



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:12 AM UTC

PDB ID : 1L5S / pdb_00001l5s
Title : Human liver glycogen phosphorylase complexed with uric acid, N-Acetyl-beta-D-glucopyranosylamine, and CP-403,700
Authors : Ekstrom, J.L.; Pauly, T.A.; Carty, M.D.; Soeller, W.C.; Culp, J.; Danley, D.E.; Hoover, D.J.; Treadway, J.L.; Gibbs, E.M.; Fletterick, R.J.; Day, Y.S.N.; Myszka, D.G.; Rath, V.L.
Deposited on : 2002-03-07
Resolution : 2.10 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

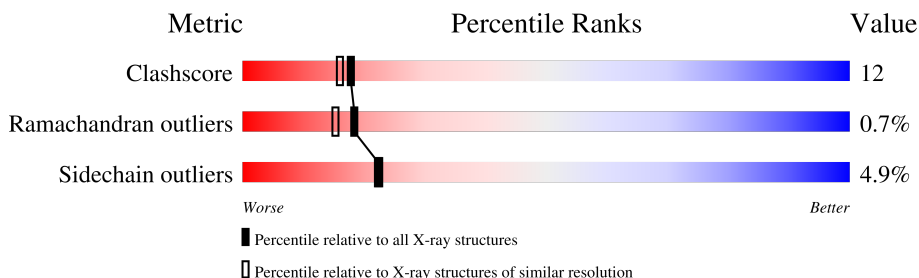
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	847	
1	B	847	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	MRD	B	903	-	-	X	-

2 Entry composition [i](#)

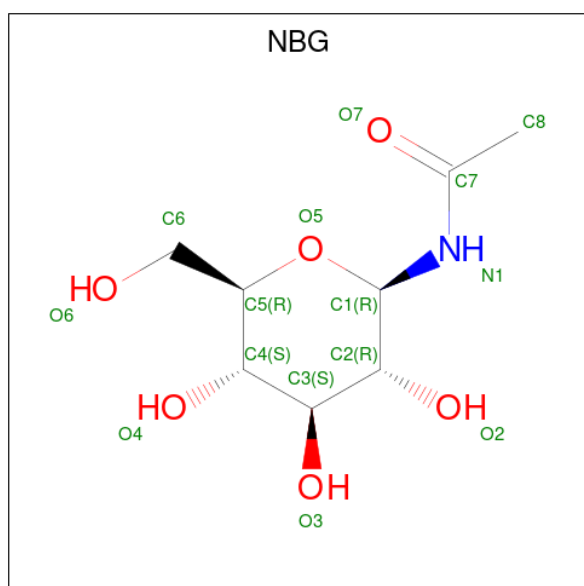
There are 7 unique types of molecules in this entry. The entry contains 13826 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glycogen phosphorylase, liver form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	793	Total	C	N	O	S	0	0	0
			6437	4134	1092	1182	29			
1	B	791	Total	C	N	O	S	0	0	0
			6420	4125	1090	1176	29			

- Molecule 2 is N-acetyl-beta-D-glucopyranosylamine (CCD ID: NBG) (formula: $C_8H_{15}NO_6$).



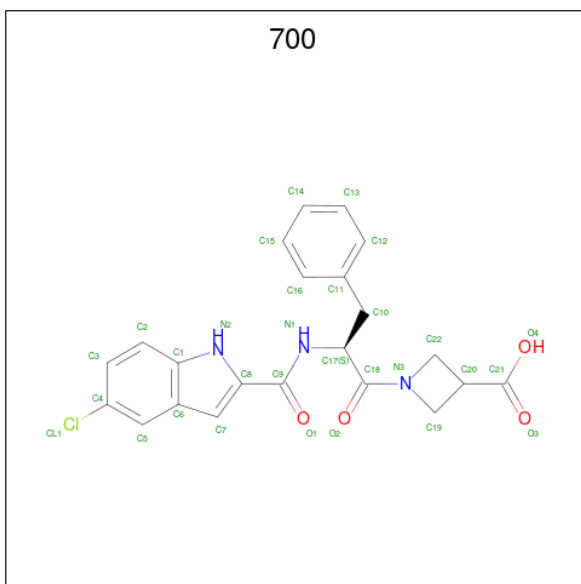
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 4 is [5-CHLORO-1H-INDOL-2-CARBONYL-PHENYLALANINYL]-AZETIDINE-3-CARBOXYLIC ACID (CCD ID: 700) (formula: $C_{22}H_{20}ClN_3O_4$).



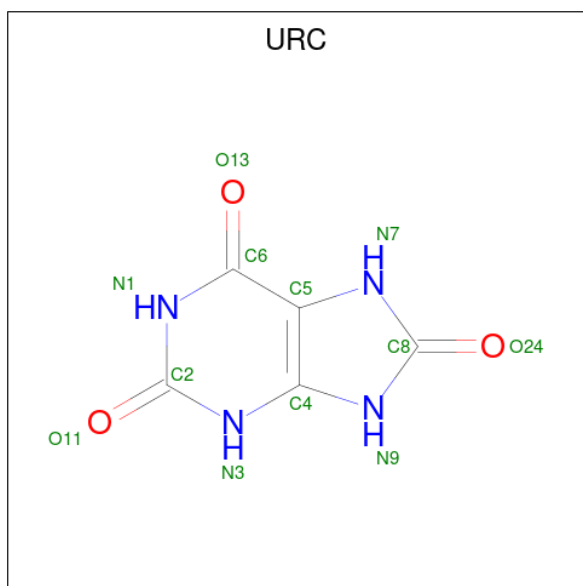
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			30	22	1	3	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	Cl	N	O	0	0
			30	22	1	3	4		

- Molecule 5 is URIC ACID (CCD ID: URC) (formula: $C_5H_4N_4O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			12	5	4	3		
5	B	1	Total	C	N	O	0	0
			12	5	4	3		

- Molecule 6 is (4R)-2-METHYLPENTANE-2,4-DIOL (CCD ID: MRD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			8	6	2		
6	A	1	Total	C	O	0	0
			8	6	2		
6	A	1	Total	C	O	0	0
			8	6	2		
6	B	1	Total	C	O	0	0
			8	6	2		
6	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 7 is water.

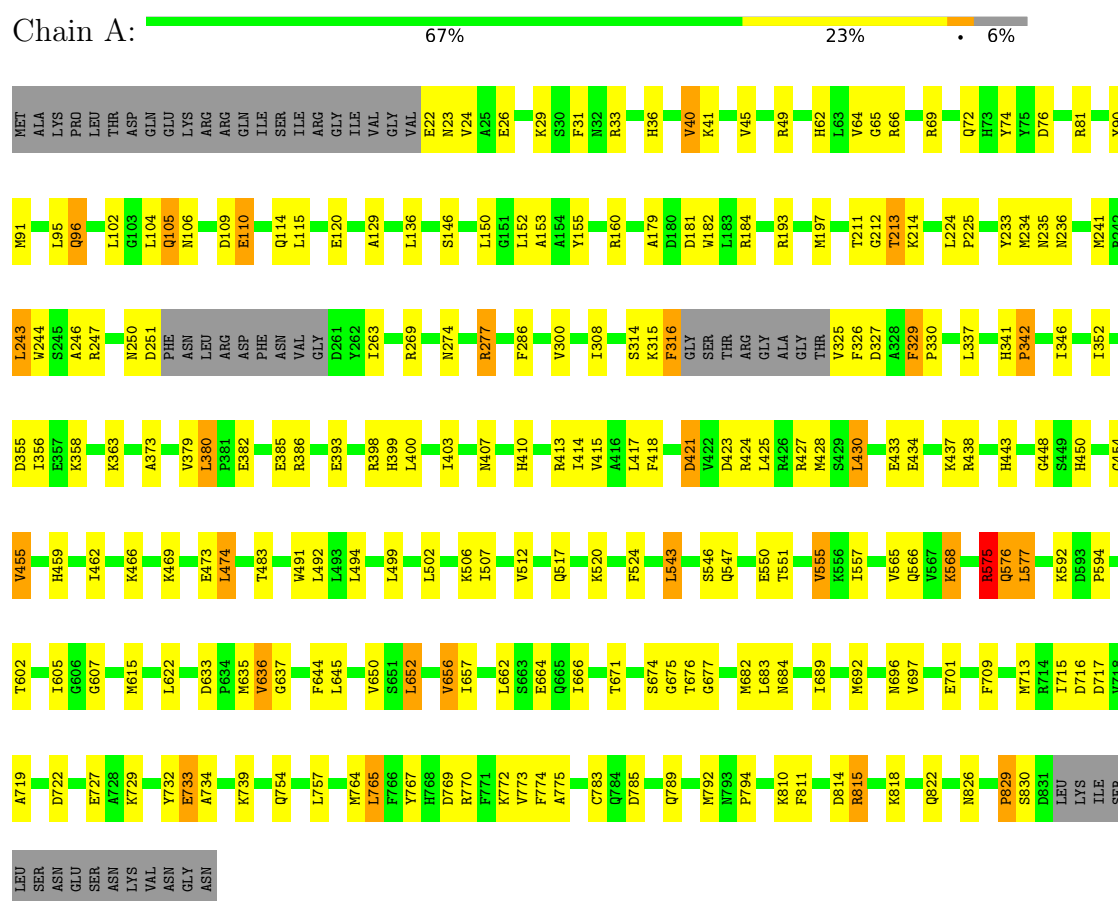
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	433	Total	O	0	0
			433	433		
7	B	352	Total	O	0	0
			352	352		

