



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:38 PM UTC

PDB ID : 1K08 / pdb_00001k08
Title : Crystallographic Binding Study of 10 mM N-benzoyl-N'-beta-D-glucopyranosyl urea to glycogen phosphorylase b
Authors : Oikonomakos, N.G.; Kosmopoulou, M.; Zographos, S.E.; Leonidas, D.D.; Chrysina, E.D.; Somsak, L.; Nagy, V.; Praly, J.P.; Docsa, T.; Toth, B.; Gergely, P.
Deposited on : 2001-09-18
Resolution : 2.26 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

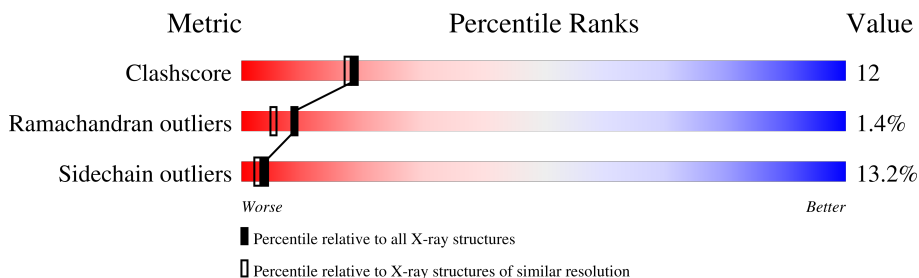
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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	842	 67% 23% 5% . .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6953 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.

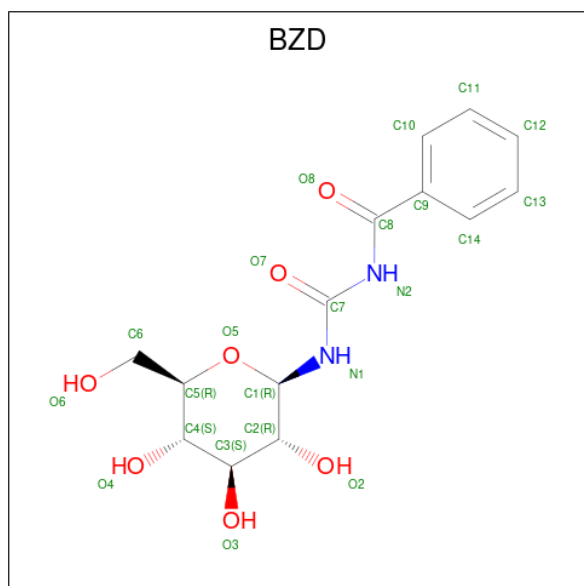
- Molecule 1 is a protein called Glycogen Phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	817	6643	4237	1169	1208	29	0	0	0

There is a discrepancy between the modelled and reference sequences:

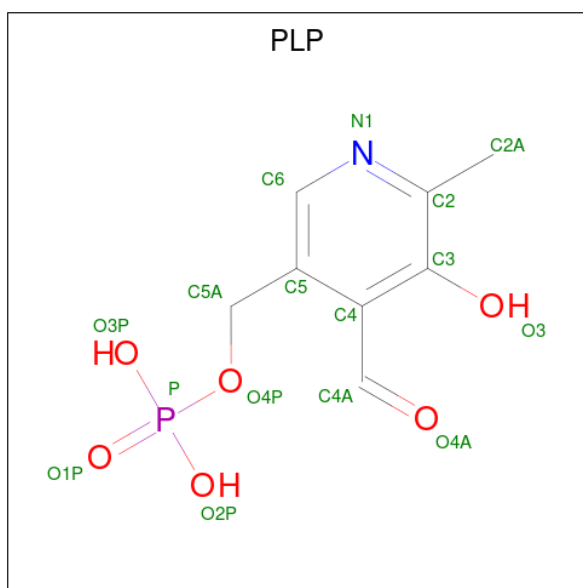
Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	SEE REMARK 999	UNP P00489

- Molecule 2 is N-[(phenylcarbonyl)carbamoyl]-beta-D-glucopyranosylamine (CCD ID: BZD) (formula: C₁₄H₁₈N₂O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	23	14	2	7	0	0
2	A	1	23	14	2	7	0	0

- 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		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	249	Total	O	0	0
			249	249		

