



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 11:33 AM BST

PDB ID : 1L7X
Title : Human liver glycogen phosphorylase b complexed with caffeine, 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 : 2002-03-18
Resolution : 2.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

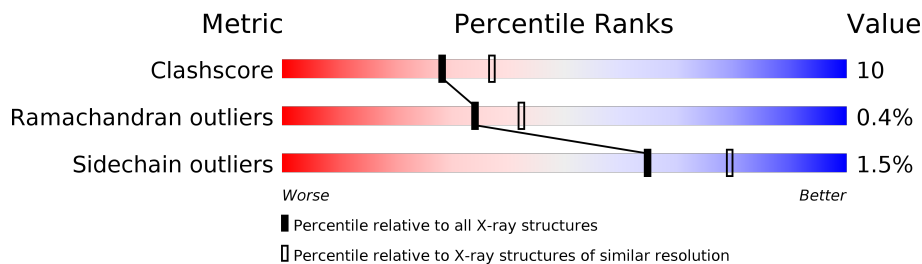
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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 on 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	

2 Entry composition i

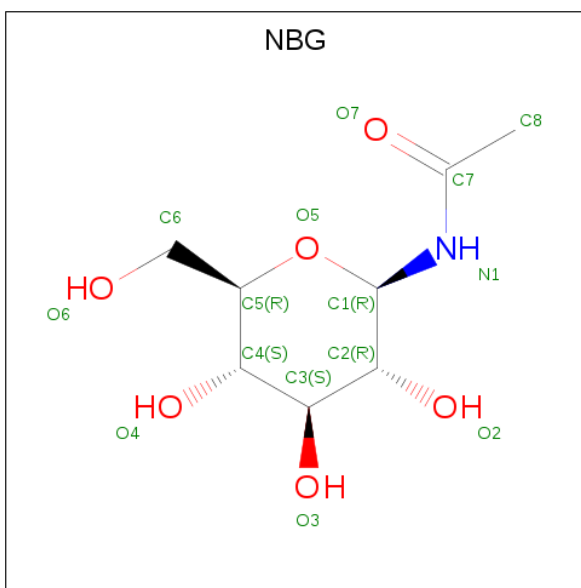
There are 7 unique types of molecules in this entry. The entry contains 13542 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	793	Total 6436	C 4135	N 1092	O 1180	S 29	0	0	0
1	B	795	Total 6446	C 4141	N 1094	O 1182	S 29	0	0	0

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



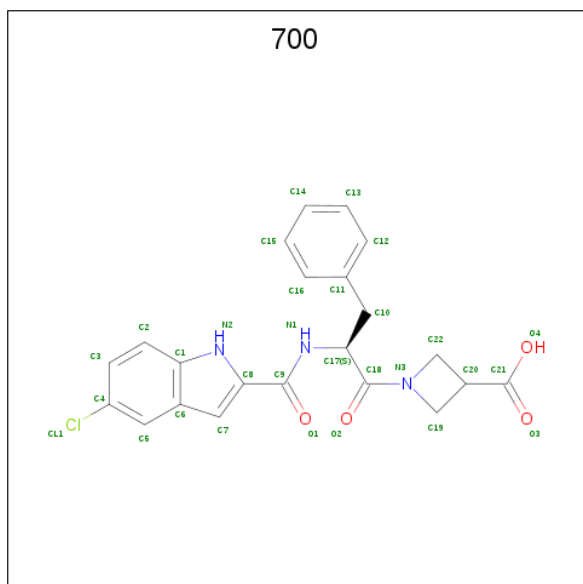
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total 15	C 8	N 1	O 6	0	0
2	B	1	Total 15	C 8	N 1	O 6	0	0

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



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

- Molecule 4 is [5-CHLORO-1H-INDOL-2-CARBONYL-PHENYLALANINYL]-AZETIDINE-3-CARBOXYLIC ACID (three-letter code: 700) (formula: C₂₂H₂₀ClN₃O₄).



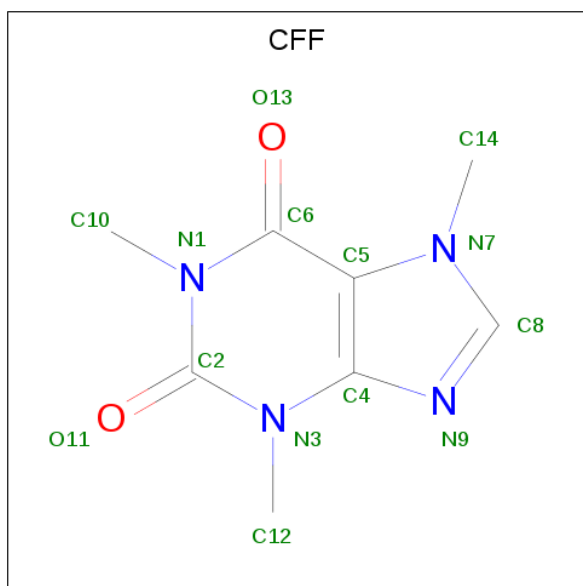
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
4	A	1	30	22	1	3	4	0	0

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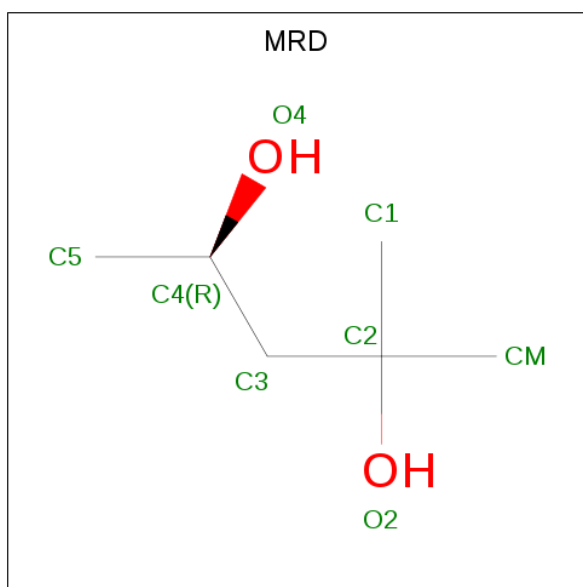
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Cl	N			O
4	B	1	30	22	1	3	4	0	0

- Molecule 5 is CAFFEINE (three-letter code: CFF) (formula: C₈H₁₀N₄O₂).