3 Residue-property plots

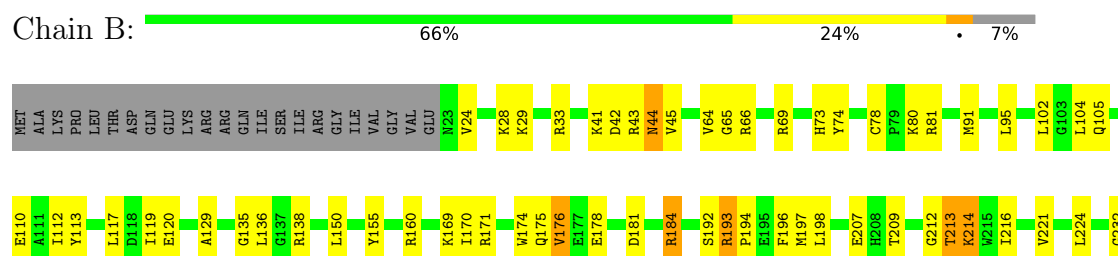
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

- Molecule 1: Glycogen phosphorylase, liver form



- Molecule 1: Glycogen phosphorylase, liver form





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	124.03Å 124.03Å 123.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.60 – 2.10	Depositor
% Data completeness (in resolution range)	87.8 (40.60-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.194 , 0.236	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13826	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PLP, 700, NBG, MRD, URC

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	2/6581 (0.0%)	1.01	36/8900 (0.4%)
1	B	0.55	0/6564	1.03	33/8877 (0.4%)
All	All	0.57	2/13145 (0.0%)	1.02	69/17777 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	657	ILE	CA-CB	7.32	1.58	1.54
1	A	682	MET	SD-CE	5.14	1.92	1.79

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	455	VAL	N-CA-C	8.94	121.06	111.77
1	A	565	VAL	N-CA-C	8.75	121.08	108.48
1	B	354	VAL	N-CA-C	8.57	118.54	110.74
1	B	64	VAL	N-CA-C	8.32	119.10	110.36
1	B	565	VAL	N-CA-C	8.23	119.63	108.11
1	A	575	ARG	N-CA-C	8.09	122.56	111.39
1	B	754	GLN	CA-C-N	7.94	129.76	119.84
1	B	754	GLN	C-N-CA	7.94	129.76	119.84
1	A	105	GLN	N-CA-C	7.93	120.62	111.11
1	B	575	ARG	N-CA-C	7.85	121.87	111.28
1	A	91	MET	N-CA-C	7.83	122.60	112.89
1	A	507	ILE	N-CA-C	7.67	119.49	112.43
1	A	329	PHE	CA-C-N	7.11	126.81	119.56
1	A	329	PHE	C-N-CA	7.11	126.81	119.56
1	B	105	GLN	N-CA-C	6.78	118.32	111.07
1	A	675	GLY	N-CA-C	-6.76	104.16	112.68
1	B	666	ILE	N-CA-C	6.72	123.32	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	VAL	N-CA-C	6.68	117.18	110.23
1	A	129	ALA	N-CA-C	-6.68	96.94	108.56
1	A	677	GLY	N-CA-C	-6.61	104.80	112.73
1	B	576	GLN	N-CA-C	-6.48	105.23	113.01
1	B	129	ALA	N-CA-C	-6.46	96.62	107.99
1	A	24	VAL	N-CA-C	6.27	116.94	110.36
1	B	216	ILE	N-CA-C	6.15	117.69	108.96
1	A	602	THR	N-CA-C	-6.14	97.28	108.02
1	A	633	ASP	CA-C-N	6.07	126.51	119.47
1	A	633	ASP	C-N-CA	6.07	126.51	119.47
1	A	650	VAL	N-CA-C	6.04	116.70	110.36
1	A	676	THR	N-CA-C	-6.02	107.17	114.75
1	B	799	THR	N-CA-C	-5.99	104.83	111.36
1	B	557	ILE	N-CA-C	5.89	117.22	109.21
1	B	650	VAL	N-CA-C	5.89	116.54	110.36
1	A	455	VAL	N-CA-C	5.84	117.72	112.17
1	A	656	VAL	N-CA-C	5.78	116.56	110.72
1	A	430	LEU	N-CA-C	-5.73	106.25	113.18
1	A	767	TYR	N-CA-C	5.71	122.06	114.12
1	A	454	GLY	N-CA-C	-5.71	103.56	112.58
1	B	91	MET	N-CA-C	5.67	119.38	112.23
1	A	666	ILE	N-CA-C	5.63	121.06	109.34
1	A	182	TRP	N-CA-C	5.63	119.25	112.38
1	B	43	ARG	N-CA-C	5.63	118.18	111.71
1	A	555	VAL	N-CA-C	5.61	121.02	109.34
1	B	684	ASN	N-CA-C	5.56	119.76	112.92
1	B	689	ILE	N-CA-C	-5.52	99.79	107.80
1	B	696	ASN	N-CA-C	-5.51	105.27	111.28
1	A	684	ASN	N-CA-C	5.51	119.00	112.72
1	B	193	ARG	CA-C-N	5.50	125.58	119.32
1	B	193	ARG	C-N-CA	5.50	125.58	119.32
1	B	333	VAL	N-CA-C	5.46	115.98	108.12
1	B	602	THR	N-CA-C	-5.42	98.41	107.99
1	A	576	GLN	N-CA-C	-5.39	106.40	112.87
1	A	380	LEU	CA-C-N	5.36	124.81	119.24
1	A	380	LEU	C-N-CA	5.36	124.81	119.24
1	B	372	PHE	N-CA-C	5.36	118.84	110.32
1	A	557	ILE	N-CA-C	5.33	116.25	108.58
1	A	491	TRP	N-CA-C	5.32	118.88	112.93
1	B	232	GLY	N-CA-C	-5.29	104.33	112.85
1	B	677	GLY	N-CA-C	-5.25	106.44	112.73
1	B	561	SER	N-CA-C	5.23	117.44	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	373	ALA	N-CA-C	-5.23	100.17	109.06
1	A	671	THR	N-CA-C	5.20	119.75	113.41
1	B	418	PHE	CA-C-N	5.13	125.17	119.32
1	B	418	PHE	C-N-CA	5.13	125.17	119.32
1	A	696	ASN	N-CA-C	-5.12	105.69	111.28
1	B	464	LYS	N-CA-C	5.11	116.66	111.14
1	B	184	ARG	N-CA-C	5.10	117.23	111.11
1	A	734	ALA	N-CA-C	5.07	118.72	112.54
1	B	551	THR	N-CA-C	-5.04	106.96	113.01
1	A	811	PHE	N-CA-C	5.03	119.14	113.15

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	6437	0	6418	155	0
1	B	6420	0	6408	160	0
2	A	15	0	15	0	0
2	B	15	0	15	1	0
3	A	15	0	7	0	0
3	B	15	0	7	1	0
4	A	30	0	18	0	0
4	B	30	0	18	0	0
5	A	12	0	4	0	0
5	B	12	0	4	0	0
6	A	24	0	42	3	0
6	B	16	0	28	9	0
7	A	433	0	0	16	0
7	B	352	0	0	21	0
All	All	13826	0	12984	320	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 12.

