



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:26 PM UTC

PDB ID : 5J87 / pdb_00005j87
Title : Discovery of N-(3-(5-((3-acrylamido-4-(morpholine-4-carbonyl)phenyl)amino)-1-methyl-6-oxo-1,6-dihydropyridin-3-yl)-2-methylphenyl)-4-(tert-butyl)benzamide (CHMFL-BTK-01) as a Highly Selective Irreversible BTK Kinase Inhibitor
Authors : Yun, C.H.; Zhang, S.
Deposited on : 2016-04-07
Resolution : 1.59 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

The following versions of software and data (see [references](#) ①) 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

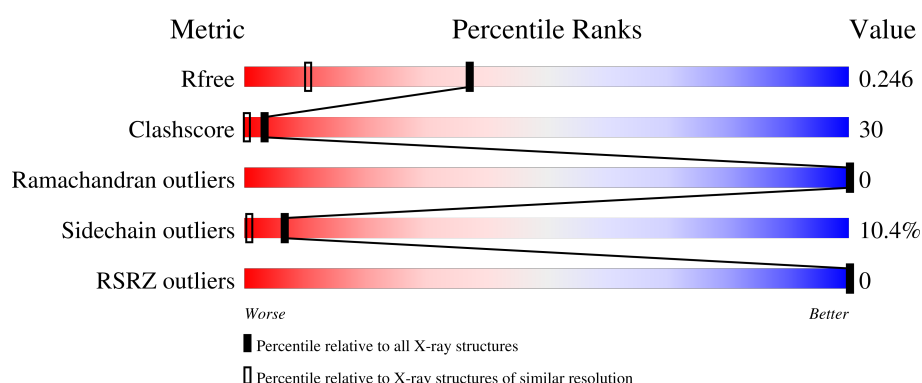
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.59 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	274	
1	B	274	
1	C	274	
1	D	274	

2 Entry composition [i](#)

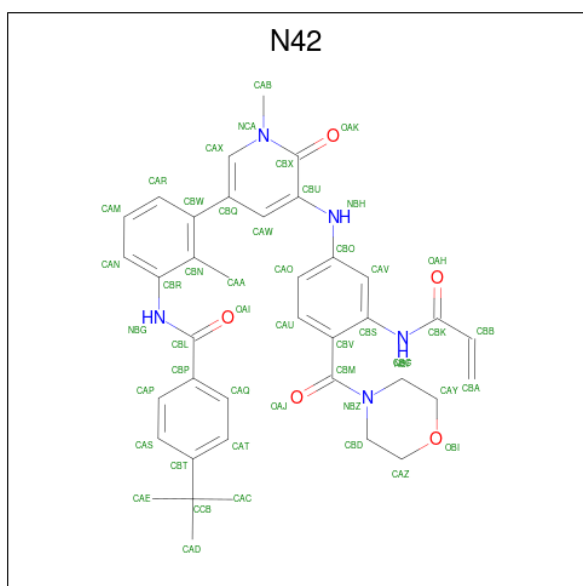
There are 3 unique types of molecules in this entry. The entry contains 9721 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Tyrosine-protein kinase BTK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	2	0
			2158	1385	352	402	19			
1	B	274	Total	C	N	O	S	0	3	0
			2239	1433	368	420	18			
1	C	261	Total	C	N	O	S	0	1	0
			2127	1365	349	394	19			
1	D	263	Total	C	N	O	S	0	1	0
			2141	1374	348	400	19			

- Molecule 2 is N-[3-(5-{[3-(acryloylamino)-4-(morpholine-4-carbonyl)phenyl]amino}-1-methyl-6-oxo-1,6-dihydropyridin-3-yl)-2-methylphenyl]-4-tert-butylbenzamide (CCD ID: N42) (formula: C₃₈H₄₁N₅O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			48	38	5	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			48	38	5	5		
2	C	1	Total	C	N	O	0	0
			48	38	5	5		
2	D	1	Total	C	N	O	0	0
			48	38	5	5		

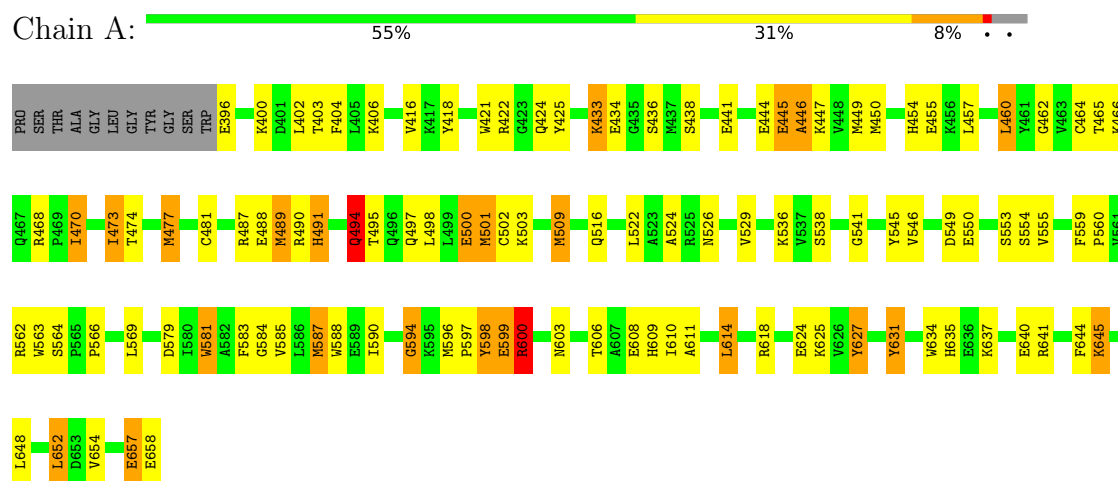
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	221	Total	O	0	0
			221	221		
3	B	235	Total	O	0	0
			235	235		
3	C	165	Total	O	0	0
			165	165		
3	D	243	Total	O	0	0
			243	243		

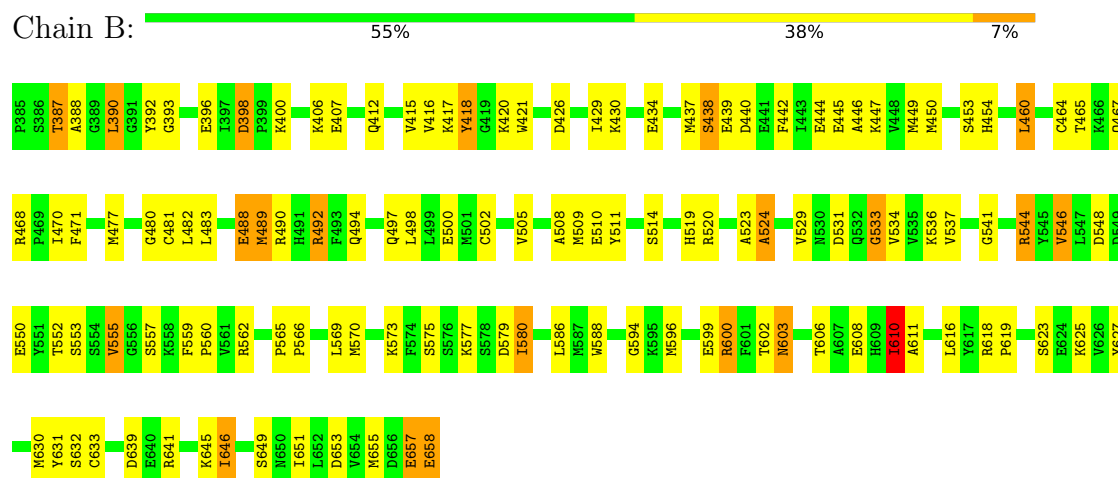
3 Residue-property plots

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: Tyrosine-protein kinase BTK

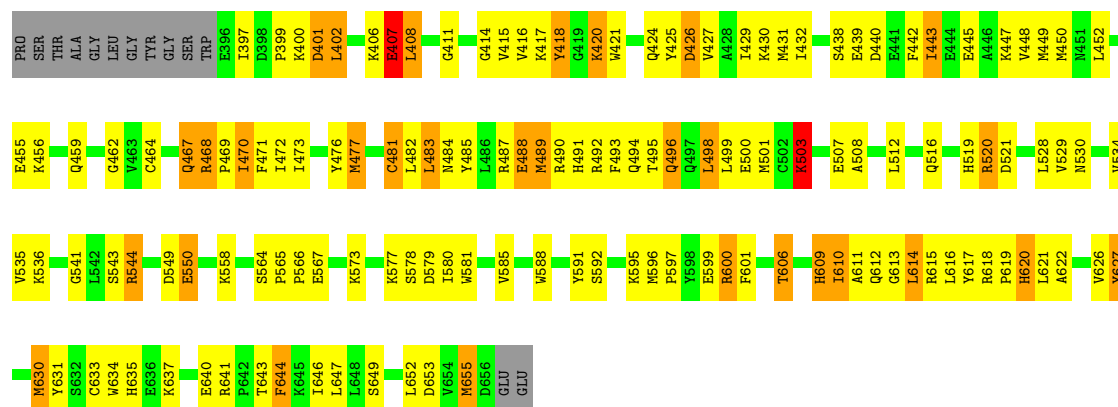


• Molecule 1: Tyrosine-protein kinase BTK

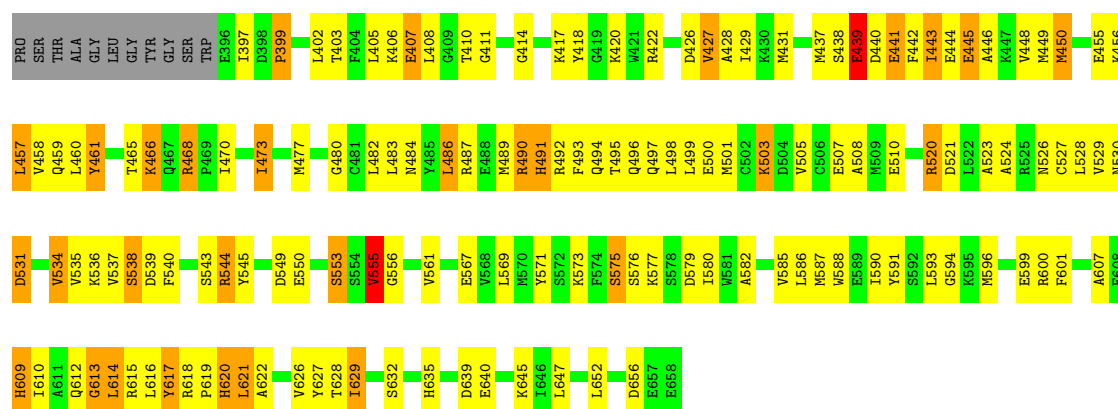


• Molecule 1: Tyrosine-protein kinase BTK





• Molecule 1: Tyrosine-protein kinase BTK



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	41.76Å 93.55Å 145.89Å 90.00° 89.94° 90.00°	Depositor
Resolution (Å)	48.63 – 1.59 48.63 – 1.59	Depositor EDS
% Data completeness (in resolution range)	90.1 (48.63-1.59) 90.3 (48.63-1.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 1.58Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.216 , 0.248 0.216 , 0.246	Depositor DCC
R_{free} test set	6882 reflections (4.53%)	wwPDB-VP
Wilson B-factor (Å ²)	13.8	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.458 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9721	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.70% 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: N42

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	1.62	42/2213 (1.9%)	1.10	6/2982 (0.2%)
1	B	1.65	52/2294 (2.3%)	1.08	8/3094 (0.3%)
1	C	1.43	16/2179 (0.7%)	1.27	15/2938 (0.5%)
1	D	1.24	11/2193 (0.5%)	1.21	9/2957 (0.3%)
All	All	1.50	121/8879 (1.4%)	1.17	38/11971 (0.3%)