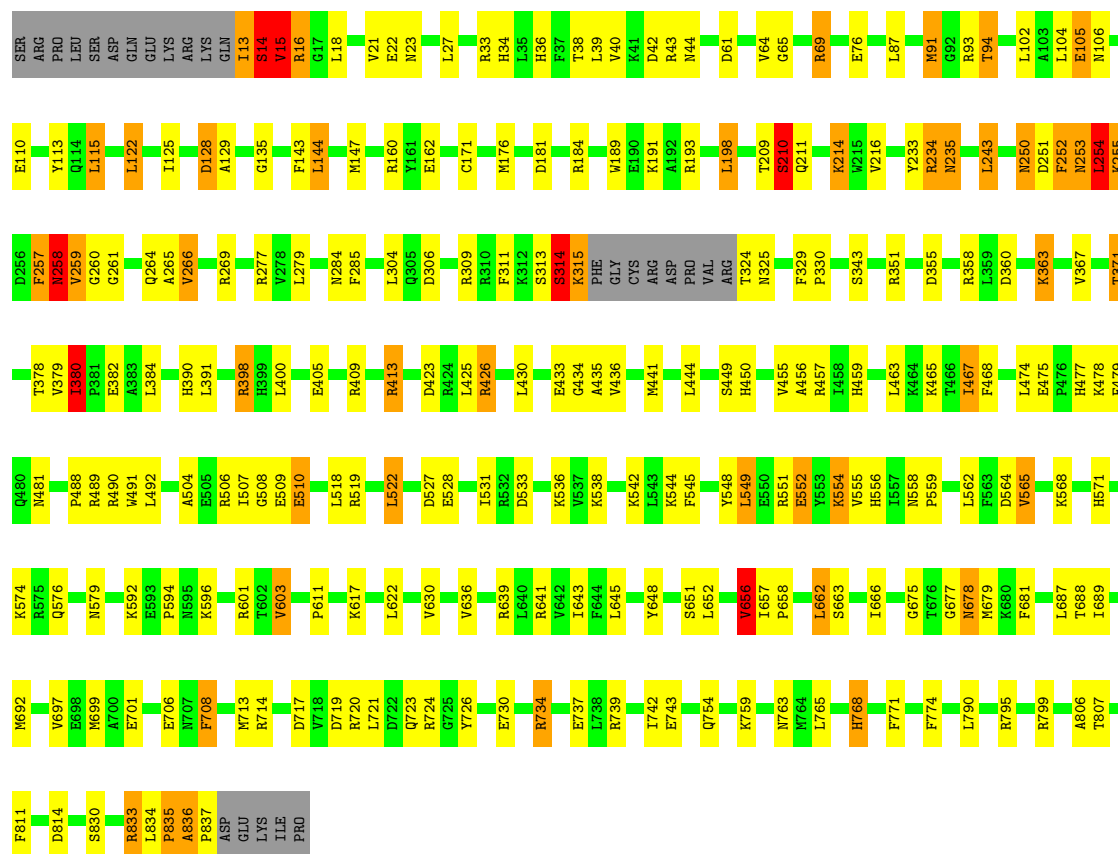
3 Residue-property plots

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

Chain A: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	128.52Å 128.52Å 116.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.75 – 2.26	Depositor
% Data completeness (in resolution range)	95.8 (28.75-2.26)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	9.60	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.180 , 0.212	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6953	wwPDB-VP
Average B, all atoms (Å ²)	33.0	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: BZD, PLP

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	0.47	2/6793 (0.0%)	0.96	31/9194 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	16	ARG	CA-CB	-7.49	1.44	1.53
1	A	16	ARG	CA-C	6.43	1.63	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	16	ARG	N-CA-C	-10.34	99.14	113.20
1	A	91	MET	N-CA-C	8.28	120.38	111.36
1	A	380	ILE	CA-C-N	7.38	127.24	119.05
1	A	380	ILE	C-N-CA	7.38	127.24	119.05
1	A	565	VAL	N-CA-C	7.07	118.99	108.46
1	A	253	ASN	N-CA-C	-7.02	103.66	113.20
1	A	576	GLN	N-CA-C	-6.67	104.25	112.38
1	A	135	GLY	N-CA-C	6.60	120.16	112.50
1	A	16	ARG	CA-C-N	-6.35	111.45	121.87
1	A	16	ARG	C-N-CA	-6.35	111.45	121.87
1	A	714	ARG	N-CA-C	-6.16	101.34	110.46
1	A	277	ARG	N-CA-C	6.14	117.77	111.14
1	A	284	ASN	N-CA-C	6.03	120.70	112.68
1	A	656	VAL	N-CA-C	5.94	116.12	110.53
1	A	675	GLY	N-CA-C	-5.82	105.44	112.48
1	A	630	VAL	N-CA-C	5.72	115.91	110.42
1	A	115	LEU	N-CA-C	-5.66	106.35	113.20
1	A	216	VAL	N-CA-C	5.59	116.89	108.96
1	A	677	GLY	N-CA-C	-5.56	106.06	112.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	771	PHE	N-CA-C	5.55	119.36	112.59
1	A	656	VAL	CB-CA-C	-5.45	104.88	112.02
1	A	666	ILE	N-CA-C	5.37	120.51	109.34
1	A	754	GLN	CA-C-N	5.28	125.60	119.47
1	A	754	GLN	C-N-CA	5.28	125.60	119.47
1	A	479	PHE	N-CA-C	5.27	118.14	109.76
1	A	491	TRP	N-CA-C	5.23	119.37	113.15
1	A	811	PHE	N-CA-C	5.23	118.79	112.93
1	A	105	GLU	N-CA-C	5.19	117.34	111.11
1	A	507	ILE	N-CA-C	5.15	117.85	112.90
1	A	688	THR	N-CA-C	5.14	117.35	109.07
1	A	430	LEU	N-CA-C	-5.02	106.66	112.89