All (320) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ASP:HB3	7:A:2741:HOH:O	1.53	1.05
1:A:49:ARG:HH22	6:A:905:MRD:H1C2	1.26	1.01
1:A:754:GLN:HG2	1:A:757:LEU:HB2	1.43	1.00
1:B:818:LYS:NZ	1:B:818:LYS:HB3	1.81	0.95
1:B:615:MET:HE2	1:B:764:MET:HE2	1.49	0.90
1:A:547:GLN:O	1:A:551:THR:HG23	1.72	0.90
1:B:110:GLU:HA	7:B:2762:HOH:O	1.79	0.82
1:A:308:ILE:HD13	1:A:352:ILE:HG21	1.61	0.81
1:A:789:GLN:HA	1:A:792:MET:HE2	1.61	0.80
1:B:770:ARG:HA	7:B:2481:HOH:O	1.81	0.79
1:A:329:PHE:HB3	1:A:330:PRO:HD3	1.65	0.78
1:B:789:GLN:HA	1:B:792:MET:HE2	1.65	0.77
1:B:592:LYS:HD3	1:B:592:LYS:C	2.09	0.77
1:B:818:LYS:HB3	1:B:818:LYS:HZ3	1.47	0.76
1:B:434:GLU:CD	1:B:434:GLU:H	1.94	0.75
1:B:169:LYS:HB2	1:B:176:VAL:HG12	1.69	0.75
1:A:29:LYS:HE2	1:A:33:ARG:HH21	1.51	0.74
1:A:29:LYS:HG2	1:A:33:ARG:NH2	2.04	0.73
1:B:729:LYS:O	1:B:733:GLU:HG2	1.90	0.72
1:A:466:LYS:HE3	7:A:2665:HOH:O	1.88	0.72
1:A:433:GLU:HG2	1:A:437:LYS:HE3	1.73	0.71
1:B:450:HIS:HD2	7:B:2730:HOH:O	1.72	0.71
1:A:592:LYS:HD3	1:A:592:LYS:C	2.14	0.71
1:B:196:PHE:CZ	6:B:903:MRD:H1C3	2.25	0.70
6:B:903:MRD:H5C1	7:B:2596:HOH:O	1.90	0.70
1:A:415:VAL:HG22	1:A:425:LEU:HD11	1.72	0.70
1:B:33:ARG:HD2	7:B:2480:HOH:O	1.90	0.70
1:A:106:ASN:ND2	7:A:2586:HOH:O	2.24	0.70
1:A:29:LYS:HE2	1:A:33:ARG:NH2	2.07	0.69
1:A:506:LYS:HD2	1:A:524:PHE:CE2	2.28	0.69
1:B:547:GLN:O	1:B:551:THR:HG23	1.92	0.69
1:A:146:SER:O	1:A:150:LEU:HD13	1.93	0.69
1:A:428:MET:HE1	1:A:474:LEU:HD12	1.73	0.69
1:A:66:ARG:HD2	1:A:236:ASN:HA	1.73	0.69
1:B:170:ILE:HG12	1:B:646:GLU:HG2	1.75	0.69
1:A:96:GLN:HG2	1:A:105:GLN:HE22	1.58	0.69
1:B:29:LYS:HG2	1:B:33:ARG:NH2	2.08	0.68
1:B:315:LYS:HE3	1:B:315:LYS:HA	1.76	0.68
1:A:421:ASP:CG	1:A:424:ARG:HB2	2.19	0.68
1:B:42:ASP:OD2	1:B:44:ASN:ND2	2.27	0.67
1:B:792:MET:O	1:B:794:PRO:HD3	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:382:GLU:CD	1:B:770:ARG:HH22	2.03	0.67
1:B:450:HIS:HE1	7:B:2135:HOH:O	1.77	0.67
1:A:455:VAL:H	1:A:459:HIS:HD2	1.44	0.66
1:A:379:VAL:HG12	1:A:379:VAL:O	1.94	0.65
1:B:433:GLU:HG3	1:B:437:LYS:HE3	1.77	0.65
1:A:382:GLU:CD	1:A:770:ARG:HH22	2.04	0.65
1:B:66:ARG:CD	1:B:236:ASN:HA	2.26	0.65
1:B:455:VAL:H	1:B:459:HIS:HD2	1.45	0.64
1:A:772:LYS:HB3	1:A:775:ALA:HB3	1.79	0.64
1:B:361:TRP:CH2	1:B:405:GLU:HG2	2.32	0.64
1:A:96:GLN:HG2	1:A:105:GLN:NE2	2.13	0.64
1:B:325:VAL:O	1:B:326:PHE:HB2	1.96	0.63
1:B:633:ASP:O	1:B:636:VAL:HG22	1.99	0.63
1:B:493:LEU:HD11	1:B:512:VAL:HG11	1.81	0.63
1:B:818:LYS:HB3	1:B:818:LYS:HZ2	1.61	0.63
1:A:65:GLY:O	1:A:69:ARG:HG3	1.98	0.62
1:B:428:MET:HE1	1:B:474:LEU:HD12	1.79	0.62
1:B:493:LEU:HD21	1:B:512:VAL:HG22	1.81	0.62
1:A:729:LYS:O	1:A:733:GLU:HG2	1.98	0.62
1:B:633:ASP:HB3	1:B:636:VAL:HG22	1.81	0.62
1:A:41:LYS:HE3	1:A:45:VAL:HG12	1.82	0.62
1:A:96:GLN:HE21	1:A:105:GLN:HE22	1.47	0.62
1:B:592:LYS:HD3	1:B:592:LYS:O	1.98	0.62
1:A:415:VAL:CG2	1:A:425:LEU:HD11	2.29	0.62
1:A:414:ILE:HD13	1:A:428:MET:SD	2.39	0.61
1:B:433:GLU:HA	1:B:437:LYS:HG2	1.82	0.61
1:A:494:LEU:HD23	1:A:494:LEU:C	2.25	0.61
1:B:421:ASP:CG	1:B:424:ARG:HB2	2.27	0.60
1:A:469:LYS:O	1:A:473:GLU:HG3	2.00	0.60
1:A:308:ILE:CD1	1:A:352:ILE:HG21	2.29	0.60
1:B:645:LEU:HD13	1:B:652:LEU:HD13	1.83	0.60
1:A:433:GLU:HA	1:A:437:LYS:HG2	1.83	0.60
1:A:23:ASN:HD21	1:A:26:GLU:CG	2.14	0.59
1:B:592:LYS:C	1:B:594:PRO:HD3	2.27	0.59
1:A:810:LYS:O	1:A:815:ARG:HD3	2.02	0.59
1:A:23:ASN:HD21	1:A:26:GLU:HG2	1.66	0.59
1:A:233:TYR:CE2	1:A:512:VAL:HG11	2.38	0.58
6:A:904:MRD:H1C3	7:A:2758:HOH:O	2.03	0.58
1:B:346:ILE:HD13	1:B:448:GLY:HA3	1.85	0.58
1:A:754:GLN:HG2	1:A:757:LEU:CB	2.28	0.58
6:B:903:MRD:H1C1	7:B:2597:HOH:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:LEU:HD23	1:A:136:LEU:C	2.29	0.58
1:B:65:GLY:O	1:B:69:ARG:HG3	2.02	0.58
1:B:363:LYS:HD2	1:B:366:GLU:OE1	2.04	0.58
1:B:432:GLU:O	1:B:437:LYS:HA	2.05	0.57
1:A:415:VAL:HG23	1:A:425:LEU:HD21	1.87	0.57
1:A:764:MET:HE1	1:A:765:LEU:HD13	1.85	0.57
1:B:81:ARG:NH1	1:B:155:TYR:OH	2.38	0.57
1:B:761:ILE:O	1:B:765:LEU:HD22	2.04	0.57
1:B:810:LYS:O	1:B:815:ARG:HD3	2.05	0.57
1:A:792:MET:O	1:A:794:PRO:HD3	2.04	0.56
1:A:325:VAL:O	1:A:326:PHE:HB2	2.04	0.56
1:B:545:PHE:O	1:B:548:PHE:HB3	2.05	0.56
1:B:160:ARG:HB2	1:B:243:LEU:HB3	1.87	0.56
1:B:392:VAL:HG21	1:B:439:ILE:HD12	1.87	0.56
1:A:179:ALA:O	1:B:250:ASN:ND2	2.38	0.56
1:B:66:ARG:HD2	1:B:236:ASN:HA	1.87	0.56
1:B:325:VAL:N	7:B:2742:HOH:O	2.38	0.56
1:A:785:ASP:O	1:A:789:GLN:HG2	2.05	0.56
1:A:213:THR:HG23	1:A:355:ASP:OD1	2.06	0.56
1:B:433:GLU:CG	1:B:437:LYS:HE3	2.36	0.55
1:A:382:GLU:OE2	1:A:770:ARG:NH2	2.39	0.55
1:A:732:TYR:CZ	1:A:739:LYS:HG3	2.41	0.55
1:B:379:VAL:HG12	1:B:379:VAL:O	2.06	0.55
1:A:433:GLU:CG	1:A:437:LYS:HE3	2.36	0.55
1:A:49:ARG:NH2	6:A:905:MRD:H1C2	2.08	0.55
1:B:136:LEU:C	1:B:136:LEU:HD23	2.32	0.55
1:A:450:HIS:HE1	7:A:2334:HOH:O	1.89	0.54
1:A:45:VAL:HG12	1:A:45:VAL:O	2.07	0.54
1:A:327:ASP:OD1	1:A:363:LYS:HE2	2.07	0.54
1:A:814:ASP:O	1:A:818:LYS:HG3	2.07	0.54
1:B:772:LYS:HB3	1:B:775:ALA:HB3	1.90	0.54
1:A:822:GLN:HB2	7:A:2748:HOH:O	2.08	0.53
1:B:785:ASP:O	1:B:789:GLN:HG2	2.08	0.53
1:B:66:ARG:HD3	1:B:236:ASN:HA	1.89	0.53
1:B:764:MET:HE1	1:B:765:LEU:HD13	1.89	0.53
1:A:592:LYS:C	1:A:594:PRO:HD3	2.34	0.53
1:B:466:LYS:NZ	1:B:715:ILE:HD11	2.23	0.53
1:A:455:VAL:HG23	1:A:674:SER:HB2	1.91	0.53
1:A:826:ASN:ND2	7:A:2682:HOH:O	2.39	0.53
1:B:463:VAL:HG13	1:B:468:PHE:CD1	2.44	0.53
1:A:407:ASN:O	1:A:410:HIS:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455:VAL:HG23	1:B:674:SER:HB2	1.92	0.52
1:B:493:LEU:HD11	1:B:512:VAL:CG1	2.39	0.52
1:A:399:HIS:O	1:A:403:ILE:HG13	2.09	0.52
1:A:713:MET:HB3	1:A:717:ASP:HB2	1.92	0.52
1:B:503:ILE:O	1:B:507:ILE:HG12	2.10	0.52
1:A:314:SER:C	1:A:316:PHE:H	2.18	0.52
6:B:902:MRD:H5C1	7:B:2274:HOH:O	2.10	0.52
1:A:269:ARG:NH2	7:A:2224:HOH:O	2.25	0.52
1:B:662:LEU:HG	1:B:787:VAL:HG11	1.92	0.51
1:B:135:GLY:HA3	7:B:2013:HOH:O	2.10	0.51
1:B:636:VAL:HG23	1:B:637:GLY:N	2.24	0.51
1:B:42:ASP:CG	1:B:44:ASN:HD21	2.18	0.51
1:A:417:LEU:HB2	1:A:418:PHE:CD1	2.46	0.51
1:A:697:VAL:O	1:A:701:GLU:HG3	2.10	0.51
1:A:727:GLU:OE1	1:A:729:LYS:HE3	2.11	0.51
6:B:903:MRD:HMC2	7:B:2100:HOH:O	2.11	0.51
1:A:462:ILE:HG23	1:A:466:LYS:HD2	1.93	0.51
1:B:197:MET:HE2	1:B:224:LEU:HD13	1.92	0.51
1:B:386:ARG:HA	1:B:439:ILE:O	2.10	0.50
1:B:536:LYS:O	1:B:540:GLU:HG3	2.11	0.50
1:B:818:LYS:NZ	1:B:818:LYS:CB	2.62	0.50
1:A:352:ILE:O	1:A:356:ILE:HB	2.11	0.50
1:B:587:TYR:O	1:B:591:LYS:HG2	2.12	0.50
1:A:466:LYS:NZ	1:A:715:ILE:HD11	2.26	0.50
1:B:434:GLU:CD	1:B:434:GLU:N	2.67	0.50
1:A:455:VAL:H	1:A:459:HIS:CD2	2.28	0.50
1:B:592:LYS:C	1:B:592:LYS:CD	2.82	0.50
1:A:213:THR:HG21	1:A:398:ARG:NH2	2.26	0.49
1:B:772:LYS:HD3	7:B:2158:HOH:O	2.12	0.49
1:B:761:ILE:HG22	1:B:765:LEU:CD2	2.42	0.49
1:A:23:ASN:ND2	1:A:26:GLU:HB2	2.27	0.49
1:A:346:ILE:HD13	1:A:448:GLY:HA3	1.95	0.49
1:B:81:ARG:NH2	7:B:2469:HOH:O	2.44	0.49
1:B:463:VAL:HG13	1:B:468:PHE:HD1	1.76	0.49
6:B:902:MRD:H5C1	6:B:903:MRD:H5C3	1.95	0.49
1:A:594:PRO:HG3	1:A:635:MET:SD	2.52	0.49
1:B:41:LYS:HE2	1:B:45:VAL:HG12	1.94	0.49
1:B:365:TRP:CD1	1:B:369:GLN:NE2	2.81	0.49
1:A:423:ASP:O	1:A:427:ARG:HG3	2.12	0.49
