



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:44 AM UTC

PDB ID : 1L5Q / pdb_0000115q
Title : Human liver glycogen phosphorylase a complexed with caffeine, N-Acetyl-beta-D-glucopyranosylamine, and CP-403700
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.; Myszkka, D.G.; Rath, V.L.
Deposited on : 2002-03-07
Resolution : 2.25 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

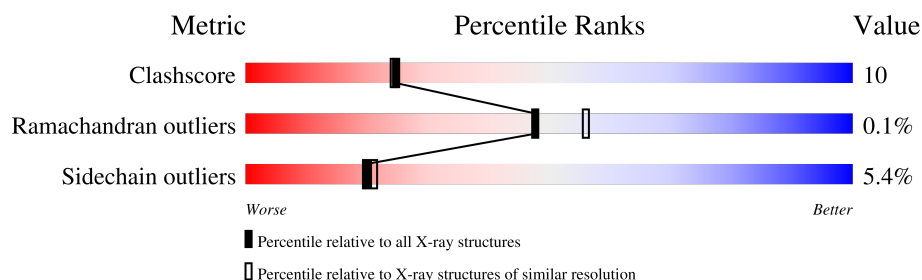
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)

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	 69% 21% • 7%
1	B	847	 70% 21% • 7%

2 Entry composition [i](#)

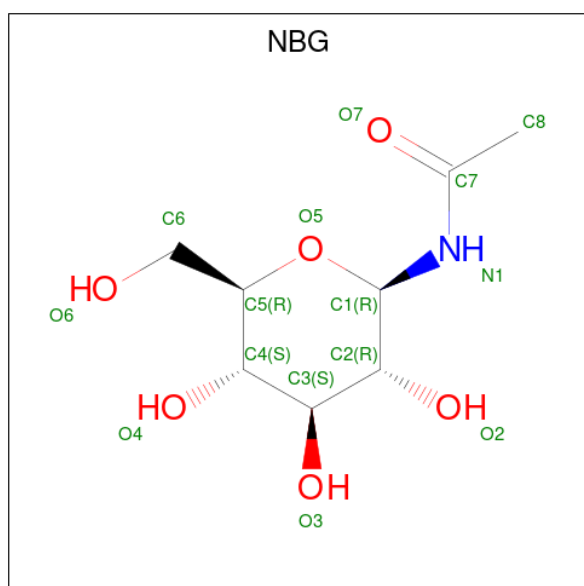
There are 6 unique types of molecules in this entry. The entry contains 13620 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

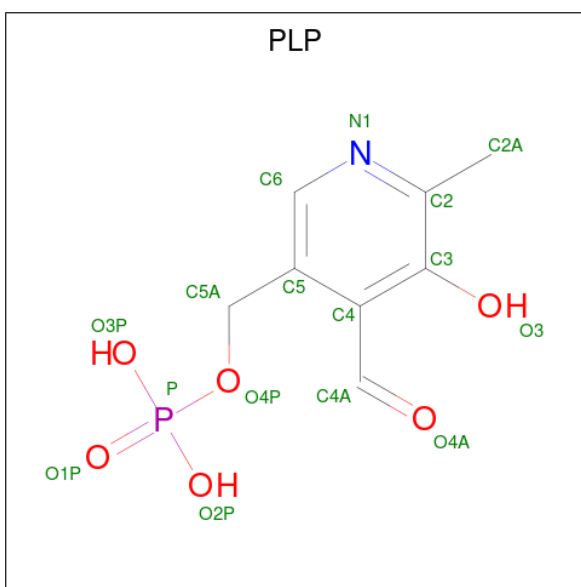
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	791	Total	C	N	O	S	0	0	0
			6423	4128	1090	1176	29			
1	B	790	Total	C	N	O	S	0	0	0
			6414	4123	1089	1173	29			

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



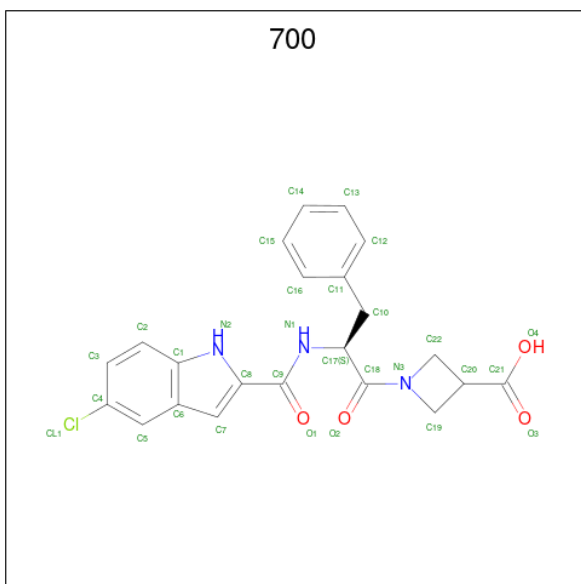
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			15	8	1	6		

- 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: $C_{22}H_{20}ClN_3O_4$).



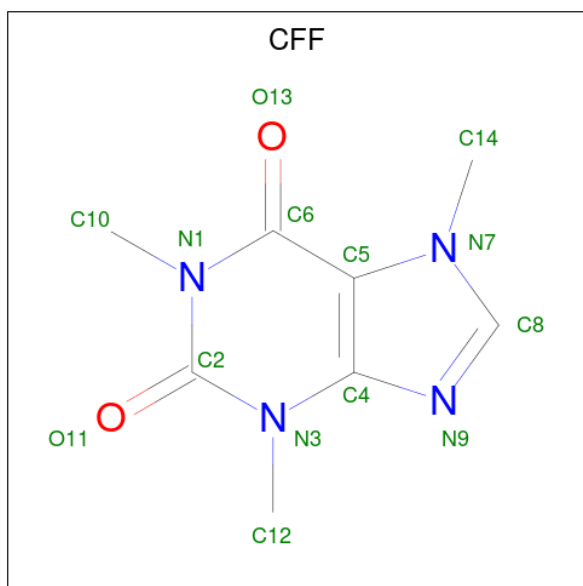
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			30	22	1	3	4		

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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 CAFFEINE (CCD ID: CFF) (formula: $C_8H_{10}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	4	2		
5	A	1	Total	C	N	O	0	0
			14	8	4	2		
5	B	1	Total	C	N	O	0	0
			14	8	4	2		
5	B	1	Total	C	N	O	0	0
			14	8	4	2		

- Molecule 6 is water.