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6643	0	6590	158	0
2	A	46	0	36	2	0
3	A	15	0	7	0	0
4	A	249	0	0	13	0
All	All	6953	0	6633	158	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 (158) 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:15:VAL:HG23	4:A:1247:HOH:O	1.13	1.28
1:A:519:ARG:HH22	1:A:807:THR:HG22	1.27	0.97
1:A:16:ARG:HD3	1:A:105:GLU:HG2	1.46	0.97
1:A:254:LEU:HD21	1:A:266:VAL:HG12	1.46	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:ASP:CG	1:A:252:PHE:H	1.73	0.94
1:A:678:ASN:HD22	1:A:679:MET:H	1.20	0.89
1:A:15:VAL:O	1:A:15:VAL:HG12	1.71	0.89
1:A:15:VAL:HG11	1:A:509:GLU:CD	2.06	0.81
1:A:519:ARG:NH2	1:A:807:THR:HG22	1.96	0.80
1:A:233:TYR:HB2	1:A:489:ARG:HD3	1.63	0.80
1:A:252:PHE:C	1:A:254:LEU:H	1.92	0.78
1:A:795:ARG:O	1:A:799:ARG:HG3	1.84	0.77
1:A:739:ARG:O	1:A:743:GLU:HG3	1.86	0.76
1:A:160:ARG:HB2	1:A:243:LEU:HB3	1.68	0.75
1:A:254:LEU:CD2	1:A:266:VAL:HG12	2.14	0.75
1:A:235:ASN:H	1:A:235:ASN:HD22	1.34	0.74
1:A:15:VAL:O	1:A:15:VAL:CG1	2.35	0.74
1:A:250:ASN:HA	1:A:269:ARG:HH21	1.54	0.72
1:A:678:ASN:HD22	1:A:679:MET:N	1.88	0.70
1:A:15:VAL:CG2	4:A:1247:HOH:O	1.91	0.70
1:A:65:GLY:O	1:A:69:ARG:HG2	1.93	0.68
1:A:13:ILE:O	1:A:14:SER:HB2	1.93	0.68
1:A:455:VAL:H	1:A:459:HIS:HD2	1.39	0.67
1:A:15:VAL:HG13	4:A:1022:HOH:O	1.94	0.67
1:A:378:THR:OG1	1:A:380:ILE:HG12	1.93	0.67
1:A:254:LEU:HD21	1:A:266:VAL:CG1	2.23	0.66
1:A:545:PHE:CZ	1:A:656:VAL:HG13	2.32	0.64
1:A:413:ARG:HG2	1:A:413:ARG:HH21	1.60	0.64
1:A:699:MET:HE2	1:A:708:PHE:HZ	1.62	0.63
1:A:259:VAL:HG12	1:A:260:GLY:N	2.13	0.63
1:A:144:LEU:HD12	1:A:147:MET:CE	2.28	0.63
1:A:198:LEU:HD21	1:A:309:ARG:NH1	2.14	0.63
1:A:571:HIS:HB2	1:A:574:LYS:HG3	1.80	0.62
1:A:257:PHE:O	1:A:258:ASN:HB2	1.98	0.62
1:A:713:MET:HB3	1:A:717:ASP:HB2	1.80	0.62
1:A:34:HIS:HE1	1:A:61:ASP:OD1	1.82	0.62
1:A:144:LEU:HD12	1:A:147:MET:HE1	1.82	0.62
1:A:251:ASP:CG	1:A:252:PHE:N	2.45	0.61
1:A:678:ASN:ND2	1:A:679:MET:H	1.96	0.61
1:A:128:ASP:OD2	1:A:651:SER:HB3	2.01	0.61
1:A:360:ASP:OD1	1:A:363:LYS:HB2	2.01	0.60
1:A:351:ARG:O	1:A:355:ASP:HB2	2.01	0.60
1:A:726:TYR:OH	1:A:774:PHE:HB2	2.02	0.60
1:A:538:LYS:O	1:A:542:LYS:HG3	2.01	0.59
1:A:719:ASP:O	1:A:723:GLN:HG2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:PHE:C	1:A:254:LEU:N	2.61	0.58
1:A:261:GLY:HA3	4:A:1181:HOH:O	2.02	0.58
1:A:329:PHE:HB3	1:A:330:PRO:HD3	1.86	0.58