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

- Molecule 6 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: C₆H₁₄O₂).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	252	Total O 252 252	0	0
7	B	222	Total O 222 222	0	0

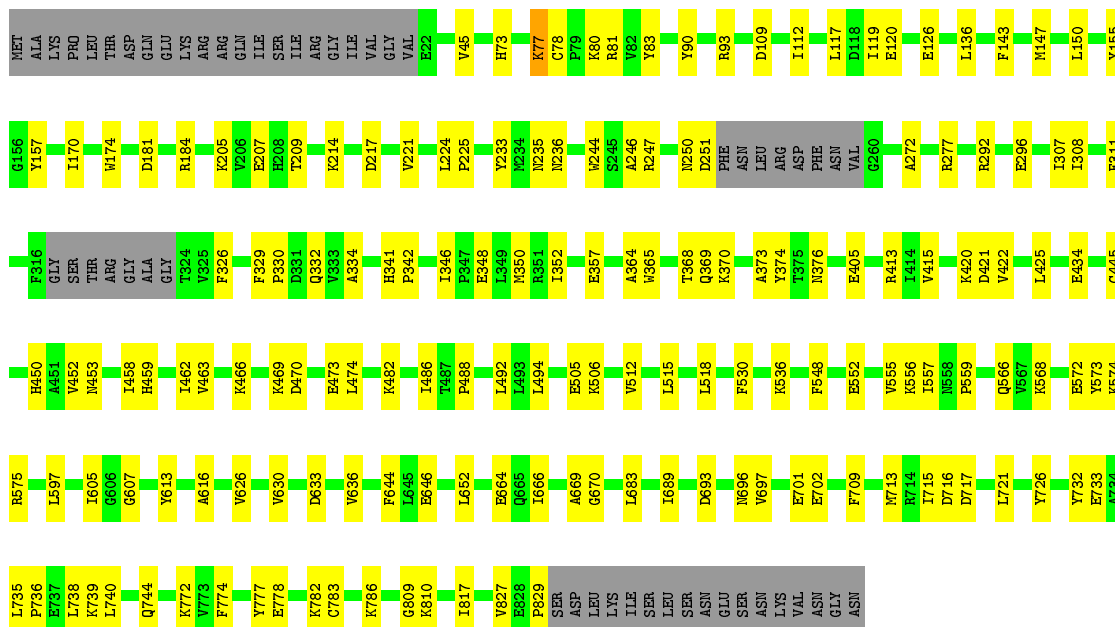
3 Residue-property plots

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.

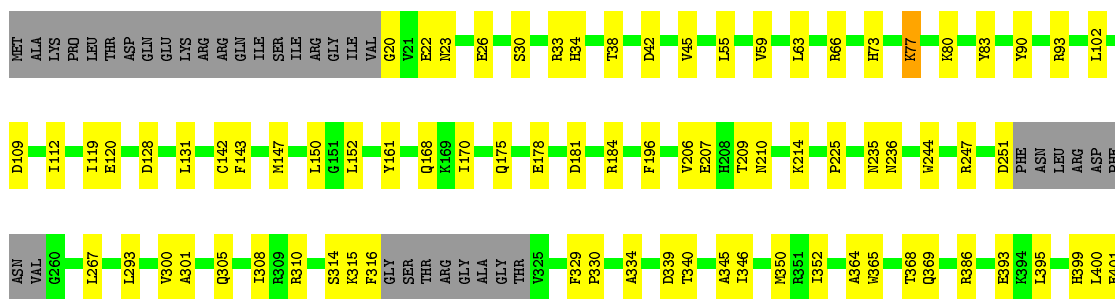
- Molecule 1: Glycogen phosphorylase, liver form

Chain A: 



- Molecule 1: Glycogen phosphorylase, liver form

Chain B: 



I402	I403	Y404	E405	K409	D421	V422	D423	R427	E432	E433	E434	K437	R438	I439	G448	V455	I458	I462	V463	F468	K469	D470	E473	L474	E475	P476	M484	T487	P488	L492	L493	I503	A504	E505	K506	E509	D510	Y511	V512	L515	L521		
F524	D528	F548	E552	V555	K556	I557	K568	Y573	K574	R575	O576	L577	K591	K592	D593	K596	L597	I605	K608	Y613	A616	V626	A627	D628	V629	V630	N631	V632	D633	V636	V642	I643	F644	L645	E646	V650	S651	L652	I657	P658			
L662	I666	S667	T668	L683	I689	M692	V697	E701	E702	A703	E706	N707	L708	F709	I710	M713	R714	I715	D716	D717	V718	Y732	E733	K739	D743	N747	F750	L765	K772	D776	Y777	V781	K782	C783	K786	V787	S812	V827	E828				
P829	S850	ASP	LEU	LYS	ILE	SER	LEU	SER	ASN	GLU	SER	ASN	LYS	VAL	ASN	GLY	ASN																										

4 Data and refinement statistics

Xtrriage (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	124.07Å 124.07Å 122.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.39 – 2.30	Depositor
% Data completeness (in resolution range)	96.6 (34.39-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.206 , 0.251	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	13542	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CFF, MRD, 700, NBG, 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	0.36	0/6580	0.59	0/8899
1	B	0.35	0/6590	0.59	0/8912
All	All	0.35	0/13170	0.59	0/17811

There are no bond length outliers.

There are no bond angle outliers.