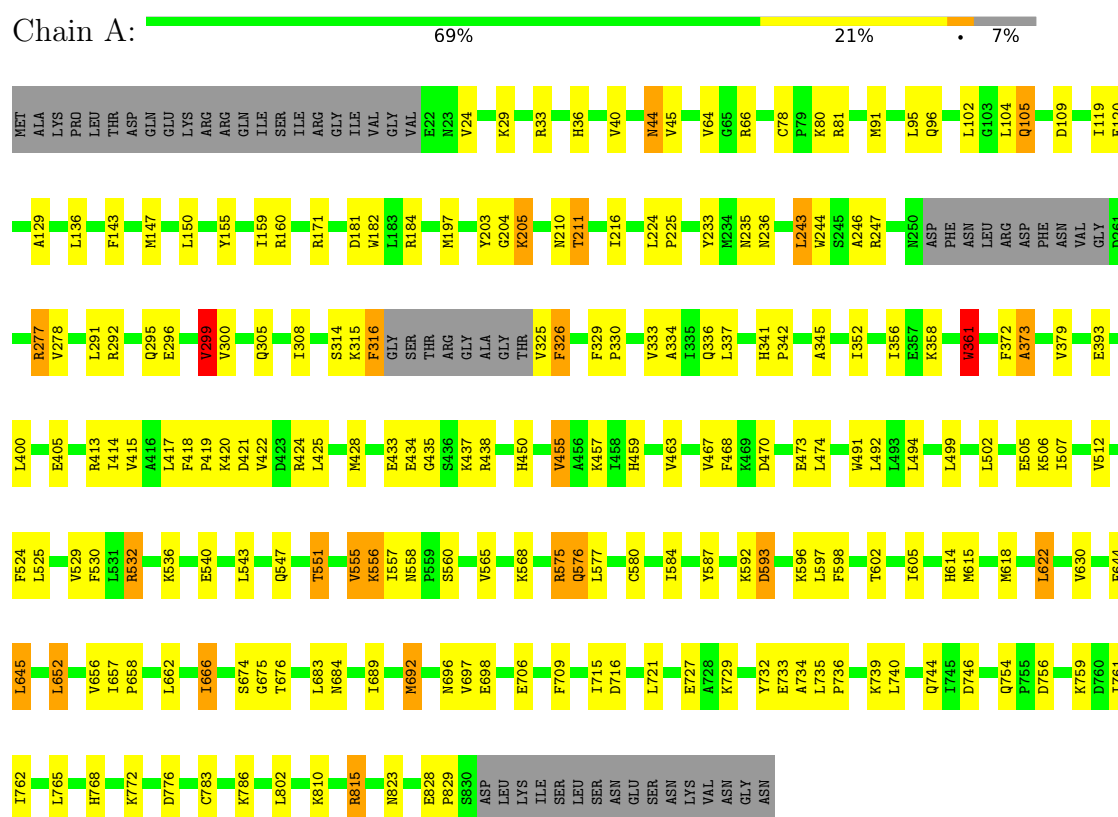
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	324	Total	O	0	0
			324	324		
6	B	283	Total	O	0	0
			283	283		

3 Residue-property plots

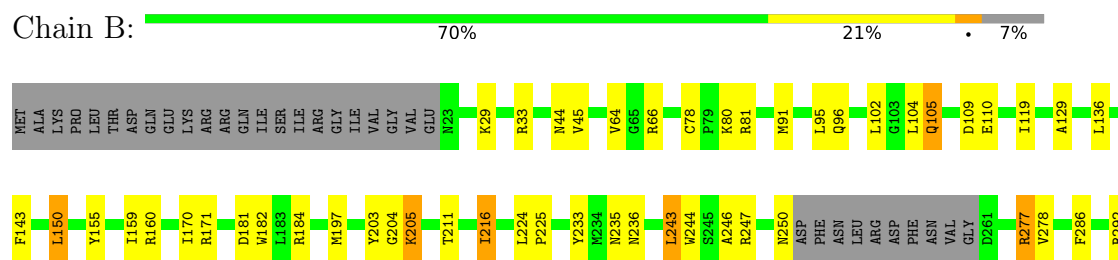
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

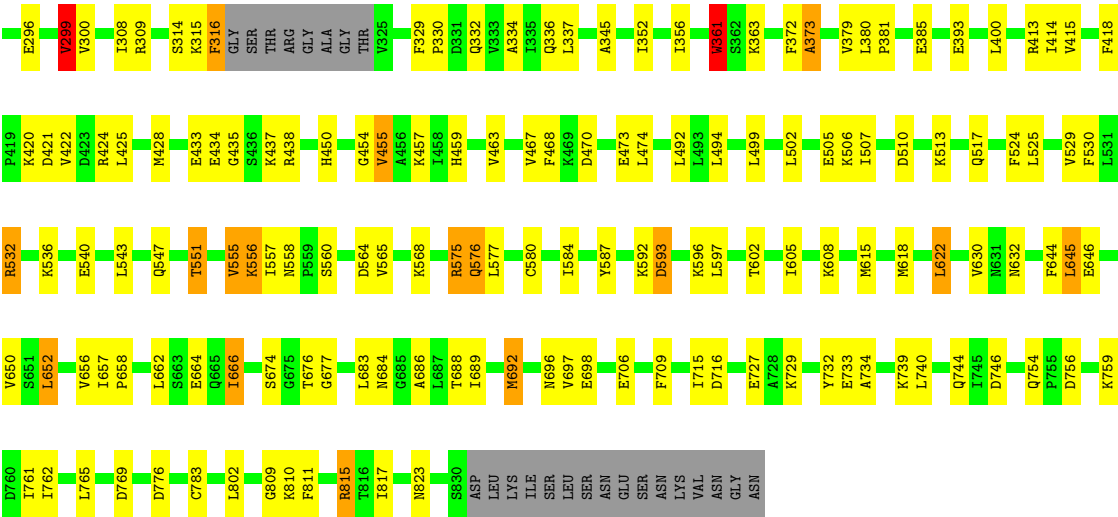
Note EDS was not executed.

- 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	124.71Å 124.71Å 124.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.82 – 2.25	Depositor
% Data completeness (in resolution range)	89.2 (40.82-2.25)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.207 , 0.240	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13620	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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: 700, PLP, NBG, CFF

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	0.56	0/6567	1.01	41/8881 (0.5%)
1	B	0.53	0/6558	1.01	42/8869 (0.5%)
All	All	0.55	0/13125	1.01	83/17750 (0.5%)

There are no bond length outliers.