1:A:522:LEU:HD13	1:A:806:ALA:CB	2.33	0.57
1:A:636:VAL:O	1:A:639:ARG:HD3	2.04	0.57
1:A:122:LEU:HA	1:A:125:ILE:HD12	1.87	0.57
1:A:235:ASN:HD22	1:A:235:ASN:N	1.99	0.57
1:A:457:ARG:HH12	1:A:701:GLU:CD	2.12	0.57
1:A:390:HIS:HD2	4:A:1245:HOH:O	1.88	0.56
1:A:252:PHE:N	1:A:255:LYS:HB3	2.21	0.56
1:A:311:PHE:O	1:A:314:SER:HB2	2.05	0.56
1:A:259:VAL:CG1	1:A:260:GLY:N	2.70	0.55
1:A:355:ASP:OD1	1:A:398:ARG:HD3	2.06	0.55
1:A:64:VAL:HG22	2:A:920:BZD:H111	1.90	0.54
1:A:730:GLU:O	1:A:734:ARG:HG2	2.08	0.54
1:A:235:ASN:HA	1:A:833:ARG:HG3	1.88	0.54
1:A:252:PHE:HA	1:A:255:LYS:HB3	1.87	0.54
1:A:251:ASP:C	1:A:255:LYS:HB3	2.33	0.54
1:A:450:HIS:HD2	4:A:1175:HOH:O	1.91	0.53
1:A:571:HIS:HB2	1:A:574:LYS:CG	2.37	0.53
1:A:34:HIS:HD2	1:A:38:THR:OG1	1.92	0.53
1:A:434:GLY:O	1:A:435:ALA:C	2.51	0.53
1:A:285:PHE:HD1	1:A:382:GLU:HB2	1.74	0.53
1:A:836:ALA:HB1	1:A:837:PRO:CD	2.39	0.52
1:A:144:LEU:HA	1:A:147:MET:CE	2.39	0.52
1:A:562:LEU:HD21	1:A:662:LEU:HB2	1.91	0.52
1:A:510:GLU:HB2	4:A:1178:HOH:O	2.09	0.51
1:A:555:VAL:HG23	1:A:556:HIS:N	2.25	0.51
1:A:144:LEU:HA	1:A:147:MET:HE3	1.92	0.51
1:A:463:LEU:HA	1:A:467:ILE:HG22	1.92	0.51
1:A:413:ARG:HG2	1:A:413:ARG:NH2	2.24	0.51
1:A:94:THR:HG22	4:A:1065:HOH:O	2.11	0.50
1:A:692:MET:HE3	1:A:697:VAL:HG22	1.92	0.50
1:A:367:VAL:O	1:A:371:THR:HG23	2.12	0.50
1:A:504:ALA:HA	1:A:508:GLY:O	2.12	0.49
1:A:522:LEU:HD13	1:A:806:ALA:HB3	1.94	0.49
1:A:285:PHE:CD1	1:A:382:GLU:HB2	2.47	0.49
1:A:574:LYS:NZ	4:A:1235:HOH:O	2.45	0.49
1:A:255:LYS:O	1:A:257:PHE:N	2.45	0.48
1:A:181:ASP:OD2	1:A:184:ARG:CZ	2.62	0.48
1:A:678:ASN:ND2	1:A:679:MET:N	2.58	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:GLY:O	1:A:69:ARG:CG	2.61	0.48
1:A:94:THR:CG2	4:A:1065:HOH:O	2.61	0.48
1:A:611:PRO:HA	1:A:617:LYS:HE3	1.95	0.48
1:A:313:SER:O	1:A:314:SER:C	2.57	0.47
1:A:343:SER:OG	1:A:441:MET:HE3	2.14	0.47
1:A:13:ILE:O	1:A:14:SER:CB	2.62	0.47
1:A:93:ARG:O	1:A:490:ARG:NH2	2.43	0.47
1:A:233:TYR:CB	1:A:489:ARG:HD3	2.38	0.47
1:A:475:GLU:HB3	1:A:477:HIS:CE1	2.49	0.47
1:A:306:ASP:OD2	1:A:309:ARG:NH1	2.49	0.46
1:A:564:ASP:O	1:A:603:VAL:HA	2.15	0.46
1:A:730:GLU:O	1:A:734:ARG:CG	2.64	0.46
1:A:209:THR:O	1:A:210:SER:C	2.58	0.46
1:A:367:VAL:O	1:A:371:THR:CG2	2.64	0.46
1:A:763:ASN:HD22	1:A:768:HIS:CE1	2.34	0.46
1:A:36:HIS:O	1:A:40:VAL:HA	2.15	0.46
1:A:379:VAL:HG22	4:A:1084:HOH:O	2.15	0.46
1:A:455:VAL:H	1:A:459:HIS:CD2	2.27	0.46