1:A:719:ALA:O	1:A:722:ASP:HB2	2.13	0.49
1:A:41:LYS:CE	1:A:45:VAL:HG12	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:LYS:NZ	7:B:2525:HOH:O	2.44	0.49
1:B:415:VAL:HG23	1:B:425:LEU:HD21	1.95	0.48
1:A:246:ALA:O	1:A:247:ARG:HD3	2.13	0.48
1:A:689:ILE:HG23	1:A:689:ILE:O	2.13	0.48
1:A:765:LEU:HG	1:A:774:PHE:CE2	2.49	0.48
1:B:221:VAL:HG22	1:B:272:ALA:HB1	1.95	0.48
1:A:66:ARG:CD	1:A:236:ASN:HA	2.42	0.48
1:A:605:ILE:O	1:A:644:PHE:HA	2.14	0.48
1:A:729:LYS:HG3	7:A:2676:HOH:O	2.14	0.48
1:A:792:MET:C	1:A:794:PRO:HD3	2.39	0.48
1:A:224:LEU:HD12	1:A:225:PRO:HD2	1.96	0.47
1:A:421:ASP:OD1	1:A:424:ARG:HD2	2.14	0.47
1:B:329:PHE:HB3	1:B:330:PRO:HD3	1.96	0.47
1:B:422:VAL:HG23	1:B:423:ASP:N	2.28	0.47
1:B:596:LYS:HG2	1:B:597:LEU:N	2.29	0.47
1:A:308:ILE:HD13	1:A:352:ILE:CG2	2.39	0.47
1:B:80:LYS:HE2	1:B:334:ALA:HB2	1.96	0.47
1:B:361:TRP:CZ3	1:B:405:GLU:HG2	2.49	0.47
1:B:235:ASN:O	1:B:236:ASN:HB2	2.14	0.47
1:B:275:ILE:O	1:B:295:GLN:HG2	2.14	0.47
1:B:308:ILE:CD1	1:B:352:ILE:HG21	2.45	0.47
1:B:729:LYS:O	1:B:732:TYR:HB3	2.15	0.47
1:B:420:LYS:O	1:B:422:VAL:N	2.48	0.47
1:A:241:MET:HE3	1:A:243:LEU:HD22	1.96	0.47
1:B:81:ARG:NE	7:B:2469:HOH:O	2.48	0.47
1:A:160:ARG:HB2	1:A:243:LEU:HB3	1.95	0.46
1:A:413:ARG:O	1:A:417:LEU:HG	2.15	0.46
1:A:546:SER:O	1:A:550:GLU:HG3	2.15	0.46
1:B:605:ILE:O	1:B:644:PHE:HA	2.14	0.46
1:A:250:ASN:CG	7:A:2224:HOH:O	2.57	0.46
1:B:689:ILE:O	1:B:689:ILE:HG23	2.14	0.46
6:B:902:MRD:H5C2	6:B:903:MRD:H3C2	1.96	0.46
1:A:393:GLU:HB2	1:A:400:LEU:HD22	1.97	0.46
1:B:170:ILE:HD13	1:B:175:GLN:HA	1.97	0.46
1:B:405:GLU:O	1:B:409:LYS:HG2	2.14	0.46
1:A:592:LYS:HD3	1:A:592:LYS:O	2.14	0.46
1:B:80:LYS:HB3	1:B:827:VAL:HG12	1.96	0.46
1:B:250:ASN:O	1:B:251:ASP:C	2.59	0.46
1:B:639:LYS:NZ	7:B:2615:HOH:O	2.48	0.46
1:B:558:ASN:OD1	1:B:560:SER:HB3	2.14	0.46
1:A:315:LYS:C	7:A:2780:HOH:O	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:GLN:HB2	1:A:664:GLU:HB2	1.98	0.46
1:A:732:TYR:CE1	1:A:739:LYS:HG3	2.50	0.46
1:A:41:LYS:HE2	1:A:45:VAL:O	2.16	0.46
1:A:197:MET:HE2	1:A:224:LEU:HD13	1.98	0.46
1:A:247:ARG:HB3	1:B:184:ARG:NH2	2.30	0.46
1:B:24:VAL:O	1:B:28:LYS:HG3	2.16	0.46
1:A:74:TYR:CZ	1:A:153:ALA:HA	2.51	0.45
1:A:235:ASN:O	1:A:236:ASN:HB2	2.16	0.45
1:A:413:ARG:HG2	1:A:413:ARG:HH11	1.81	0.45
1:A:543:LEU:HD12	1:A:543:LEU:HA	1.74	0.45
1:B:45:VAL:HG12	1:B:45:VAL:O	2.16	0.45
1:B:494:LEU:C	1:B:494:LEU:HD23	2.41	0.45
1:A:314:SER:O	1:A:316:PHE:HD2	1.98	0.45
1:A:770:ARG:HA	7:A:2270:HOH:O	2.17	0.45
1:B:739:LYS:HG2	1:B:743:ASP:OD2	2.16	0.45
1:A:212:GLY:O	1:A:214:LYS:HD3	2.16	0.45
1:A:66:ARG:HG3	1:A:69:ARG:HH12	1.80	0.45
1:A:225:PRO:HB3	1:A:244:TRP:CZ3	2.51	0.45
1:B:575:ARG:HD3	1:B:666:ILE:O	2.16	0.45
1:B:413:ARG:HA	1:B:413:ARG:NE	2.31	0.45
1:A:251:ASP:HB3	1:B:178:GLU:OE1	2.16	0.45
1:A:592:LYS:O	1:A:594:PRO:HD3	2.17	0.45
1:A:709:PHE:HB3	1:A:783:CYS:SG	2.57	0.45
1:A:772:LYS:CE	7:A:2270:HOH:O	2.65	0.44
1:B:113:TYR:HB3	7:B:2762:HOH:O	2.16	0.44
1:B:315:LYS:O	1:B:316:PHE:C	2.60	0.44
1:B:530:PHE:HE2	1:B:802:LEU:HD22	1.82	0.44
1:B:764:MET:CE	1:B:765:LEU:HD13	2.48	0.44
1:A:29:LYS:HG2	1:A:33:ARG:HH21	1.76	0.44
1:B:138:ARG:HD2	1:B:138:ARG:HA	1.82	0.44
1:B:553:TYR:CD1	1:B:553:TYR:N	2.85	0.44
1:A:81:ARG:NH1	1:A:155:TYR:OH	2.51	0.44
1:B:286:PHE:CD1	1:B:385:GLU:HG2	2.52	0.44
1:B:764:MET:HE3	1:B:764:MET:HB3	1.81	0.44
1:B:405:GLU:OE1	1:B:409:LYS:HE3	2.17	0.44
1:B:772:LYS:HD2	1:B:772:LYS:N	2.33	0.44
1:B:802:LEU:O	1:B:802:LEU:HD12	2.18	0.44
2:B:1861:NBG:H3	7:B:2452:HOH:O	2.17	0.44
1:A:379:VAL:O	1:A:379:VAL:CG1	2.64	0.44
1:A:22:GLU:HB3	1:A:62:HIS:CE1	2.52	0.43
1:A:286:PHE:CD1	1:A:385:GLU:HG2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:THR:O	1:A:815:ARG:NH2	2.47	0.43
1:A:517:GLN:OE1	1:A:520:LYS:HE3	2.18	0.43
1:B:309:ARG:HD2	7:B:2744:HOH:O	2.18	0.43
1:A:772:LYS:N	1:A:772:LYS:HD2	2.33	0.43
1:A:652:LEU:O	1:A:656:VAL:HG12	2.18	0.43
1:A:109:ASP:CB	7:A:2741:HOH:O	2.33	0.43
1:B:212:GLY:O	1:B:214:LYS:HD2	2.18	0.43
1:B:682:MET:HB2	1:B:699:MET:HE3	2.01	0.42
1:A:74:TYR:HB3	1:A:81:ARG:HH12	1.84	0.42
1:A:615:MET:HE2	1:A:764:MET:HE2	2.01	0.42
1:B:192:SER:C	1:B:194:PRO:HD3	2.44	0.42
1:B:196:PHE:CE2	6:B:903:MRD:H1C3	2.54	0.42
1:A:263:ILE:HG12	7:A:2568:HOH:O	2.18	0.42
1:B:393:GLU:HB2	1:B:400:LEU:HD22	2.00	0.42
1:B:678:ASN:HB2	1:B:699:MET:SD	2.59	0.42
1:B:80:LYS:HE3	1:B:330:PRO:O	2.20	0.42
1:B:181:ASP:OD2	1:B:184:ARG:NE	2.52	0.42
1:B:274:ASN:OD1	1:B:277:ARG:HD2	2.20	0.42
1:B:527:ASP:OD2	1:B:529:VAL:HB	2.19	0.42
1:A:764:MET:C	1:A:764:MET:SD	3.02	0.42
1:B:198:LEU:HD21	1:B:309:ARG:CZ	2.49	0.42
1:B:420:LYS:O	1:B:422:VAL:HG13	2.20	0.42
1:A:152:LEU:HD23	1:A:829:PRO:HA	2.00	0.42
1:A:575:ARG:C	1:A:577:LEU:N	2.75	0.42
1:B:308:ILE:HD13	1:B:352:ILE:HG21	2.02	0.42
1:B:379:VAL:O	1:B:379:VAL:CG1	2.68	0.42
1:B:555:VAL:HG21	1:B:631:ASN:ND2	2.35	0.42
1:B:716:ASP:O	1:B:719:ALA:HB3	2.20	0.42
1:B:170:ILE:HA	1:B:174:TRP:O	2.19	0.42
1:B:207:GLU:HG2	1:B:209:THR:HG23	2.02	0.42
1:A:72:GLN:HE21	1:A:76:ASP:CG	2.27	0.42
1:A:235:ASN:O	1:A:236:ASN:CB	2.67	0.42
1:A:769:ASP:OD2	1:A:773:VAL:HG23	2.20	0.41
1:B:213:THR:O	1:B:213:THR:HG23	2.19	0.41
1:A:110:GLU:OE1	1:A:114:GLN:NE2	2.47	0.41
1:A:764:MET:CE	1:A:765:LEU:HD13	2.48	0.41
1:A:193:ARG:HB2	1:A:225:PRO:HG2	2.03	0.41
1:B:74:TYR:HB3	1:B:81:ARG:NH1	2.36	0.41
1:A:233:TYR:CZ	1:A:512:VAL:HG11	2.56	0.41
1:B:233:TYR:CZ	1:B:512:VAL:HG11	2.56	0.41
1:B:598:PHE:HE2	1:B:639:LYS:O	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:ASP:CG	1:B:44:ASN:ND2	2.78	0.41
1:B:119:ILE:HG23	1:B:120:GLU:N	2.35	0.41
1:B:728:ALA:HB3	1:B:766:PHE:HA	2.03	0.41
1:A:341:HIS:HB2	1:A:342:PRO:HD3	2.02	0.41
1:A:430:LEU:HD23	1:A:443:HIS:HB3	2.03	0.41
1:B:112:ILE:HG23	1:B:117:LEU:HB2	2.01	0.41
1:B:193:ARG:HH12	6:B:903:MRD:HMC1	1.86	0.41
1:B:680:LYS:NZ	3:B:1860:PLP:O3	2.53	0.41
1:A:733:GLU:HG2	1:A:733:GLU:H	1.65	0.41
1:B:380:LEU:HA	1:B:381:PRO:HD3	1.85	0.41
1:A:211:THR:O	1:A:358:LYS:NZ	2.47	0.41
1:A:274:ASN:OD1	1:A:277:ARG:HD2	2.20	0.41
1:A:421:ASP:OD1	1:A:424:ARG:HB2	2.21	0.41
1:A:494:LEU:C	1:A:494:LEU:CD2	2.93	0.41
1:B:73:HIS:HA	7:B:2595:HOH:O	2.21	0.41
1:B:304:LEU:HD22	1:B:349:LEU:HD13	2.01	0.41
1:B:630:VAL:O	1:B:636:VAL:HG21	2.21	0.41
1:B:682:MET:HG2	1:B:808:SER:HB3	2.03	0.41
1:A:234:MET:HE2	7:A:2456:HOH:O	2.20	0.41
1:A:715:ILE:HG23	1:A:716:ASP:N	2.35	0.41
1:B:315:LYS:O	1:B:315:LYS:HD3	2.20	0.41
1:A:36:HIS:O	1:A:40:VAL:HA	2.21	0.40
1:A:181:ASP:OD2	1:A:184:ARG:NE	2.54	0.40
1:A:568:LYS:O	1:A:607:GLY:HA3	2.21	0.40
1:A:636:VAL:CG2	1:A:637:GLY:N	2.83	0.40
1:B:386:ARG:NH2	1:B:438:ARG:HD2	2.36	0.40
1:A:31:PHE:CD1	1:A:115:LEU:HD13	2.57	0.40
1:B:678:ASN:OD1	1:B:679:MET:N	2.50	0.40
1:A:386:ARG:HB3	1:A:438:ARG:HD3	2.03	0.40
1:A:417:LEU:HB2	1:A:418:PHE:CE1	2.56	0.40
1:B:44:ASN:HD22	1:B:45:VAL:HG23	1.86	0.40
1:B:759:LYS:HA	1:B:759:LYS:HD2	1.92	0.40
1:B:81:ARG:CZ	7:B:2469:HOH:O	2.68	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	787/847 (93%)	743 (94%)	38 (5%)	6 (1%)	16	12
1	B	785/847 (93%)	747 (95%)	33 (4%)	5 (1%)	21	18
All	All	1572/1694 (93%)	1490 (95%)	71 (4%)	11 (1%)	18	15

