0.56
1:B:662:CYS:HB3	1:B:665:SER:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:CA	1:B:12:ARG:HH11	2.20	0.55
1:B:49:SER:O	1:B:49:SER:OG	2.23	0.55
1:B:391:TYR:HD2	1:B:717:TYR:CD1	2.24	0.55
1:B:312:LEU:HD21	1:B:393:ILE:HA	1.89	0.55
1:B:214:GLN:HE21	1:B:244:SER:HB2	1.72	0.55
1:A:397:GLN:HB3	1:A:739:LEU:CD1	2.36	0.54
1:A:687:SER:OG	1:A:689:LYS:HD2	2.07	0.54
1:B:495:ASN:OD1	1:B:495:ASN:O	2.25	0.54
1:B:699:GLY:HA2	1:B:702:ILE:HD12	1.89	0.54
1:A:404:TYR:CE2	1:A:737:TYR:HE1	2.24	0.54
1:A:537:TYR:CE1	1:A:584:LEU:HD13	2.42	0.54
1:A:339:MET:HB2	1:A:728:TRP:CZ2	2.42	0.54
1:B:528:ASN:HD21	1:B:698:ARG:NH2	2.05	0.54
1:A:389:LEU:HD23	1:A:393:ILE:HD11	1.90	0.54
1:A:214:GLN:NE2	1:A:487:PRO:HD3	2.23	0.54
1:A:372:ALA:HA	1:A:375:GLU:HB2	1.90	0.54
1:B:304:TRP:HH2	1:B:353:PRO:HB3	1.72	0.54
1:B:709:ASN:N	1:B:709:ASN:HD22	2.05	0.54
1:A:285:TYR:CZ	1:B:275:MET:HG3	2.43	0.54
1:A:535:ILE:HG22	1:A:599:ILE:HD12	1.90	0.53
1:A:537:TYR:HB2	1:A:581:TRP:CH2	2.42	0.53
1:B:23:GLN:OE1	1:B:36:PRO:HG2	2.07	0.53
1:B:342:VAL:HG13	1:B:387:GLN:HG2	1.90	0.53
1:B:171:LEU:HD23	1:B:194:SER:HA	1.91	0.53
1:A:334:ILE:O	1:A:408:LYS:N	2.41	0.53
1:B:308:ILE:HG13	1:B:389:LEU:HD21	1.90	0.53
1:B:377:GLN:CD	1:B:379:ARG:HH21	2.15	0.53
1:B:223:MET:HG2	1:B:255:ILE:HD11	1.91	0.53
1:B:301:LEU:HD11	1:B:305:HIS:HB3	1.91	0.53
1:A:495:ASN:OD1	1:A:500:PRO:HD2	2.08	0.53
1:B:384:VAL:HB	1:B:388:GLN:OE1	2.09	0.53
1:A:130:ARG:HE	1:A:187:ILE:CD1	2.22	0.52
1:A:333:TRP:NE1	1:A:408:LYS:HG3	2.24	0.52
1:A:434:GLU:HG2	1:A:597:LEU:HD12	1.91	0.52
1:A:59:LEU:HA	1:A:62:GLU:HB2	1.91	0.52
1:A:26:CYS:HA	1:A:29:LEU:HD12	1.90	0.52
1:A:301:LEU:HD11	1:A:305:HIS:HB3	1.91	0.52
1:A:602:MET:HB2	1:A:604:THR:HG23	1.90	0.52
1:B:1:MET:HE1	1:B:47:LEU:O	2.10	0.52
1:B:240:LEU:O	1:B:243:LYS:HB3	2.09	0.52
1:B:667:GLN:HE22	1:B:681:LYS:HA	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:MET:O	1:A:735:GLY:N	2.43	0.52
1:A:18:ILE:O	1:A:22:ILE:HG12	2.10	0.52
1:A:339:MET:HG3	1:A:728:TRP:CD1	2.45	0.52
1:A:616:SER:OG	1:A:617:ILE:N	2.43	0.52
1:B:474:VAL:HG21	1:B:539:ALA:HA	1.90	0.52
1:A:599:ILE:HB	1:A:702:ILE:HA	1.91	0.52
1:B:347:ASP:HA	1:B:385:LYS:HA	1.91	0.52
1:B:518:PRO:HA	1:B:679:LEU:HA	1.91	0.52
1:B:199:THR:HG22	1:B:448:SER:HB2	1.92	0.52
1:A:695:ALA:HB1	1:A:708:LEU:HD11	1.91	0.51
1:A:537:TYR:HE2	1:A:579:TRP:HB3	1.72	0.51
1:B:709:ASN:ND2	1:B:737:TYR:HD2	2.09	0.51
1:B:57:ASP:HB2	1:B:85:ASN:HD22	1.76	0.51
1:B:214:GLN:HE21	1:B:244:SER:CB	2.23	0.51
1:B:709:ASN:ND2	1:B:737:TYR:HB3	2.25	0.51
1:A:720:LEU:HD21	1:A:739:LEU:HD11	1.92	0.51
1:A:130:ARG:HE	1:A:187:ILE:HD12	1.76	0.51
1:A:499:ARG:HG3	1:A:553:TYR:HB2	1.91	0.51
1:A:407:TYR:CD1	1:A:728:TRP:HB2	2.46	0.51
1:A:407:TYR:CE1	1:A:728:TRP:HB2	2.45	0.51
1:B:146:PHE:HE1	1:B:634:PHE:HB2	1.76	0.51
1:B:364:GLY:H	1:B:409:ASP:CG	2.19	0.51
1:B:96:ASP:O	1:B:100:ASP:HB2	2.11	0.50
1:B:492:CYS:O	1:B:496:LYS:HB2	2.11	0.50
1:A:498:HIS:HB2	1:A:500:PRO:HD3	1.94	0.50
1:B:238:CYS:HB2	1:B:248:ILE:HD13	1.93	0.50
1:B:449:LEU:HB2	1:B:505:VAL:HG12	1.93	0.50
1:B:571:TRP:CD1	1:B:700:ALA:HA	2.47	0.50
1:A:167:PRO:O	1:A:171:LEU:HD12	2.11	0.50
1:B:718:GLY:HA2	1:B:721:THR:HB	1.92	0.50
1:A:649:GLY:O	1:A:651:TRP:N	2.40	0.50
1:A:650:LEU:HD12	1:A:671:GLU:HB2	1.94	0.50
1:B:341:ARG:HA	1:B:344:THR:OG1	2.11	0.50
1:B:200:HIS:HB3	1:B:204:THR:HB	1.93	0.50
1:B:315:LYS:HE3	1:B:329:PHE:HA	1.94	0.50
1:B:436:THR:HG23	1:B:441:VAL:HA	1.94	0.50
1:A:277:ARG:HH11	1:B:284:ARG:HH12	1.60	0.50
1:A:395:GLU:HG3	1:A:717:TYR:CE1	2.40	0.50
1:B:44:ILE:HG12	1:B:47:LEU:HD12	1.94	0.50
1:B:221:LEU:HB2	1:B:250:VAL:HG22	1.94	0.50
1:A:341:ARG:O	1:A:386:ALA:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:634:PHE:CD1	1:B:634:PHE:N	2.80	0.49
1:A:52:THR:H	1:A:55:GLU:CG	2.16	0.49
1:A:173:ARG:NH1	1:A:208:ALA:O	2.45	0.49
1:A:241:ILE:HB	1:A:248:ILE:HD11	1.93	0.49
1:A:526:LEU:O	1:A:529:LYS:HB2	2.12	0.49
1:A:629:VAL:HB	1:A:634:PHE:HE1	1.77	0.49
1:A:276:LEU:HD21	1:A:299:ILE:HG21	1.94	0.49
1:A:499:ARG:HE	1:A:594:ARG:CD	2.24	0.49
1:B:3:VAL:HG12	1:B:51:VAL:O	2.13	0.49
1:B:4:ILE:HG13	1:B:9:ARG:O	2.12	0.49
1:B:497:ARG:CG	1:B:554:GLU:HG2	2.21	0.49
1:B:681:LYS:HD3	1:B:686:ILE:HG12	1.95	0.49
1:A:349:SER:HB3	1:A:380:VAL:HG21	1.94	0.49
1:B:179:HIS:NE2	1:B:476:ASN:OD1	2.46	0.49
1:B:400:THR:OG1	1:B:401:GLY:N	2.45	0.49
1:A:288:GLN:HG3	1:B:265:THR:HG22	1.94	0.49
1:B:91:LYS:HE2	1:B:96:ASP:OD2	2.13	0.49
1:A:544:CYS:HA	1:A:592:GLY:O	2.11	0.49
1:B:363:TRP:CE3	1:B:364:GLY:HA3	2.48	0.49
1:B:416:ASN:H	1:B:597:LEU:HD21	1.77	0.49
1:B:121:LEU:HD22	1:B:125:LEU:CD1	2.42	0.49
1:A:420:LEU:HD13	1:A:498:HIS:CD2	2.48	0.49
1:A:93:VAL:HG13	1:A:96:ASP:HB2	1.95	0.49
1:B:5:LYS:HB3	1:B:6:ARG:H	1.24	0.49
1:B:273:VAL:HB	1:B:274:PRO:HD3	1.95	0.49
1:B:690:THR:C	1:B:693:LYS:HB3	2.38	0.49
1:B:1:MET:N	1:B:12:ARG:NE	2.52	0.48
1:B:29:LEU:HD21	1:B:80:ARG:HH21	1.78	0.48
1:A:333:TRP:CD1	1:A:408:LYS:HG3	2.48	0.48
1:A:530:GLN:HG2	1:A:578:LEU:HD22	1.94	0.48
3:A:802:3X4:O1	3:A:802:3X4:N	2.46	0.48
1:B:130:ARG:HH21	1:B:183:ILE:HG22	1.78	0.48
1:B:332:LEU:HG	1:B:403:PRO:HB2	1.95	0.48
1:B:626:THR:HG22	1:B:635:GLN:HA	1.93	0.48
1:B:690:THR:HA	1:B:693:LYS:HB3	1.96	0.48
1:A:201:ALA:HB2	1:A:446:LEU:HB2	1.94	0.48
1:B:664:GLY:O	1:B:666:ILE:N	2.47	0.48
1:A:247:GLY:HA3	1:A:428:LEU:CD2	2.43	0.48
1:A:705:SER:OG	1:A:706:GLN:N	2.40	0.48
1:B:415:SER:O	1:B:418:GLN:HG3	2.13	0.48
1:B:431:GLU:HG2	1:B:432:ILE:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:540:LEU:HD11	1:B:566:LEU:HD21	1.96	0.48