All (121) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	608	GLU	C-O	-8.39	1.14	1.24
1	D	647	LEU	C-O	-8.18	1.14	1.24
1	A	498	LEU	C-O	-8.05	1.14	1.24
1	A	416	VAL	C-O	-7.77	1.16	1.24
1	B	646	ILE	C-O	-7.45	1.15	1.24
1	B	606	THR	C-O	-7.42	1.15	1.24
1	D	505	VAL	C-O	-7.07	1.15	1.24
1	A	644	PHE	C-O	-7.06	1.15	1.24
1	A	581	TRP	C-O	-7.05	1.15	1.24
1	B	529	VAL	C-O	-7.03	1.16	1.24
1	B	579	ASP	C-O	-6.86	1.16	1.24
1	B	498	LEU	C-O	-6.81	1.16	1.24
1	A	631	TYR	C-O	-6.79	1.15	1.24
1	B	482	LEU	C-O	-6.76	1.16	1.24
1	A	608	GLU	C-O	-6.68	1.16	1.24
1	A	495	THR	C-O	-6.64	1.15	1.24
1	A	457	LEU	C-O	-6.52	1.16	1.24
1	A	500	GLU	C-O	-6.50	1.15	1.24
1	A	524	ALA	C-O	-6.49	1.15	1.24
1	B	453	SER	C-O	-6.44	1.16	1.24
1	A	579	ASP	C-O	-6.43	1.16	1.24
1	C	477	MET	C-O	-6.39	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	529	VAL	C-O	-6.38	1.17	1.24
1	C	498	LEU	C-O	-6.31	1.16	1.24
1	B	505	VAL	C-O	-6.31	1.16	1.24
1	A	460	LEU	C-O	-6.31	1.16	1.24
1	A	624	GLU	C-O	-6.30	1.16	1.24
1	B	454	HIS	C-O	-6.29	1.16	1.23
1	B	580	ILE	C-O	-6.29	1.16	1.24
1	B	619	PRO	C-O	-6.15	1.16	1.23
1	A	566	PRO	C-O	-6.14	1.16	1.24
1	A	598	TYR	C-O	-6.14	1.15	1.23
1	C	601	PHE	C-O	-6.10	1.16	1.23
1	A	652	LEU	C-O	-6.05	1.17	1.24
1	B	497	GLN	C-O	-5.99	1.17	1.24
1	B	502	CYS	C-O	-5.98	1.17	1.24
1	A	641	ARG	C-O	-5.91	1.16	1.24
1	B	610	ILE	C-O	-5.91	1.17	1.24
1	B	429	ILE	C-O	-5.89	1.17	1.24
1	B	575	SER	C-O	-5.88	1.17	1.23
1	B	398	ASP	C-O	-5.88	1.16	1.24
1	B	625	LYS	C-O	-5.86	1.17	1.24
1	A	585	VAL	C-O	-5.85	1.17	1.24
1	C	630	MET	C-O	-5.85	1.17	1.24
1	A	597	PRO	C-O	-5.84	1.17	1.23
1	B	447	LYS	C-O	-5.83	1.16	1.24
1	B	388	ALA	C-O	-5.83	1.17	1.23
1	B	510	GLU	C-O	-5.82	1.17	1.24
1	B	509	MET	C-O	-5.78	1.17	1.24
1	B	603	ASN	C-O	-5.76	1.17	1.24
1	A	541	GLY	C-O	-5.74	1.16	1.24
1	C	597	PRO	C-O	-5.69	1.16	1.23
1	B	533	GLY	C-O	-5.67	1.16	1.24
1	D	459	GLN	C-O	-5.66	1.17	1.24
1	B	537	VAL	C-O	-5.65	1.17	1.24
1	A	606	THR	C-O	-5.62	1.17	1.24
1	A	473	ILE	C-O	-5.60	1.18	1.24
1	B	631	TYR	C-O	-5.60	1.17	1.24
1	B	546	VAL	C-O	-5.59	1.18	1.24
1	B	418	TYR	C-O	-5.58	1.17	1.23
1	C	564	SER	C-O	-5.58	1.16	1.24
1	A	477	MET	C-O	-5.56	1.17	1.24
1	A	404	PHE	C-O	-5.51	1.17	1.23
1	A	603	ASN	C-O	-5.51	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	565	PRO	C-O	-5.50	1.18	1.24
1	A	587	MET	C-O	-5.50	1.17	1.24
1	B	442	PHE	C-O	-5.50	1.17	1.24
1	A	446	ALA	C-O	-5.49	1.17	1.24
1	C	447	LYS	C-O	-5.47	1.17	1.24
1	B	464	CYS	C-O	-5.45	1.17	1.24
1	B	438	SER	C-O	-5.44	1.17	1.23
1	C	528	LEU	C-O	-5.43	1.17	1.24
1	D	399	PRO	C-O	-5.43	1.16	1.24
1	D	427	VAL	C-O	-5.42	1.17	1.23
1	A	627	TYR	C-O	-5.41	1.17	1.24
1	C	580	ILE	C-O	-5.41	1.17	1.24
1	A	433	LYS	C-O	-5.39	1.17	1.23
1	A	588	TRP	C-O	-5.37	1.17	1.24
1	B	450	MET	C-O	-5.36	1.17	1.24
1	A	584	GLY	C-O	-5.36	1.17	1.23
1	D	529	VAL	C-O	-5.35	1.18	1.24
1	B	446	ALA	C-O	-5.35	1.17	1.24
1	B	480	GLY	C-O	-5.34	1.16	1.23
1	B	611	ALA	C-O	-5.34	1.17	1.24
1	A	400	LYS	C-O	-5.33	1.17	1.24
1	B	524	ALA	C-O	-5.33	1.17	1.24
1	A	509	MET	C-O	-5.32	1.17	1.24
1	B	421	TRP	C-O	-5.32	1.17	1.24
1	C	442	PHE	C-O	-5.32	1.17	1.24
1	B	508	ALA	C-O	-5.32	1.17	1.24
1	B	544	ARG	C-O	-5.28	1.17	1.24
1	D	629	ILE	C-O	-5.27	1.18	1.24
1	D	473	ILE	C-O	-5.27	1.18	1.24
1	A	600	ARG	C-O	-5.25	1.17	1.24
1	B	550	GLU	C-O	-5.24	1.17	1.24
1	C	503	LYS	C-O	-5.22	1.18	1.24
1	A	454	HIS	C-O	-5.21	1.17	1.23
1	C	579	ASP	C-O	-5.21	1.18	1.24
1	A	501	MET	C-O	-5.18	1.18	1.24
1	A	522	LEU	C-O	-5.18	1.17	1.23
1	D	457	LEU	C-O	-5.18	1.17	1.23
1	A	474	THR	C-O	-5.16	1.17	1.23
1	C	644	PHE	C-O	-5.16	1.18	1.24
1	A	583	PHE	C-O	-5.14	1.18	1.24
1	B	630	MET	C-O	-5.14	1.18	1.24
1	B	519	HIS	C-O	-5.12	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	632	SER	C-O	-5.12	1.17	1.24
1	C	470	ILE	C-O	-5.11	1.17	1.24
1	B	562	ARG	C-O	-5.08	1.17	1.24
1	B	541	GLY	C-O	-5.08	1.17	1.23
1	C	544	ARG	C-O	-5.07	1.17	1.24
1	B	393	GLY	C-O	-5.07	1.17	1.24
1	B	434	GLU	C-O	-5.06	1.17	1.23
1	A	546	VAL	C-O	-5.05	1.18	1.24
1	A	503	LYS	C-O	-5.04	1.18	1.24
1	C	627	TYR	C-O	-5.04	1.18	1.24
1	D	626	VAL	C-O	-5.03	1.18	1.24
1	D	523	ALA	C-O	-5.03	1.18	1.23
1	B	523	ALA	C-O	-5.02	1.18	1.23
1	B	437	MET	C-O	-5.01	1.18	1.23
1	B	570	MET	C-O	-5.01	1.18	1.24

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	439	GLU	N-CA-C	9.36	121.57	111.36
1	D	491	HIS	N-CA-C	7.39	119.42	111.36
1	C	408	LEU	N-CA-C	6.94	118.92	111.36
1	D	613	GLY	N-CA-C	6.93	123.10	114.37
1	C	655	MET	CA-C-N	-6.74	109.57	121.70
1	C	655	MET	C-N-CA	-6.74	109.57	121.70
1	C	614	LEU	N-CA-C	6.56	120.19	110.48
1	C	443	ILE	N-CA-C	6.50	117.25	110.62
1	D	561	VAL	N-CA-C	6.40	117.92	110.62
1	D	450	MET	N-CA-C	6.37	118.31	111.36
1	C	613	GLY	N-CA-C	5.99	121.92	114.37
1	C	415	VAL	N-CA-C	5.97	118.23	109.63
1	C	653	ASP	N-CA-C	-5.96	104.78	111.28
1	B	552	THR	N-CA-C	5.84	117.45	111.14
1	C	462	GLY	N-CA-C	5.83	118.73	110.74
1	A	590	ILE	N-CA-C	5.83	116.02	110.42
1	D	441	GLU	N-CA-C	-5.63	106.62	112.93
1	C	567	GLU	N-CA-C	5.53	117.39	111.36
1	A	491	HIS	N-CA-C	-5.45	99.85	108.73
1	B	489	MET	N-CA-C	-5.40	106.53	113.01
1	C	606	THR	N-CA-C	-5.36	105.43	111.28
1	A	490	ARG	N-CA-C	-5.36	105.44	111.28
1	D	497	GLN	N-CA-C	5.34	117.19	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	594	GLY	N-CA-C	5.33	123.43	115.64
1	C	627	TYR	N-CA-C	5.33	117.17	111.36
1	C	496	GLN	N-CA-C	-5.30	105.50	111.28
1	A	489	MET	N-CA-C	-5.28	106.52	113.17
1	C	407	GLU	N-CA-C	5.28	118.15	109.76
1	C	577	LYS	N-CA-C	5.22	117.88	111.82
1	D	484	ASN	N-CA-C	5.13	116.95	111.36
1	D	555	VAL	N-CA-C	5.13	116.47	111.91
1	A	494	GLN	N-CA-C	-5.12	103.64	110.55
1	B	557	SER	N-CA-C	5.10	117.58	111.71
1	A	594	GLY	N-CA-C	5.05	122.80	115.32
1	B	497	GLN	N-CA-C	5.04	116.77	111.28
1	B	657	GLU	CA-C-N	-5.04	112.64	121.70
1	B	657	GLU	C-N-CA	-5.04	112.64	121.70
1	B	392	TYR	N-CA-C	5.00	117.63	111.82

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	2158	0	2129	61	0
1	B	2239	0	2188	78	0
1	C	2127	0	2091	210	0
1	D	2141	0	2096	238	0
2	A	48	0	0	3	0
2	B	48	0	0	1	0
2	C	48	0	0	5	0
2	D	48	0	0	2	0
3	A	221	0	0	12	0
3	B	235	0	0	24	0
3	C	165	0	0	43	0
3	D	243	0	0	41	0
All	All	9721	0	8504	528	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 30.