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	565	VAL	N-CA-C	9.98	122.09	108.11
1	B	565	VAL	N-CA-C	9.45	121.33	108.11
1	B	64	VAL	N-CA-C	8.86	119.45	110.23
1	A	64	VAL	N-CA-C	8.33	118.89	110.23
1	A	91	MET	N-CA-C	8.10	121.22	111.82
1	B	299	VAL	CB-CA-C	-7.95	101.79	111.97
1	A	299	VAL	CB-CA-C	-7.88	101.88	111.97
1	B	455	VAL	N-CA-C	7.76	119.85	111.77
1	B	575	ARG	N-CA-C	7.61	121.89	111.39
1	A	356	ILE	N-CA-C	7.47	118.77	111.67
1	B	129	ALA	N-CA-C	-7.27	95.19	107.99
1	A	455	VAL	N-CA-C	7.26	119.07	112.17
1	A	24	VAL	N-CA-C	7.11	117.25	110.42
1	A	593	ASP	CA-C-N	7.09	127.69	119.47
1	A	593	ASP	C-N-CA	7.09	127.69	119.47
1	A	575	ARG	N-CA-C	7.02	121.08	111.39
1	A	754	GLN	CA-C-N	6.86	127.14	119.32
1	A	754	GLN	C-N-CA	6.86	127.14	119.32
1	B	754	GLN	CA-C-N	6.75	127.02	119.32
1	B	754	GLN	C-N-CA	6.75	127.02	119.32
1	A	656	VAL	N-CA-C	6.60	117.39	110.72
1	B	91	MET	N-CA-C	6.60	120.54	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	GLN	N-CA-C	6.60	119.03	111.11
1	B	356	ILE	N-CA-C	6.57	117.91	111.67
1	B	593	ASP	CA-C-N	6.56	127.08	119.47
1	B	593	ASP	C-N-CA	6.56	127.08	119.47
1	B	656	VAL	N-CA-C	6.46	117.25	110.72
1	B	277	ARG	N-CA-C	6.31	119.09	111.40
1	B	684	ASN	N-CA-C	6.19	119.78	112.72
1	A	277	ARG	N-CA-C	6.17	118.93	111.40
1	A	684	ASN	N-CA-C	6.13	119.71	112.72
1	A	372	PHE	N-CA-C	6.07	120.16	109.96
1	B	216	ILE	N-CA-C	6.00	117.55	108.80
1	B	557	ILE	N-CA-C	5.97	116.71	107.99
1	A	666	ILE	N-CA-C	5.97	121.76	109.34
1	B	373	ALA	N-CA-C	-5.96	100.00	109.23
1	A	216	ILE	N-CA-C	5.89	117.40	108.80
1	A	557	ILE	N-CA-C	5.88	116.57	107.99
1	A	675	GLY	N-CA-C	-5.82	105.44	112.48
1	B	467	VAL	N-CA-C	5.81	116.55	110.62
1	A	676	THR	N-CA-C	-5.80	107.44	114.75
1	B	666	ILE	N-CA-C	5.80	121.41	109.34
1	A	734	ALA	N-CA-C	5.77	119.58	112.54
1	B	734	ALA	N-CA-C	5.73	119.53	112.54
1	A	467	VAL	N-CA-C	5.71	116.44	110.62
1	B	602	THR	N-CA-C	-5.68	98.08	108.02
1	B	105	GLN	N-CA-C	5.67	117.91	111.11
1	A	576	GLN	N-CA-C	-5.66	106.22	113.01
1	B	418	PHE	CA-C-N	5.65	126.02	119.47
1	B	418	PHE	C-N-CA	5.65	126.02	119.47
1	A	418	PHE	CA-C-N	5.59	125.95	119.47
1	A	418	PHE	C-N-CA	5.59	125.95	119.47
1	A	326	PHE	N-CA-C	-5.59	105.67	112.88
1	A	630	VAL	N-CA-C	5.52	115.72	110.42
1	B	507	ILE	N-CA-C	5.51	120.80	109.34
1	B	811	PHE	N-CA-C	5.50	119.09	112.93
1	A	203	TYR	CB-CA-C	-5.48	110.27	116.63
1	B	676	THR	N-CA-C	-5.46	107.87	114.75
1	A	602	THR	N-CA-C	-5.46	98.47	108.02
1	B	182	TRP	N-CA-C	5.43	119.00	112.38
1	B	630	VAL	N-CA-C	5.42	115.62	110.42
1	A	491	TRP	N-CA-C	5.41	119.51	113.02
1	A	182	TRP	N-CA-C	5.40	118.97	112.38
1	B	372	PHE	N-CA-C	5.40	118.91	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	507	ILE	N-CA-C	5.40	120.57	109.34
1	B	361	TRP	N-CA-C	5.38	117.57	111.11
1	B	677	GLY	N-CA-C	-5.38	106.27	112.73
1	A	333	VAL	N-CA-C	5.38	116.41	108.45
1	A	555	VAL	N-CA-C	5.35	120.47	109.34
1	B	555	VAL	N-CA-C	5.34	120.44	109.34
1	B	688	THR	N-CA-C	5.32	117.64	109.07
1	B	696	ASN	N-CA-C	-5.29	105.52	111.28
1	B	650	VAL	N-CA-C	5.28	115.90	110.36
1	B	454	GLY	N-CA-C	-5.27	104.26	112.58
1	B	576	GLN	N-CA-C	-5.25	106.71	113.01
1	B	203	TYR	CB-CA-C	-5.23	110.56	116.63
1	B	809	GLY	N-CA-C	5.22	119.19	112.83
1	A	361	TRP	N-CA-C	5.18	117.33	111.11
1	A	823	ASN	N-CA-C	5.18	119.69	113.17
1	A	129	ALA	N-CA-C	-5.07	98.45	107.98
1	A	373	ALA	N-CA-C	-5.06	100.79	109.24
1	B	823	ASN	N-CA-C	5.05	119.53	113.17
1	A	696	ASN	N-CA-C	-5.03	105.80	111.28

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	6423	0	6417	129	0
1	B	6414	0	6411	123	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	0	0
4	A	30	0	18	0	0
4	B	30	0	18	0	0
5	A	28	0	20	1	0
5	B	28	0	20	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	324	0	0	16	0
6	B	283	0	0	20	0
All	All	13620	0	12948	253	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 10.