1:A:79:ALA:HB2	1:A:145:TYR:N	2.28	0.48
1:A:107:PRO:HG3	1:A:160:ASN:HD21	1.78	0.48
1:A:338:PHE:O	1:A:342:VAL:HG23	2.13	0.48
1:B:669:ILE:H	1:B:669:ILE:HG13	1.49	0.48
1:B:414:LYS:HB2	1:B:733:LYS:HE2	1.96	0.48
1:B:530:GLN:HA	1:B:533:GLU:HB2	1.94	0.48
1:B:656:LYS:O	1:B:660:ILE:HG13	2.13	0.48
1:B:665:SER:C	1:B:667:GLN:H	2.22	0.48
1:A:102:TYR:OH	1:A:118:LYS:HD2	2.13	0.48
1:B:645:LEU:HB3	1:B:651:TRP:HB2	1.96	0.48
1:B:695:ALA:O	1:B:699:GLY:N	2.45	0.48
1:A:397:GLN:HG3	1:A:403:PRO:HD2	1.96	0.48
1:B:486:TYR:OH	1:B:495:ASN:ND2	2.47	0.48
1:A:427:ASN:OD1	1:A:430:THR:N	2.48	0.47
1:A:516:ARG:HH11	1:A:679:LEU:HD13	1.76	0.47
1:A:561:VAL:HG21	1:A:593:ILE:HD11	1.94	0.47
1:A:39:ILE:O	1:A:43:VAL:HG23	2.14	0.47
1:A:204:THR:HA	1:A:215:LEU:HD22	1.96	0.47
1:B:624:ILE:HD13	1:B:660:ILE:HG12	1.96	0.47
1:A:274:PRO:HB2	1:B:285:TYR:HD2	1.79	0.47
1:B:602:MET:O	1:B:602:MET:HG3	2.14	0.47
1:A:33:PHE:CD1	1:A:33:PHE:N	2.82	0.47
1:A:97:VAL:HG21	1:A:169:HIS:ND1	2.30	0.47
1:B:41:MET:O	1:B:45:GLN:HB2	2.13	0.47
1:B:356:CYS:HB3	1:B:374:TYR:CE1	2.50	0.47
1:B:471:LYS:HG2	1:B:475:ARG:HH21	1.80	0.47
1:A:117:ALA:O	1:A:121:LEU:N	2.36	0.47
1:A:225:ASP:HB2	1:A:230:GLY:HA3	1.97	0.47
1:A:478:ASN:HD21	1:A:499:ARG:NH2	2.13	0.47
1:B:124:VAL:HG22	1:B:176:VAL:HG11	1.95	0.47
1:A:23:GLN:C	1:A:25:LEU:N	2.73	0.47
1:A:223:MET:SD	1:A:231:ILE:HA	2.55	0.47
1:A:480:ILE:O	1:A:484:ASN:HB2	2.15	0.47
1:A:650:LEU:HD11	1:A:672:ILE:HA	1.97	0.47
1:B:222:SER:OG	1:B:436:THR:HB	2.14	0.47
1:B:468:GLU:O	1:B:468:GLU:HG2	2.14	0.47
1:A:137:TYR:OH	1:A:169:HIS:NE2	2.45	0.47
1:B:202:SER:HB2	1:B:203:PRO:HD3	1.97	0.47
1:B:319:GLY:HA3	1:B:324:ARG:HH11	1.79	0.47
1:B:710:ILE:HG21	1:B:723:MET:HE2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:LEU:HD22	1:A:234:THR:HG23	1.97	0.47
1:B:200:HIS:HE1	1:B:476:ASN:HB3	1.79	0.47
1:A:207:ASN:HB3	1:A:210:THR:OG1	2.14	0.47
1:A:356:CYS:HB3	1:A:374:TYR:CD1	2.49	0.47
1:A:499:ARG:HB2	1:A:594:ARG:O	2.15	0.47
1:B:196:ARG:O	1:B:453:MET:HG3	2.15	0.47
1:B:320:LYS:H	1:B:324:ARG:HD2	1.80	0.47
1:A:66:THR:HA	1:A:634:PHE:HD2	1.80	0.46
1:A:456:THR:C	1:A:458:GLU:H	2.23	0.46
1:A:687:SER:O	1:A:690:THR:OG1	2.31	0.46
1:B:5:LYS:HZ3	1:B:9:ARG:NE	2.13	0.46
1:B:52:THR:HG23	1:B:55:GLU:HB2	1.97	0.46
1:B:208:ALA:HA	1:B:215:LEU:HD21	1.97	0.46
1:B:300:TYR:CE2	1:B:406:LEU:HD13	2.47	0.46
1:B:391:TYR:HD2	1:B:717:TYR:HD1	1.61	0.46
1:B:497:ARG:O	1:B:553:TYR:HB2	2.15	0.46
1:B:256:ARG:NH1	1:B:262:ILE:HA	2.28	0.46
1:B:602:MET:HA	1:B:603:PRO:HD3	1.81	0.46
1:B:200:HIS:HD1	1:B:204:THR:HG21	1.81	0.46
1:B:220:LEU:HD21	1:B:432:ILE:HG22	1.96	0.46
1:B:308:ILE:HG21	1:B:389:LEU:HD11	1.97	0.46
1:B:296:ALA:C	1:B:297:PHE:HD1	2.24	0.46
1:A:14:MET:SD	1:A:15:PHE:N	2.89	0.46
1:A:469:VAL:O	1:A:473:VAL:HG23	2.16	0.46
1:B:1:MET:N	1:B:12:ARG:HH11	2.14	0.46
1:B:102:TYR:CB	1:B:121:LEU:HD12	2.46	0.46
1:B:340:LYS:O	1:B:344:THR:HG23	2.16	0.46
1:B:529:LYS:CE	1:B:697:GLU:HG2	2.45	0.46
1:A:224:LYS:HE3	1:A:237:GLN:NE2	2.31	0.46
1:A:604:THR:HB	1:A:607:THR:HG22	1.97	0.46
1:B:173:ARG:O	1:B:177:GLY:N	2.43	0.46
1:B:420:LEU:HD22	1:B:498:HIS:NE2	2.31	0.46
1:B:471:LYS:HA	1:B:542:ALA:HB2	1.98	0.46
1:B:553:TYR:O	1:B:555:THR:N	2.49	0.46
1:B:553:TYR:O	1:B:554:GLU:C	2.59	0.45
1:A:94:PHE:HA	1:A:169:HIS:CD2	2.51	0.45
1:A:304:TRP:HH2	1:A:353:PRO:HB3	1.80	0.45
1:A:553:TYR:CZ	1:A:556:TYR:HA	2.50	0.45
1:B:86:LEU:HD11	1:B:163:VAL:HG21	1.97	0.45
1:A:513:ILE:HA	1:A:679:LEU:HD21	1.99	0.45
1:B:313:ASP:HA	1:B:316:LYS:HE3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:ASN:ND2	1:B:500:PRO:O	2.49	0.45
1:A:667:GLN:HA	1:A:677:LYS:HD2	1.99	0.45
1:B:311:PHE:CE1	1:B:330:PHE:HD1	2.35	0.45
1:B:516:ARG:NH2	1:B:644:ASP:OD2	2.44	0.45
1:B:672:ILE:O	1:B:677:LYS:NZ	2.41	0.45
1:A:306:LEU:CD2	1:A:381:ARG:HH21	2.29	0.45
1:A:341:ARG:NH1	1:A:346:GLN:HE21	2.14	0.45
1:A:584:LEU:C	1:A:586:GLU:H	2.25	0.45
1:B:57:ASP:CB	1:B:85:ASN:HD22	2.29	0.45
1:A:652:HIS:O	1:A:656:LYS:HB2	2.16	0.45
1:B:94:PHE:HB2	1:B:135:ILE:HD12	1.98	0.45
1:A:545:ASP:O	1:A:549:GLU:HG3	2.17	0.45
1:B:5:LYS:HZ3	1:B:9:ARG:HE	1.64	0.45
1:A:78:ALA:HA	1:A:81:ILE:HD12	1.99	0.45
1:A:94:PHE:HB2	1:A:135:ILE:HD12	1.99	0.45
1:A:280:ASN:HA	1:A:328:LEU:HG	1.99	0.45
1:A:400:THR:OG1	1:A:401:GLY:N	2.49	0.45
1:A:470:THR:O	1:A:474:VAL:HG23	2.17	0.45
1:B:117:ALA:HB2	1:B:210:THR:C	2.42	0.45
1:B:508:LEU:HD12	1:B:508:LEU:O	2.17	0.45
1:B:519:PHE:CD2	1:B:619:PRO:HB3	2.52	0.45
1:B:709:ASN:N	1:B:709:ASN:ND2	2.65	0.45
1:A:247:GLY:HA3	1:A:428:LEU:HD22	1.99	0.44
1:B:599:ILE:HG22	1:B:601:PRO:HD3	1.98	0.44
1:A:37:ALA:O	1:A:41:MET:HB2	2.17	0.44
1:B:232:TYR:HA	1:B:235:LEU:HB3	2.00	0.44
1:A:203:PRO:HG2	1:A:217:SER:HB3	1.98	0.44
1:A:341:ARG:HB3	1:A:346:GLN:CG	2.47	0.44
1:B:609:GLN:CB	1:B:627:ARG:NH1	2.81	0.44
1:A:67:LEU:C	1:A:69:THR:N	2.76	0.44
1:A:195:GLU:HB3	1:A:197:TRP:CD1	2.52	0.44
1:B:336:ASP:CG	1:B:409:ASP:HB2	2.42	0.44
1:B:104:TYR:CE1	1:B:159:ILE:HG23	2.53	0.44
1:B:334:ILE:O	1:B:408:LYS:N	2.51	0.44
1:A:500:PRO:HB3	1:A:596:SER:OG	2.18	0.44
1:B:448:SER:O	1:B:449:LEU:HD23	2.18	0.44
1:A:31:MET:HE1	1:A:36:PRO:HD3	2.00	0.44
1:A:684:TRP:CZ3	1:A:711:HIS:HB3	2.53	0.44
1:B:446:LEU:HB3	1:B:602:MET:SD	2.58	0.44
1:A:576:THR:HG22	1:A:578:LEU:H	1.82	0.43
1:A:645:LEU:HB3	1:A:651:TRP:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:GLN:HA	1:B:41:MET:SD	2.58	0.43
1:B:241:ILE:HB	1:B:248:ILE:HD11	1.98	0.43
1:B:315:LYS:HD2	1:B:330:PHE:CE2	2.52	0.43
1:B:514:LEU:HD23	1:B:514:LEU:O	2.17	0.43
1:B:634:PHE:N	1:B:634:PHE:HD1	2.16	0.43