All (528) 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:C:620:HIS:N	1:D:617:TYR:HB3	1.21	1.46
1:C:618:ARG:CB	1:D:618:ARG:HG2	1.60	1.30
1:B:492:ARG:HH21	1:B:492:ARG:HG3	1.01	1.17
1:C:455:GLU:O	1:C:536:LYS:HE2	1.43	1.16
1:C:489:MET:HG3	3:C:866:HOH:O	1.40	1.15
1:D:490:ARG:HB2	1:D:490:ARG:NH2	1.61	1.14
1:D:429:ILE:HG13	3:D:889:HOH:O	1.48	1.13
1:D:499:LEU:HD22	3:D:820:HOH:O	1.47	1.11
1:C:618:ARG:HB3	1:D:618:ARG:HG2	1.27	1.11
1:D:620:HIS:HB3	1:D:621:LEU:HD12	1.32	1.11
1:D:486:LEU:HD23	3:D:881:HOH:O	1.51	1.11
1:C:620:HIS:N	1:D:617:TYR:CB	2.14	1.09
1:C:618:ARG:HB2	1:D:618:ARG:HG2	1.35	1.06
1:A:614:LEU:C	1:A:614:LEU:HD12	1.79	1.05
1:C:620:HIS:CA	1:D:617:TYR:HB3	1.86	1.05
1:D:490:ARG:HB2	1:D:490:ARG:CZ	1.85	1.04
1:A:614:LEU:HD12	1:A:614:LEU:O	1.57	1.04
1:D:620:HIS:HB3	1:D:621:LEU:CD1	1.92	1.00
1:D:486:LEU:HD11	1:D:590:ILE:HA	1.44	0.98
1:D:486:LEU:HA	3:D:881:HOH:O	1.61	0.97
1:C:616:LEU:HD23	1:D:620:HIS:HE1	1.27	0.97
1:C:617:TYR:HB3	1:D:620:HIS:N	1.79	0.96
1:C:618:ARG:HB3	1:D:618:ARG:CG	1.97	0.95
1:C:529:VAL:HG22	1:C:535:VAL:HG22	1.45	0.94
1:C:616:LEU:HA	1:D:620:HIS:CE1	2.03	0.93
1:C:477:MET:HG2	3:C:807:HOH:O	1.67	0.93
1:C:620:HIS:HA	1:D:617:TYR:CA	1.99	0.92
1:C:620:HIS:H	1:D:617:TYR:HB3	1.34	0.91
1:C:581:TRP:HE3	1:C:641:ARG:NH1	1.69	0.90
1:C:619:PRO:C	1:D:617:TYR:HB3	1.96	0.90
1:C:464:CYS:HB2	1:C:471:PHE:HB2	1.53	0.89
1:C:618:ARG:NH2	1:D:627:TYR:CE1	2.40	0.89
1:A:614:LEU:C	1:A:614:LEU:CD1	2.44	0.89
1:D:490:ARG:NH2	1:D:490:ARG:CB	2.36	0.88
1:B:492:ARG:HG3	1:B:492:ARG:NH2	1.80	0.88
1:C:429:ILE:HG23	3:C:902:HOH:O	1.71	0.87
1:C:620:HIS:HA	1:D:617:TYR:N	1.90	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:621:LEU:CD1	1:D:621:LEU:N	2.38	0.87
1:C:615:ARG:HD2	1:C:634:TRP:HE3	1.38	0.87
1:C:616:LEU:HD23	1:D:620:HIS:CE1	2.11	0.86
1:C:485:TYR:CE2	1:C:491:HIS:CE1	2.65	0.84
1:D:440:ASP:O	1:D:444:GLU:HG3	1.77	0.83
1:D:618:ARG:CB	1:D:627:TYR:CD1	2.62	0.82
1:B:600:ARG:HG3	1:D:407:GLU:OE2	1.79	0.82
1:A:598:TYR:CE2	1:A:614:LEU:HD11	2.14	0.82
1:C:491:HIS:ND1	1:C:493:PHE:CE2	2.47	0.81
1:A:445:GLU:HG2	1:A:545:TYR:OH	1.79	0.81
1:C:476:TYR:CD2	3:C:834:HOH:O	2.33	0.81
1:C:501:MET:SD	3:C:940:HOH:O	2.38	0.81
1:C:617:TYR:HB3	1:D:620:HIS:CA	2.10	0.81
1:B:534:VAL:HA	3:B:807:HOH:O	1.80	0.80
1:D:490:ARG:CG	1:D:490:ARG:HH21	1.95	0.80
1:C:617:TYR:HB3	1:D:619:PRO:C	2.06	0.80
1:C:596:MET:HE2	1:C:599:GLU:HA	1.62	0.80
1:B:494:GLN:HG2	3:B:860:HOH:O	1.80	0.79
1:C:592:SER:HB2	3:C:839:HOH:O	1.82	0.79
1:D:405:LEU:HD12	1:D:418:TYR:CE2	2.17	0.79
1:C:491:HIS:HD1	1:C:493:PHE:HE2	1.29	0.79
1:D:549:ASP:O	1:D:553:SER:HB3	1.82	0.79
1:D:490:ARG:CZ	1:D:490:ARG:CB	2.60	0.79
1:D:417:LYS:NZ	1:D:431:MET:SD	2.56	0.79
1:D:503:LYS:HE3	1:D:507:GLU:OE1	1.82	0.79
1:C:581:TRP:HB2	1:C:641:ARG:NH1	1.97	0.78
1:C:618:ARG:HH21	1:D:627:TYR:HE1	1.31	0.78
1:D:465:THR:HA	1:D:470:ILE:HG12	1.65	0.78
1:C:615:ARG:HD2	1:C:634:TRP:CE3	2.17	0.78
1:C:631:TYR:HA	3:C:894:HOH:O	1.84	0.78
1:C:611:ALA:HB2	3:C:877:HOH:O	1.84	0.77
1:C:485:TYR:HB3	3:C:855:HOH:O	1.84	0.77
1:B:460:LEU:HD12	3:B:862:HOH:O	1.84	0.77
1:C:530:ASN:HB2	3:C:808:HOH:O	1.84	0.77
1:C:406:LYS:HG2	1:C:418:TYR:HD2	1.50	0.76
1:C:498:LEU:HD12	3:C:884:HOH:O	1.86	0.76
1:B:641:ARG:HD2	3:B:856:HOH:O	1.86	0.75
1:D:621:LEU:HD12	1:D:621:LEU:N	1.99	0.75
1:D:618:ARG:HB3	1:D:627:TYR:CD1	2.21	0.75
1:C:473:ILE:HG13	3:C:902:HOH:O	1.87	0.75
1:B:610:ILE:HD12	3:B:849:HOH:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:618:ARG:O	1:D:617:TYR:HB2	1.88	0.74
1:B:488:GLU:OE1	1:B:490:ARG:HD3	1.87	0.74
1:C:503:LYS:O	1:C:507:GLU:HG3	1.87	0.74
1:C:618:ARG:HG3	1:C:627:TYR:HB2	1.69	0.74
1:C:581:TRP:CE3	1:C:641:ARG:NH1	2.55	0.74
1:C:489:MET:HG2	3:C:889:HOH:O	1.86	0.73
1:D:439:GLU:OE2	1:D:470:ILE:HD12	1.87	0.73
1:C:619:PRO:C	1:D:617:TYR:CB	2.56	0.73
1:D:403:THR:HB	3:D:802:HOH:O	1.87	0.73
1:D:618:ARG:HB2	1:D:627:TYR:CD1	2.24	0.72
1:C:617:TYR:HB2	1:D:618:ARG:O	1.90	0.72
1:C:618:ARG:NH2	1:D:618:ARG:H	1.88	0.72
1:A:509:MET:SD	3:A:919:HOH:O	2.48	0.72
1:D:486:LEU:HA	1:D:493:PHE:HE2	1.55	0.72
1:C:617:TYR:CA	1:D:620:HIS:HA	2.20	0.71
1:C:620:HIS:CA	1:D:617:TYR:CB	2.66	0.71
1:D:420:LYS:HG2	1:D:426:ASP:OD1	1.89	0.71
1:C:617:TYR:HB3	1:D:620:HIS:HA	1.71	0.71
1:A:402:LEU:HB3	3:A:823:HOH:O	1.90	0.70
1:C:620:HIS:ND1	1:D:617:TYR:CD2	2.58	0.70
1:C:401:ASP:HB2	1:C:421:TRP:HD1	1.55	0.70
1:C:408:LEU:HD21	1:C:418:TYR:HB3	1.72	0.70
1:D:442:PHE:HD2	1:D:443:ILE:HD13	1.57	0.70
1:C:635:HIS:CD2	1:C:637:LYS:HG3	2.27	0.70
1:D:455:GLU:HG2	1:D:456:LYS:HG2	1.74	0.69
1:B:398:ASP:OD1	1:B:400:LYS:HB2	1.92	0.69
1:C:418:TYR:CD1	3:C:834:HOH:O	2.46	0.69
1:C:585:VAL:HG22	1:C:634:TRP:HZ2	1.58	0.69
1:D:501:MET:SD	3:D:994:HOH:O	2.50	0.69
1:D:620:HIS:CB	1:D:621:LEU:CD1	2.70	0.69
1:D:490:ARG:HH21	1:D:490:ARG:HG3	1.56	0.69
1:C:491:HIS:HB2	1:C:493:PHE:CD2	2.28	0.68
1:C:618:ARG:NE	1:D:618:ARG:HB3	2.08	0.68
1:B:534:VAL:CA	3:B:807:HOH:O	2.37	0.68
1:D:473:ILE:HG22	3:D:832:HOH:O	1.93	0.68
1:C:618:ARG:HB3	1:D:618:ARG:CB	2.23	0.68
1:D:618:ARG:CD	1:D:622:ALA:HB3	2.24	0.68
1:C:464:CYS:SG	3:C:933:HOH:O	2.53	0.67
1:D:483:LEU:O	1:D:487:ARG:HG3	1.95	0.67
1:B:470:ILE:HD11	3:B:801:HOH:O	1.93	0.67
1:D:503:LYS:HE3	1:D:507:GLU:CD	2.20	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:GLU:HB2	3:A:991:HOH:O	1.96	0.66
1:D:418:TYR:HE1	1:D:426:ASP:HB3	1.60	0.66
1:D:621:LEU:HD13	1:D:621:LEU:H	1.61	0.65
1:C:430:LYS:HB2	1:C:472:ILE:HB	1.78	0.65
1:D:441:GLU:O	1:D:545:TYR:CE1	2.50	0.65
1:C:620:HIS:HA	1:D:617:TYR:HA	1.78	0.65
1:B:412:GLN:HG3	3:B:876:HOH:O	1.96	0.65
1:D:427:VAL:HG23	3:D:889:HOH:O	1.97	0.65
1:D:569:LEU:CD1	1:D:610:ILE:HD11	2.26	0.65
1:D:534:VAL:HG13	3:D:828:HOH:O	1.96	0.65
1:C:618:ARG:CZ	1:D:618:ARG:H	2.10	0.65
1:C:482:LEU:HD12	3:C:855:HOH:O	1.97	0.64
1:C:503:LYS:HD3	3:C:864:HOH:O	1.97	0.64
1:C:635:HIS:HD2	1:C:637:LYS:HG3	1.62	0.64
1:C:476:TYR:CG	3:C:834:HOH:O	2.47	0.64
1:D:582:ALA:HA	3:D:856:HOH:O	1.98	0.64
1:C:618:ARG:NH1	1:C:619:PRO:O	2.31	0.64
1:D:495:THR:HG22	1:D:621:LEU:HB3	1.80	0.64
1:B:468:ARG:NH2	3:B:801:HOH:O	2.32	0.63
1:C:407:GLU:HG2	1:C:416:VAL:O	1.98	0.63
1:D:455:GLU:CG	1:D:456:LYS:HG2	2.28	0.63
1:C:418:TYR:HD1	3:C:834:HOH:O	1.82	0.63
1:D:596:MET:CE	1:D:599:GLU:HA	2.29	0.63
1:D:618:ARG:CD	1:D:622:ALA:CB	2.77	0.63
1:A:596:MET:HE3	1:A:599:GLU:HA	1.79	0.63
1:C:406:LYS:HG2	1:C:418:TYR:CD2	2.33	0.63
1:C:618:ARG:NH1	1:C:622:ALA:O	2.32	0.63
1:D:618:ARG:HB2	1:D:627:TYR:HD1	1.62	0.63
1:B:449:MET:HG2	1:B:460:LEU:HD11	1.81	0.62
1:C:620:HIS:CD2	3:C:860:HOH:O	2.52	0.62
1:D:635:HIS:CG	1:D:640:GLU:HB2	2.35	0.62
1:C:618:ARG:HE	1:D:618:ARG:HB3	1.62	0.62
1:C:616:LEU:CD2	1:D:620:HIS:HE1	2.09	0.62
1:D:573:LYS:NZ	1:D:575:SER:OG	2.33	0.62
1:D:613:GLY:HA3	3:D:807:HOH:O	1.98	0.62
1:C:617:TYR:CB	1:D:620:HIS:HA	2.29	0.61
1:A:494:GLN:HG3	1:A:497:GLN:HG3	1.82	0.61
1:C:618:ARG:NH2	1:D:618:ARG:N	2.49	0.61
1:D:490:ARG:NE	3:D:809:HOH:O	2.34	0.61
1:C:520:ARG:HH11	1:C:544:ARG:HD3	1.66	0.61
1:D:468:ARG:NH1	1:D:470:ILE:HG13	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:477:MET:HE3	1:C:530:ASN:HB3	1.83	0.61
1:C:618:ARG:CB	1:D:618:ARG:CG	2.53	0.61
1:C:618:ARG:NE	1:D:627:TYR:CE1	2.69	0.61
1:D:456:LYS:NZ	1:D:507:GLU:OE2	2.32	0.60
1:C:599:GLU:OE1	1:C:600:ARG:NH2	2.34	0.60
1:A:433:LYS:HE2	1:A:436:SER:HB3	1.82	0.60
1:B:618:ARG:HH11	1:B:618:ARG:HG2	1.65	0.60
1:D:482:LEU:HD12	1:D:527:CYS:HB2	1.82	0.60
1:C:620:HIS:HA	1:D:617:TYR:CB	2.29	0.60
1:D:569:LEU:HD11	1:D:610:ILE:HD11	1.83	0.60
1:A:481:CYS:HB2	3:A:821:HOH:O	2.01	0.60
1:C:616:LEU:HD12	1:C:634:TRP:CH2	2.37	0.60
1:D:550:GLU:O	1:D:556:GLY:HA3	2.01	0.60
1:B:449:MET:HG2	1:B:460:LEU:CD1	2.32	0.60
1:C:616:LEU:HA	1:D:620:HIS:ND1	2.17	0.60
1:C:585:VAL:HG22	1:C:634:TRP:CZ2	2.36	0.60
1:D:397:ILE:HD12	1:D:473:ILE:HG13	1.84	0.60
1:D:490:ARG:CB	1:D:490:ARG:HH21	2.13	0.60