1:A:171:CYS:HB2	1:A:176:MET:HG3	1.98	0.45
1:A:648:TYR:HA	1:A:652:LEU:HD23	1.98	0.45
1:A:110:GLU:O	1:A:113:TYR:HB3	2.16	0.45
1:A:255:LYS:O	1:A:255:LYS:HG3	2.16	0.45
1:A:663:SER:HB2	1:A:681:PHE:CG	2.51	0.45
1:A:834:LEU:O	1:A:836:ALA:N	2.50	0.45
1:A:579:ASN:C	1:A:579:ASN:HD22	2.24	0.45
1:A:13:ILE:HD12	1:A:106:ASN:OD1	2.16	0.45
1:A:189:TRP:O	2:A:920:BZD:H131	2.17	0.45
1:A:252:PHE:CA	1:A:255:LYS:HB3	2.47	0.45
1:A:489:ARG:NH2	1:A:814:ASP:OD2	2.50	0.45
1:A:549:LEU:HD12	1:A:549:LEU:HA	1.82	0.45
1:A:551:ARG:NH1	1:A:552:GLU:OE1	2.49	0.45
1:A:564:ASP:OD1	1:A:601:ARG:NH1	2.49	0.44
1:A:91:MET:HB2	1:A:129:ALA:HB3	2.00	0.44
1:A:405:GLU:O	1:A:409:ARG:HG3	2.17	0.44
1:A:564:ASP:HB3	1:A:603:VAL:HA	1.99	0.44
1:A:259:VAL:CG1	1:A:260:GLY:H	2.31	0.44
1:A:488:PRO:O	1:A:492:LEU:HB3	2.17	0.44
1:A:251:ASP:O	1:A:255:LYS:N	2.48	0.44
1:A:726:TYR:HH	1:A:774:PHE:HB2	1.82	0.44
1:A:449:SER:O	1:A:478:LYS:HE2	2.19	0.43
1:A:423:ASP:O	1:A:426:ARG:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:689:ILE:HG23	1:A:689:ILE:O	2.17	0.43
1:A:506:ARG:NH1	1:A:533:ASP:OD2	2.52	0.42
1:A:657:ILE:HB	1:A:658:PRO:HD3	2.01	0.42
1:A:235:ASN:H	1:A:235:ASN:ND2	2.10	0.42
1:A:527:ASP:O	1:A:531:ILE:HG13	2.19	0.42
1:A:304:LEU:HD23	1:A:304:LEU:HA	1.85	0.42
1:A:592:LYS:HD2	1:A:592:LYS:O	2.20	0.42
1:A:678:ASN:HD22	1:A:678:ASN:N	2.17	0.42
1:A:835:PRO:O	1:A:836:ALA:O	2.38	0.42
1:A:233:TYR:CZ	1:A:234:ARG:HD3	2.55	0.42
1:A:214:LYS:HE2	1:A:214:LYS:HB3	1.59	0.42
1:A:456:ALA:C	1:A:481:ASN:HD21	2.28	0.42
1:A:594:PRO:O	1:A:639:ARG:NH1	2.51	0.42
1:A:548:TYR:CD1	1:A:548:TYR:C	2.97	0.41
1:A:254:LEU:HD22	1:A:265:ALA:CB	2.50	0.41
1:A:314:SER:HB3	1:A:315:LYS:H	1.46	0.41
1:A:391:LEU:HD12	1:A:391:LEU:HA	1.85	0.41
1:A:42:ASP:O	1:A:44:ASN:N	2.53	0.41
1:A:16:ARG:O	1:A:106:ASN:HB2	2.20	0.41
1:A:678:ASN:ND2	1:A:678:ASN:N	2.67	0.41
1:A:641:ARG:HG3	4:A:1198:HOH:O	2.19	0.41
1:A:737:GLU:HG3	4:A:1135:HOH:O	2.20	0.41
1:A:42:ASP:OD1	1:A:44:ASN:HB2	2.21	0.41
1:A:198:LEU:HD21	1:A:309:ARG:HH11	1.84	0.41
1:A:558:ASN:HA	1:A:559:PRO:HD3	1.95	0.41
1:A:489:ARG:HH22	1:A:814:ASP:CG	2.29	0.40
1:A:467:ILE:HG23	1:A:468:PHE:CG	2.57	0.40
1:A:143:PHE:C	1:A:147:MET:HE2	2.46	0.40
1:A:13:ILE:HD12	1:A:106:ASN:CG	2.47	0.40
1:A:254:LEU:HD22	1:A:265:ALA:HB1	2.04	0.40
1:A:522:LEU:HD12	1:A:522:LEU:HA	1.96	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	813/842 (97%)	763 (94%)	39 (5%)	11 (1%)	9 5