1:A:136:ILE:HD12	1:A:139:ARG:CZ	2.48	0.43
1:A:638:ASN:HB3	1:A:641:LEU:HB3	2.00	0.43
1:B:1:MET:HG2	1:B:2:HIS:CB	2.44	0.43
1:B:713:ALA:HB2	1:B:742:ARG:HH22	1.83	0.43
1:A:351:MET:HB3	1:A:356:CYS:SG	2.58	0.43
1:A:431:GLU:OE2	1:A:603:PRO:HD3	2.18	0.43
1:B:441:VAL:HG22	1:B:490:GLU:HB2	1.99	0.43
1:B:508:LEU:HA	1:B:511:ALA:HB3	2.01	0.43
1:A:91:LYS:NZ	1:A:100:ASP:OD1	2.41	0.43
1:A:92:LYS:HA	1:A:166:ARG:CZ	2.49	0.43
1:A:309:PHE:C	1:A:311:PHE:H	2.27	0.43
1:A:392:ALA:HA	1:A:395:GLU:OE1	2.18	0.43
1:B:120:THR:O	1:B:124:VAL:HG23	2.19	0.43
1:B:599:ILE:HB	1:B:702:ILE:HA	2.01	0.43
1:A:326:ARG:HG3	1:A:326:ARG:HH11	1.82	0.43
1:A:362:VAL:HG13	1:A:367:PHE:HD2	1.83	0.43
1:A:394:ILE:HG23	1:A:720:LEU:HD13	2.00	0.43
1:A:645:LEU:HD13	1:A:651:TRP:CE3	2.53	0.43
1:B:534:THR:HA	1:B:579:TRP:HE1	1.84	0.43
1:B:716:ASN:HB3	1:B:719:LYS:HB3	2.00	0.43
1:A:25:LEU:HD22	1:A:80:ARG:HB3	2.01	0.43
1:A:29:LEU:CD1	1:A:77:LEU:HB2	2.49	0.43
1:A:226:ASP:OD1	1:A:256:ARG:HG2	2.19	0.43
1:A:227:SER:O	1:A:231:ILE:N	2.49	0.43
1:B:561:VAL:HG21	1:B:593:ILE:HD11	2.01	0.43
1:A:306:LEU:HD22	1:A:381:ARG:HE	1.84	0.43
1:A:519:PHE:CZ	1:A:619:PRO:HG3	2.54	0.43
1:A:655:MET:O	1:A:659:ILE:HG13	2.19	0.43
1:B:432:ILE:HG13	1:B:444:CYS:SG	2.59	0.43
1:B:456:THR:C	1:B:458:GLU:H	2.27	0.43
1:A:33:PHE:CD2	1:A:646:THR:HB	2.54	0.43
1:B:716:ASN:HB3	1:B:719:LYS:CB	2.49	0.43
1:A:29:LEU:O	1:A:31:MET:N	2.52	0.42
1:A:449:LEU:HB2	1:A:505:VAL:HG12	1.99	0.42
1:A:529:LYS:NZ	1:A:697:GLU:OE1	2.51	0.42
1:B:219:PHE:N	1:B:247:GLY:O	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:GLY:HA2	1:A:739:LEU:HB2	2.01	0.42
1:A:18:ILE:O	1:A:21:ARG:HB2	2.20	0.42
1:A:390:TRP:NE1	1:A:394:ILE:HD11	2.34	0.42
1:A:18:ILE:HB	1:A:40:THR:HG23	2.02	0.42
1:A:120:THR:O	1:A:124:VAL:HG23	2.20	0.42
1:B:341:ARG:CD	1:B:347:ASP:O	2.66	0.42
1:B:635:GLN:HE22	1:B:660:ILE:HD11	1.84	0.42
1:A:253:SER:OG	1:A:302:GLU:HG3	2.20	0.42
1:B:300:TYR:CE2	1:B:426:SER:HB3	2.54	0.42
1:A:204:THR:HG23	1:A:215:LEU:HD22	2.02	0.42
1:A:300:TYR:CZ	1:A:426:SER:HB3	2.55	0.42
1:A:405:MET:HB2	1:A:736:MET:N	2.35	0.42
1:B:306:LEU:HA	1:B:350:LEU:HB3	2.02	0.42
1:B:313:ASP:HB3	1:B:324:ARG:NH2	2.34	0.42
1:A:429:CYS:HB2	1:A:431:GLU:OE2	2.20	0.42
1:A:439:ASP:HB3	1:A:490:GLU:HG3	2.01	0.42
1:A:669:ILE:HA	1:A:670:PRO:HD3	1.54	0.42
1:B:512:PHE:CZ	1:B:524:ALA:HB1	2.54	0.42
1:A:261:TYR:HA	1:A:268:ASN:ND2	2.33	0.42
1:A:306:LEU:C	1:A:308:ILE:H	2.28	0.42
1:A:402:THR:HG22	1:A:404:TYR:HE1	1.82	0.42
1:B:123:ILE:HG21	1:B:181:GLU:HA	2.01	0.42
1:B:417:GLN:NE2	1:B:596:SER:OG	2.51	0.42
1:A:642:LEU:HA	1:A:645:LEU:HB2	2.01	0.42
1:B:20:SER:HA	1:B:23:GLN:HB2	2.00	0.42
1:B:117:ALA:HB2	1:B:211:ASN:N	2.34	0.42
1:B:362:VAL:HG11	1:B:370:LEU:CD2	2.50	0.42
1:A:79:ALA:O	1:A:83:VAL:HG23	2.19	0.41
1:B:512:PHE:HD2	1:B:519:PHE:CD2	2.37	0.41
1:A:227:SER:HA	2:A:801:TTP:O3'	2.19	0.41
1:B:5:LYS:HA	1:B:53:THR:HG23	2.01	0.41
1:B:228:ILE:HG12	2:B:801:TTP:H5'2	2.03	0.41
1:A:220:LEU:CD1	1:A:434:GLU:HB2	2.50	0.41
1:B:221:LEU:O	1:B:250:VAL:HA	2.20	0.41
1:B:300:TYR:CZ	1:B:426:SER:HB3	2.56	0.41
1:A:69:THR:HG21	1:A:656:LYS:HZ3	1.83	0.41
1:A:155:TYR:HB3	1:A:170:MET:HE2	2.01	0.41
1:A:343:GLU:C	1:A:345:ASN:H	2.27	0.41
1:A:472:VAL:HG12	1:A:476:ASN:OD1	2.20	0.41
1:B:272:LEU:HD12	1:B:307:ASP:HB2	2.03	0.41
1:B:456:THR:C	1:B:458:GLU:N	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:597:LEU:HD13	1:B:704:GLN:HG2	2.02	0.41
1:A:33:PHE:N	1:A:33:PHE:HD1	2.18	0.41
1:A:532:PHE:CE2	1:A:698:ARG:HD3	2.56	0.41
1:B:275:MET:HE3	1:B:279:TYR:CE2	2.54	0.41
1:B:628:ARG:CB	1:B:633:GLU:HG2	2.51	0.41
1:A:646:THR:C	1:A:648:ARG:H	2.27	0.41
1:A:652:HIS:H	1:A:655:MET:HB3	1.86	0.41
1:B:195:GLU:HG3	1:B:197:TRP:CD1	2.55	0.41
1:B:407:TYR:CZ	1:B:728:TRP:HB2	2.55	0.41
1:A:304:TRP:CH2	1:A:353:PRO:HB3	2.55	0.41
1:A:426:SER:OG	1:A:427:ASN:N	2.54	0.41
1:A:308:ILE:O	1:A:312:LEU:HD12	2.21	0.41
1:A:466:LEU:O	1:A:470:THR:OG1	2.20	0.41
1:A:477:LEU:O	1:A:481:ILE:HG13	2.20	0.41
1:B:104:TYR:HE1	1:B:159:ILE:HG23	1.86	0.41
1:B:469:VAL:O	1:B:473:VAL:HG23	2.21	0.41
1:B:512:PHE:CE2	1:B:524:ALA:HB1	2.56	0.41
1:B:621:THR:O	1:B:682:THR:HB	2.20	0.41
1:B:675:ASP:OD1	1:B:675:ASP:C	2.64	0.41
1:B:698:ARG:HG3	1:B:706:GLN:HE22	1.86	0.41
1:A:405:MET:HE3	1:A:405:MET:HB3	1.94	0.41
1:B:3:VAL:CG2	1:B:13:VAL:HG13	2.51	0.41
1:B:407:TYR:O	1:B:411:CYS:N	2.54	0.41
1:B:662:CYS:O	1:B:663:ASN:HB2	2.19	0.41
1:A:121:LEU:HD23	1:A:121:LEU:O	2.21	0.40
1:B:474:VAL:HG22	1:B:503:ILE:HD11	2.02	0.40
1:A:304:TRP:CH2	1:A:359:LEU:HB3	2.56	0.40
1:A:391:TYR:CD2	1:A:394:ILE:HD12	2.56	0.40
1:A:710:ILE:CG1	1:A:736:MET:HG3	2.51	0.40
1:B:223:MET:HE3	1:B:231:ILE:HA	2.03	0.40
1:A:220:LEU:HD13	1:A:434:GLU:HB2	2.03	0.40
1:A:337:LEU:O	1:A:341:ARG:HG3	2.21	0.40
3:A:802:3X4:C12	3:A:802:3X4:H27	2.33	0.40
1:B:736:MET:SD	1:B:739:LEU:HG	2.61	0.40
1:A:683:VAL:HA	1:A:686:ILE:HB	2.02	0.40
1:B:204:THR:O	1:B:208:ALA:HB2	2.20	0.40
1:B:394:ILE:HG23	1:B:720:LEU:HD13	2.02	0.40
1:B:667:GLN:N	1:B:667:GLN:OE1	2.54	0.40
1:A:298:ALA:CB	1:A:428:LEU:HA	2.52	0.40
1:A:405:MET:HG3	1:A:724:HIS:CE1	2.55	0.40
1:A:553:TYR:HE1	1:A:555:THR:HG23	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:702:ILE:HD12	1:A:706:GLN:NE2	2.37	0.40
1:B:385:LYS:O	1:B:388:GLN:HB2	2.21	0.40
1:B:488:VAL:HA	1:B:489:PRO:HD3	1.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	708/792 (89%)	607 (86%)	82 (12%)	19 (3%)	4	27
1	B	732/792 (92%)	619 (85%)	88 (12%)	25 (3%)	3	25
All	All	1440/1584 (91%)	1226 (85%)	170 (12%)	44 (3%)	3	26