1:C:618:ARG:NH2	1:D:616:LEU:O	2.32	0.59
1:A:465:THR:HA	1:A:470:ILE:HG12	1.84	0.59
1:C:467:GLN:HB2	1:C:469:PRO:O	2.03	0.59
2:C:701:N42:CAA	2:C:701:N42:CAX	2.80	0.59
1:C:530:ASN:HD21	1:C:534:VAL:HB	1.67	0.59
1:C:618:ARG:NE	1:D:627:TYR:CZ	2.70	0.59
1:B:544:ARG:HD2	3:B:866:HOH:O	2.03	0.59
1:C:455:GLU:O	1:C:536:LYS:CE	2.34	0.59
1:A:406:LYS:HB3	1:A:418:TYR:HB3	1.85	0.59
1:D:499:LEU:HB2	3:D:820:HOH:O	2.01	0.59
1:C:565:PRO:HB3	1:C:641:ARG:HH12	1.68	0.59
1:D:455:GLU:HG3	1:D:456:LYS:HE3	1.84	0.58
1:C:588:TRP:HA	3:C:870:HOH:O	2.01	0.58
1:C:401:ASP:HB2	1:C:421:TRP:CD1	2.37	0.58
1:C:600:ARG:NE	3:C:806:HOH:O	2.34	0.58
1:D:422:ARG:NH2	3:D:816:HOH:O	2.36	0.58
1:D:442:PHE:CD2	1:D:443:ILE:HD13	2.39	0.58
1:C:519:HIS:CE1	1:C:521:ASP:O	2.56	0.58
1:B:524:ALA:N	1:B:586[A]:LEU:HD13	2.18	0.58
1:B:534:VAL:N	3:B:807:HOH:O	2.37	0.58
1:C:617:TYR:CB	1:D:619:PRO:C	2.75	0.58
1:C:618:ARG:NH2	1:D:627:TYR:CZ	2.72	0.58
1:C:620:HIS:ND1	1:D:617:TYR:CG	2.61	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:609:HIS:ND1	3:A:805:HOH:O	2.33	0.58
1:D:500:GLU:HB3	3:D:867:HOH:O	2.04	0.58
1:B:600:ARG:NH1	3:B:804:HOH:O	2.36	0.57
1:C:516:GLN:NE2	3:C:801:HOH:O	2.31	0.57
1:C:424:GLN:HG2	1:C:425:TYR:CD2	2.39	0.57
1:C:627:TYR:HA	1:C:630:MET:HE3	1.86	0.57
1:D:544:ARG:NH2	1:D:545:TYR:OH	2.34	0.57
1:D:621:LEU:CD1	1:D:621:LEU:H	2.12	0.57
1:A:645:LYS:NZ	3:A:801:HOH:O	2.31	0.57
1:B:599:GLU:HG3	1:D:407:GLU:OE2	2.04	0.57
1:C:618:ARG:CZ	1:D:627:TYR:CE1	2.88	0.57
1:D:406:LYS:HG2	1:D:418:TYR:HD2	1.69	0.57
1:C:445:GLU:CD	1:C:544:ARG:HH22	2.12	0.57
1:D:496:GLN:NE2	3:D:819:HOH:O	2.37	0.57
1:C:485:TYR:HE2	1:C:491:HIS:CE1	2.19	0.57
1:C:417:LYS:O	1:C:429:ILE:N	2.38	0.56
1:C:618:ARG:CZ	1:D:627:TYR:CZ	2.88	0.56
1:D:618:ARG:O	1:D:618:ARG:HG3	2.03	0.56
1:D:635:HIS:CD2	1:D:640:GLU:HB2	2.41	0.56
1:A:424:GLN:HG2	1:A:425:TYR:N	2.20	0.56
1:C:617:TYR:N	1:D:620:HIS:ND1	2.53	0.56
1:C:630:MET:SD	3:C:870:HOH:O	2.58	0.56
2:C:701:N42:CAB	3:C:807:HOH:O	2.53	0.56
1:D:618:ARG:CD	1:D:627:TYR:HB2	2.36	0.56
1:C:401:ASP:N	1:C:401:ASP:OD2	2.38	0.56
1:D:571:TYR:HB2	3:D:823:HOH:O	2.05	0.56
1:D:427:VAL:CG2	3:D:889:HOH:O	2.52	0.56
1:A:625:LYS:HE2	1:A:654:VAL:HG22	1.88	0.56
1:D:483:LEU:HD13	1:D:524:ALA:HB3	1.87	0.55
1:C:445:GLU:O	1:C:448:VAL:N	2.39	0.55
1:D:591:TYR:HB3	1:D:619:PRO:HB2	1.88	0.55
1:C:581:TRP:HB2	1:C:641:ARG:HH12	1.70	0.55
1:B:477:MET:HE2	1:B:536:LYS:HB2	1.88	0.55
1:D:486:LEU:HA	1:D:493:PHE:CE2	2.38	0.55
1:A:610:ILE:C	1:A:610:ILE:HD12	2.31	0.55
1:B:651:ILE:O	1:B:655:MET:HG3	2.06	0.55
1:D:487:ARG:HE	1:D:594:GLY:HA3	1.71	0.54
1:A:445:GLU:HG2	1:A:545:TYR:HH	1.71	0.54
1:A:598:TYR:HE2	1:A:614:LEU:HD11	1.67	0.54
1:C:595:LYS:NZ	1:D:617:TYR:CD2	2.75	0.54
1:D:540:PHE:HD1	3:D:874:HOH:O	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:609:HIS:CD2	3:C:814:HOH:O	2.59	0.54
1:D:456:LYS:C	3:D:830:HOH:O	2.50	0.54
1:D:521:ASP:O	1:D:526:ASN:ND2	2.36	0.54
1:C:618:ARG:HG3	1:C:627:TYR:CD1	2.43	0.54
1:C:620:HIS:ND1	1:D:617:TYR:N	2.52	0.53
1:B:580:ILE:HB	3:B:856:HOH:O	2.08	0.53
1:D:510:GLU:OE1	1:D:645:LYS:HA	2.08	0.53
1:C:618:ARG:HB3	1:D:618:ARG:HB3	1.90	0.53
1:D:508:ALA:CB	3:D:830:HOH:O	2.56	0.53
1:D:620:HIS:CB	1:D:621:LEU:HD12	2.23	0.53
1:A:635:HIS:NE2	1:A:640:GLU:OE1	2.41	0.53
1:C:581:TRP:HB2	1:C:641:ARG:HH11	1.74	0.53
1:C:599:GLU:HG3	1:C:600:ARG:HG2	1.91	0.53
1:C:592:SER:HB3	1:C:595:LYS:HB2	1.90	0.53
1:C:617:TYR:N	1:D:620:HIS:HA	2.23	0.53
1:D:482:LEU:HD12	1:D:527:CYS:CB	2.38	0.53
1:C:489:MET:SD	3:C:954:HOH:O	2.59	0.53
1:A:635:HIS:HB2	3:A:944:HOH:O	2.08	0.53
1:C:618:ARG:HG2	1:C:618:ARG:HH11	1.74	0.53
1:D:555:VAL:CG2	3:D:843:HOH:O	2.57	0.53
1:C:615:ARG:HB3	1:C:634:TRP:CZ3	2.44	0.53
1:C:620:HIS:HD1	1:D:617:TYR:CB	2.21	0.53
1:D:493:PHE:HB3	1:D:498:LEU:HD21	1.90	0.53
1:D:588:TRP:NE1	1:D:617:TYR:O	2.42	0.53
2:C:701:N42:CAU	2:C:701:N42:CBD	2.88	0.52
2:C:701:N42:CAV	2:C:701:N42:CAW	2.86	0.52
1:D:586:LEU:HD23	1:D:586:LEU:O	2.09	0.52
1:D:585:VAL:HB	3:D:856:HOH:O	2.08	0.52
1:C:616:LEU:HD12	1:C:634:TRP:HH2	1.74	0.52
1:D:486:LEU:CA	3:D:881:HOH:O	2.37	0.52
1:A:600:ARG:HG2	1:A:600:ARG:HH21	1.75	0.52
1:B:492:ARG:NH2	1:B:492:ARG:CG	2.62	0.52
1:C:620:HIS:HD2	3:C:860:HOH:O	1.88	0.52
1:D:461:TYR:HD2	1:D:461:TYR:N	2.07	0.52
1:C:606:THR:O	1:C:610:ILE:HG23	2.10	0.52
1:B:407:GLU:HG2	3:B:883:HOH:O	2.09	0.52
1:C:609:HIS:HE1	3:C:881:HOH:O	1.93	0.52
1:D:599:GLU:HG3	1:D:600:ARG:HG3	1.91	0.52
1:C:439:GLU:OE2	1:C:468:ARG:CZ	2.58	0.52
1:C:464:CYS:CB	1:C:471:PHE:HB2	2.33	0.52
1:C:520:ARG:NH1	1:C:544:ARG:HD3	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:615:ARG:HB3	1:C:634:TRP:CE3	2.45	0.52
1:D:458:VAL:HB	1:D:538:SER:OG	2.10	0.51
1:B:420:LYS:NZ	1:B:426:ASP:OD1	2.43	0.51
1:C:445:GLU:OE2	1:C:544:ARG:NH2	2.44	0.51
1:D:591:TYR:CB	1:D:619:PRO:HG2	2.41	0.51
1:A:549:ASP:O	1:A:553:SER:HB3	2.11	0.51
1:D:596:MET:HE2	1:D:599:GLU:HA	1.91	0.51
1:C:476:TYR:HA	3:C:807:HOH:O	2.09	0.51
1:D:455:GLU:O	1:D:536:LYS:HE2	2.10	0.51
1:C:489:MET:O	1:C:492:ARG:N	2.44	0.51
1:B:416:VAL:HG22	1:B:430:LYS:HG2	1.93	0.51
1:B:488:GLU:HG3	1:B:490:ARG:HG2	1.92	0.51
1:C:424:GLN:HG2	1:C:425:TYR:CE2	2.46	0.51
1:B:533:GLY:C	3:B:807:HOH:O	2.53	0.50
1:C:609:HIS:HA	1:C:612:GLN:HB2	1.93	0.50
1:D:461:TYR:N	1:D:461:TYR:CD2	2.79	0.50
1:C:477:MET:CE	1:C:530:ASN:HB3	2.40	0.50
1:D:490:ARG:HD3	3:D:824:HOH:O	2.11	0.50
1:D:491:HIS:HB3	1:D:493:PHE:CE1	2.45	0.50
1:D:486:LEU:O	1:D:493:PHE:CE2	2.65	0.50
1:B:553:SER:OG	1:B:555:VAL:HG23	2.11	0.50
1:D:612:GLN:NE2	3:D:825:HOH:O	2.45	0.50
1:B:600:ARG:H	1:B:600:ARG:NE	2.09	0.50
1:B:600:ARG:H	1:B:600:ARG:CD	2.25	0.50
1:C:611:ALA:CB	3:C:877:HOH:O	2.51	0.50
1:C:635:HIS:CD2	1:C:640:GLU:HB2	2.47	0.49
1:A:550:GLU:HA	1:A:550:GLU:OE1	2.12	0.49
1:B:618:ARG:HG2	1:B:618:ARG:NH1	2.27	0.49
1:C:550:GLU:HB2	1:C:558:LYS:HD2	1.93	0.49
1:A:637:LYS:HG2	1:A:640:GLU:HG3	1.94	0.49
1:A:581:TRP:CD1	1:A:581:TRP:C	2.89	0.49
1:B:658:GLU:CD	1:B:658:GLU:C	2.80	0.49
1:C:439:GLU:OE2	1:C:468:ARG:NE	2.46	0.49
1:B:439:GLU:HB3	3:B:801:HOH:O	2.13	0.49
1:B:467:GLN:O	1:B:468:ARG:HD3	2.13	0.49
1:D:443:ILE:HG21	1:D:465:THR:HG21	1.95	0.49
1:A:403:THR:N	3:A:823:HOH:O	2.46	0.49
1:D:457:LEU:HG	3:D:830:HOH:O	2.12	0.49
1:D:466:LYS:NZ	3:D:826:HOH:O	2.45	0.49
1:A:562:ARG:HB2	1:A:563:TRP:CZ3	2.48	0.48
1:C:616:LEU:H	1:C:634:TRP:HZ3	1.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:397:ILE:HD12	1:C:473:ILE:HG21	1.96	0.48
1:B:602:THR:HG22	1:D:410:THR:HG21	1.94	0.48
1:C:617:TYR:HA	1:D:620:HIS:HA	1.95	0.48
1:C:619:PRO:C	1:D:617:TYR:HB2	2.38	0.48
1:C:500:GLU:OE2	1:C:503:LYS:NZ	2.47	0.48
1:C:508:ALA:O	1:C:512:LEU:HG	2.13	0.48
1:C:620:HIS:CA	1:D:617:TYR:CA	2.82	0.48
1:D:535:VAL:N	3:D:828:HOH:O	2.47	0.48
1:D:571:TYR:HD1	3:D:823:HOH:O	1.94	0.48
1:C:635:HIS:NE2	1:C:637:LYS:HE2	2.28	0.48
1:D:503:LYS:CE	1:D:507:GLU:CD	2.85	0.48
1:D:402:LEU:HD22	1:D:473:ILE:HD12	1.95	0.48
1:D:406:LYS:HG2	1:D:418:TYR:CD2	2.49	0.48
1:A:488:GLU:O	1:A:491:HIS:O	2.32	0.48
1:C:530:ASN:ND2	1:C:534:VAL:HB	2.29	0.48
1:A:421:TRP:CD1	1:A:422:ARG:HG3	2.49	0.48
1:A:516:GLN:HG2	3:A:969:HOH:O	2.12	0.48
1:D:609:HIS:HE1	1:D:614:LEU:HB3	1.79	0.48
1:C:643:THR:H	1:C:646:ILE:HD12	1.78	0.47
1:D:528:LEU:HB3	3:D:884:HOH:O	2.14	0.47
1:D:530:ASN:OD1	1:D:534:VAL:HB	2.13	0.47
1:C:489:MET:HA	3:C:889:HOH:O	2.14	0.47
1:B:546:VAL:HG12	1:B:548:ASP:H	1.80	0.47
2:A:701:N42:CBM	2:A:701:N42:CBK	2.92	0.47
1:C:421:TRP:HB3	1:C:427:VAL:HG11	1.97	0.47
1:C:477:MET:HE1	1:C:530:ASN:HD22	1.80	0.47
1:C:485:TYR:CE2	1:C:491:HIS:HE1	2.27	0.47
1:D:449:MET:HG2	1:D:460:LEU:HD12	1.96	0.47
1:D:596:MET:HE3	1:D:599:GLU:HA	1.96	0.47
1:D:629:ILE:O	1:D:632:SER:OG	2.31	0.47
1:D:482:LEU:CD1	1:D:527:CYS:HB2	2.45	0.47
1:C:493:PHE:HD2	1:C:493:PHE:H	1.62	0.47
1:A:500:GLU:O	1:A:500:GLU:HG3	2.14	0.47
1:A:657:GLU:OE2	1:A:658:GLU:HG3	2.15	0.47
1:C:619:PRO:HG2	3:C:870:HOH:O	2.14	0.47