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	SER
1	A	210	SER
1	A	254	LEU
1	A	259	VAL
1	A	314	SER
1	A	835	PRO
1	A	836	ALA
1	A	43	ARG
1	A	258	ASN
1	A	554	LYS
1	A	15	VAL

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	707/731 (97%)	614 (87%)	93 (13%)	4 2

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ILE
1	A	14	SER
1	A	15	VAL
1	A	18	LEU
1	A	21	VAL
1	A	22	GLU
1	A	23	ASN
1	A	27	LEU

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Mol	Chain	Res	Type
1	A	33	ARG
1	A	39	LEU
1	A	69	ARG
1	A	76	GLU
1	A	87	LEU
1	A	94	THR
1	A	102	LEU
1	A	104	LEU
1	A	115	LEU
1	A	122	LEU
1	A	128	ASP
1	A	144	LEU
1	A	162	GLU
1	A	191	LYS
1	A	193	ARG
1	A	198	LEU
1	A	210	SER
1	A	211	GLN
1	A	214	LYS
1	A	234	ARG
1	A	235	ASN
1	A	243	LEU
1	A	250	ASN
1	A	252	PHE
1	A	253	ASN
1	A	254	LEU
1	A	255	LYS
1	A	257	PHE
1	A	258	ASN
1	A	264	GLN
1	A	266	VAL
1	A	279	LEU
1	A	314	SER
1	A	315	LYS
1	A	324	THR
1	A	325	ASN
1	A	358	ARG
1	A	363	LYS
1	A	371	THR
1	A	380	ILE
1	A	384	LEU
1	A	398	ARG

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Mol	Chain	Res	Type
1	A	400	LEU
1	A	413	ARG
1	A	425	LEU
1	A	426	ARG
1	A	433	GLU
1	A	436	VAL
1	A	444	LEU
1	A	465	LYS
1	A	467	ILE
1	A	474	LEU
1	A	510	GLU
1	A	518	LEU
1	A	522	LEU
1	A	528	GLU
1	A	536	LYS
1	A	544	LYS
1	A	549	LEU
1	A	552	GLU
1	A	554	LYS
1	A	565	VAL
1	A	568	LYS
1	A	596	LYS
1	A	603	VAL
1	A	622	LEU
1	A	643	ILE
1	A	645	LEU
1	A	656	VAL
1	A	662	LEU
1	A	678	ASN
1	A	687	LEU
1	A	706	GLU
1	A	708	PHE
1	A	720	ARG
1	A	721	LEU
1	A	724	ARG
1	A	734	ARG
1	A	742	ILE
1	A	759	LYS
1	A	765	LEU
1	A	768	HIS
1	A	790	LEU
1	A	830	SER

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Mol	Chain	Res	Type
1	A	833	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	72	GLN
1	A	235	ASN
1	A	253	ASN
1	A	325	ASN
1	A	412	ASN
1	A	450	HIS
1	A	459	HIS
1	A	481	ASN
1	A	484	ASN
1	A	560	ASN
1	A	566	GLN
1	A	579	ASN
1	A	678	ASN
1	A	763	ASN
1	A	832	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	BZD	A	920	-	24,24,24	2.30	10 (41%)	33,33,33	1.48	7 (21%)
2	BZD	A	998	-	24,24,24	1.71	7 (29%)	33,33,33	1.08	4 (12%)
3	PLP	A	999	1	15,15,16	1.70	4 (26%)	21,22,23	1.17	3 (14%)