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	218	CYS
1	A	219	PHE
1	A	263	ALA
1	A	615	GLU
1	A	656	LYS
1	B	7	ASP
1	B	12	ARG
1	B	52	THR
1	B	525	GLN
1	B	554	GLU
1	B	602	MET
1	B	640	HIS
1	B	648	ARG
1	A	30	ASN
1	A	51	VAL

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Mol	Chain	Res	Type
1	A	530	GLN
1	A	572	ASN
1	A	650	LEU
1	B	5	LYS
1	B	23	GLN
1	B	49	SER
1	B	180	LYS
1	B	288	GLN
1	B	317	ASN
1	B	639	PRO
1	A	382	LYS
1	A	404	TYR
1	A	590	LYS
1	B	116	VAL
1	B	529	LYS
1	B	665	SER
1	A	116	VAL
1	A	529	LYS
1	B	51	VAL
1	B	321	GLU
1	B	737	TYR
1	A	62	GLU
1	A	224	LYS
1	A	715	PRO
1	B	316	LYS
1	A	605	ALA
1	B	217	SER
1	B	666	ILE
1	B	601	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	581/693 (84%)	511 (88%)	70 (12%)	5	23
1	B	607/693 (88%)	537 (88%)	70 (12%)	5	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1188/1386 (86%)	1048 (88%)	140 (12%)	5 23