1:D:586:LEU:HD23	1:D:586:LEU:C	2.40	0.47
1:D:618:ARG:HB2	1:D:627:TYR:HB2	1.96	0.47
1:C:591:TYR:CZ	1:C:626:VAL:HG11	2.49	0.46
1:C:620:HIS:HD1	1:D:617:TYR:H	1.61	0.46
1:D:420:LYS:N	3:D:802:HOH:O	2.31	0.46
1:A:473:ILE:N	1:A:473:ILE:HD12	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:701:N42:CAX	2:A:701:N42:CAA	2.90	0.46
1:C:483:LEU:O	1:C:487:ARG:HG3	2.16	0.46
1:A:610:ILE:HD12	1:A:611:ALA:N	2.30	0.46
1:C:477:MET:N	3:C:807:HOH:O	2.48	0.46
1:D:457:LEU:N	3:D:830:HOH:O	2.48	0.46
1:A:487:ARG:NH2	1:A:594:GLY:O	2.41	0.46
1:C:618:ARG:HG3	1:C:627:TYR:CB	2.43	0.46
1:D:456:LYS:HB2	1:D:508:ALA:HB2	1.96	0.46
1:A:600:ARG:HD2	3:A:942:HOH:O	2.15	0.46
2:B:701:N42:CAA	2:B:701:N42:CAX	2.93	0.46
1:C:449:MET:HE1	1:C:541:GLY:O	2.15	0.46
1:A:560:PRO:O	1:A:564:SER:OG	2.33	0.46
1:D:445:GLU:O	1:D:445:GLU:HG3	2.01	0.46
1:B:481:CYS:HB3	3:B:926:HOH:O	2.16	0.46
1:B:520:ARG:NH2	3:B:821:HOH:O	2.48	0.46
1:D:492:ARG:HA	3:D:957:HOH:O	2.15	0.46
1:D:569:LEU:HD12	1:D:610:ILE:HD11	1.96	0.46
1:A:477:MET:HE1	1:A:536:LYS:HG3	1.98	0.46
1:B:406:LYS:HB2	3:B:943:HOH:O	2.16	0.46
1:B:633:CYS:O	1:B:641:ARG:HD3	2.15	0.46
1:C:449:MET:HA	1:C:452:LEU:HD12	1.97	0.46
1:B:387:THR:HG21	1:B:396:GLU:HB2	1.97	0.46
1:A:502:CYS:SG	1:A:587:MET:HG2	2.57	0.45
1:C:485:TYR:CE2	1:C:491:HIS:NE2	2.84	0.45
1:D:599:GLU:HG3	1:D:600:ARG:N	2.31	0.45
1:A:468:ARG:NH2	3:A:809:HOH:O	2.34	0.45
1:A:559:PHE:CG	1:A:560:PRO:HD2	2.51	0.45
1:D:576:SER:HA	1:D:579:ASP:HB2	1.98	0.45
1:B:489:MET:HA	1:B:492:ARG:HE	1.81	0.45
1:D:615:ARG:NH2	3:D:827:HOH:O	2.45	0.45
1:D:620:HIS:C	1:D:621:LEU:HD12	2.42	0.45
1:C:425:TYR:O	1:C:427:VAL:HG13	2.16	0.45
1:D:406:LYS:HE2	1:D:408:LEU:CD2	2.46	0.45
1:D:538:SER:O	1:D:539:ASP:HB2	2.17	0.45
1:B:618:ARG:HG3	1:B:627:TYR:HB2	1.98	0.45
1:C:614:LEU:CD2	1:C:615:ARG:H	2.30	0.45
1:D:482:LEU:HD22	1:D:524:ALA:HB1	1.97	0.45
1:D:531:ASP:OD1	1:D:531:ASP:N	2.42	0.45
1:B:599:GLU:HG3	1:D:407:GLU:HG2	1.99	0.45
1:D:411:GLY:N	1:D:414:GLY:O	2.39	0.45
1:D:486:LEU:CG	3:D:881:HOH:O	2.61	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:567:GLU:HB2	3:D:823:HOH:O	2.16	0.45
1:D:569:LEU:HD13	1:D:607:ALA:HA	1.98	0.45
1:A:446:ALA:O	1:A:450:MET:HG2	2.17	0.45
1:B:387:THR:HB	1:B:465:THR:OG1	2.17	0.45
1:C:439:GLU:HG2	1:C:470:ILE:HD12	1.99	0.45
1:D:486:LEU:CA	1:D:493:PHE:HE2	2.27	0.45
1:D:495:THR:HB	3:D:806:HOH:O	2.16	0.45
1:C:476:TYR:CB	3:C:834:HOH:O	2.65	0.44
1:C:484:ASN:O	1:C:488:GLU:HG2	2.17	0.44
1:D:621:LEU:N	1:D:621:LEU:HD13	2.19	0.44
1:A:618:ARG:HG3	1:A:627:TYR:HB2	1.99	0.44
1:B:577:LYS:HB3	3:B:856:HOH:O	2.17	0.44
1:D:486:LEU:O	1:D:493:PHE:HE2	1.99	0.44
1:A:438:SER:OG	1:A:441:GLU:OE1	2.35	0.44
1:B:599:GLU:H	1:B:600:ARG:HH11	1.64	0.44
2:D:701:N42:CAX	2:D:701:N42:CAA	2.93	0.44
1:B:488:GLU:HG3	1:B:490:ARG:CG	2.48	0.44
1:C:495:THR:HG22	3:C:884:HOH:O	2.18	0.44
1:C:618:ARG:NH1	1:C:618:ARG:HG2	2.32	0.44
1:D:439:GLU:HG2	1:D:468:ARG:NH2	2.32	0.44
1:D:493:PHE:HD2	1:D:593:LEU:HD22	1.82	0.44
1:A:631:TYR:HA	1:A:634:TRP:CE3	2.53	0.44
1:C:467:GLN:C	1:C:469:PRO:O	2.61	0.44
1:C:481:CYS:HB2	2:C:701:N42:OAH	2.18	0.44
1:A:450:MET:HE1	1:A:462:GLY:HA2	2.00	0.44
1:B:449:MET:HE3	1:B:449:MET:HB2	1.75	0.44
1:B:511:TYR:O	1:B:514:SER:OG	2.30	0.44
1:C:565:PRO:HG3	1:C:578:SER:HA	2.00	0.44
1:D:428:ALA:HB3	2:D:701:N42:CAB	2.48	0.43
1:D:480:GLY:HA2	3:D:884:HOH:O	2.18	0.43
1:C:581:TRP:HE3	1:C:641:ARG:CZ	2.29	0.43
1:D:576:SER:O	1:D:580:ILE:N	2.51	0.43
1:B:417:LYS:NZ	1:C:600:ARG:O	2.46	0.43
1:C:596:MET:CE	1:C:599:GLU:HA	2.40	0.43
1:B:488:GLU:CG	1:B:490:ARG:HG2	2.47	0.43
1:B:406:LYS:HG2	1:B:418:TYR:HD2	1.83	0.43
1:B:602:THR:HG22	1:D:410:THR:CG2	2.49	0.43
1:B:646:ILE:O	1:B:649[A]:SER:OG	2.35	0.43
1:C:620:HIS:HA	1:D:616:LEU:C	2.43	0.43
1:C:644:PHE:HA	1:C:647:LEU:HD12	2.00	0.43
1:D:635:HIS:CE1	1:D:640:GLU:HG3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:LYS:O	1:A:418:TYR:N	2.43	0.43
1:B:653:ASP:O	1:B:657:GLU:HG3	2.18	0.43
1:D:587:MET:HG2	3:D:952:HOH:O	2.18	0.43
1:D:449:MET:HG2	1:D:460:LEU:CD1	2.49	0.43
1:A:466:LYS:HA	1:A:466:LYS:HD3	1.90	0.43
1:A:600:ARG:NH2	3:A:829:HOH:O	2.52	0.43
1:B:603:ASN:HA	3:B:814:HOH:O	2.18	0.43
1:B:390:LEU:HD12	1:B:390:LEU:HA	1.87	0.43
1:C:432:ILE:O	1:C:469:PRO:HB3	2.18	0.43
1:C:482:LEU:HD11	3:C:901:HOH:O	2.18	0.43
1:C:618:ARG:HG3	1:C:627:TYR:CG	2.54	0.43
1:D:445:GLU:OE1	1:D:448:VAL:HB	2.19	0.43
1:D:482:LEU:C	1:D:482:LEU:HD23	2.44	0.43
1:D:588:TRP:CD1	1:D:616:LEU:HB3	2.54	0.43
1:A:494:GLN:HG3	1:A:497:GLN:CG	2.48	0.42
1:C:618:ARG:O	1:D:618:ARG:O	2.37	0.42
1:D:520:ARG:HB2	1:D:520:ARG:NH1	2.33	0.42
1:C:456:LYS:HA	1:C:536:LYS:HG2	2.00	0.42
1:B:596:MET:HG3	3:B:1001:HOH:O	2.19	0.42
1:D:399:PRO:HA	1:D:402:LEU:HD12	2.01	0.42
1:D:477:MET:HE1	1:D:530:ASN:HB3	2.01	0.42
1:C:470:ILE:CG2	1:C:471:PHE:N	2.80	0.42
1:D:439:GLU:CD	1:D:470:ILE:HD12	2.43	0.42
1:A:598:TYR:HE2	1:A:614:LEU:CD1	2.31	0.42
1:B:430:LYS:O	1:B:471:PHE:HA	2.19	0.42
1:C:420:LYS:HD2	3:C:909:HOH:O	2.19	0.42
1:C:618:ARG:NE	1:D:627:TYR:CE2	2.88	0.42
1:D:445:GLU:O	1:D:446:ALA:C	2.62	0.42
1:B:488:GLU:OE1	1:B:490:ARG:CD	2.63	0.42
1:B:559:PHE:CD1	1:B:560:PRO:HD2	2.54	0.42
1:C:481:CYS:HB3	1:C:484:ASN:H	1.84	0.42
1:D:408:LEU:HD11	1:D:418:TYR:HB2	2.01	0.42
1:C:418:TYR:HE1	1:C:426:ASP:OD2	2.03	0.42
1:D:470:ILE:HD11	3:D:900:HOH:O	2.20	0.42
1:D:569:LEU:HD23	1:D:569:LEU:HA	1.76	0.42
1:D:652:LEU:O	1:D:656:ASP:N	2.53	0.42
1:A:449:MET:HG2	1:A:460:LEU:HD13	2.00	0.42
1:B:524:ALA:HB2	1:B:586[A]:LEU:CD1	2.49	0.42
1:B:559:PHE:CG	1:B:560:PRO:HD2	2.55	0.42
1:B:588:TRP:CE2	1:B:616:LEU:HD22	2.55	0.42
1:B:602:THR:HA	1:D:410:THR:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:524:ALA:HA	1:B:586[A]:LEU:HD11	2.01	0.42
1:A:569:LEU:HD12	1:A:610:ILE:HD11	2.02	0.41
1:A:600:ARG:HD2	1:A:600:ARG:H	1.85	0.41
1:D:577:LYS:HD3	1:D:580:ILE:HG13	2.02	0.41
1:C:477:MET:HE2	1:C:536:LYS:HB2	2.02	0.41
1:B:623:SER:N	3:B:826:HOH:O	2.54	0.41
2:A:701:N42:CAU	2:A:701:N42:CBD	2.98	0.41
1:D:468:ARG:HD3	1:D:468:ARG:HA	1.84	0.41
1:B:569:LEU:HD11	1:B:610:ILE:CD1	2.51	0.41
1:D:486:LEU:HD13	1:D:593:LEU:HA	2.01	0.41
1:D:618:ARG:HA	1:D:619:PRO:HD3	1.75	0.41
1:B:534:VAL:CG2	3:B:807:HOH:O	2.69	0.41
1:C:430:LYS:N	3:C:832:HOH:O	2.53	0.41
1:C:618:ARG:H	1:D:618:ARG:HG3	1.85	0.41
1:A:497:GLN:O	1:A:501:MET:HG3	2.21	0.41
1:C:430:LYS:HG3	3:C:832:HOH:O	2.19	0.41
1:C:652:LEU:HD23	1:C:652:LEU:HA	1.89	0.41
1:B:599:GLU:OE1	1:D:407:GLU:HB3	2.20	0.41
1:C:431:MET:HE2	1:C:471:PHE:CE1	2.55	0.41
1:D:397:ILE:HG21	1:D:402:LEU:HD21	2.03	0.41
1:D:468:ARG:HH12	1:D:470:ILE:HG13	1.86	0.41
1:D:491:HIS:CB	1:D:493:PHE:CE1	3.04	0.41
1:D:617:TYR:O	1:D:617:TYR:HD1	2.03	0.41
1:A:396:GLU:OE1	1:A:464:CYS:HA	2.21	0.41
1:B:445:GLU:O	1:B:445:GLU:HG3	2.21	0.41
1:C:411:GLY:N	1:C:414:GLY:O	2.52	0.41
1:C:543:SER:HB3	3:C:822:HOH:O	2.21	0.41
1:A:526:ASN:O	1:A:538[A]:SER:OG	2.33	0.40
1:C:499:LEU:HB3	3:C:850:HOH:O	2.21	0.40
1:C:591:TYR:HB2	3:C:870:HOH:O	2.21	0.40
1:D:618:ARG:CD	1:D:622:ALA:HB1	2.51	0.40
1:A:648:LEU:O	1:A:652:LEU:HG	2.21	0.40
1:B:488:GLU:OE2	1:B:488:GLU:HA	2.18	0.40
1:C:610:ILE:HG13	1:C:611:ALA:H	1.86	0.40
1:C:633:CYS:O	1:C:641:ARG:HD3	2.21	0.40
1:D:437:MET:HG2	1:D:438:SER:N	2.36	0.40
1:D:482:LEU:HB3	1:D:524:ALA:O	2.22	0.40
1:C:399:PRO:HA	1:C:402:LEU:HB2	2.04	0.40
1:C:456:LYS:HA	1:C:456:LYS:HD3	2.00	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	263/274 (96%)	259 (98%)	4 (2%)	0	100	100
1	B	275/274 (100%)	272 (99%)	3 (1%)	0	100	100
1	C	260/274 (95%)	253 (97%)	7 (3%)	0	100	100
1	D	262/274 (96%)	253 (97%)	9 (3%)	0	100	100
All	All	1060/1096 (97%)	1037 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	239/245 (98%)	225 (94%)	14 (6%)	18	4
1	B	245/245 (100%)	226 (92%)	19 (8%)	11	2
1	C	234/245 (96%)	200 (86%)	34 (14%)	3	0
1	D	235/245 (96%)	204 (87%)	31 (13%)	4	0
All	All	953/980 (97%)	855 (90%)	98 (10%)	7	1