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	BZD	A	920	-	-	0/14/34/34	0/2/2/2
2	BZD	A	998	-	-	2/14/34/34	0/2/2/2
3	PLP	A	999	1	-	1/6/6/8	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	920	BZD	C10-C9	5.04	1.47	1.39
2	A	998	BZD	C2-C1	4.33	1.57	1.53
2	A	920	BZD	C14-C9	4.05	1.45	1.39
2	A	920	BZD	C4-C5	3.72	1.61	1.53
2	A	920	BZD	C13-C12	3.31	1.45	1.38
2	A	920	BZD	C13-C14	3.24	1.44	1.38
2	A	920	BZD	C12-C11	3.19	1.45	1.38
3	A	999	PLP	C3-C2	-3.05	1.37	1.41
3	A	999	PLP	C4A-C4	3.03	1.57	1.51
2	A	920	BZD	O5-C1	3.02	1.48	1.43
3	A	999	PLP	C5A-C5	2.91	1.58	1.50
2	A	998	BZD	C14-C9	2.76	1.43	1.39
2	A	920	BZD	C11-C10	2.69	1.43	1.38
2	A	998	BZD	C10-C9	2.54	1.43	1.39
2	A	920	BZD	C4-C3	2.34	1.58	1.52
2	A	998	BZD	C13-C14	2.27	1.42	1.38
3	A	999	PLP	C2-N1	2.14	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	998	BZD	C12-C11	2.10	1.42	1.38
2	A	998	BZD	C11-C10	2.08	1.42	1.38
2	A	998	BZD	C1-N1	2.05	1.46	1.43
2	A	920	BZD	C3-C2	2.03	1.57	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	920	BZD	C9-C8-N2	4.06	122.10	116.25
2	A	920	BZD	O5-C1-C2	3.36	113.50	109.72
2	A	920	BZD	O8-C8-C9	-2.92	115.12	120.90
2	A	920	BZD	C8-N2-C7	-2.72	125.55	128.13
2	A	998	BZD	N2-C7-N1	2.70	121.19	116.06
2	A	920	BZD	N2-C7-N1	2.61	121.01	116.06
2	A	920	BZD	C2-C1-N1	-2.60	107.90	111.25
2	A	998	BZD	C9-C8-N2	2.52	119.87	116.25
3	A	999	PLP	O3P-P-O1P	2.27	119.67	110.83
3	A	999	PLP	O4P-C5A-C5	2.22	113.51	109.36
2	A	998	BZD	O7-C7-N1	-2.20	117.98	122.67
3	A	999	PLP	C5-C6-N1	-2.16	120.32	123.83
2	A	998	BZD	O8-C8-C9	-2.15	116.65	120.90
2	A	920	BZD	O7-C7-N1	-2.05	118.29	122.67

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	998	BZD	O7-C7-N2-C8
2	A	998	BZD	N1-C7-N2-C8
3	A	999	PLP	C4-C5-C5A-O4P

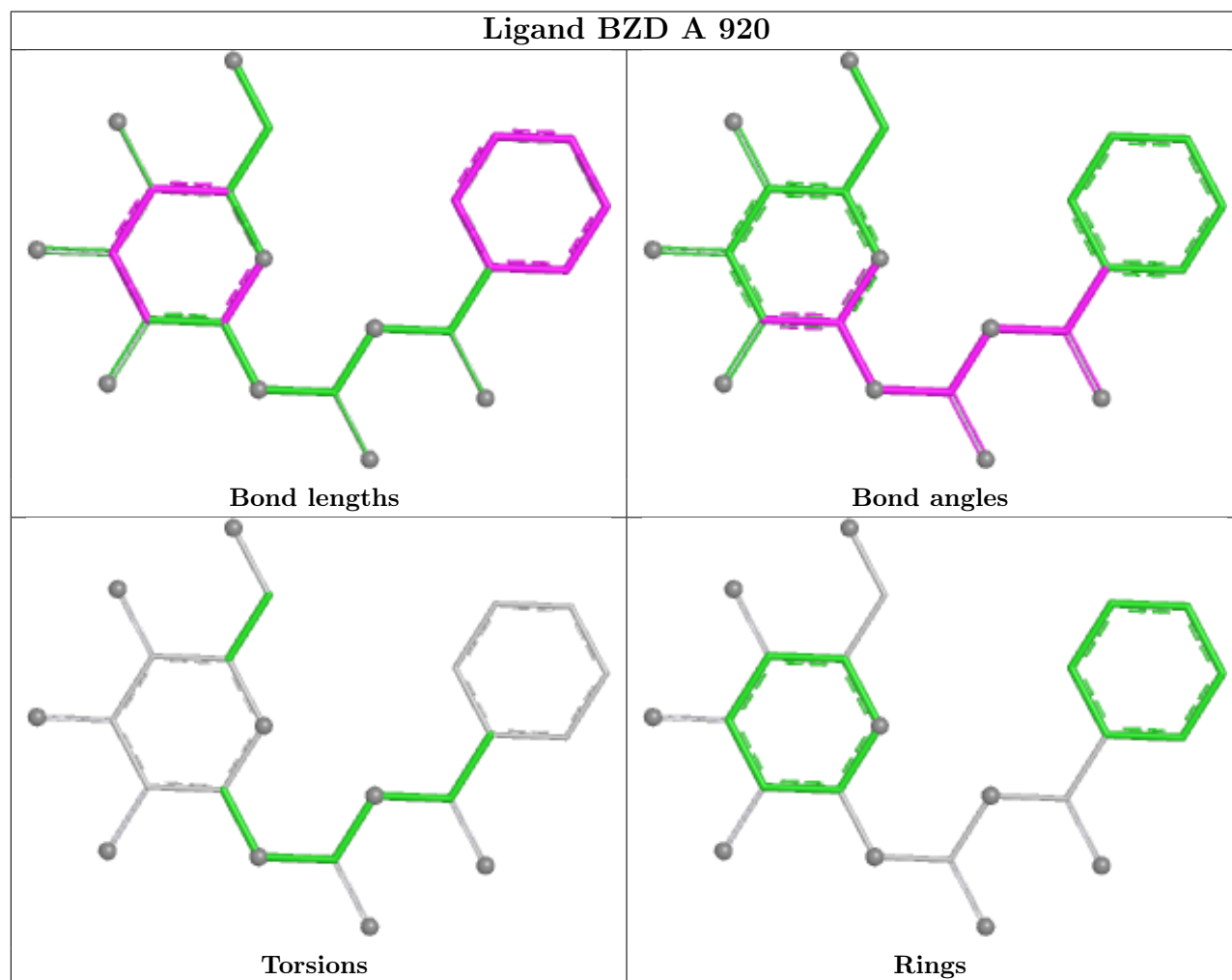
There are no ring outliers.