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	32	ASP
1	A	41	MET
1	A	55	GLU
1	A	59	LEU
1	A	62	GLU
1	A	69	THR
1	A	91	LYS
1	A	93	VAL
1	A	119	SER
1	A	122	ASP
1	A	130	ARG
1	A	158	LYS
1	A	171	LEU
1	A	184	ASP
1	A	214	GLN
1	A	220	LEU
1	A	221	LEU
1	A	225	ASP
1	A	229	GLU
1	A	243	LYS
1	A	270	ASN
1	A	282	THR
1	A	287	ASP
1	A	288	GLN
1	A	310	GLU
1	A	341	ARG
1	A	343	GLU
1	A	344	THR
1	A	361	GLU
1	A	375	GLU
1	A	380	VAL
1	A	381	ARG
1	A	382	LYS
1	A	383	VAL
1	A	389	LEU
1	A	404	TYR

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Mol	Chain	Res	Type
1	A	413	ARG
1	A	414	LYS
1	A	428	LEU
1	A	443	VAL
1	A	455	VAL
1	A	465	LYS
1	A	475	ARG
1	A	499	ARG
1	A	508	LEU
1	A	516	ARG
1	A	523	GLU
1	A	526	LEU
1	A	527	LEU
1	A	546	LEU
1	A	565	ILE
1	A	572	ASN
1	A	583	VAL
1	A	587	LYS
1	A	591	TYR
1	A	594	ARG
1	A	602	MET
1	A	606	SER
1	A	607	THR
1	A	650	LEU
1	A	669	ILE
1	A	671	GLU
1	A	677	LYS
1	A	679	LEU
1	A	681	LYS
1	A	685	GLU
1	A	688	GLN
1	A	728	TRP
1	A	739	LEU
1	B	7	ASP
1	B	9	ARG
1	B	13	VAL
1	B	16	ASP
1	B	27	TYR
1	B	31	MET
1	B	33	PHE
1	B	47	LEU
1	B	51	VAL