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	421	ASP
1	A	555	VAL
1	B	421	ASP
1	B	435	GLY
1	A	829	PRO
1	A	434	GLU
1	A	830	SER
1	B	213	THR
1	B	829	PRO
1	B	755	PRO
1	A	342	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	694/740 (94%)	660 (95%)	34 (5%)	22	22
1	B	692/740 (94%)	658 (95%)	34 (5%)	22	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1386/1480 (94%)	1318 (95%)	68 (5%)	22	22

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	VAL
1	A	90	TYR
1	A	95	LEU
1	A	96	GLN
1	A	102	LEU
1	A	104	LEU
1	A	110	GLU
1	A	120	GLU
1	A	213	THR
1	A	243	LEU
1	A	277	ARG
1	A	300	VAL
1	A	316	PHE
1	A	337	LEU
1	A	380	LEU
1	A	474	LEU
1	A	492	LEU
1	A	499	LEU
1	A	502	LEU
1	A	543	LEU
1	A	568	LYS
1	A	575	ARG
1	A	576	GLN
1	A	577	LEU
1	A	622	LEU
1	A	636	VAL
1	A	645	LEU
1	A	652	LEU
1	A	662	LEU
1	A	683	LEU
1	A	692	MET
1	A	733	GLU
1	A	765	LEU
1	A	815	ARG
1	B	44	ASN
1	B	78	CYS
1	B	95	LEU