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	6436	0	6426	126	0
1	B	6446	0	6436	133	0
2	A	15	0	15	0	0
2	B	15	0	15	0	0
3	A	15	0	7	0	0
3	B	15	0	7	0	0
4	A	30	0	19	0	0
4	B	30	0	19	0	0
5	A	28	0	20	0	0
5	B	14	0	10	0	0
6	B	24	0	42	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	252	0	0	7	0
7	B	222	0	0	4	0
All	All	13542	0	13016	256	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 (256) 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:350:MET:HE1	1:A:364:ALA:HB1	1.56	0.86
1:B:77:LYS:HA	1:B:77:LYS:HE3	1.59	0.84
1:A:80:LYS:HB3	1:A:827:VAL:HG12	1.60	0.83
1:A:721:LEU:HD23	1:A:772:LYS:HD3	1.60	0.83
1:B:80:LYS:HB3	1:B:827:VAL:HG12	1.62	0.82
1:B:170:ILE:HG12	1:B:646:GLU:HG2	1.61	0.81
1:A:597:LEU:H	1:A:597:LEU:HD22	1.45	0.80
1:B:597:LEU:HD22	1:B:597:LEU:H	1.47	0.79
1:A:329:PHE:HB3	1:A:330:PRO:HD3	1.63	0.79
1:A:308:ILE:HD13	1:A:352:ILE:HG21	1.64	0.78
1:B:350:MET:HE1	1:B:364:ALA:HB1	1.64	0.78
1:A:308:ILE:CD1	1:A:352:ILE:HG21	2.14	0.77
1:B:633:ASP:O	1:B:636:VAL:HG12	1.84	0.76
1:B:181:ASP:OD2	1:B:184:ARG:HB2	1.85	0.76
1:B:30:SER:HA	1:B:33:ARG:NH1	2.02	0.75
1:B:575:ARG:HD3	1:B:666:ILE:O	1.88	0.74
1:A:209:THR:HG21	1:A:214:LYS:HE2	1.70	0.72
1:B:170:ILE:HG22	7:B:2366:HOH:O	1.89	0.71
1:A:77:LYS:HA	1:A:77:LYS:HE3	1.73	0.70
1:B:329:PHE:HB3	1:B:330:PRO:HD3	1.73	0.69
1:A:350:MET:HE3	1:A:364:ALA:O	1.92	0.69
1:B:568:LYS:HD3	1:B:574:LYS:HD3	1.74	0.69
1:A:633:ASP:O	1:A:636:VAL:HG12	1.94	0.68
1:A:350:MET:HA	1:A:350:MET:CE	2.24	0.67
1:B:575:ARG:NH2	1:B:776:ASP:HB2	2.09	0.67
1:A:568:LYS:HD3	1:A:574:LYS:HD3	1.78	0.66
1:B:575:ARG:HH22	1:B:776:ASP:HB2	1.61	0.65
1:B:247:ARG:HD2	7:B:2449:HOH:O	1.96	0.65
1:A:613:TYR:CD2	1:A:616:ALA:HB2	2.32	0.65
1:A:786:LYS:NZ	1:A:786:LYS:HB3	2.10	0.65
1:A:150:LEU:O	1:A:829:PRO:HB3	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:MET:HE3	1:B:364:ALA:O	1.97	0.64
1:B:142:CYS:SG	1:B:487:THR:HG22	2.37	0.64
1:A:415:VAL:HG22	1:A:425:LEU:HD11	1.80	0.63
1:B:93:ARG:HG3	1:B:128:ASP:OD2	1.97	0.63
1:A:732:TYR:CE1	1:A:739:LYS:HG3	2.33	0.62
1:A:713:MET:HB3	1:A:717:ASP:HB2	1.81	0.62
1:B:548:PHE:O	1:B:552:GLU:HG2	2.01	0.61
1:A:365:TRP:CD1	1:A:369:GLN:NE2	2.69	0.60
1:A:515:LEU:HG	1:A:809:GLY:HA2	1.82	0.60
1:A:462:ILE:HG12	1:A:466:LYS:NZ	2.16	0.60
1:A:181:ASP:OD2	1:A:184:ARG:NE	2.34	0.60
1:B:469:LYS:O	1:B:473:GLU:HG3	2.02	0.60
1:A:209:THR:CG2	1:A:214:LYS:HE2	2.32	0.59
1:B:109:ASP:OD1	1:B:119:ILE:HD13	2.03	0.58
1:B:207:GLU:HG2	1:B:209:THR:HG23	1.85	0.58
1:A:462:ILE:HA	1:A:466:LYS:HD2	1.84	0.58
1:A:548:PHE:O	1:A:552:GLU:HG2	2.03	0.58
1:B:386:ARG:HD2	1:B:432:GLU:OE2	2.04	0.58
1:B:697:VAL:O	1:B:701:GLU:HG3	2.03	0.58
1:A:292:ARG:O	1:A:296:GLU:HG3	2.02	0.58
1:B:66:ARG:HD2	1:B:236:ASN:HA	1.85	0.57
1:B:555:VAL:CG2	1:B:631:ASN:HD22	2.17	0.57
1:B:662:LEU:HD22	1:B:787:VAL:HG11	1.85	0.57
1:A:365:TRP:NE1	1:A:369:GLN:NE2	2.53	0.57
1:A:597:LEU:H	1:A:597:LEU:CD2	2.17	0.57
1:B:458:ILE:O	1:B:462:ILE:HG13	2.04	0.57
1:A:45:VAL:O	1:A:45:VAL:HG12	2.05	0.57
1:A:556:LYS:HD3	1:A:557:ILE:N	2.20	0.57
1:A:170:ILE:HG12	1:A:646:GLU:HG2	1.86	0.57
1:A:357:GLU:HA	1:A:357:GLU:OE2	2.04	0.56
1:A:250:ASN:HD21	1:B:184:ARG:NH1	2.02	0.56
1:A:458:ILE:HG22	7:A:2145:HOH:O	2.04	0.56
1:A:494:LEU:HD23	1:A:494:LEU:C	2.25	0.56
1:B:30:SER:HA	1:B:33:ARG:HH12	1.70	0.56
1:A:224:LEU:HD12	1:A:225:PRO:HD2	1.88	0.56
1:B:20:GLY:HA2	1:B:23:ASN:HD22	1.71	0.56
1:A:350:MET:HE3	1:A:364:ALA:C	2.26	0.56
1:B:150:LEU:O	1:B:829:PRO:HB3	2.07	0.55
1:A:109:ASP:OD1	1:A:119:ILE:HD13	2.05	0.55
1:A:505:GLU:HG3	7:A:2296:HOH:O	2.05	0.55
1:B:597:LEU:HD22	1:B:597:LEU:N	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:777:TYR:O	1:B:781:VAL:HG23	2.06	0.55
1:B:515:LEU:HD22	1:B:812:SER:HB2	1.88	0.55
1:A:469:LYS:O	1:A:473:GLU:HG3	2.07	0.54
1:A:73:HIS:CE1	1:A:77:LYS:HG3	2.43	0.54
1:B:350:MET:CE	1:B:368:THR:OG1	2.56	0.54
1:B:575:ARG:HH22	1:B:776:ASP:CB	2.20	0.54
1:B:597:LEU:CD2	1:B:597:LEU:H	2.17	0.54