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Mol	Chain	Res	Type
1	B	54	VAL
1	B	59	LEU
1	B	86	LEU
1	B	91	LYS
1	B	108	HIS
1	B	119	SER
1	B	121	LEU
1	B	123	ILE
1	B	128	LYS
1	B	130	ARG
1	B	140	ASP
1	B	158	LYS
1	B	162	LYS
1	B	180	LYS
1	B	199	THR
1	B	207	ASN
1	B	212	ARG
1	B	214	GLN
1	B	220	LEU
1	B	223	MET
1	B	272	LEU
1	B	287	ASP
1	B	297	PHE
1	B	315	LYS
1	B	324	ARG
1	B	343	GLU
1	B	355	GLU
1	B	365	GLU
1	B	366	GLU
1	B	369	LYS
1	B	379	ARG
1	B	380	VAL
1	B	389	LEU
1	B	391	TYR
1	B	422	THR
1	B	436	THR
1	B	457	SER
1	B	465	LYS
1	B	478	ASN
1	B	479	LYS
1	B	497	ARG
1	B	508	LEU

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Mol	Chain	Res	Type
1	B	516	ARG
1	B	523	GLU
1	B	526	LEU
1	B	554	GLU
1	B	563	LYS
1	B	566	LEU
1	B	578	LEU
1	B	590	LYS
1	B	604	THR
1	B	611	LEU
1	B	629	VAL
1	B	648	ARG
1	B	669	ILE
1	B	671	GLU
1	B	674	ASP
1	B	675	ASP
1	B	681	LYS
1	B	697	GLU
1	B	709	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	ASN
1	A	268	ASN
1	A	346	GLN
1	A	445	ASN
1	A	478	ASN
1	A	525	GLN
1	A	530	GLN
1	A	595	ASN
1	A	657	ASN
1	A	667	GLN
1	A	678	GLN
1	B	2	HIS
1	B	85	ASN
1	B	200	HIS
1	B	214	GLN
1	B	291	ASN
1	B	323	GLN
1	B	418	GLN
1	B	445	ASN

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Mol	Chain	Res	Type
1	B	459	HIS
1	B	478	ASN
1	B	495	ASN
1	B	525	GLN
1	B	635	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](#)

3 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	TTP	B	801	-	29,30,30	1.30	5 (17%)	43,47,47	1.82	8 (18%)
2	TTP	A	801	-	29,30,30	1.42	7 (24%)	43,47,47	1.92	10 (23%)
3	3X4	A	802	-	30,31,31	2.31	7 (23%)	41,44,44	2.05	9 (21%)

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	TTP	B	801	-	-	8/22/34/34	0/2/2/2
2	TTP	A	801	-	-	6/22/34/34	0/2/2/2
3	3X4	A	802	-	-	9/27/43/43	0/2/2/2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	3X4	O2-C5	6.46	1.35	1.22
3	A	802	3X4	O1-C12	6.41	1.35	1.22
3	A	802	3X4	C11-C12	-5.63	1.39	1.48
3	A	802	3X4	C6-C5	-3.54	1.43	1.48
3	A	802	3X4	O6-C24	3.02	1.31	1.22
2	A	801	TTP	C4-N3	-3.02	1.33	1.38
2	A	801	TTP	C2-N1	2.99	1.43	1.38
2	B	801	TTP	C4-N3	-2.65	1.33	1.38
2	A	801	TTP	C6-N1	-2.61	1.33	1.38
3	A	802	3X4	O7-C24	-2.60	1.22	1.30
2	A	801	TTP	C6-C5	2.41	1.38	1.34
2	B	801	TTP	C6-C5	2.39	1.38	1.34
3	A	802	3X4	C4-C3	2.38	1.56	1.52
2	B	801	TTP	C2-N1	2.28	1.42	1.38
2	B	801	TTP	C6-N1	-2.26	1.34	1.38
2	A	801	TTP	C4-C5	2.25	1.48	1.44
2	A	801	TTP	C2-N3	-2.12	1.34	1.38
2	B	801	TTP	PA-O3A	2.07	1.61	1.59
2	A	801	TTP	PA-O3A	2.02	1.61	1.59

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	3X4	C12-N1-C5	-6.31	106.63	112.02
3	A	802	3X4	C4-N1-C12	5.75	128.79	123.71
2	A	801	TTP	N3-C2-N1	5.52	122.08	114.89
2	A	801	TTP	C4-N3-C2	-5.09	120.66	127.34
2	B	801	TTP	C4-N3-C2	-5.06	120.71	127.34
2	B	801	TTP	O4-C4-C5	-4.88	119.33	124.92
2	B	801	TTP	C5-C4-N3	4.73	119.44	115.32
2	B	801	TTP	N3-C2-N1	4.62	120.90	114.89
3	A	802	3X4	O1-C12-N1	-4.56	120.18	124.79
3	A	802	3X4	C11-C12-N1	4.29	109.06	105.88
3	A	802	3X4	C6-C5-N1	3.91	108.77	105.88
2	A	801	TTP	C5-C6-N1	-3.63	119.37	123.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	3X4	O2-C5-N1	-3.60	121.15	124.79
2	A	801	TTP	C5-C4-N3	3.42	118.29	115.32
2	A	801	TTP	O4-C4-C5	-3.36	121.07	124.92
2	B	801	TTP	C5-C6-N1	-3.24	119.79	123.31
2	A	801	TTP	C1'-N1-C2	2.98	123.48	117.66
2	A	801	TTP	O2-C2-N3	-2.94	116.06	121.49
2	A	801	TTP	C5M-C5-C6	-2.57	119.37	122.85
2	A	801	TTP	C1'-N1-C6	-2.35	116.80	120.74
3	A	802	3X4	C10-C11-C6	-2.26	118.48	121.06
2	A	801	TTP	C6-C5-C4	2.26	119.88	118.02
2	B	801	TTP	C1'-N1-C2	2.16	121.88	117.66
3	A	802	3X4	O-C3-C4	-2.02	117.47	121.02
3	A	802	3X4	C4-C3-N	2.02	118.58	114.94
2	B	801	TTP	C1'-N1-C6	-2.02	117.35	120.74
2	B	801	TTP	O2-C2-N1	-2.01	120.18	122.80