All (253) 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:615:MET:HE1	1:A:761:ILE:HG12	1.24	1.17
1:B:615:MET:HE1	1:B:761:ILE:HG12	1.25	1.16
1:B:170:ILE:HG12	1:B:646:GLU:HG2	1.56	0.86
1:A:205:LYS:HG3	6:A:2509:HOH:O	1.76	0.84
1:A:532:ARG:HB2	1:A:532:ARG:HH11	1.44	0.82
1:A:547:GLN:O	1:A:551:THR:HG23	1.82	0.80
1:B:532:ARG:HH11	1:B:532:ARG:HB2	1.46	0.80
1:B:547:GLN:O	1:B:551:THR:HG23	1.84	0.78
1:A:325:VAL:HG23	1:A:326:PHE:H	1.47	0.77
1:A:205:LYS:HB2	6:A:2426:HOH:O	1.88	0.74
1:B:170:ILE:CG1	1:B:646:GLU:HG2	2.20	0.72
1:B:363:LYS:HE2	6:B:2345:HOH:O	1.91	0.71
1:B:455:VAL:H	1:B:459:HIS:HD2	1.39	0.70
1:A:29:LYS:HG2	1:A:33:ARG:NH2	2.06	0.70
1:A:316:PHE:H	1:A:316:PHE:HD2	1.39	0.70
1:A:551:THR:HG22	6:A:2359:HOH:O	1.91	0.70
1:B:29:LYS:HG2	1:B:33:ARG:NH2	2.06	0.70
1:B:363:LYS:HG2	6:B:2345:HOH:O	1.93	0.69
1:B:510:ASP:HB2	6:B:2325:HOH:O	1.91	0.69
1:B:29:LYS:HE2	1:B:33:ARG:HH21	1.59	0.68
1:B:450:HIS:HD2	6:B:2385:HOH:O	1.75	0.68
1:B:224:LEU:HD21	6:B:2088:HOH:O	1.93	0.68
1:B:433:GLU:HG3	1:B:437:LYS:HZ3	1.59	0.67
1:B:615:MET:CE	1:B:761:ILE:HG12	2.14	0.67
1:A:615:MET:CE	1:A:761:ILE:HG12	2.15	0.66
1:A:532:ARG:HB2	1:A:532:ARG:NH1	2.10	0.66
1:A:277:ARG:HD3	6:B:2102:HOH:O	1.96	0.66
1:B:532:ARG:HB2	1:B:532:ARG:NH1	2.10	0.66
1:A:455:VAL:H	1:A:459:HIS:HD2	1.42	0.65
1:A:29:LYS:HE2	1:A:33:ARG:HH21	1.60	0.65
1:B:592:LYS:O	1:B:592:LYS:HD3	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:PHE:HB3	1:A:330:PRO:HD3	1.78	0.64
1:B:532:ARG:HD2	6:B:2339:HOH:O	1.98	0.63
1:B:329:PHE:HB3	1:B:330:PRO:HD3	1.81	0.62
1:B:732:TYR:CE1	1:B:739:LYS:HG3	2.35	0.62
1:A:506:LYS:HD2	1:A:524:PHE:CE2	2.35	0.61
1:A:592:LYS:O	1:A:592:LYS:HD3	2.00	0.61
1:B:308:ILE:HD12	1:B:352:ILE:HG21	1.83	0.61
1:B:66:ARG:HD2	1:B:236:ASN:HA	1.83	0.61
2:B:1861:NBG:H3	6:B:2323:HOH:O	2.01	0.61
1:A:316:PHE:N	1:A:316:PHE:CD2	2.67	0.60
1:B:29:LYS:HE2	1:B:33:ARG:NH2	2.16	0.60
1:A:66:ARG:HD2	1:A:236:ASN:HA	1.84	0.60
1:A:414:ILE:HD13	1:A:428:MET:SD	2.42	0.60
1:A:235:ASN:O	1:A:236:ASN:HB2	2.02	0.59
1:A:420:LYS:N	1:A:420:LYS:HD2	2.18	0.59
1:B:433:GLU:HG3	1:B:437:LYS:NZ	2.17	0.59
1:A:433:GLU:HG3	1:A:437:LYS:NZ	2.18	0.59
1:A:732:TYR:CE1	1:A:739:LYS:HG3	2.37	0.58
1:A:29:LYS:HE2	1:A:33:ARG:NH2	2.18	0.58
1:B:308:ILE:CD1	1:B:352:ILE:HG21	2.34	0.58
1:A:29:LYS:HG2	1:A:33:ARG:HH21	1.69	0.58
1:A:379:VAL:HG12	1:A:379:VAL:O	2.02	0.58
1:B:506:LYS:HD2	1:B:524:PHE:CE2	2.39	0.58
1:B:810:LYS:O	1:B:815:ARG:HD3	2.03	0.58
1:B:421:ASP:CG	1:B:424:ARG:HB2	2.28	0.58
1:A:598:PHE:HE1	6:A:2197:HOH:O	1.86	0.58
1:A:325:VAL:HG23	1:A:326:PHE:N	2.18	0.57
1:A:421:ASP:CG	1:A:424:ARG:HB2	2.29	0.57
1:B:235:ASN:O	1:B:236:ASN:HB2	2.04	0.57
1:B:420:LYS:HD2	1:B:420:LYS:N	2.20	0.57
1:B:29:LYS:HG2	1:B:33:ARG:HH21	1.70	0.57
1:B:316:PHE:H	1:B:316:PHE:HD2	1.52	0.57
1:A:592:LYS:HD3	1:A:592:LYS:C	2.31	0.56
1:B:433:GLU:O	1:B:435:GLY:N	2.39	0.56
1:A:159:ILE:HD11	1:A:299:VAL:HG22	1.87	0.56
1:A:316:PHE:HD2	1:A:316:PHE:N	1.99	0.56
1:A:614:HIS:HE1	5:A:864:CFF:H81	1.69	0.56
1:A:433:GLU:HG2	1:A:437:LYS:HZ1	1.71	0.56
1:B:645:LEU:HD13	1:B:652:LEU:HD13	1.86	0.56
1:A:470:ASP:O	1:A:474:LEU:HD13	2.06	0.56
1:A:305:GLN:HG3	6:A:2535:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:592:LYS:HD3	1:B:592:LYS:C	2.30	0.55
1:B:470:ASP:O	1:B:474:LEU:HD13	2.06	0.55
1:B:170:ILE:HG12	1:B:646:GLU:CG	2.33	0.55
1:A:96:GLN:HE21	1:A:105:GLN:HE22	1.54	0.54
1:B:379:VAL:HG12	1:B:379:VAL:O	2.07	0.54
1:A:433:GLU:CG	1:A:437:LYS:NZ	2.71	0.54
1:B:66:ARG:CD	1:B:236:ASN:HA	2.37	0.54
1:B:433:GLU:CG	1:B:437:LYS:NZ	2.71	0.54
1:A:433:GLU:O	1:A:435:GLY:N	2.40	0.54
1:A:361:TRP:NE1	6:A:2346:HOH:O	2.40	0.54
1:A:645:LEU:HD13	1:A:652:LEU:HD13	1.89	0.54
1:A:450:HIS:HE1	6:A:2180:HOH:O	1.91	0.53
6:A:2530:HOH:O	1:B:277:ARG:HD3	2.07	0.53
1:A:66:ARG:CD	1:A:236:ASN:HA	2.37	0.53
1:A:593:ASP:OD2	1:A:596:LYS:HB2	2.09	0.53
1:A:692:MET:HG3	1:A:697:VAL:HG22	1.90	0.53
1:B:300:VAL:HG13	1:B:345:ALA:HA	1.90	0.52
1:B:692:MET:HG3	1:B:697:VAL:HG22	1.91	0.52
1:B:463:VAL:HG13	1:B:468:PHE:CD1	2.45	0.52
1:A:494:LEU:HD23	1:A:494:LEU:C	2.34	0.52
1:A:810:LYS:O	1:A:815:ARG:HD3	2.10	0.52
1:B:530:PHE:HE2	1:B:802:LEU:HD13	1.75	0.52
1:B:314:SER:O	1:B:315:LYS:C	2.53	0.51
1:B:159:ILE:HD11	1:B:299:VAL:HG22	1.92	0.51
1:B:450:HIS:HE1	6:B:2049:HOH:O	1.93	0.51
1:A:233:TYR:CE2	1:A:512:VAL:HG11	2.45	0.51
1:A:308:ILE:HD12	1:A:352:ILE:HG21	1.92	0.51
1:A:308:ILE:CD1	1:A:352:ILE:HG21	2.40	0.51
1:B:316:PHE:N	1:B:316:PHE:CD2	2.78	0.51
1:A:433:GLU:CG	1:A:437:LYS:HZ1	2.23	0.51
1:B:96:GLN:HE21	1:B:105:GLN:HE22	1.59	0.51
1:A:455:VAL:HG23	1:A:674:SER:HB2	1.93	0.50
1:B:110:GLU:OE2	6:B:2040:HOH:O	2.19	0.50
1:A:160:ARG:HB2	1:A:243:LEU:HB3	1.94	0.50
1:A:292:ARG:O	1:A:296:GLU:HG3	2.11	0.50
1:B:413:ARG:HA	1:B:413:ARG:NE	2.26	0.50
1:B:593:ASP:OD2	1:B:596:LYS:HB2	2.11	0.50
1:B:414:ILE:HD13	1:B:428:MET:SD	2.51	0.50
1:B:729:LYS:HG3	6:B:2463:HOH:O	2.11	0.50
1:B:292:ARG:O	1:B:296:GLU:HG3	2.11	0.50
1:B:314:SER:C	1:B:316:PHE:N	2.67	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:580:CYS:SG	1:B:622:LEU:HD13	2.52	0.50
1:A:314:SER:O	1:A:315:LYS:C	2.55	0.49
1:A:424:ARG:HH12	1:A:474:LEU:HD11	1.77	0.49
1:B:494:LEU:C	1:B:494:LEU:HD23	2.37	0.49
1:B:181:ASP:OD2	1:B:184:ARG:NE	2.44	0.49
1:B:424:ARG:HH12	1:B:474:LEU:HD11	1.76	0.49
1:B:250:ASN:O	6:B:2168:HOH:O	2.20	0.49
1:A:575:ARG:HD3	1:A:666:ILE:O	2.12	0.49
1:A:433:GLU:HG3	1:A:437:LYS:HZ2	1.77	0.49
1:A:413:ARG:HA	1:A:413:ARG:NE	2.26	0.49
1:B:575:ARG:HD3	1:B:666:ILE:O	2.12	0.49
1:B:455:VAL:HG23	1:B:674:SER:HB2	1.95	0.48
1:B:536:LYS:O	1:B:540:GLU:HG3	2.13	0.48
1:A:181:ASP:OD2	1:A:184:ARG:NE	2.46	0.48
1:A:580:CYS:SG	1:A:622:LEU:HD13	2.53	0.48