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Mol	Chain	Res	Type
1	B	102	LEU
1	B	104	LEU
1	B	150	LEU
1	B	171	ARG
1	B	176	VAL
1	B	214	LYS
1	B	243	LEU
1	B	277	ARG
1	B	337	LEU
1	B	366	GLU
1	B	474	LEU
1	B	492	LEU
1	B	499	LEU
1	B	502	LEU
1	B	532	ARG
1	B	543	LEU
1	B	568	LYS
1	B	575	ARG
1	B	576	GLN
1	B	577	LEU
1	B	615	MET
1	B	622	LEU
1	B	628	ASP
1	B	645	LEU
1	B	652	LEU
1	B	662	LEU
1	B	683	LEU
1	B	692	MET
1	B	755	PRO
1	B	765	LEU
1	B	815	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	62	HIS
1	A	72	GLN
1	A	96	GLN
1	A	105	GLN
1	A	250	ASN
1	A	450	HIS

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Mol	Chain	Res	Type
1	A	459	HIS
1	A	804	ASN
1	B	44	ASN
1	B	96	GLN
1	B	97	ASN
1	B	105	GLN
1	B	332	GLN
1	B	443	HIS
1	B	450	HIS
1	B	459	HIS
1	B	539	GLN
1	B	822	GLN
1	B	823	ASN
1	B	826	ASN

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](#)