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	TTP	C5'-O5'-PA-O2A
2	B	801	TTP	O4'-C4'-C5'-O5'
3	A	802	3X4	C3-C4-N1-C5
3	A	802	3X4	C3-C4-N1-C12
2	A	801	TTP	O4'-C1'-N1-C2
2	B	801	TTP	C3'-C4'-C5'-O5'
2	B	801	TTP	C4'-C5'-O5'-PA
2	A	801	TTP	O4'-C1'-N1-C6
3	A	802	3X4	N2-C14-C15-C16
3	A	802	3X4	N3-C18-C24-O7
3	A	802	3X4	C-C1-C13-N2
3	A	802	3X4	C2-C1-C13-N2
3	A	802	3X4	C16-C17-C18-N3
2	B	801	TTP	C5'-O5'-PA-O1A
2	B	801	TTP	C5'-O5'-PA-O3A
3	A	802	3X4	C-C1-C13-O3
2	A	801	TTP	PG-O3B-PB-O3A
3	A	802	3X4	C2-C1-C13-O3
2	A	801	TTP	PA-O3A-PB-O2B
2	B	801	TTP	PG-O3B-PB-O1B
2	A	801	TTP	PG-O3B-PB-O1B
2	B	801	TTP	PG-O3B-PB-O2B

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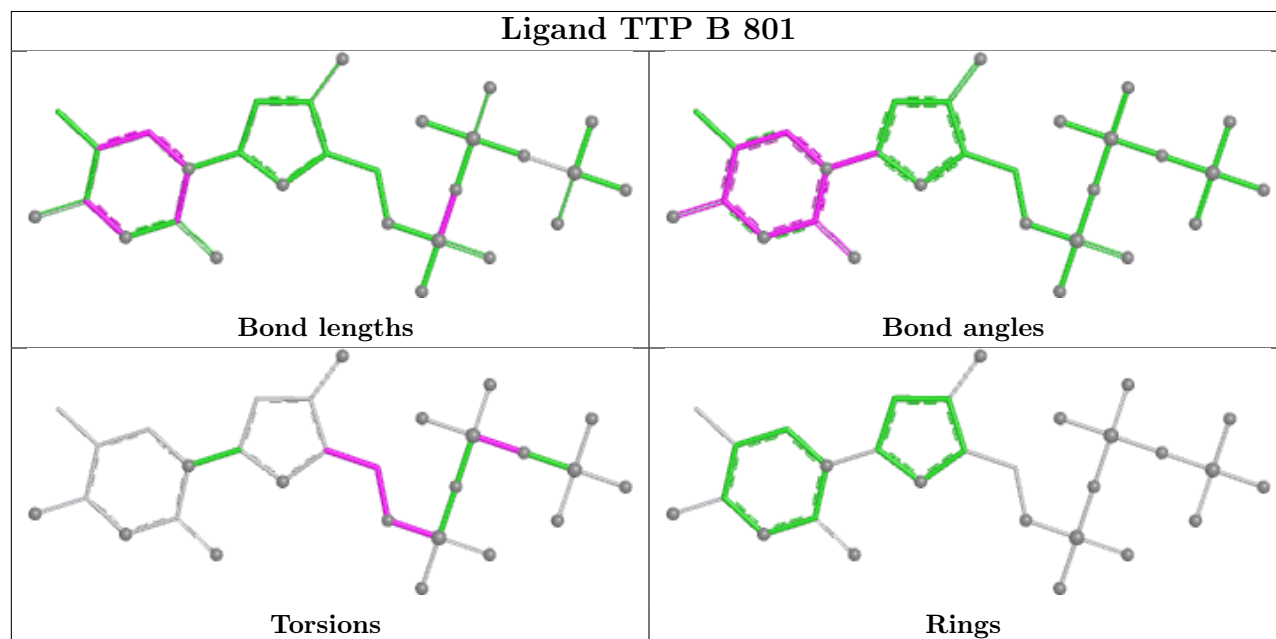
Mol	Chain	Res	Type	Atoms
2	A	801	TTP	O4'-C4'-C5'-O5'

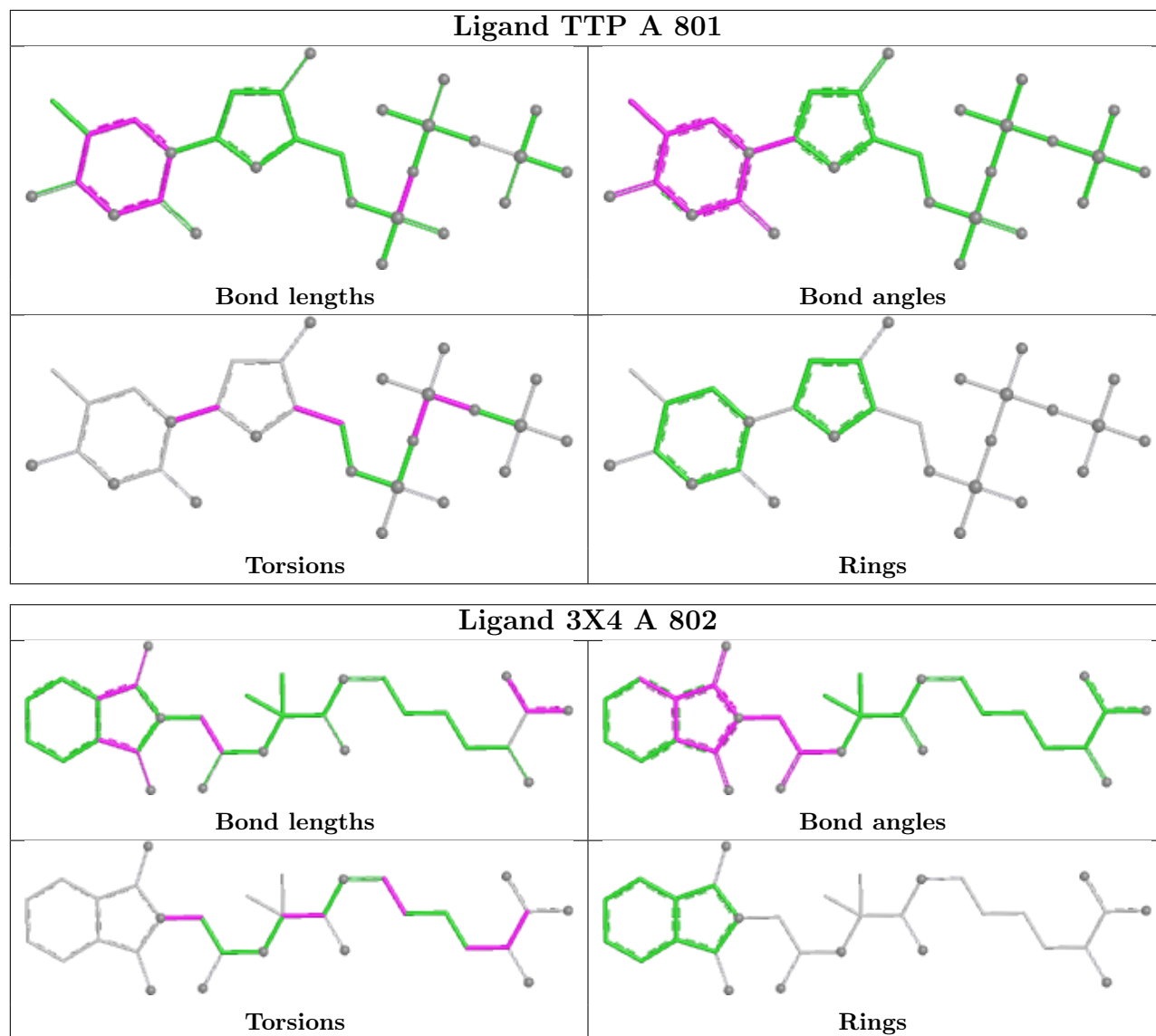
There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	TTP	4	0
2	A	801	TTP	4	0
3	A	802	3X4	3	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	714/792 (90%)	-0.33	0 100 100	35, 115, 140, 165	2 (0%)
1	B	738/792 (93%)	-0.35	0 100 100	90, 125, 154, 173	0
All	All	1452/1584 (91%)	-0.34	0 100 100	35, 119, 148, 173	2 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