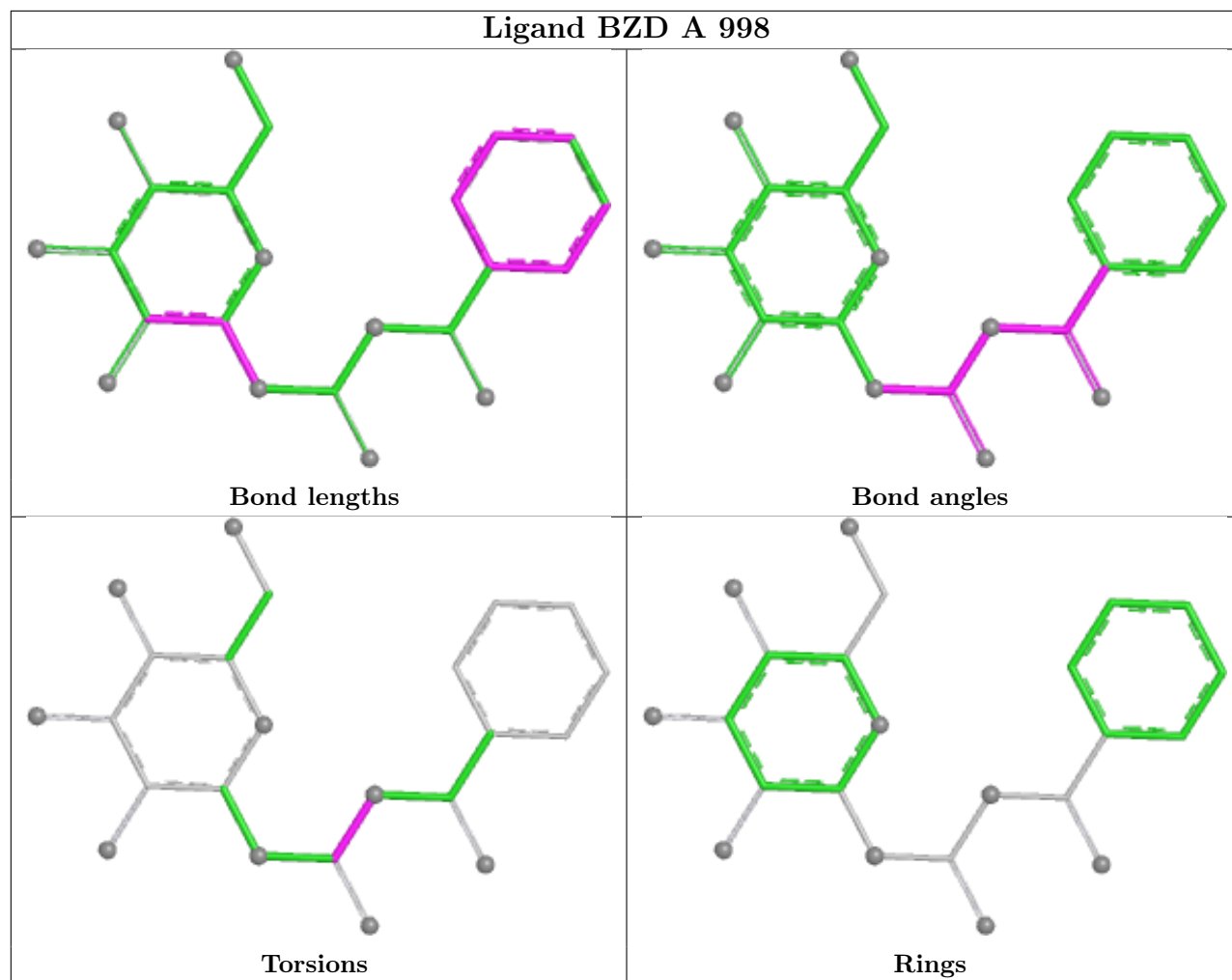
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	920	BZD	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.