1:A:463:VAL:HG13	1:A:468:PHE:CD1	2.48	0.48
1:B:746:ASP:OD1	1:B:762:ILE:HG13	2.13	0.48
1:B:160:ARG:HB2	1:B:243:LEU:HB3	1.94	0.48
1:A:536:LYS:O	1:A:540:GLU:HG3	2.13	0.48
1:A:558:ASN:OD1	1:A:560:SER:HB3	2.13	0.48
1:B:81:ARG:NH1	1:B:155:TYR:OH	2.47	0.48
1:A:81:ARG:NH1	1:A:155:TYR:OH	2.47	0.47
1:B:336:GLN:OE1	1:B:373:ALA:HB3	2.14	0.47
1:B:517:GLN:HG3	6:B:2325:HOH:O	2.13	0.47
1:A:136:LEU:HD23	1:A:136:LEU:C	2.40	0.47
1:B:615:MET:HE3	1:B:618:MET:HB2	1.97	0.47
1:A:689:ILE:HG23	1:A:689:ILE:O	2.14	0.47
1:B:224:LEU:HD12	1:B:225:PRO:HD2	1.96	0.47
1:B:433:GLU:CG	1:B:437:LYS:HZ3	2.23	0.47
1:B:686:ALA:HB2	6:B:2571:HOH:O	2.15	0.47
1:B:361:TRP:HZ2	6:B:2488:HOH:O	1.97	0.47
1:A:210:ASN:ND2	6:A:2384:HOH:O	2.48	0.47
1:B:463:VAL:HG13	1:B:468:PHE:HD1	1.79	0.47
1:A:305:GLN:NE2	6:A:2535:HOH:O	2.49	0.46
1:B:575:ARG:HH22	1:B:776:ASP:HB2	1.81	0.46
1:B:45:VAL:HG12	1:B:45:VAL:O	2.15	0.46
1:A:438:ARG:HE	1:A:438:ARG:HB3	1.54	0.46
1:A:575:ARG:HH22	1:A:776:ASP:HB2	1.81	0.46
1:B:740:LEU:O	1:B:744:GLN:HG3	2.14	0.46
1:A:746:ASP:OD1	1:A:762:ILE:HG13	2.15	0.46
1:B:225:PRO:HB3	1:B:244:TRP:CZ3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:ARG:HA	1:A:171:ARG:HD3	1.71	0.46
1:A:224:LEU:HD12	1:A:225:PRO:HD2	1.97	0.46
1:A:615:MET:HE3	1:A:618:MET:HB2	1.97	0.45
1:A:109:ASP:OD1	1:A:119:ILE:HD13	2.16	0.45
1:A:314:SER:C	1:A:316:PHE:N	2.72	0.45
1:B:393:GLU:HB2	1:B:400:LEU:HD22	1.99	0.45
1:A:740:LEU:O	1:A:744:GLN:HG3	2.17	0.45
1:B:361:TRP:NE1	6:B:2488:HOH:O	2.48	0.45
1:B:575:ARG:NH2	1:B:776:ASP:HB2	2.32	0.45
1:B:143:PHE:CG	1:B:817:ILE:HD11	2.51	0.45
1:A:393:GLU:HB2	1:A:400:LEU:HD22	1.98	0.45
1:B:109:ASP:OD1	1:B:119:ILE:HD13	2.16	0.44
1:B:393:GLU:HB2	1:B:400:LEU:CD2	2.47	0.44
1:A:828:GLU:HA	1:A:829:PRO:HD3	1.89	0.44
1:A:197:MET:HE2	1:A:224:LEU:HD13	1.99	0.44
1:B:171:ARG:HA	1:B:171:ARG:HD3	1.79	0.44
1:A:457:LYS:HE2	1:A:698:GLU:HG2	2.00	0.44
1:B:197:MET:HE2	1:B:224:LEU:HD13	2.00	0.44
1:B:204:GLY:C	1:B:205:LYS:HE2	2.43	0.44
1:A:543:LEU:HD12	1:A:543:LEU:HA	1.84	0.44
1:A:732:TYR:CZ	1:A:739:LYS:HG3	2.52	0.44
1:A:336:GLN:OE1	1:A:373:ALA:HB3	2.18	0.44
1:A:405:GLU:HG2	6:A:2346:HOH:O	2.18	0.44
1:A:205:LYS:CG	6:A:2509:HOH:O	2.48	0.43
1:A:233:TYR:CZ	1:A:512:VAL:HG11	2.53	0.43
1:A:204:GLY:C	1:A:205:LYS:HE2	2.43	0.43
1:A:463:VAL:HG13	1:A:468:PHE:HD1	1.82	0.43
1:A:735:LEU:HA	1:A:736:PRO:HD2	1.90	0.43
1:B:78:CYS:SG	1:B:332:GLN:NE2	2.91	0.43
1:A:120:GLU:HB2	6:A:2358:HOH:O	2.17	0.43
1:A:530:PHE:HE2	1:A:802:LEU:HD13	1.84	0.43
1:B:529:VAL:HA	1:B:532:ARG:HD3	1.99	0.43
1:B:657:ILE:HB	1:B:658:PRO:HD3	2.00	0.43
1:B:756:ASP:HA	1:B:759:LYS:HD3	2.00	0.43
1:A:727:GLU:OE1	1:A:729:LYS:HE2	2.19	0.43
1:B:136:LEU:C	1:B:136:LEU:HD23	2.43	0.43
1:B:150:LEU:HD12	1:B:150:LEU:HA	1.80	0.43
1:A:45:VAL:O	1:A:45:VAL:HG12	2.18	0.43
1:A:721:LEU:HD23	1:A:772:LYS:HD3	2.00	0.43
1:B:732:TYR:CZ	1:B:739:LYS:HG3	2.53	0.43
1:B:632:ASN:C	6:B:2423:HOH:O	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:ARG:HE	1:B:438:ARG:HB3	1.52	0.42
1:B:605:ILE:O	1:B:644:PHE:HA	2.19	0.42
1:B:689:ILE:O	1:B:689:ILE:HG23	2.19	0.42
1:B:715:ILE:HG23	1:B:716:ASP:N	2.34	0.42
1:A:246:ALA:O	1:A:247:ARG:HD2	2.19	0.42
1:A:715:ILE:HG23	1:A:716:ASP:N	2.34	0.42
1:A:828:GLU:HG3	1:A:829:PRO:HD2	2.01	0.42
1:A:300:VAL:HG13	1:A:345:ALA:HA	2.00	0.42
1:A:657:ILE:HB	1:A:658:PRO:HD3	2.02	0.42
1:A:768:HIS:HB2	6:A:2411:HOH:O	2.18	0.42
1:B:584:ILE:O	1:B:587:TYR:HB3	2.19	0.42
1:B:769:ASP:OD1	1:B:769:ASP:C	2.62	0.42
1:B:608:LYS:NZ	6:B:2606:HOH:O	2.51	0.42
1:B:216:ILE:HA	6:B:2372:HOH:O	2.19	0.42
1:B:455:VAL:H	1:B:459:HIS:CD2	2.26	0.42
1:A:575:ARG:NH2	1:A:776:ASP:HB2	2.35	0.42
1:B:433:GLU:HG2	1:B:437:LYS:HZ2	1.85	0.42
1:B:622:LEU:HD22	1:B:622:LEU:O	2.20	0.42
1:B:709:PHE:HB3	1:B:783:CYS:SG	2.59	0.42
1:A:325:VAL:CG2	1:A:326:PHE:H	2.26	0.42
1:B:380:LEU:HA	1:B:381:PRO:HD3	1.91	0.42
1:B:424:ARG:HH12	1:B:474:LEU:CD1	2.32	0.42
1:A:171:ARG:NH1	6:A:2240:HOH:O	2.52	0.42
1:A:415:VAL:HG22	1:A:425:LEU:HD11	2.01	0.42
1:B:525:LEU:HD23	1:B:802:LEU:HD23	2.01	0.42
1:A:44:ASN:HD22	1:A:45:VAL:HG23	1.84	0.42
1:A:393:GLU:HB2	1:A:400:LEU:CD2	2.49	0.42
1:A:786:LYS:HE2	1:A:786:LYS:HB3	1.85	0.42
1:B:555:VAL:HG12	1:B:556:LYS:N	2.34	0.42
1:A:225:PRO:HB3	1:A:244:TRP:CZ3	2.55	0.42
1:B:558:ASN:OD1	1:B:560:SER:HB3	2.20	0.42
1:B:246:ALA:O	1:B:247:ARG:HD2	2.19	0.41
1:B:457:LYS:HE2	1:B:698:GLU:HG2	2.02	0.41
1:B:564:ASP:OD1	1:B:664:GLU:OE2	2.38	0.41
1:B:415:VAL:HG22	1:B:425:LEU:HD11	2.02	0.41
1:A:341:HIS:HB2	1:A:342:PRO:HD3	2.02	0.41
1:A:80:LYS:HE2	1:A:334:ALA:HB2	2.02	0.41
1:A:143:PHE:O	1:A:147:MET:HG3	2.21	0.41
1:A:361:TRP:HZ2	6:A:2346:HOH:O	2.00	0.41
1:B:286:PHE:CD1	1:B:385:GLU:HG2	2.55	0.41
1:A:291:LEU:O	1:A:295:GLN:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:LEU:HD23	1:A:802:LEU:HD23	2.01	0.41
1:A:555:VAL:HG12	1:A:556:LYS:N	2.34	0.41
1:B:233:TYR:HD2	1:B:513:LYS:HE3	1.86	0.41
1:B:727:GLU:OE1	1:B:729:LYS:HE2	2.20	0.41
1:A:36:HIS:O	1:A:40:VAL:HA	2.21	0.41
1:A:181:ASP:OD2	1:A:184:ARG:CZ	2.69	0.41
1:B:96:GLN:HB2	6:B:2184:HOH:O	2.20	0.41
1:A:424:ARG:NH1	1:A:474:LEU:HD11	2.36	0.41
1:A:584:ILE:O	1:A:587:TYR:HB3	2.21	0.41
1:A:211:THR:O	1:A:358:LYS:NZ	2.54	0.40
1:A:756:ASP:HA	1:A:759:LYS:HD3	2.02	0.40
1:A:417:LEU:C	1:A:419:PRO:HD3	2.47	0.40
1:B:80:LYS:HE2	1:B:334:ALA:HB2	2.04	0.40
1:A:424:ARG:HH12	1:A:474:LEU:CD1	2.34	0.40
1:A:529:VAL:HA	1:A:532:ARG:HD3	2.02	0.40
1:A:605:ILE:O	1:A:644:PHE:HA	2.21	0.40
1:A:709:PHE:HB3	1:A:783:CYS:SG	2.61	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	785/847 (93%)	754 (96%)	30 (4%)	1 (0%)	48	56
1	B	784/847 (93%)	749 (96%)	34 (4%)	1 (0%)	48	56
All	All	1569/1694 (93%)	1503 (96%)	64 (4%)	2 (0%)	48	56