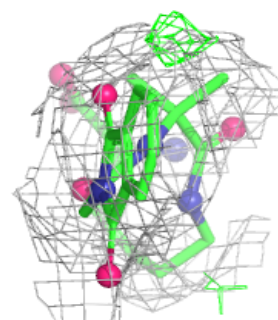
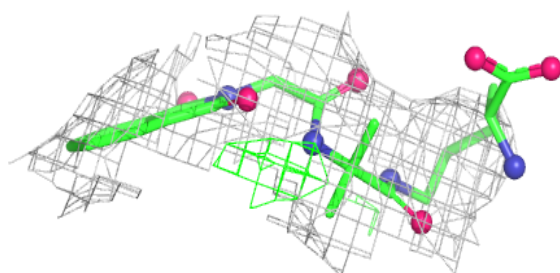
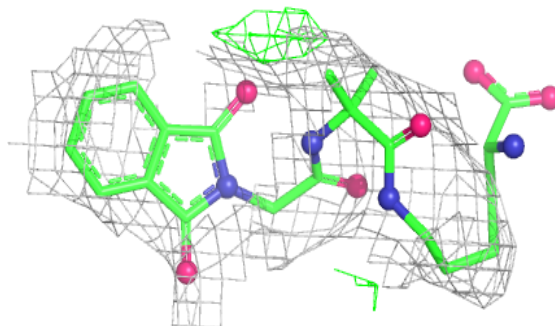
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	3X4	A	802	30/30	0.62	0.10	103,119,126,129	0
2	TTP	A	801	29/29	0.65	0.12	101,127,159,165	0
2	TTP	B	801	29/29	0.92	0.07	93,111,129,132	0

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.

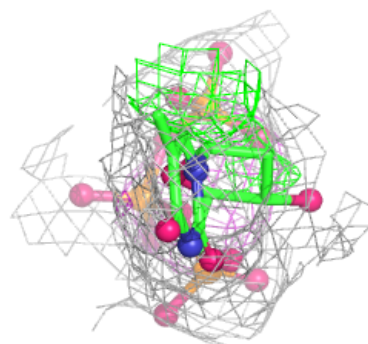
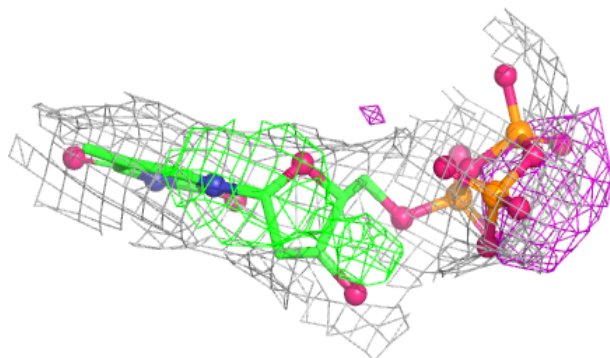
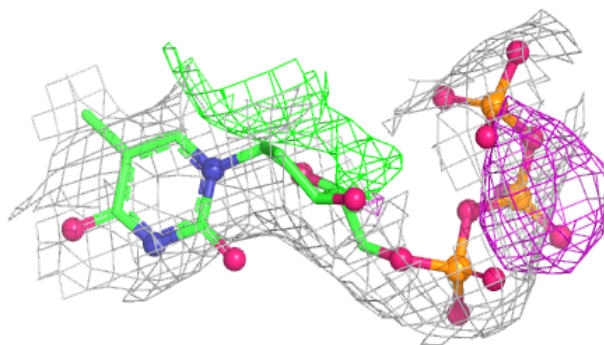
Electron density around 3X4 A 802:

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



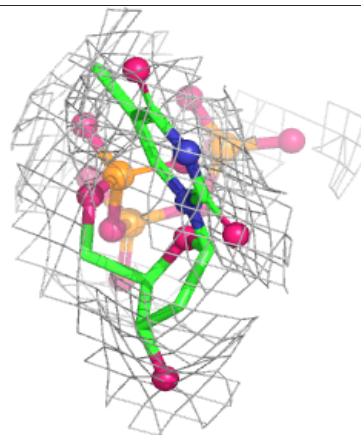
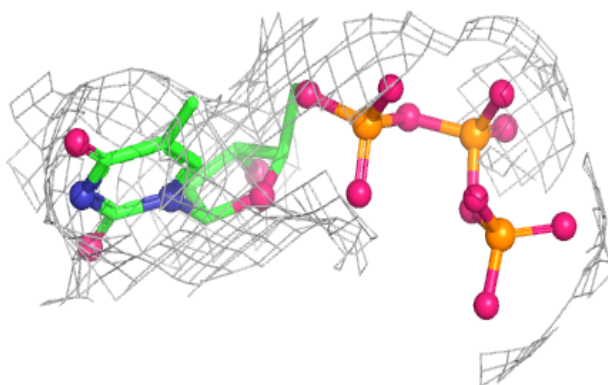
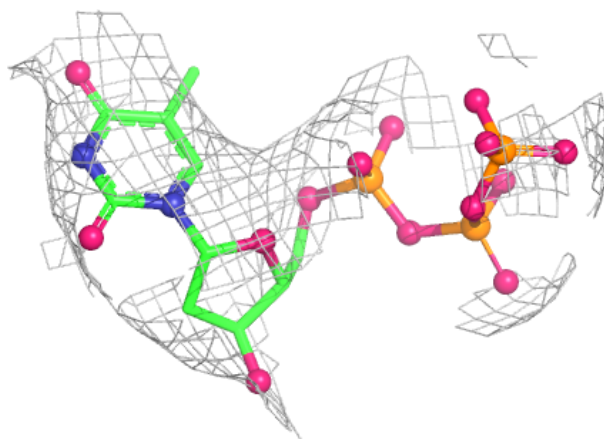
Electron density around TTP A 801:

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



Electron density around TTP B 801:

$2mF_o - DF_c$ (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.