13 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	NBG	A	861	-	15,15,15	1.39	4 (26%)	21,21,21	1.21	3 (14%)
4	700	A	862	-	31,33,33	1.99	12 (38%)	44,47,47	1.91	11 (25%)
5	URC	B	1863	-	13,13,13	2.33	8 (61%)	17,19,19	1.72	3 (17%)
3	PLP	A	860	1	15,15,16	2.36	9 (60%)	21,22,23	1.21	2 (9%)
4	700	B	1862	-	31,33,33	1.92	10 (32%)	44,47,47	1.86	9 (20%)
2	NBG	B	1861	-	15,15,15	1.60	4 (26%)	21,21,21	1.37	3 (14%)
6	MRD	A	1902	-	7,7,7	0.50	0	9,10,10	0.75	0
6	MRD	B	903	-	7,7,7	1.35	1 (14%)	9,10,10	1.05	1 (11%)
5	URC	A	863	-	13,13,13	2.34	7 (53%)	17,19,19	1.77	4 (23%)
6	MRD	B	902	-	7,7,7	0.64	0	9,10,10	0.67	0
3	PLP	B	1860	1	15,15,16	2.04	4 (26%)	21,22,23	1.12	1 (4%)
6	MRD	A	904	-	7,7,7	0.88	0	9,10,10	0.91	0
6	MRD	A	905	-	7,7,7	0.72	0	9,10,10	0.95	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NBG	A	861	-	-	0/6/26/26	0/1/1/1
4	700	A	862	-	-	0/22/32/32	0/4/4/4
5	URC	B	1863	-	-	-	0/2/2/2
3	PLP	A	860	1	-	0/6/6/8	0/1/1/1
4	700	B	1862	-	-	2/22/32/32	0/4/4/4
2	NBG	B	1861	-	-	0/6/26/26	0/1/1/1
6	MRD	A	1902	-	-	4/5/5/5	-
6	MRD	B	903	-	-	1/5/5/5	-
5	URC	A	863	-	-	-	0/2/2/2
6	MRD	B	902	-	-	2/5/5/5	-
3	PLP	B	1860	1	-	2/6/6/8	0/1/1/1
6	MRD	A	904	-	-	4/5/5/5	-
6	MRD	A	905	-	-	2/5/5/5	-

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1860	PLP	C4A-C4	-5.97	1.39	1.51
4	A	862	700	C8-N2	-5.33	1.30	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1862	700	C8-N2	-5.25	1.31	1.38
5	A	863	URC	C5-N7	-4.56	1.30	1.37
3	A	860	PLP	C4A-C4	-4.39	1.42	1.51
5	B	1863	URC	C5-N7	-4.18	1.31	1.37
4	B	1862	700	C5-C4	3.46	1.43	1.38
3	A	860	PLP	C2-N1	3.36	1.39	1.33
2	B	1861	NBG	C1-N1	3.22	1.47	1.43
3	A	860	PLP	C2A-C2	3.18	1.55	1.50
2	B	1861	NBG	C2-C1	3.14	1.56	1.53
5	A	863	URC	C4-N9	-3.11	1.30	1.35
3	A	860	PLP	C3-C4	3.06	1.46	1.40
4	A	862	700	C5-C4	3.05	1.43	1.38
4	B	1862	700	C22-N3	-3.02	1.44	1.47
5	A	863	URC	C8-N9	-3.02	1.31	1.38
5	A	863	URC	C8-N7	-3.01	1.31	1.38
5	B	1863	URC	C8-N7	-2.97	1.31	1.38
4	A	862	700	C3-C4	2.86	1.43	1.38
5	B	1863	URC	C4-N9	-2.85	1.30	1.35
4	A	862	700	C1-N2	-2.85	1.33	1.38
5	B	1863	URC	C6-N1	-2.83	1.33	1.38
4	B	1862	700	C12-C11	2.80	1.44	1.38
5	B	1863	URC	C5-C6	2.75	1.50	1.41
5	B	1863	URC	C8-N9	-2.74	1.32	1.38
4	A	862	700	C12-C11	2.67	1.44	1.38
4	B	1862	700	C16-C11	2.66	1.44	1.38
3	A	860	PLP	C5A-C5	2.66	1.57	1.50
2	A	861	NBG	C2-C1	2.55	1.55	1.53
5	A	863	URC	C5-C6	2.46	1.49	1.41
3	A	860	PLP	P-O4P	2.44	1.68	1.60
4	B	1862	700	C15-C14	2.36	1.43	1.38
5	B	1863	URC	C4-N3	-2.35	1.33	1.37
2	B	1861	NBG	C4-C5	2.26	1.57	1.53
4	B	1862	700	C3-C4	2.26	1.42	1.38
3	A	860	PLP	P-O3P	-2.25	1.46	1.54
2	B	1861	NBG	C3-C2	2.23	1.58	1.52
4	B	1862	700	C6-C7	2.23	1.50	1.44
4	A	862	700	C17-N1	2.22	1.50	1.45
2	A	861	NBG	C1-N1	2.20	1.46	1.43
2	A	861	NBG	C3-C2	2.19	1.58	1.52
3	B	1860	PLP	C5-C4	-2.18	1.38	1.40
5	A	863	URC	C6-N1	-2.18	1.34	1.38
5	A	863	URC	C4-N3	-2.16	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	860	PLP	O3-C3	2.16	1.41	1.36
4	A	862	700	C15-C16	2.15	1.42	1.38
3	B	1860	PLP	C3-C2	-2.15	1.38	1.41
5	B	1863	URC	C2-N1	-2.13	1.34	1.37
4	A	862	700	C10-C11	2.12	1.56	1.51
4	A	862	700	C6-C7	2.11	1.50	1.44
3	A	860	PLP	C6-N1	2.07	1.38	1.34
4	B	1862	700	O4-C21	-2.07	1.24	1.30
3	B	1860	PLP	P-O3P	-2.07	1.47	1.54
4	B	1862	700	C14-C13	2.05	1.42	1.38
4	A	862	700	O4-C21	-2.05	1.24	1.30
4	A	862	700	C10-C17	2.02	1.58	1.54
2	A	861	NBG	O5-C1	2.02	1.46	1.43
4	A	862	700	C13-C12	2.02	1.42	1.38
6	B	903	MRD	CM-C2	-2.01	1.46	1.52

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1862	700	C1-C6-C7	-5.31	102.45	106.80
4	A	862	700	C1-C6-C7	-5.28	102.47	106.80
4	B	1862	700	C8-C9-N1	4.61	123.02	116.86
4	A	862	700	C8-C9-N1	4.50	122.87	116.86
4	A	862	700	C5-C6-C1	4.44	121.88	119.13
4	B	1862	700	O1-C9-C8	-4.32	115.53	121.09
2	B	1861	NBG	C5-O5-C1	4.23	118.35	112.47
4	A	862	700	O1-C9-C8	-4.11	115.79	121.09
4	B	1862	700	C5-C6-C1	3.79	121.47	119.13
4	A	862	700	O3-C21-C20	-3.66	113.14	122.86
5	A	863	URC	N3-C2-N1	3.43	121.13	115.74
2	A	861	NBG	C5-O5-C1	3.41	117.20	112.47
4	B	1862	700	O3-C21-C20	-3.36	113.93	122.86
5	B	1863	URC	N3-C2-N1	3.34	120.99	115.74
4	B	1862	700	O4-C21-O3	3.20	131.34	124.08
4	A	862	700	O4-C21-O3	3.13	131.18	124.08
5	A	863	URC	O13-C6-C5	-3.10	119.78	127.26
4	A	862	700	C1-N2-C8	2.98	112.21	109.01
5	B	1863	URC	O13-C6-C5	-2.83	120.43	127.26
5	A	863	URC	C6-N1-C2	-2.83	122.47	126.37
3	A	860	PLP	O4P-C5A-C5	-2.82	104.07	109.36
4	B	1862	700	C6-C5-C4	-2.80	117.04	120.40
5	B	1863	URC	C6-N1-C2	-2.68	122.67	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	862	700	C6-C5-C4	-2.65	117.22	120.40
3	B	1860	PLP	O4P-P-O1P	-2.56	99.51	106.44
2	B	1861	NBG	C3-C2-C1	2.55	113.61	109.86
4	B	1862	700	C1-N2-C8	2.50	111.69	109.01
3	A	860	PLP	O3P-P-O2P	2.41	116.83	107.80
2	B	1861	NBG	C2-C1-N1	-2.25	108.34	111.25
4	A	862	700	C22-C20-C21	2.20	121.60	116.40
5	A	863	URC	O13-C6-N1	2.18	124.22	120.11
6	B	903	MRD	O2-C2-C3	2.17	117.38	109.27
4	A	862	700	C10-C17-C18	-2.16	105.41	109.94
2	A	861	NBG	C2-C1-N1	-2.12	108.52	111.25
2	A	861	NBG	C3-C2-C1	2.11	112.96	109.86
4	B	1862	700	C10-C17-C18	-2.04	105.66	109.94
4	A	862	700	C19-C20-C21	2.02	121.17	116.40

There are no chirality outliers.