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	434	GLU

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Mol	Chain	Res	Type
1	B	434	GLU

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	693/740 (94%)	656 (95%)	37 (5%)	20	22
1	B	692/740 (94%)	654 (94%)	38 (6%)	19	20
All	All	1385/1480 (94%)	1310 (95%)	75 (5%)	20	21

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	78	CYS
1	A	95	LEU
1	A	102	LEU
1	A	104	LEU
1	A	150	LEU
1	A	205	LYS
1	A	211	THR
1	A	243	LEU
1	A	278	VAL
1	A	299	VAL
1	A	316	PHE
1	A	337	LEU
1	A	361	TRP
1	A	422	VAL
1	A	473	GLU
1	A	492	LEU
1	A	499	LEU
1	A	502	LEU
1	A	505	GLU
1	A	532	ARG
1	A	551	THR

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Mol	Chain	Res	Type
1	A	556	LYS
1	A	568	LYS
1	A	576	GLN
1	A	577	LEU
1	A	597	LEU
1	A	622	LEU
1	A	645	LEU
1	A	652	LEU
1	A	662	LEU
1	A	683	LEU
1	A	692	MET
1	A	706	GLU
1	A	733	GLU
1	A	765	LEU
1	A	815	ARG
1	B	44	ASN
1	B	95	LEU
1	B	102	LEU
1	B	104	LEU
1	B	150	LEU
1	B	205	LYS
1	B	211	THR
1	B	243	LEU
1	B	278	VAL
1	B	299	VAL
1	B	309	ARG
1	B	316	PHE
1	B	337	LEU
1	B	361	TRP
1	B	422	VAL
1	B	473	GLU
1	B	492	LEU
1	B	499	LEU
1	B	502	LEU
1	B	505	GLU
1	B	532	ARG
1	B	543	LEU
1	B	551	THR
1	B	556	LYS
1	B	568	LYS
1	B	576	GLN
1	B	577	LEU

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Mol	Chain	Res	Type
1	B	597	LEU
1	B	622	LEU
1	B	645	LEU
1	B	652	LEU
1	B	662	LEU
1	B	683	LEU
1	B	692	MET
1	B	706	GLU
1	B	733	GLU
1	B	765	LEU
1	B	815	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	44	ASN
1	A	62	HIS
1	A	96	GLN
1	A	210	ASN
1	A	219	GLN
1	A	250	ASN
1	A	332	GLN
1	A	450	HIS
1	A	459	HIS
1	A	804	ASN
1	B	32	ASN
1	B	44	ASN
1	B	62	HIS
1	B	71	GLN
1	B	105	GLN
1	B	219	GLN
1	B	250	ASN
1	B	332	GLN
1	B	450	HIS
1	B	459	HIS
1	B	632	ASN
1	B	822	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

10 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$
4	700	A	862	-	31,33,33	1.99	8 (25%)	44,47,47	1.90	10 (22%)
2	NBG	B	1861	-	15,15,15	2.03	3 (20%)	21,21,21	1.20	2 (9%)
5	CFF	B	1863	-	15,15,15	2.67	5 (33%)	23,23,23	2.01	5 (21%)
3	PLP	A	860	1	15,15,16	1.97	4 (26%)	21,22,23	1.45	4 (19%)
3	PLP	B	1860	1	15,15,16	2.56	4 (26%)	21,22,23	1.26	1 (4%)
2	NBG	A	861	-	15,15,15	1.86	3 (20%)	21,21,21	1.06	1 (4%)
5	CFF	B	1864	-	15,15,15	2.81	7 (46%)	23,23,23	2.11	6 (26%)
4	700	B	1862	-	31,33,33	2.05	15 (48%)	44,47,47	1.89	10 (22%)
5	CFF	A	863	-	15,15,15	2.56	7 (46%)	23,23,23	2.07	8 (34%)
5	CFF	A	864	-	15,15,15	2.72	6 (40%)	23,23,23	2.06	6 (26%)

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
4	700	A	862	-	-	0/22/32/32	0/4/4/4
2	NBG	B	1861	-	-	0/6/26/26	0/1/1/1
5	CFF	B	1863	-	-	-	0/2/2/2
3	PLP	A	860	1	-	2/6/6/8	0/1/1/1
3	PLP	B	1860	1	-	1/6/6/8	0/1/1/1
2	NBG	A	861	-	-	0/6/26/26	0/1/1/1
5	CFF	B	1864	-	-	-	0/2/2/2
4	700	B	1862	-	-	0/22/32/32	0/4/4/4
5	CFF	A	863	-	-	-	0/2/2/2
5	CFF	A	864	-	-	-	0/2/2/2