1:A:246:ALA:O	1:A:247:ARG:HD3	2.07	0.54
1:A:350:MET:HA	1:A:350:MET:HE2	1.89	0.54
1:B:22:GLU:O	1:B:26:GLU:HG2	2.08	0.54
1:B:293:LEU:HD23	1:B:395:LEU:HD23	1.90	0.54
1:B:556:LYS:HD3	1:B:557:ILE:N	2.22	0.54
1:B:207:GLU:OE1	1:B:214:LYS:HE3	2.08	0.53
1:B:209:THR:OG1	1:B:214:LYS:HE2	2.08	0.53
1:B:463:VAL:HG13	1:B:468:PHE:CD1	2.44	0.53
1:B:786:LYS:HB3	1:B:786:LYS:NZ	2.24	0.53
1:A:225:PRO:HB3	1:A:244:TRP:CZ3	2.44	0.53
1:A:536:LYS:HD3	7:A:2237:HOH:O	2.08	0.53
1:B:308:ILE:CD1	1:B:352:ILE:HG21	2.39	0.53
1:B:591:LYS:HD3	1:B:633:ASP:OD1	2.09	0.53
1:A:470:ASP:O	1:A:474:LEU:HD13	2.09	0.53
1:A:143:PHE:CG	1:A:817:ILE:HD11	2.44	0.52
1:B:657:ILE:HB	1:B:658:PRO:HD3	1.91	0.52
1:A:575:ARG:HD3	1:A:666:ILE:O	2.09	0.52
1:A:740:LEU:O	1:A:744:GLN:HG3	2.10	0.52
1:B:510:ASP:OD2	1:B:510:ASP:N	2.38	0.52
1:B:555:VAL:HG21	1:B:631:ASN:HD22	1.75	0.52
1:B:315:LYS:O	1:B:316:PHE:O	2.27	0.52
1:A:374:TYR:O	1:A:452:VAL:HA	2.10	0.52
1:B:405:GLU:OE1	1:B:409:LYS:NZ	2.42	0.52
1:B:80:LYS:HB3	1:B:827:VAL:CG1	2.39	0.52
1:B:492:LEU:HD22	1:B:683:LEU:HD11	1.92	0.51
1:B:45:VAL:HG12	1:B:45:VAL:O	2.10	0.51
1:B:575:ARG:HD2	1:B:668:THR:N	2.26	0.51
1:B:555:VAL:HG21	1:B:631:ASN:ND2	2.25	0.51
1:B:732:TYR:CE1	1:B:739:LYS:HG3	2.46	0.51
1:B:350:MET:HE3	1:B:368:THR:OG1	2.11	0.51
1:B:506:LYS:HD2	1:B:524:PHE:CE2	2.46	0.51
1:A:506:LYS:HE2	1:A:530:PHE:CD1	2.46	0.51
1:B:77:LYS:HA	1:B:77:LYS:CE	2.34	0.51
1:B:22:GLU:HG2	1:B:22:GLU:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:ALA:O	1:B:305:GLN:HG3	2.11	0.50
1:B:350:MET:HE3	1:B:364:ALA:C	2.30	0.50
1:B:470:ASP:O	1:B:474:LEU:HD13	2.12	0.50
1:A:112:ILE:HG23	1:A:117:LEU:HB2	1.93	0.50
1:A:506:LYS:HE2	1:A:530:PHE:HD1	1.77	0.50
1:A:515:LEU:HD11	1:A:518:LEU:HD11	1.94	0.50
1:A:136:LEU:C	1:A:136:LEU:HD23	2.32	0.49
1:A:330:PRO:HB3	1:A:370:LYS:HB3	1.92	0.49
1:A:453:ASN:ND2	1:A:482:LYS:HB2	2.27	0.49
1:A:786:LYS:HB3	1:A:786:LYS:HZ2	1.76	0.49
1:B:488:PRO:O	1:B:492:LEU:HB3	2.12	0.49
1:A:221:VAL:HG22	1:A:272:ALA:HB1	1.94	0.49
1:A:488:PRO:O	1:A:492:LEU:HB3	2.11	0.49
1:B:718:VAL:HG13	1:B:772:LYS:HE2	1.94	0.49
1:B:168:GLN:HG3	1:B:175:GLN:HG3	1.95	0.49
1:B:423:ASP:OD1	1:B:427:ARG:NH1	2.46	0.49
1:B:593:ASP:OD1	1:B:596:LYS:N	2.46	0.49
1:A:415:VAL:CG2	1:A:425:LEU:HD11	2.42	0.49
1:A:369:GLN:O	1:A:450:HIS:HB3	2.13	0.49
1:B:626:VAL:HA	1:B:750:PHE:CD1	2.48	0.49
1:B:196:PHE:CZ	6:B:903:MRD:H1C3	2.47	0.49
1:B:743:ASP:O	1:B:747:ASN:ND2	2.46	0.49
1:B:346:ILE:HD13	1:B:448:GLY:HA3	1.94	0.49
1:A:207:GLU:OE1	1:A:214:LYS:HE3	2.12	0.49
1:A:81:ARG:HD3	1:A:83:TYR:OH	2.13	0.48
1:B:613:TYR:CD2	1:B:616:ALA:HB2	2.48	0.48
1:B:73:HIS:CE1	1:B:77:LYS:HG3	2.48	0.48
1:A:462:ILE:HG12	1:A:466:LYS:HZ3	1.78	0.48
1:B:474:LEU:O	1:B:476:PRO:HD3	2.12	0.48
1:B:455:VAL:CG1	1:B:484:ASN:HD21	2.26	0.48
1:B:713:MET:HB3	1:B:717:ASP:HB2	1.95	0.48
1:B:393:GLU:HB2	1:B:400:LEU:CD2	2.44	0.48
1:A:459:HIS:O	1:A:463:VAL:HG23	2.14	0.48
1:A:348:GLU:O	1:A:352:ILE:HG13	2.13	0.48
1:B:493:LEU:HD21	1:B:512:VAL:HG11	1.96	0.48
1:B:515:LEU:CD2	1:B:812:SER:HB2	2.44	0.48
1:A:605:ILE:O	1:A:644:PHE:HA	2.14	0.48
1:B:350:MET:HA	1:B:350:MET:CE	2.44	0.47
1:B:63:LEU:HD23	1:B:102:LEU:HD11	1.96	0.47
1:A:350:MET:CE	1:A:368:THR:OG1	2.62	0.47
1:A:557:ILE:O	1:A:559:PRO:HD3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:ASP:OD1	1:B:340:THR:N	2.43	0.47
1:B:689:ILE:HG23	1:B:689:ILE:O	2.14	0.47
1:B:83:TYR:OH	1:B:310:ARG:HD2	2.15	0.47
1:B:386:ARG:HA	1:B:439:ILE:O	2.14	0.47
1:A:205:LYS:HE2	1:A:217:ASP:OD2	2.14	0.47
1:B:80:LYS:HE2	1:B:334:ALA:HB2	1.95	0.47
1:B:568:LYS:HB3	1:B:568:LYS:NZ	2.30	0.47
1:B:365:TRP:CD1	1:B:369:GLN:NE2	2.83	0.47
1:B:505:GLU:HG2	1:B:505:GLU:O	2.15	0.47
1:A:157:TYR:HD2	1:A:244:TRP:HE1	1.63	0.47
1:A:566:GLN:HB2	1:A:664:GLU:HB2	1.96	0.47
1:A:726:TYR:OH	1:A:774:PHE:HB2	2.15	0.47
1:B:66:ARG:CD	1:B:236:ASN:HA	2.44	0.47
1:B:577:LEU:HD13	1:B:765:LEU:HD21	1.96	0.47
1:A:233:TYR:CE2	1:A:512:VAL:HG11	2.50	0.46
1:A:308:ILE:HD12	1:A:352:ILE:HD13	1.96	0.46