All (17) torsion outliers are listed below:

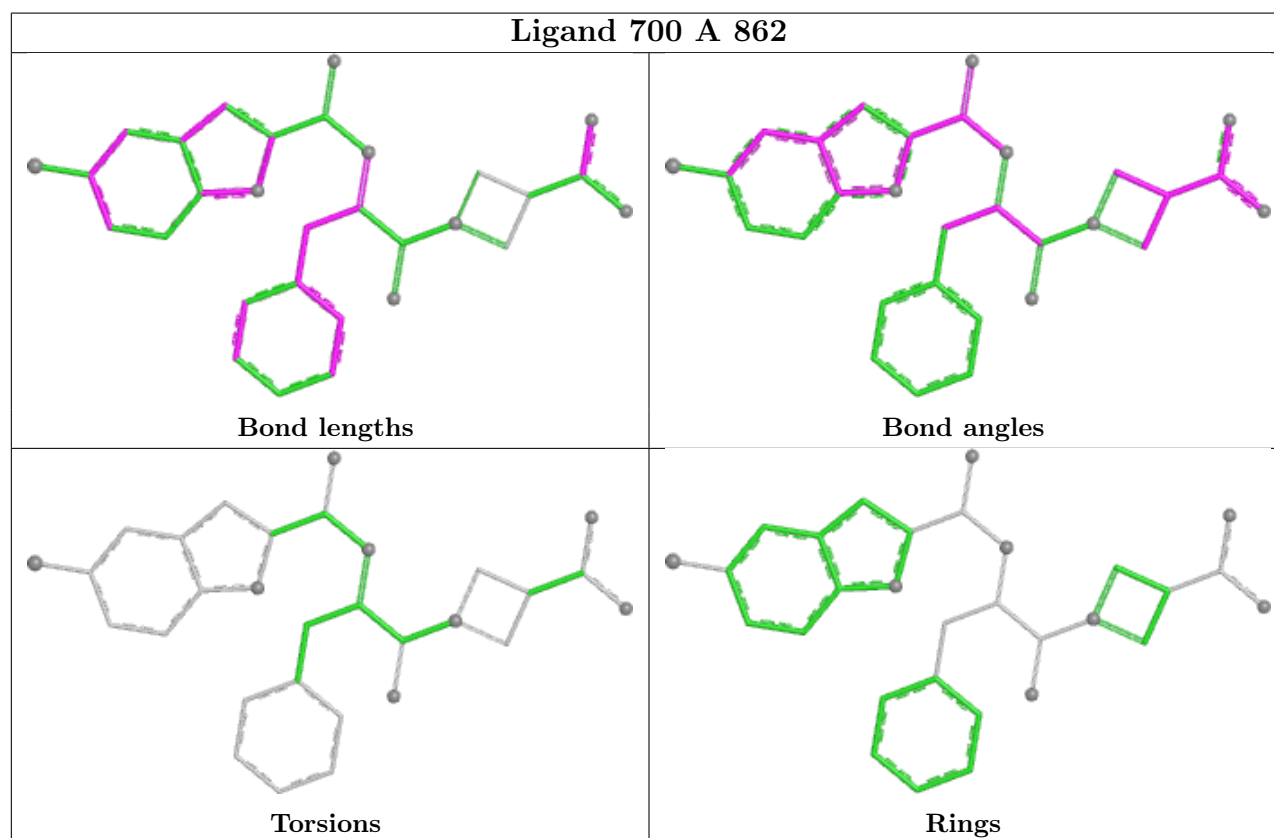
Mol	Chain	Res	Type	Atoms
6	A	904	MRD	O2-C2-C3-C4
6	A	904	MRD	CM-C2-C3-C4
6	A	904	MRD	C2-C3-C4-C5
6	B	902	MRD	C2-C3-C4-O4
3	B	1860	PLP	C6-C5-C5A-O4P
6	A	905	MRD	C2-C3-C4-C5
6	B	902	MRD	C2-C3-C4-C5
4	B	1862	700	C22-C20-C21-O3
4	B	1862	700	C22-C20-C21-O4
3	B	1860	PLP	C4-C5-C5A-O4P
6	A	1902	MRD	O2-C2-C3-C4
6	A	1902	MRD	C2-C3-C4-O4
6	A	905	MRD	C2-C3-C4-O4
6	A	1902	MRD	C1-C2-C3-C4
6	A	1902	MRD	CM-C2-C3-C4
6	A	904	MRD	C1-C2-C3-C4
6	B	903	MRD	C1-C2-C3-C4

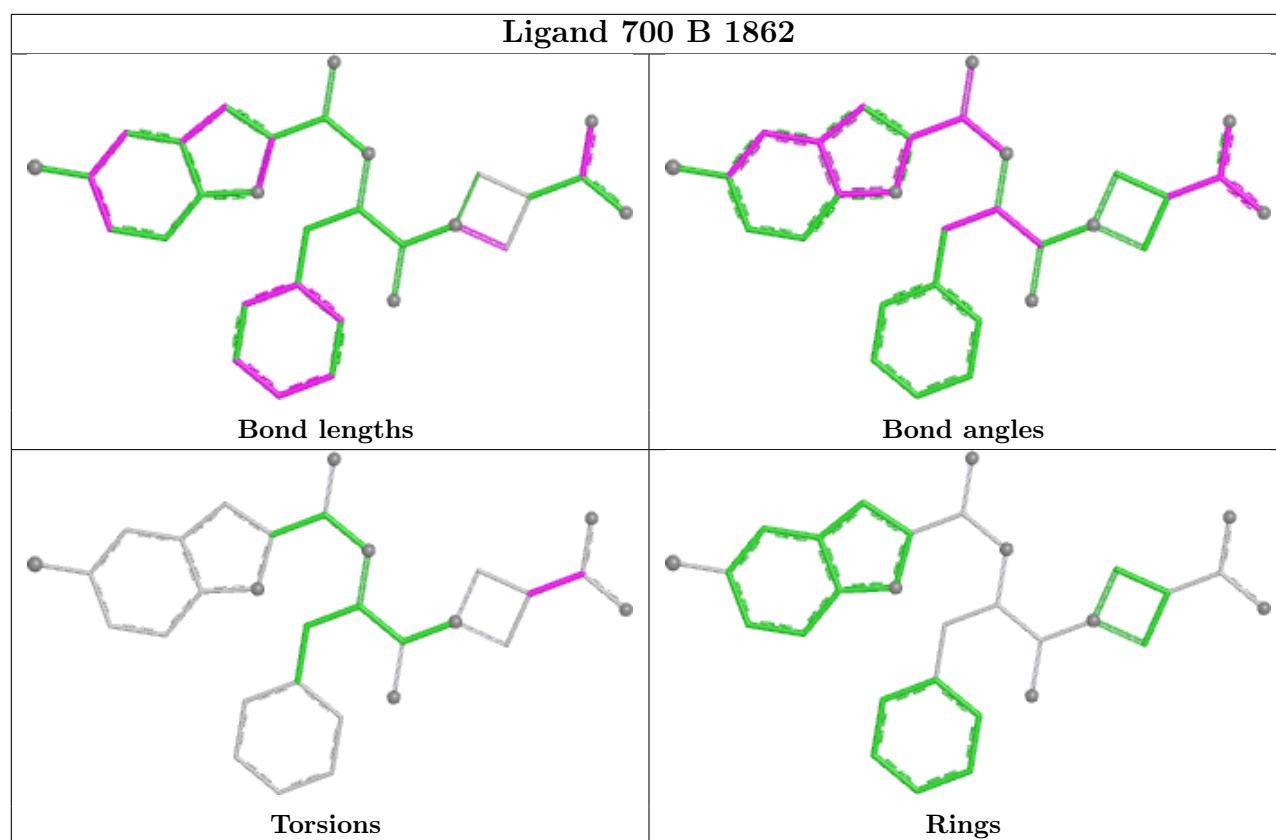
There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1861	NBG	1	0
6	B	903	MRD	8	0
6	B	902	MRD	3	0
3	B	1860	PLP	1	0
6	A	904	MRD	1	0
6	A	905	MRD	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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.