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	444	GLU
1	A	445	GLU

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Mol	Chain	Res	Type
1	A	447	LYS
1	A	455	GLU
1	A	470	ILE
1	A	489	MET
1	A	494	GLN
1	A	554	SER
1	A	555	VAL
1	A	599	GLU
1	A	600	ARG
1	A	614	LEU
1	A	645	LYS
1	A	657	GLU
1	B	387	THR
1	B	390	LEU
1	B	415	VAL
1	B	438	SER
1	B	440	ASP
1	B	444	GLU
1	B	460	LEU
1	B	483	LEU
1	B	488	GLU
1	B	492	ARG
1	B	500	GLU
1	B	531	ASP
1	B	555	VAL
1	B	566	PRO
1	B	573	LYS
1	B	600	ARG
1	B	610	ILE
1	B	645	LYS
1	B	658	GLU
1	C	400	LYS
1	C	401	ASP
1	C	402	LEU
1	C	407	GLU
1	C	418	TYR
1	C	420	LYS
1	C	426	ASP
1	C	438	SER
1	C	440	ASP
1	C	443	ILE
1	C	450	MET

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Mol	Chain	Res	Type
1	C	459	GLN
1	C	467	GLN
1	C	468	ARG
1	C	481	CYS
1	C	483	LEU
1	C	488	GLU
1	C	489	MET
1	C	490	ARG
1	C	494	GLN
1	C	496	GLN
1	C	503	LYS
1	C	520	ARG
1	C	549	ASP
1	C	550	GLU
1	C	566	PRO
1	C	573	LYS
1	C	600	ARG
1	C	609	HIS
1	C	610	ILE
1	C	620	HIS
1	C	621	LEU
1	C	649	SER
1	C	655	MET
1	D	407	GLU
1	D	439	GLU
1	D	443	ILE
1	D	445	GLU
1	D	450	MET
1	D	461	TYR
1	D	466	LYS
1	D	468	ARG
1	D	486	LEU
1	D	489	MET
1	D	490	ARG
1	D	494	GLN
1	D	503	LYS
1	D	520	ARG
1	D	531	ASP
1	D	534	VAL
1	D	537	VAL
1	D	538	SER
1	D	543	SER

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Mol	Chain	Res	Type
1	D	544	ARG
1	D	553	SER
1	D	555	VAL
1	D	575	SER
1	D	601	PHE
1	D	609	HIS
1	D	614	LEU
1	D	617	TYR
1	D	620	HIS
1	D	621	LEU
1	D	628	THR
1	D	639	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	491	HIS
1	A	532	GLN
1	B	491	HIS
1	C	467	GLN
1	C	497	GLN
1	D	496	GLN
1	D	609	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	N42	C	701	1	52,52,52	2.62	12 (23%)	71,75,75	1.71	9 (12%)
2	N42	B	701	1	52,52,52	2.38	13 (25%)	71,75,75	1.91	10 (14%)
2	N42	A	701	1	52,52,52	2.38	13 (25%)	71,75,75	2.39	10 (14%)
2	N42	D	701	1	52,52,52	2.47	13 (25%)	71,75,75	1.94	12 (16%)