1:A:626:VAL:O	1:A:630:VAL:HG23	2.16	0.46
1:A:492:LEU:HD22	1:A:683:LEU:HD11	1.97	0.46
1:A:78:CYS:HB3	1:A:332:GLN:HE22	1.80	0.46
1:B:630:VAL:O	1:B:636:VAL:HG11	2.14	0.46
1:B:605:ILE:O	1:B:644:PHE:HA	2.15	0.46
1:A:506:LYS:HG3	1:A:530:PHE:CE1	2.49	0.46
1:A:420:LYS:O	1:A:422:VAL:HG13	2.15	0.46
1:B:55:LEU:HD13	1:B:112:ILE:HD11	1.96	0.46
1:A:778:GLU:CG	1:A:782:LYS:HE2	2.46	0.46
1:B:308:ILE:HD13	1:B:352:ILE:HG21	1.98	0.46
1:B:463:VAL:HG13	1:B:468:PHE:HD1	1.79	0.46
1:B:55:LEU:O	1:B:59:VAL:HG23	2.15	0.46
1:A:341:HIS:HB2	1:A:342:PRO:HD3	1.97	0.45
1:B:181:ASP:OD2	1:B:184:ARG:NE	2.49	0.45
1:A:693:ASP:O	1:A:696:ASN:HB2	2.16	0.45
1:A:376:ASN:O	1:A:459:HIS:HE1	1.98	0.45
1:B:225:PRO:HB3	1:B:244:TRP:CZ3	2.52	0.45
1:B:293:LEU:HD23	1:B:395:LEU:CD2	2.47	0.45
1:A:732:TYR:CZ	1:A:739:LYS:HG3	2.52	0.45
1:A:405:GLU:HA	1:A:405:GLU:OE2	2.16	0.45
1:A:83:TYR:CD1	1:A:155:TYR:HB2	2.53	0.44
1:B:300:VAL:HG13	1:B:345:ALA:HA	1.99	0.44
1:A:670:GLY:H	1:A:693:ASP:CG	2.21	0.44
1:B:131:LEU:HD22	1:B:161:TYR:HB2	2.00	0.44
1:B:152:LEU:HD23	1:B:829:PRO:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:PHE:HB3	1:A:783:CYS:SG	2.58	0.44
1:B:393:GLU:HB2	1:B:400:LEU:HD22	2.00	0.44
1:B:715:ILE:HG23	1:B:716:ASP:N	2.32	0.44
1:A:93:ARG:HG2	1:A:126:GLU:HG2	1.99	0.44
1:A:568:LYS:O	1:A:607:GLY:HA3	2.17	0.43
1:B:650:VAL:HB	7:B:2328:HOH:O	2.18	0.43
1:A:209:THR:HG21	1:A:214:LYS:CE	2.43	0.43
1:A:307:ILE:HG23	7:A:2398:HOH:O	2.18	0.43
1:A:486:ILE:O	1:A:486:ILE:HG13	2.16	0.43
1:A:778:GLU:HG3	1:A:782:LYS:HE2	2.00	0.43
1:B:399:HIS:O	1:B:403:ILE:HG13	2.19	0.43
1:B:42:ASP:C	1:B:42:ASP:OD2	2.57	0.43
1:A:277:ARG:HG2	1:B:267:LEU:HD23	2.01	0.43
1:A:697:VAL:O	1:A:701:GLU:HG3	2.19	0.43
1:A:669:ALA:HA	1:A:693:ASP:HB2	2.00	0.43
1:B:432:GLU:O	1:B:437:LYS:HA	2.19	0.43
1:A:689:ILE:O	1:A:689:ILE:HG23	2.19	0.43
1:B:692:MET:HG2	1:B:710:ILE:HG21	2.01	0.43
1:A:373:ALA:HB3	7:A:2194:HOH:O	2.18	0.43
1:A:572:GLU:HG3	1:A:613:TYR:OH	2.18	0.42
1:A:738:LEU:HB2	1:A:777:TYR:CE2	2.53	0.42
1:A:80:LYS:HE2	1:A:334:ALA:HB2	2.00	0.42
1:A:326:PHE:CZ	1:A:357:GLU:HG3	2.55	0.42
1:A:346:ILE:CD1	1:A:445:CYS:HA	2.49	0.42
1:A:515:LEU:CG	1:A:809:GLY:HA2	2.48	0.42
1:B:350:MET:HE2	1:B:368:THR:OG1	2.19	0.42
1:A:556:LYS:C	1:A:556:LYS:HD3	2.40	0.42
1:B:405:GLU:OE2	1:B:405:GLU:HA	2.20	0.42
1:B:235:ASN:O	1:B:236:ASN:HB2	2.19	0.42
1:B:170:ILE:CG1	1:B:646:GLU:HG2	2.39	0.42
1:A:715:ILE:HG22	7:A:2297:HOH:O	2.19	0.42
1:B:143:PHE:O	1:B:147:MET:HG3	2.20	0.42
1:B:34:HIS:O	1:B:38:THR:HB	2.20	0.42
1:A:702:GLU:CD	1:A:810:LYS:HD2	2.40	0.42
1:B:315:LYS:O	1:B:316:PHE:C	2.58	0.42
1:B:703:ALA:O	1:B:707:ASN:ND2	2.48	0.42
1:A:311:PHE:CE1	1:A:329:PHE:HA	2.55	0.42
1:B:350:MET:HE1	1:B:364:ALA:CB	2.44	0.42
1:A:235:ASN:O	1:A:236:ASN:HB2	2.19	0.41
1:B:503:ILE:HG23	1:B:521:LEU:HD21	2.02	0.41
1:A:143:PHE:O	1:A:147:MET:HG3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:PHE:CZ	1:A:552:GLU:HG3	2.55	0.41
1:A:735:LEU:HA	1:A:736:PRO:HD2	1.97	0.41
1:A:109:ASP:OD1	1:A:119:ILE:HG21	2.20	0.41
1:A:251:ASP:HA	1:B:178:GLU:OE1	2.20	0.41
1:B:314:SER:HB3	7:B:2199:HOH:O	2.20	0.41
1:A:170:ILE:HA	1:A:174:TRP:O	2.21	0.41
1:B:627:ALA:HA	1:B:642:VAL:HB	2.03	0.41
1:A:413:ARG:HH11	1:A:413:ARG:HG2	1.85	0.41
1:A:181:ASP:OD2	1:A:184:ARG:HB2	2.21	0.41
1:A:566:GLN:HA	7:A:2209:HOH:O	2.20	0.41
1:B:455:VAL:HG12	1:B:484:ASN:HD21	1.83	0.41
1:A:715:ILE:HG23	1:A:716:ASP:OD1	2.20	0.41
1:B:168:GLN:NE2	1:B:608:LYS:HA	2.35	0.41
1:A:474:LEU:N	1:A:474:LEU:HD12	2.36	0.41
1:B:206:VAL:HG11	1:B:401:GLU:OE1	2.20	0.41
1:A:136:LEU:O	1:A:136:LEU:HD23	2.21	0.40
1:B:555:VAL:HG22	1:B:631:ASN:HD22	1.86	0.40
1:B:509:GLU:O	1:B:512:VAL:HG23	2.21	0.40
1:B:709:PHE:HB3	1:B:783:CYS:SG	2.61	0.40
1:A:170:ILE:CG1	1:A:646:GLU:HG2	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	787/847 (93%)	752 (96%)	32 (4%)	3 (0%)	34 42
1	B	789/847 (93%)	743 (94%)	43 (5%)	3 (0%)	34 42
All	All	1576/1694 (93%)	1495 (95%)	75 (5%)	6 (0%)	34 42