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1863	CFF	C2-N1	7.62	1.54	1.39
5	B	1864	CFF	C2-N1	7.29	1.53	1.39
5	A	863	CFF	C2-N1	7.00	1.52	1.39
3	B	1860	PLP	C4A-C4	-6.88	1.37	1.51
5	A	864	CFF	C2-N1	6.69	1.52	1.39
4	A	862	700	C8-N2	-5.47	1.30	1.38
5	B	1864	CFF	C4-N3	5.47	1.47	1.38
5	A	864	CFF	C4-N3	4.85	1.46	1.38
2	B	1861	NBG	C2-C1	4.67	1.57	1.53
4	A	862	700	C5-C4	4.65	1.45	1.38
2	B	1861	NBG	C1-N1	4.58	1.49	1.43
3	A	860	PLP	C4A-C4	-4.50	1.42	1.51
4	B	1862	700	C8-N2	-4.39	1.32	1.38
3	B	1860	PLP	C5A-C5	4.19	1.61	1.50
3	B	1860	PLP	C3-C2	-4.10	1.36	1.41
2	A	861	NBG	C1-N1	3.96	1.48	1.43
2	A	861	NBG	C2-C1	3.69	1.56	1.53
5	B	1863	CFF	C4-N3	3.50	1.43	1.38
5	A	864	CFF	C2-N3	-3.49	1.32	1.39
5	A	864	CFF	O13-C6	3.29	1.29	1.23
5	B	1863	CFF	C2-N3	-3.23	1.32	1.39
5	A	863	CFF	C2-N3	-3.15	1.32	1.39
4	B	1862	700	C12-C11	3.15	1.45	1.38
5	B	1863	CFF	O13-C6	3.13	1.29	1.23
5	A	863	CFF	O13-C6	3.10	1.29	1.23
4	B	1862	700	C3-C2	3.09	1.43	1.38
4	B	1862	700	C3-C4	3.08	1.43	1.38
2	A	861	NBG	C3-C2	3.01	1.60	1.52
5	A	863	CFF	C4-N3	2.93	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1862	700	C5-C4	2.93	1.43	1.38
3	A	860	PLP	C5A-C5	2.91	1.58	1.50
4	B	1862	700	C10-C11	2.84	1.58	1.51
5	B	1864	CFF	C2-N3	-2.81	1.33	1.39
5	B	1864	CFF	O13-C6	2.81	1.28	1.23
3	A	860	PLP	C2-N1	2.76	1.38	1.33
3	B	1860	PLP	C2-N1	2.68	1.38	1.33
4	B	1862	700	C6-C7	2.67	1.52	1.44
5	A	863	CFF	C4-N9	-2.64	1.30	1.36
4	B	1862	700	C13-C12	2.61	1.43	1.38
4	A	862	700	C3-C2	2.58	1.43	1.38
4	A	862	700	C6-C7	2.56	1.51	1.44
5	B	1864	CFF	C12-N3	2.51	1.51	1.47
4	A	862	700	C3-C4	2.49	1.42	1.38
4	B	1862	700	C16-C11	2.49	1.43	1.38
2	B	1861	NBG	C3-C2	2.47	1.58	1.52
4	B	1862	700	C22-N3	-2.42	1.45	1.47
5	A	863	CFF	C12-N3	2.33	1.51	1.47
4	B	1862	700	C2-C1	2.31	1.43	1.39
4	A	862	700	C22-N3	-2.27	1.45	1.47
5	B	1864	CFF	C5-N7	2.26	1.42	1.38
4	B	1862	700	C10-C17	2.21	1.59	1.54
3	A	860	PLP	P-O2P	-2.21	1.46	1.54
4	A	862	700	O4-C21	-2.20	1.23	1.30
5	A	864	CFF	C12-N3	2.16	1.50	1.47
5	B	1863	CFF	C4-N9	-2.15	1.31	1.36
4	A	862	700	C4-CL1	-2.15	1.69	1.74
4	B	1862	700	O4-C21	-2.11	1.23	1.30
5	A	863	CFF	O11-C2	-2.08	1.18	1.22
4	B	1862	700	C14-C13	2.06	1.42	1.38
5	B	1864	CFF	C10-N1	2.06	1.50	1.47
4	B	1862	700	C15-C14	2.03	1.42	1.38
5	A	864	CFF	C5-N7	2.02	1.42	1.38

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1864	CFF	O11-C2-N3	6.28	130.02	121.33
5	A	863	CFF	O11-C2-N3	6.15	129.84	121.33
5	A	864	CFF	O11-C2-N3	6.12	129.80	121.33
5	B	1863	CFF	O11-C2-N3	5.99	129.62	121.33
4	A	862	700	C1-C6-C7	-5.98	101.90	106.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1862	700	C1-C6-C7	-5.20	102.54	106.80
4	B	1862	700	C5-C6-C1	4.85	122.13	119.13
4	A	862	700	C8-C9-N1	4.65	123.07	116.86
4	B	1862	700	C8-C9-N1	4.52	122.89	116.86
2	B	1861	NBG	C5-O5-C1	3.91	117.90	112.47
4	B	1862	700	O1-C9-C8	-3.90	116.07	121.09
4	A	862	700	C5-C6-C1	3.82	121.49	119.13
5	B	1864	CFF	N3-C2-N1	-3.82	112.36	117.14
5	B	1864	CFF	C2-N3-C4	3.77	124.42	119.58
5	A	864	CFF	C2-N3-C4	3.73	124.38	119.58
5	B	1863	CFF	C2-N3-C4	3.72	124.36	119.58
5	A	863	CFF	C2-N3-C4	3.66	124.28	119.58
5	B	1863	CFF	N3-C2-N1	-3.63	112.59	117.14
4	A	862	700	O3-C21-C20	-3.48	113.62	122.86
4	A	862	700	O1-C9-C8	-3.47	116.61	121.09
5	A	864	CFF	N3-C2-N1	-3.44	112.84	117.14
5	A	863	CFF	N3-C2-N1	-3.43	112.84	117.14
2	A	861	NBG	C5-O5-C1	3.28	117.03	112.47
4	B	1862	700	O4-C21-O3	3.10	131.11	124.08
4	A	862	700	C1-N2-C8	3.02	112.25	109.01
4	A	862	700	O4-C21-O3	2.95	130.77	124.08
4	B	1862	700	C1-N2-C8	2.92	112.15	109.01
5	A	863	CFF	O11-C2-N1	-2.90	117.32	121.33
4	B	1862	700	C10-C17-C18	-2.89	103.88	109.94
5	A	864	CFF	O11-C2-N1	-2.87	117.36	121.33
4	B	1862	700	C19-C20-C21	2.82	123.06	116.40
3	A	860	PLP	O3P-P-O4P	-2.73	99.55	106.67
4	B	1862	700	O3-C21-C20	-2.69	115.72	122.86
5	B	1864	CFF	O11-C2-N1	-2.68	117.62	121.33
3	A	860	PLP	O3P-P-O2P	2.59	117.53	107.80
5	B	1863	CFF	O11-C2-N1	-2.57	117.79	121.33
5	B	1864	CFF	C6-C5-C4	-2.50	119.76	122.92
4	A	862	700	C6-C5-C4	-2.44	117.47	120.40
5	A	864	CFF	C6-C5-C4	-2.42	119.88	122.92
4	A	862	700	C19-C20-C21	2.41	122.09	116.40
3	A	860	PLP	O4P-C5A-C5	-2.36	104.94	109.36
5	B	1864	CFF	C5-C6-N1	2.34	116.34	112.06
2	B	1861	NBG	C3-C2-C1	2.29	113.22	109.86
5	A	863	CFF	C10-N1-C6	2.24	121.12	117.64
3	A	860	PLP	C6-C5-C4	2.19	119.89	118.10
4	A	862	700	C10-C17-C18	-2.19	105.34	109.94
5	A	863	CFF	C6-C5-C4	-2.19	120.16	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	863	CFF	C10-N1-C2	-2.14	113.61	117.33
5	A	863	CFF	C12-N3-C4	-2.08	117.69	120.75
5	B	1863	CFF	C6-C5-C4	-2.07	120.31	122.92
3	B	1860	PLP	C5-C6-N1	-2.06	120.47	123.83
5	A	864	CFF	C5-C6-N1	2.05	115.81	112.06
4	B	1862	700	C6-C5-C4	-2.03	117.96	120.40