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	N42	C	701	1	-	7/36/44/44	0/5/5/5
2	N42	B	701	1	-	6/36/44/44	0/5/5/5
2	N42	A	701	1	-	6/36/44/44	0/5/5/5
2	N42	D	701	1	-	7/36/44/44	0/5/5/5

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	701	N42	CAA-CBN	-8.13	1.35	1.51
2	C	701	N42	CCB-CBT	-7.62	1.38	1.53
2	D	701	N42	CBV-CBM	-7.51	1.39	1.50
2	C	701	N42	CBV-CBM	-7.14	1.40	1.50
2	A	701	N42	CBV-CBM	-7.02	1.40	1.50
2	A	701	N42	CCB-CBT	-6.89	1.40	1.53
2	B	701	N42	CBV-CBM	-6.80	1.40	1.50
2	A	701	N42	CAA-CBN	-6.69	1.38	1.51
2	D	701	N42	CCB-CBT	-6.65	1.40	1.53
2	B	701	N42	CAA-CBN	-6.49	1.38	1.51
2	D	701	N42	CAA-CBN	-6.13	1.39	1.51
2	B	701	N42	CCB-CBT	-6.02	1.41	1.53
2	B	701	N42	CBW-CBQ	-5.92	1.40	1.48
2	C	701	N42	CBX-NCA	-5.87	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	701	N42	CBW-CBQ	-5.73	1.41	1.48
2	C	701	N42	CBP-CBL	-5.52	1.38	1.50
2	C	701	N42	CBA-CBB	5.43	1.56	1.30
2	A	701	N42	CBA-CBB	4.97	1.54	1.30
2	D	701	N42	CBA-CBB	4.95	1.54	1.30
2	C	701	N42	CBW-CBQ	-4.74	1.42	1.48
2	A	701	N42	CBW-CBQ	-4.61	1.42	1.48
2	B	701	N42	CBA-CBB	4.61	1.52	1.30
2	A	701	N42	CBP-CBL	-4.54	1.40	1.50
2	D	701	N42	CBO-NBH	-4.39	1.32	1.41
2	B	701	N42	CBS-NBF	-4.28	1.33	1.41
2	A	701	N42	CBX-NCA	-4.18	1.33	1.39
2	A	701	N42	CBS-NBF	-4.05	1.33	1.41
2	D	701	N42	CBB-CBK	3.96	1.54	1.48
2	B	701	N42	CBP-CBL	-3.91	1.41	1.50
2	B	701	N42	CBU-CBX	-3.88	1.38	1.48
2	D	701	N42	CBP-CBL	-3.87	1.41	1.50
2	B	701	N42	CBX-NCA	-3.77	1.34	1.39
2	A	701	N42	CBU-CBX	-3.75	1.39	1.48
2	D	701	N42	CBX-NCA	-3.71	1.34	1.39
2	D	701	N42	CBS-NBF	-3.70	1.34	1.41
2	B	701	N42	CBR-NBG	-3.68	1.34	1.41
2	D	701	N42	CBU-CBX	-3.63	1.39	1.48
2	D	701	N42	CBR-NBG	-3.60	1.34	1.41
2	B	701	N42	CBO-NBH	-3.35	1.34	1.41
2	C	701	N42	CBU-CBX	-3.28	1.40	1.48
2	A	701	N42	CBO-NBH	-2.96	1.35	1.41
2	B	701	N42	CBB-CBK	2.87	1.52	1.48
2	C	701	N42	CBR-NBG	-2.83	1.36	1.41
2	C	701	N42	CBS-NBF	-2.77	1.36	1.41
2	A	701	N42	CBR-NBG	-2.76	1.36	1.41
2	C	701	N42	CBO-NBH	-2.69	1.36	1.41
2	A	701	N42	CBB-CBK	2.61	1.52	1.48
2	C	701	N42	CBB-CBK	2.56	1.52	1.48
2	D	701	N42	CAW-CBU	2.38	1.41	1.36
2	A	701	N42	CAW-CBU	2.31	1.41	1.36
2	B	701	N42	CAW-CBU	2.01	1.40	1.36

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	N42	CBA-CBB-CBK	-15.51	105.17	122.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	701	N42	CBA-CBB-CBK	-11.60	109.48	122.22
2	B	701	N42	CBA-CBB-CBK	-10.54	110.64	122.22
2	C	701	N42	CBA-CBB-CBK	-5.57	116.10	122.22
2	C	701	N42	CBU-CBX-NCA	5.07	121.17	116.41
2	C	701	N42	CBX-CBU-NBH	4.79	116.53	112.05
2	A	701	N42	CBW-CBN-CBR	4.69	121.54	117.30
2	C	701	N42	CBW-CBN-CBR	4.52	121.39	117.30
2	A	701	N42	CBU-CBX-NCA	4.52	120.65	116.41
2	A	701	N42	CAR-CBW-CBN	-4.42	117.59	120.74
2	B	701	N42	CAR-CBW-CBN	-4.40	117.60	120.74
2	D	701	N42	CBW-CBN-CBR	4.37	121.25	117.30
2	B	701	N42	CBW-CBN-CBR	4.31	121.19	117.30
2	D	701	N42	CAR-CBW-CBN	-4.14	117.78	120.74
2	C	701	N42	CBB-CBK-NBF	4.10	116.62	113.84
2	C	701	N42	CAR-CBW-CBN	-3.67	118.12	120.74
2	B	701	N42	CBU-CBX-NCA	3.62	119.80	116.41
2	D	701	N42	CBU-CBX-NCA	3.45	119.65	116.41
2	B	701	N42	CAU-CAO-CBO	3.34	124.15	120.30
2	B	701	N42	CBS-CBV-CBM	3.29	125.30	120.72
2	A	701	N42	CBD-NBZ-CBC	3.25	119.31	112.68
2	C	701	N42	OAH-CBK-CBB	-3.18	117.93	122.70
2	A	701	N42	OAH-CBK-NBF	3.03	127.11	123.11
2	D	701	N42	CBB-CBK-NBF	2.99	115.87	113.84
2	D	701	N42	CBS-NBF-CBK	-2.97	119.82	126.88
2	A	701	N42	CBV-CBM-NBZ	2.79	122.57	118.24
2	B	701	N42	CBV-CBM-NBZ	2.69	122.41	118.24
2	D	701	N42	CBS-CBV-CBM	2.50	124.21	120.72
2	B	701	N42	CBS-NBF-CBK	-2.40	121.17	126.88
2	D	701	N42	CBD-NBZ-CBC	2.37	117.52	112.68
2	D	701	N42	CAA-CBN-CBW	-2.27	118.91	122.29
2	C	701	N42	CBV-CBM-NBZ	2.25	121.74	118.24
2	B	701	N42	CBR-NBG-CBL	-2.24	120.68	126.90
2	D	701	N42	CAB-NCA-CBX	2.24	120.21	117.14
2	A	701	N42	CBB-CBK-NBF	-2.22	112.33	113.84
2	A	701	N42	CAU-CAO-CBO	2.22	122.86	120.30
2	D	701	N42	CBR-NBG-CBL	-2.20	120.78	126.90
2	B	701	N42	CAV-CBS-CBV	2.19	122.23	118.86
2	C	701	N42	CAA-CBN-CBW	-2.15	119.08	122.29
2	A	701	N42	CAO-CBO-CAV	-2.08	117.14	119.66
2	D	701	N42	OBI-CAY-CBC	-2.06	107.33	111.77

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	N42	CBA-CBB-CBK-OAH
2	A	701	N42	CBA-CBB-CBK-NBF
2	B	701	N42	CBA-CBB-CBK-OAH
2	B	701	N42	CBA-CBB-CBK-NBF
2	D	701	N42	CBA-CBB-CBK-OAH
2	D	701	N42	CBA-CBB-CBK-NBF
2	B	701	N42	CAN-CBR-NBG-CBL
2	A	701	N42	CAN-CBR-NBG-CBL
2	C	701	N42	CAN-CBR-NBG-CBL
2	D	701	N42	CAN-CBR-NBG-CBL
2	C	701	N42	CBN-CBR-NBG-CBL
2	C	701	N42	CBA-CBB-CBK-OAH
2	D	701	N42	CBN-CBR-NBG-CBL
2	B	701	N42	CBN-CBR-NBG-CBL
2	A	701	N42	CBN-CBR-NBG-CBL
2	A	701	N42	CAW-CBQ-CBW-CBN
2	B	701	N42	CAW-CBQ-CBW-CBN
2	C	701	N42	CAW-CBQ-CBW-CBN
2	C	701	N42	CAX-CBQ-CBW-CAR
2	A	701	N42	CBV-CBS-NBF-CBK
2	D	701	N42	CAW-CBQ-CBW-CAR
2	B	701	N42	CBV-CBS-NBF-CBK
2	C	701	N42	CAV-CBS-NBF-CBK
2	D	701	N42	CBV-CBS-NBF-CBK
2	D	701	N42	CAW-CBQ-CBW-CBN
2	C	701	N42	CBV-CBS-NBF-CBK

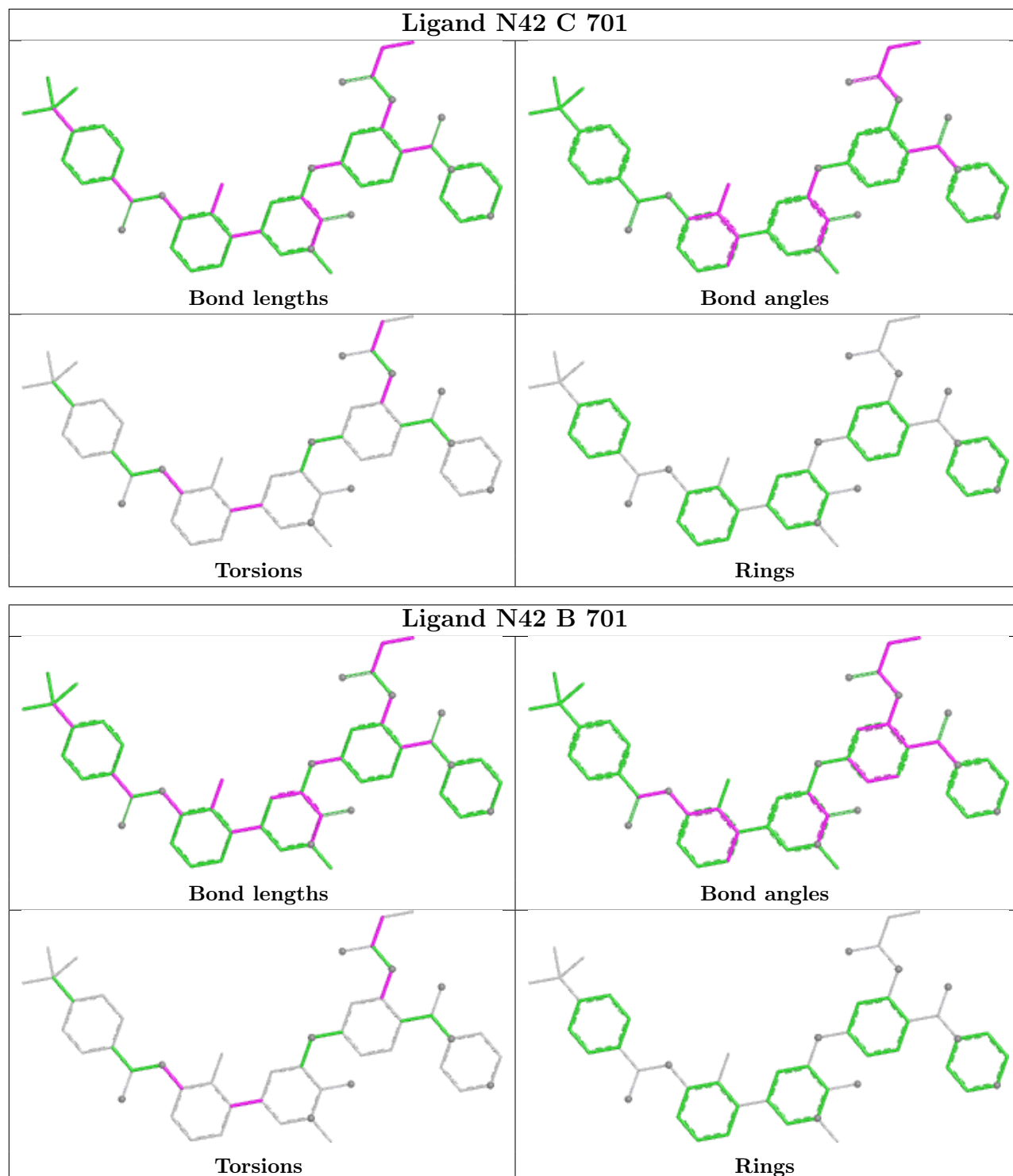
There are no ring outliers.