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	421	ASP
1	A	555	VAL
1	B	421	ASP
1	A	434	GLU
1	B	434	GLU
1	B	829	PRO

5.3.2 Protein sidechains [i](#)

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%)	688 (99%)	6 (1%)	78 89
1	B	695/740 (94%)	680 (98%)	15 (2%)	52 69
All	All	1389/1480 (94%)	1368 (98%)	21 (2%)	65 79

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	LYS
1	A	90	TYR
1	A	120	GLU
1	A	573	TYR
1	A	652	LEU
1	A	733	GLU
1	B	77	LYS
1	B	90	TYR
1	B	120	GLU
1	B	210	ASN
1	B	251	ASP
1	B	510	ASP
1	B	528	ASP
1	B	568	LYS
1	B	573	TYR
1	B	613	TYR
1	B	628	ASP
1	B	652	LEU

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Mol	Chain	Res	Type
1	B	706	GLU
1	B	716	ASP
1	B	733	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	73	HIS
1	A	96	GLN
1	A	105	GLN
1	A	250	ASN
1	A	332	GLN
1	A	369	GLN
1	A	484	ASN
1	A	517	GLN
1	A	822	GLN
1	B	23	ASN
1	B	62	HIS
1	B	73	HIS
1	B	219	GLN
1	B	332	GLN
1	B	369	GLN
1	B	484	ASN
1	B	539	GLN
1	B	747	ASN
1	B	793	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 monosaccharides in this entry.

5.6 Ligand geometry i

12 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
6	MRD	B	903	-	7,7,7	0.71	0	9,10,10	0.90	0
5	CFF	B	1863	-	8,15,15	1.35	1 (12%)	8,23,23	1.14	1 (12%)
2	NBG	B	1861	-	15,15,15	1.65	2 (13%)	21,21,21	1.34	2 (9%)
5	CFF	A	864	-	8,15,15	1.47	1 (12%)	8,23,23	1.18	2 (25%)
2	NBG	A	861	-	15,15,15	1.47	3 (20%)	21,21,21	1.20	1 (4%)
5	CFF	A	863	-	8,15,15	1.39	1 (12%)	8,23,23	1.15	2 (25%)
6	MRD	B	1902	-	7,7,7	0.56	0	9,10,10	0.69	0
6	MRD	B	902	-	7,7,7	0.60	0	9,10,10	0.66	0
3	PLP	B	1860	1	15,15,16	1.72	2 (13%)	20,22,23	1.42	4 (20%)
4	700	A	862	-	28,33,33	1.94	10 (35%)	32,47,47	1.65	5 (15%)
3	PLP	A	860	1	15,15,16	2.00	4 (26%)	20,22,23	1.11	1 (5%)
4	700	B	1862	-	28,33,33	2.12	8 (28%)	32,47,47	1.62	6 (18%)