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	860	PLP	C4-C5-C5A-O4P
3	A	860	PLP	C6-C5-C5A-O4P
3	B	1860	PLP	C4-C5-C5A-O4P

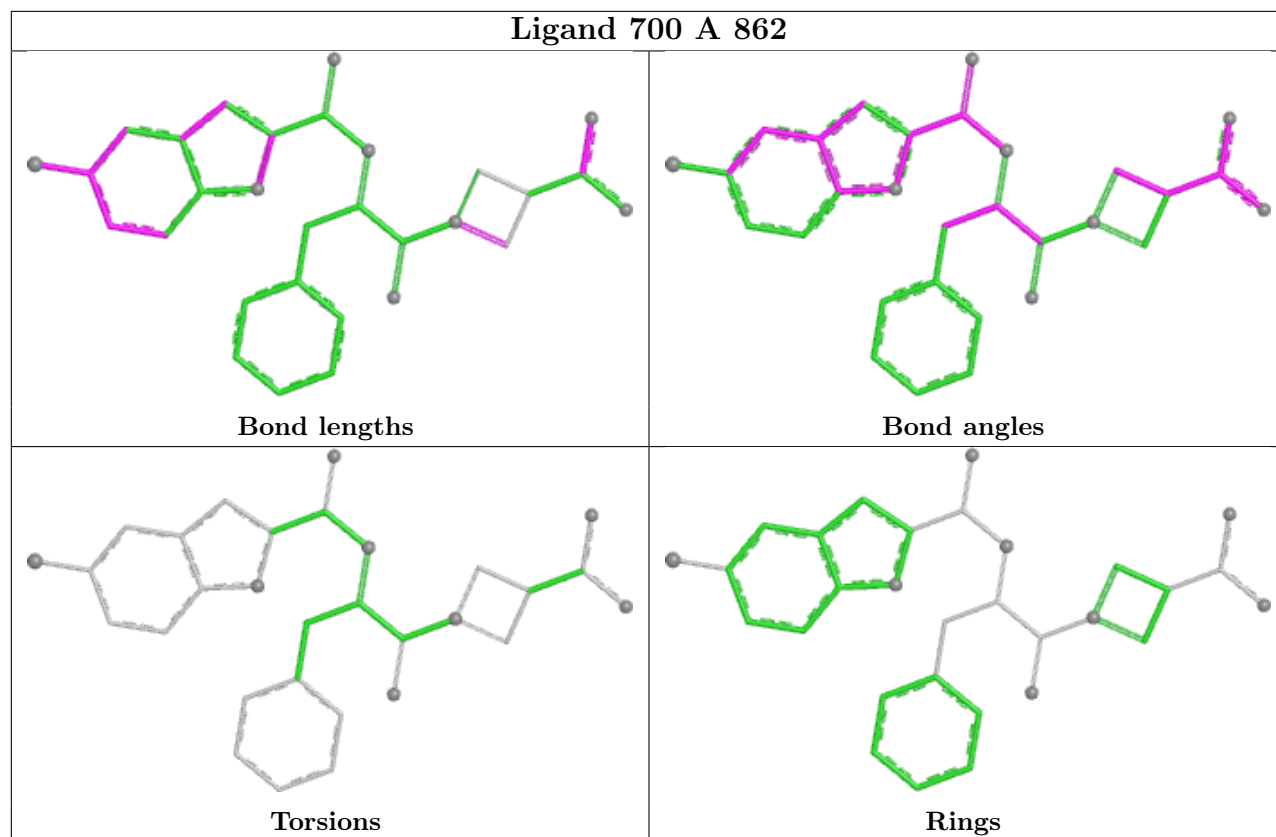
There are no ring outliers.

2 monomers are involved in 2 short contacts:

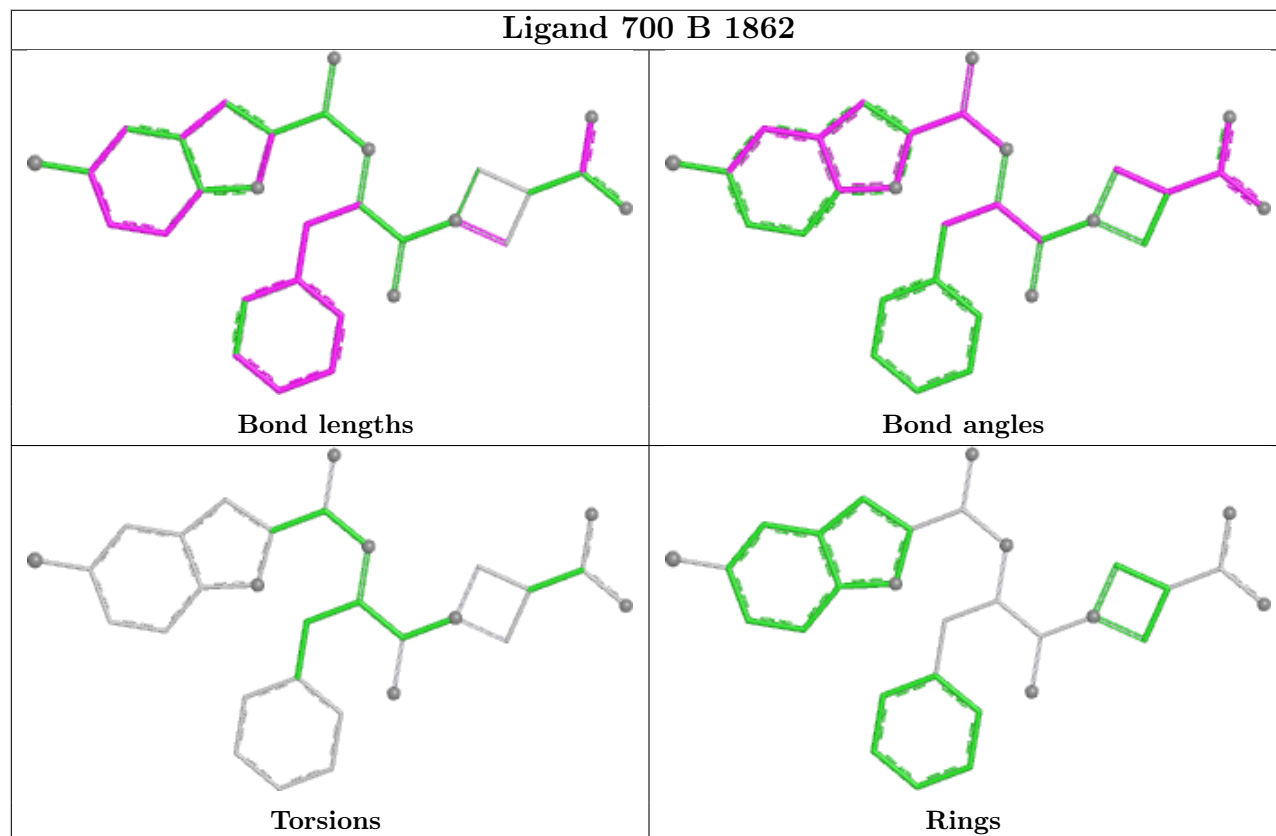
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1861	NBG	1	0
5	A	864	CFF	1	0

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.

Ligand 700 A 862



Ligand 700 B 1862



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.