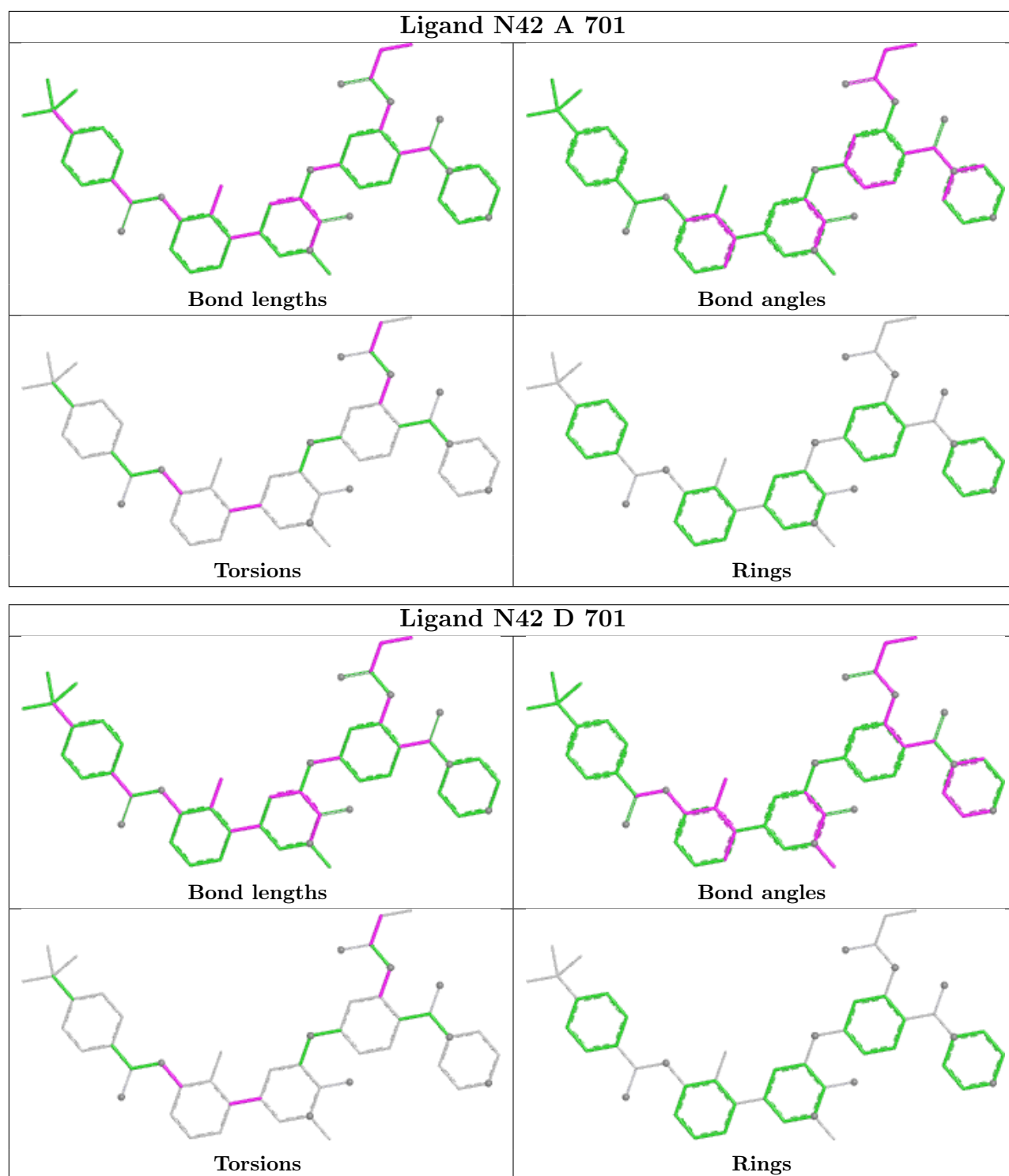
4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	701	N42	5	0
2	B	701	N42	1	0
2	A	701	N42	3	0
2	D	701	N42	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	263/274 (95%)	-1.23	0 100 100	4, 10, 19, 37	2 (0%)
1	B	274/274 (100%)	-1.28	0 100 100	2, 9, 18, 40	3 (1%)
1	C	261/274 (95%)	-0.72	0 100 100	13, 19, 29, 36	1 (0%)
1	D	263/274 (95%)	-0.81	0 100 100	11, 19, 27, 33	1 (0%)
All	All	1061/1096 (96%)	-1.01	0 100 100	2, 15, 26, 40	7 (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](#)

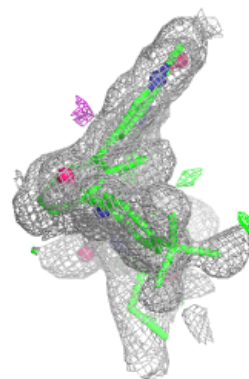
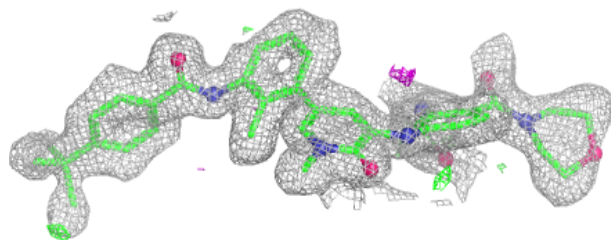
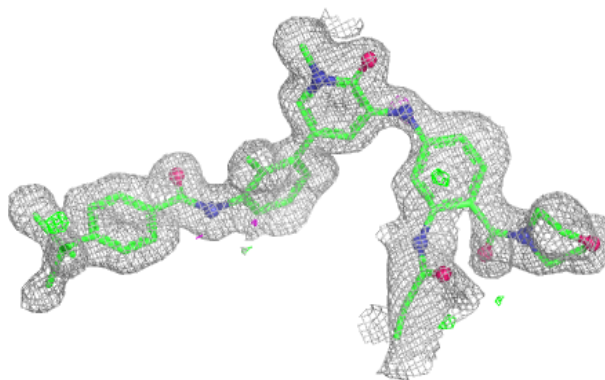
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	N42	C	701	48/48	0.98	0.05	13,18,28,33	0
2	N42	D	701	48/48	0.98	0.05	10,18,34,37	0
2	N42	A	701	48/48	0.99	0.03	6,9,17,21	0
2	N42	B	701	48/48	0.99	0.03	5,9,13,20	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.

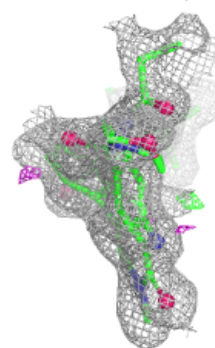
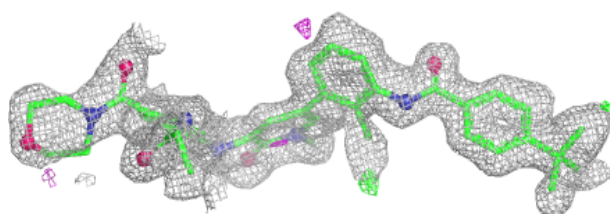
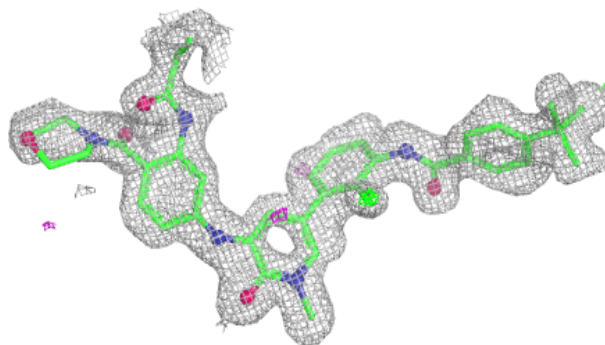
Electron density around N42 C 701:

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

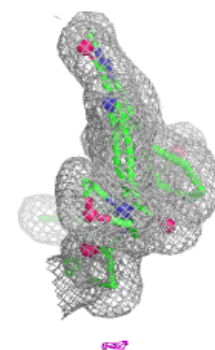
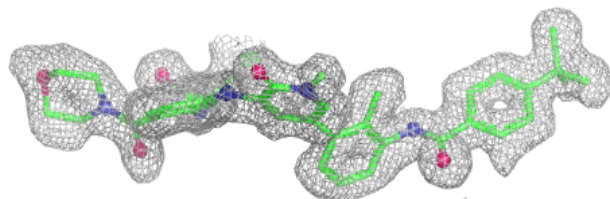
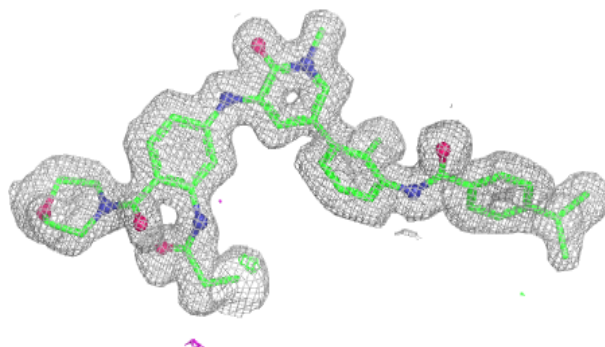


Electron density around N42 D 701:

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

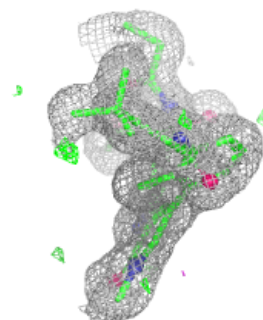
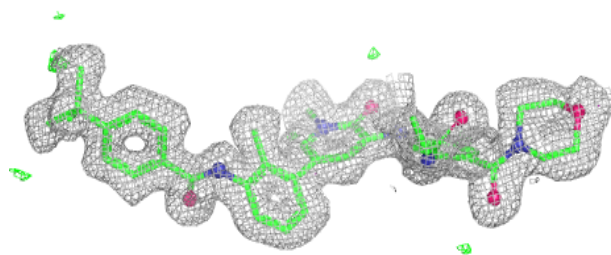
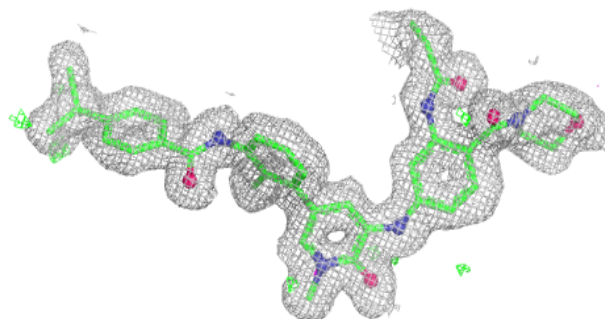
**Electron density around N42 A 701:**

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



Electron density around N42 B 701:

$2mF_o-DF_c$ (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.