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
5	CFF	A	863	-	-	-	0/2/2/2
6	MRD	B	1902	-	-	2/5/5/5	-
5	CFF	B	1863	-	-	-	0/2/2/2
2	NBG	B	1861	-	-	0/6/26/26	0/1/1/1
5	CFF	A	864	-	-	-	0/2/2/2
2	NBG	A	861	-	-	0/6/26/26	0/1/1/1
6	MRD	B	903	-	-	0/5/5/5	-
3	PLP	B	1860	1	-	3/6/6/8	0/1/1/1
6	MRD	B	902	-	-	2/5/5/5	-
3	PLP	A	860	1	-	1/6/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	700	A	862	-	-	0/15/32/32	0/4/4/4
4	700	B	1862	-	-	0/15/32/32	0/4/4/4

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1862	700	C22-C20	5.59	1.60	1.55
3	B	1860	PLP	C4A-C4	-5.05	1.41	1.51
3	A	860	PLP	C4A-C4	-5.02	1.41	1.51
4	A	862	700	C22-C20	4.60	1.59	1.55
2	B	1861	NBG	C2-C1	4.40	1.57	1.52
4	B	1862	700	C5-C4	3.53	1.43	1.36
4	A	862	700	C5-C4	3.45	1.43	1.36
4	B	1862	700	C12-C11	3.11	1.45	1.38
3	A	860	PLP	C3-C2	-3.01	1.37	1.40
2	A	861	NBG	C2-C1	2.91	1.56	1.52
2	B	1861	NBG	C1-N1	2.90	1.46	1.43
4	B	1862	700	C19-C20	-2.90	1.52	1.55
4	A	862	700	C2-C3	2.79	1.42	1.36
4	B	1862	700	C2-C3	2.74	1.42	1.36
4	A	862	700	C7-C6	2.72	1.51	1.41
2	A	861	NBG	C1-N1	2.69	1.46	1.43
4	B	1862	700	C7-C6	2.67	1.51	1.41
4	A	862	700	C3-C4	2.56	1.42	1.38
4	B	1862	700	C3-C4	2.51	1.42	1.38
2	A	861	NBG	C3-C2	2.45	1.58	1.52
3	A	860	PLP	C5-C4	2.25	1.43	1.40
5	A	864	CFF	C6-C5	2.24	1.44	1.41
4	B	1862	700	C7-C8	-2.23	1.35	1.39
4	A	862	700	C13-C12	2.18	1.43	1.38
5	B	1863	CFF	C5-C4	-2.14	1.36	1.39
4	A	862	700	C15-C14	2.12	1.43	1.38
4	A	862	700	C12-C11	2.10	1.43	1.38
3	B	1860	PLP	P-O2P	-2.06	1.46	1.54
4	A	862	700	C16-C11	2.05	1.43	1.38
5	A	863	CFF	C5-C4	-2.05	1.36	1.39
4	A	862	700	C17-N1	2.03	1.50	1.45
3	A	860	PLP	C2-N1	2.01	1.37	1.33

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	862	700	C7-C6-C1	-4.49	102.36	106.27
2	B	1861	NBG	C5-O5-C1	4.46	118.57	112.52
4	A	862	700	C8-C9-N1	4.43	123.43	115.20
4	B	1862	700	C7-C6-C1	-4.41	102.43	106.27
4	B	1862	700	C8-C9-N1	4.01	122.64	115.20
2	A	861	NBG	C5-O5-C1	3.93	117.85	112.52
4	B	1862	700	C8-N2-C1	3.82	112.42	104.45
4	A	862	700	C8-N2-C1	3.75	112.27	104.45
3	B	1860	PLP	O4P-C5A-C5	2.96	114.99	109.35
3	B	1860	PLP	O4P-P-O1P	-2.85	98.48	106.47
4	B	1862	700	C3-C2-C1	-2.79	117.33	120.84
4	A	862	700	C3-C2-C1	-2.64	117.51	120.84
4	A	862	700	O1-C9-C8	-2.60	115.42	121.08
4	B	1862	700	O1-C9-C8	-2.56	115.52	121.08
3	B	1860	PLP	C6-C5-C4	2.21	119.90	118.16
5	A	864	CFF	C10-N1-C2	-2.20	114.15	119.61
5	A	863	CFF	C5-C6-N1	-2.19	115.87	118.20
2	B	1861	NBG	C2-C1-N1	-2.19	108.74	111.30
5	A	864	CFF	C5-C6-N1	-2.12	115.94	118.20
5	B	1863	CFF	C5-C6-N1	-2.11	115.95	118.20
5	A	863	CFF	C10-N1-C2	-2.07	114.46	119.61
3	B	1860	PLP	O2P-P-O1P	2.06	118.75	110.68
4	B	1862	700	O2-C18-N3	2.05	124.07	121.67
3	A	860	PLP	O2P-P-O4P	-2.01	101.39	106.73

There are no chirality outliers.

All (8) torsion outliers are listed below:

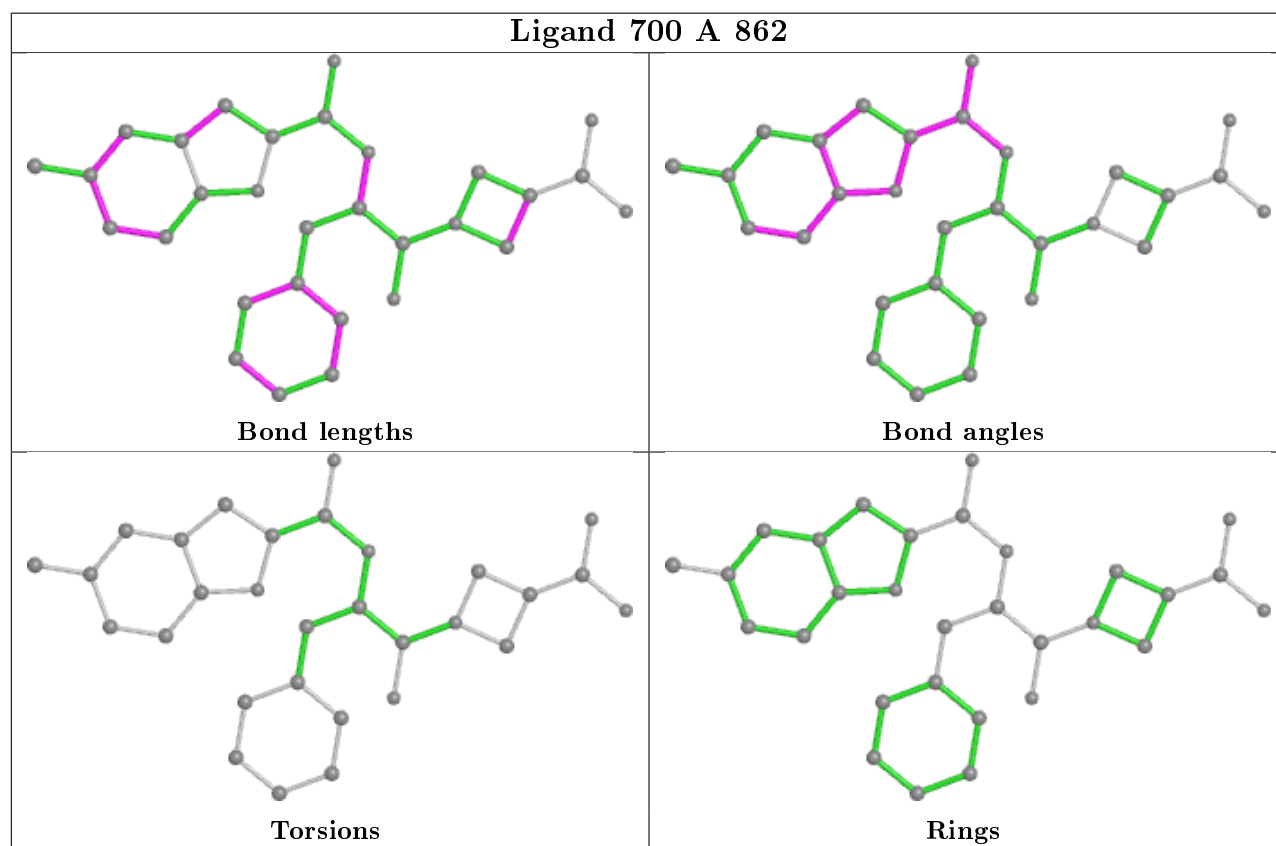
Mol	Chain	Res	Type	Atoms
3	B	1860	PLP	C5A-O4P-P-O1P
3	B	1860	PLP	C5A-O4P-P-O2P
3	B	1860	PLP	C5A-O4P-P-O3P
6	B	1902	MRD	C2-C3-C4-O4
6	B	902	MRD	C2-C3-C4-O4
3	A	860	PLP	C5A-O4P-P-O1P
6	B	1902	MRD	C2-C3-C4-C5
6	B	902	MRD	C2-C3-C4-C5

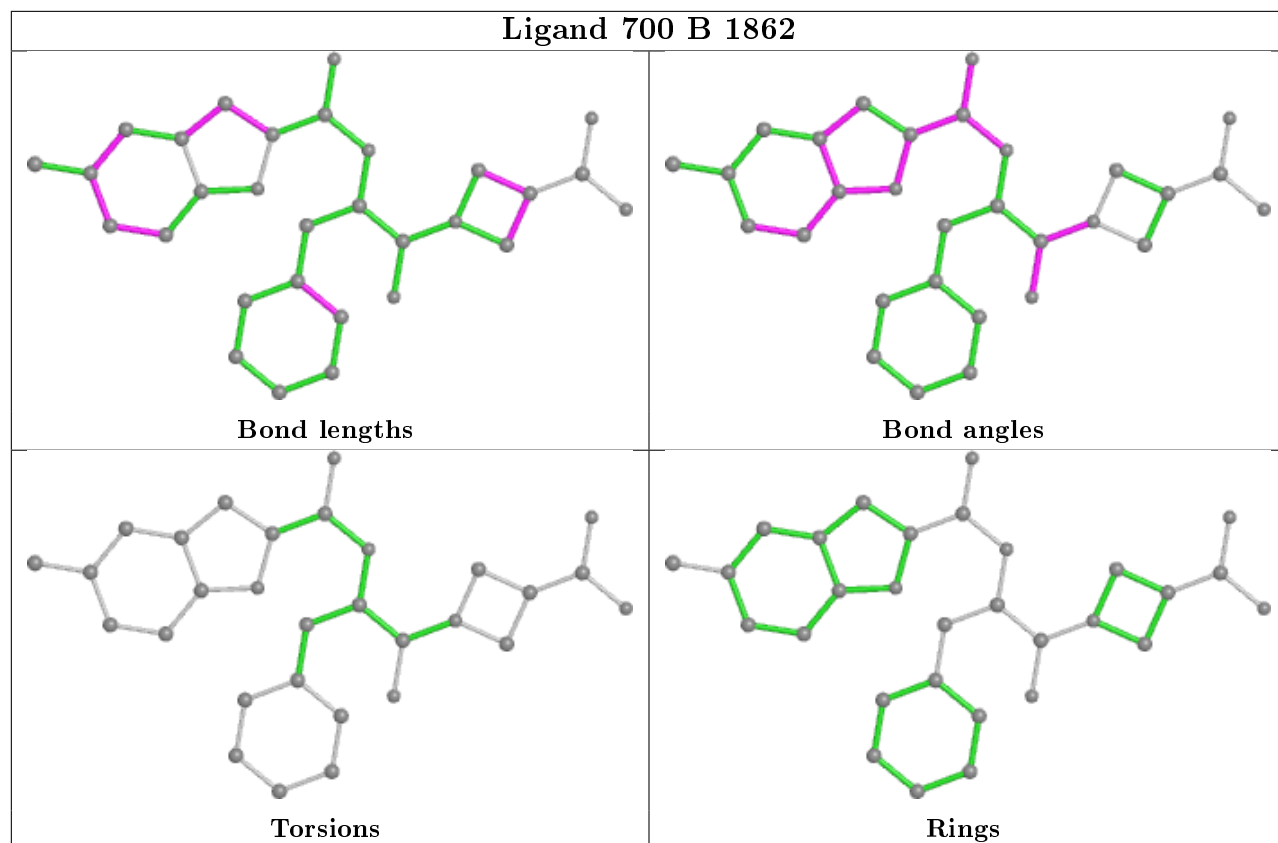
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	903	MRD	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.





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.